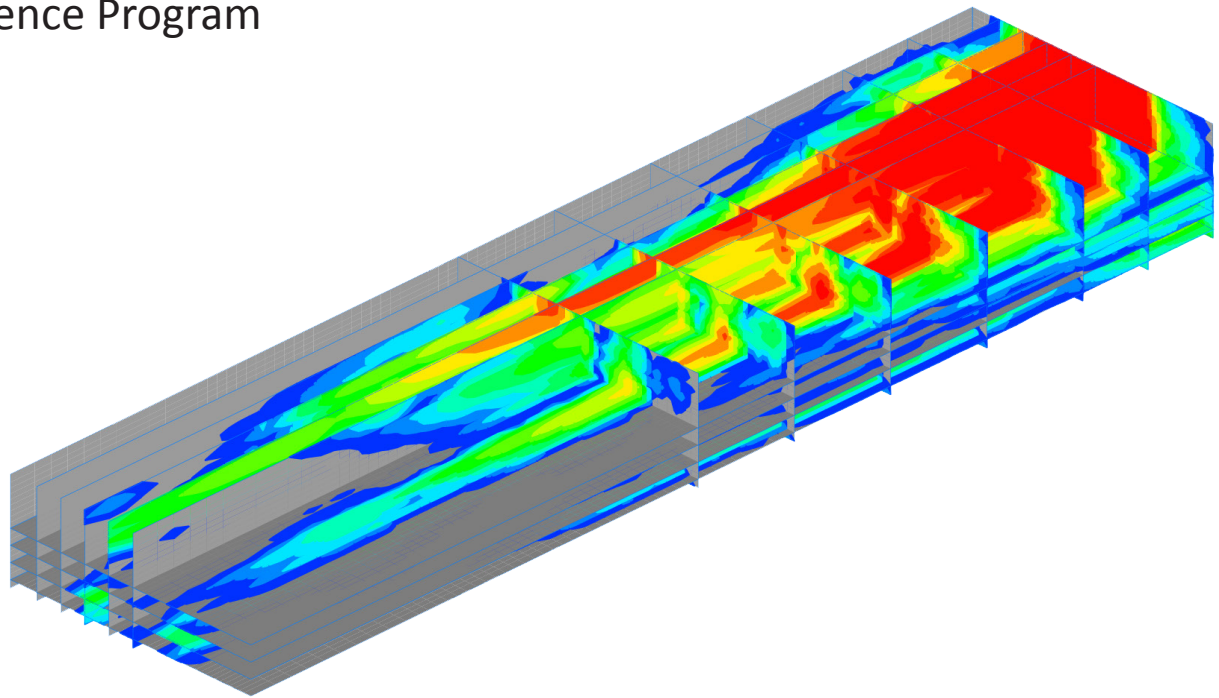# Computational Methods in Water Resources 2016

XXI International Conference

University of Toronto
June 20-24th 2016
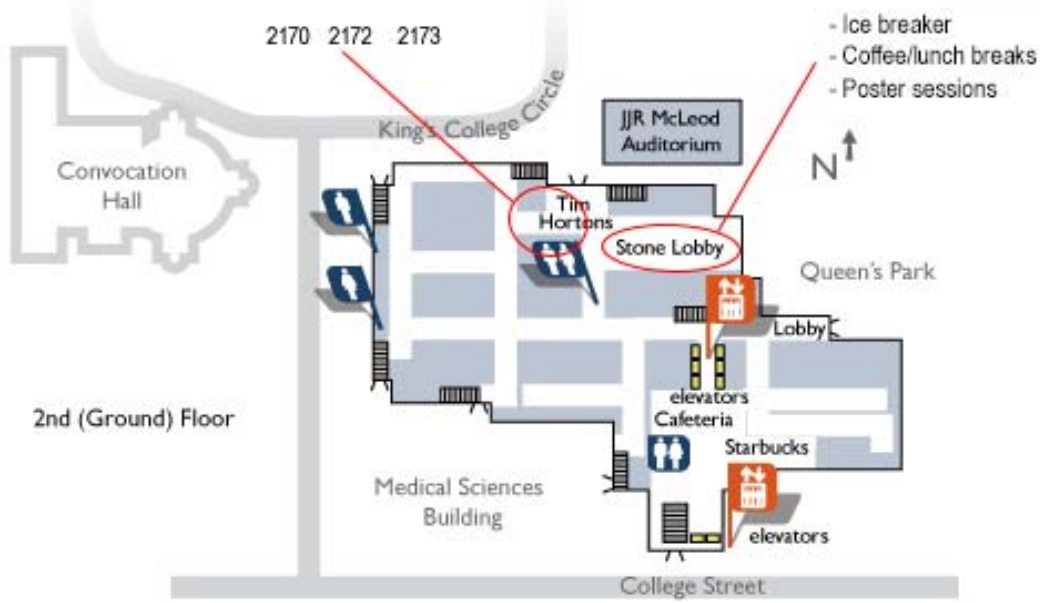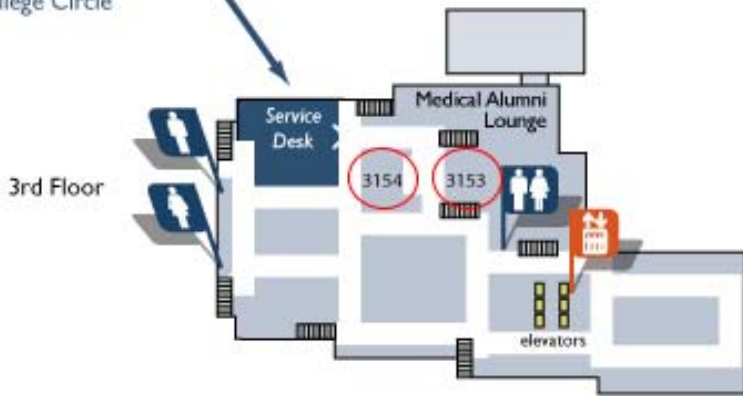Conference Program

CMWR
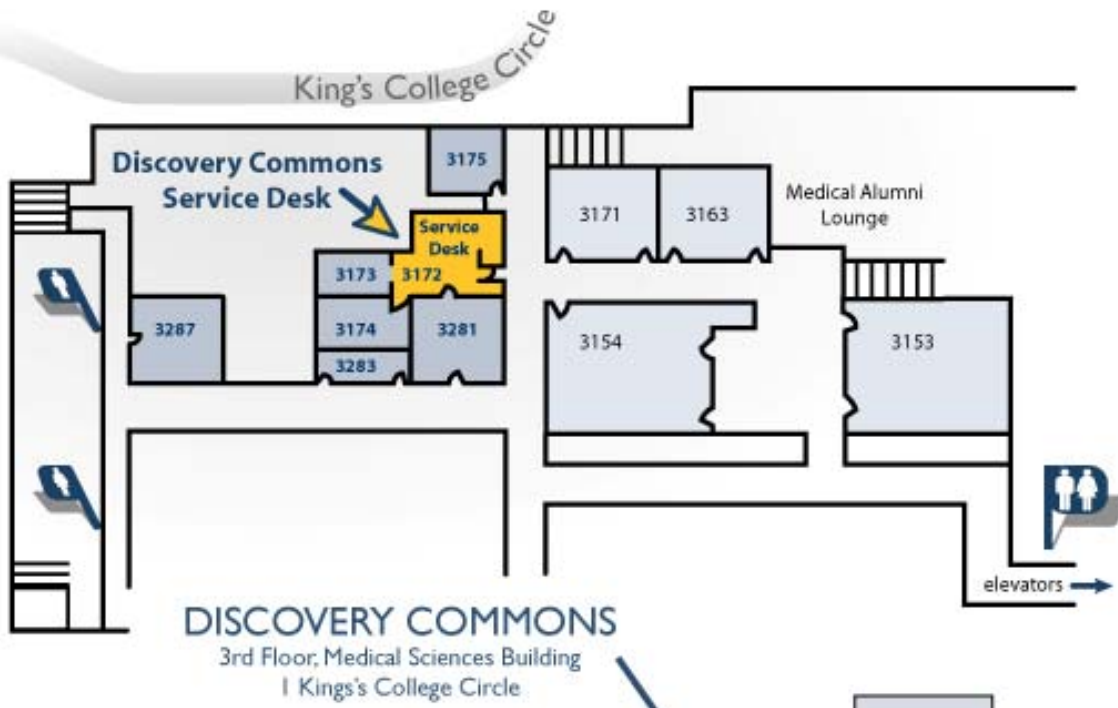Computational Methods
in Water Resources 2016

UNIVERSITY OF
TORONTO

King's College Circle

Discovery Commons Service Desk

3175

3171 3163 Medical Alumni Lounge

Service Desk 3172

3173

3287 3174 3281

3283

3154 3153

elevators →

DISCOVERY COMMONS
3rd Floor, Medical Sciences Building
I Kings's College Circle

3rd Floor

Service Desk

Medical Alumni Lounge

3154 3153

elevators

2170 2172 2173

- Ice breaker
- Coffee/lunch breaks
- Poster sessions

King's College Circle

JJR McLeod Auditorium

N↑

Convocation Hall

Tim Hortons

Stone Lobby

Queen's Park

Lobby

elevators
Cafeteria

2nd (Ground) Floor

Starbucks

Medical Sciences Building

elevators

College Street

Monday, 20/Jun/2016				
6:00pm - 8:00pm	**W-1: Welcome Reception** Location: **Stone Lobby** ~~Galbraith Building~~ Medical Science Building			

Tuesday, 21/Jun/2016				
8:15am - 8:30am	**Opening: Introduction to CMWR2016** Location: **Med Sci 3153**			
8:30am - 9:30am	**Keynote-1: David DiCarlo: Measurements of Three-Phase Flow and How Three-Phase Flow is Both More Complicated and Simpler Than Two-Phase Flow** Location: **Med Sci 3153**			
9:40am - 10:40am	**11-1: Computational Ecohydrology** Location: **Med Sci 2170** Conveners: Valeriy Y. Ivanov, University of Michigan and Edoardo Daly, Monash University	**4-1: Parameter Estimation and Uncertainty Analyses in Water Resource Models** Location: **Med Sci 2172** Conveners: Walter A. Illman, University of Waterloo and Sabine Attinger, Helmholtz Centre for Environmental Research – UFZ	**1-1: The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media** Location: **Med Sci 3153** Conveners: Florian Doster, Heriot-Watt University and Mark Porter, Los Alamos National Laboratory	**2-1: Mixing and Reaction Across Scales in Hydrological Systems** Location: **Med Sci 3154** Conveners: Marco Dentz, Institute of Environmental Assessment and Water Research and Tanguy Le Borgne, University of Rennes
10:40am - 11:00am	**CB-1: Morning Coffee Break** Location: **Stone Lobby**			
11:00am - 12:20pm	**11-2: Computational Ecohydrology** Location: **Med Sci 2170** Conveners: Valeriy Y. Ivanov, University of Michigan and Edoardo Daly, Monash University	**4-2: Parameter Estimation and Uncertainty Analyses in Water Resource Models** Location: **Med Sci 2172** Conveners: Walter A. Illman, University of Waterloo and Sabine Attinger, Helmholtz Centre for Environmental Research – UFZ	**1-2: The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media** Location: **Med Sci 3153** Conveners: Florian Doster, Heriot-Watt University and Mark Porter, Los Alamos National Laboratory	**2-2: Mixing and Reaction Across Scales in Hydrological Systems** Location: **Med Sci 3154** Conveners: Marco Dentz, Institute of Environmental Assessment and Water Research and Tanguy Le Borgne, University of Rennes
12:20pm - 1:20pm	**L-1: Lunch Break** Location: **Stone Lobby**			
1:20pm - 2:20pm	**Keynote-2: Christine Shoemaker: Efficient Surrogate Methods for Global Optimization and Uncertainty Quantification of Computationally Expensive Nonconvex Models of Hydrogeologic Systems** Location: **Med Sci 3153**			
2:30pm - 3:30pm		**4-3: Parameter Estimation and Uncertainty Analyses in Water Resource Models** Location: **Med Sci 2172** Conveners: Walter A. Illman, University of Waterloo and Sabine Attinger, Helmholtz Centre for Environmental Research – UFZ	**1-3: The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media** Location: **Med Sci 3153** Conveners: Florian Doster, Heriot-Watt University and Mark Porter, Los Alamos National Laboratory	**2-3: Mixing and Reaction Across Scales in Hydrological Systems** Location: **Med Sci 3154** Conveners: Marco Dentz, Institute of Environmental Assessment and Water Research and Tanguy Le Borgne, University of Rennes
3:30pm - 3:50pm	**CB-2: Afternoon Coffee Break** Location: **Stone Lobby**			
3:50pm - 5:30pm	**13-1: Targeting Evolving Computational Environments to Advance Hydrological Models** Location: **Med Sci 2170** Conveners: Katherine Evans and Matthew Norman, Oak Ridge National Laboratory	**4-4: Parameter Estimation and Uncertainty Analyses in Water Resource Models** Location: **Med Sci 2172** Conveners: Walter A. Illman, University of Waterloo and Sabine Attinger, Helmholtz Centre for Environmental Research – UFZ	**1-4: The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media** Location: **Med Sci 3153** Conveners: Florian Doster, Heriot-Watt University and Mark Porter, Los Alamos National Laboratory	**2-4: Mixing and Reaction Across Scales in Hydrological Systems** Location: **Med Sci 3154** Conveners: Marco Dentz, Institute of Environmental Assessment and Water Research and Tanguy Le Borgne, University of Rennes
6:00pm - 8:00pm	**P-1: Poster Session 1** Location: **Stone Lobby**	**Short Course: Christine Shoemaker: Python & Matlab Software for Surrogate Global Optimization Toolbox in Water Resources** Location: **Med Sci 2173**		

Wednesday, 22/Jun/2016			
8:30am - 9:30am	**Keynote-3: Ruben Juanes: Induced Seismicity in Subsurface Technologies: New Operational Constraints in Need of New Computational Models.** Location: **Med Sci 3153**		
9:40am - 10:40am	**6-1: Hybrid Multiscale Modelling of Subsurface Flow and Reactive Transport** Location: **Med Sci 2170** Conveners: Tim Scheibe, Pacific Northwest National Laboratory and Ilenia Battiato, San Diego State University	**8-1: Hydro-Mechanical and Thermo-Hydro-Mechanical Modelling of Subsurface Processes** Location: **Med Sci 2172** Conveners: Joshua White Lawrence Livermore National Laboratory and Nicola Castelleto, Stanford University	**5-1: Advances in Numerical Solvers for Water Resources Applications** Location: **Med Sci 3153** Conveners: Carol Woodward, Lawrence Livermore National Laboratory and Peter Bastian, Universität Heidelberg	**7-1: Novel Developments and Data-Integration in Complex Biogeochemical and Hydrological Process Models** Location: **Med Sci 3154** Conveners: Li Li, Pennsylvania State University and Christof Meile, University of Georgia
10:40am - 11:00am	**CB-3: Morning Coffee Break** Location: **Stone Lobby**			
11:00am - 12:20pm	**15-1: Advances in Fluvial Eco-Hydraulics and Morphodynamics** Location: **Med Sci 2170** Conveners: Donatella Termini, University of Palermo; Grant Gordon, OSU Oregon State University	**8-2: Hydro-Mechanical and Thermo-Hydro-Mechanical Modelling of Subsurface Processes** Location: **Med Sci 2172** Conveners: Joshua White Lawrence Livermore National Laboratory and Nicola Castelleto, Stanford University	**1-5: The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media** Location: **Med Sci 3153** Conveners: Florian Doster, Heriot-Watt University and Mark Porter, Los Alamos National Laboratory	**2-5: Mixing and Reaction Across Scales in Hydrological Systems** Location: **Med Sci 3154** Conveners: Marco Dentz, Institute of Environmental Assessment and Water Research and Tanguy Le Borgne, University of Rennes
12:20pm - 1:20pm	**L-2: Lunch Break** Location: **Stone Lobby**			
1:20pm - 2:20pm	**Keynote-4: Stéphane Zaleski: The simulation of droplets, bubbles and interfaces** Location: **Med Sci 3153**			
2:30pm - 3:30pm	**6-2: Hybrid Multiscale Modelling of Subsurface Flow and Reactive Transport** Location: **Med Sci 2170** Conveners: Tim Scheibe, Pacific Northwest National Laboratory and Ilenia Battiato, San Diego State University	**14-1: General Session on Advances in Computational Methods for Subsurface Water Resources** Location: **Med Sci 2172** Convener: Valeriy Y. Ivanov, University of Michigan	**5-2: Advances in Numerical Solvers for Water Resources Applications** Location: **Med Sci 3153** Conveners: Carol Woodward, Lawrence Livermore National Laboratory and Peter Bastian, Universität Heidelberg	**7-2: Novel Developments and Data-Integration in Complex Biogeochemical and Hydrological Process Models** Location: **Med Sci 3154** Conveners: Li Li, Pennsylvania State University and Christof Meile, University of Georgia
3:30pm - 3:50pm	**CB-4: Afternoon Coffee Break** Location: **Stone Lobby**			
3:50pm - 5:30pm	**8-3: Hydro-Mechanical and Thermo-Hydro-Mechanical Modelling of Subsurface Processes** Location: **Med Sci 2170** Conveners: Joshua White Lawrence Livermore National Laboratory and Nicola Castelleto, Stanford University	**5-3: Advances in Numerical Solvers for Water Resources Applications** Location: **Med Sci 3153** Conveners: Carol Woodward, Lawrence Livermore National Laboratory and Peter Bastian, Universität Heidelberg	**7-3: Novel Developments and Data-Integration in Complex Biogeochemical and Hydrological Process Models** Location: **Med Sci 3154** Conveners: Li Li, Pennsylvania State University and Christof Meile, University of Georgia	**14-2: General Session on Advances in Computational Methods for Subsurface Water Resources** Location: **Med Sci 2173** Convener: Valeriy Y. Ivanov, University of Michigan
6:00pm - 8:00pm	**P-2: Poster Session 2** Location: **Stone Lobby**			

	Thursday, 23/Jun/2016			
8:30am - 9:30am	**Keynote-5: Randall Leveque: Multi-scale Tsunami Modeling and Probabilistic Hazard Assessment.** Location: **Med Sci 3153**			
9:40am - 10:40am	**20-1: Advances in Computational Methods for Surface Hydrological Processes** Location: **Med Sci 2170** Conveners: Matteo Camporese, University of Padua; Florian Doster, Heriot-Watt University	**3-1: Recent Advances in Coastal Ocean Modelling of Waves, Circulation and Transport** Location: **Med Sci 2172** Conveners: Casey Dietrich, North Carolina State University; Clint Dawson, University of Texas at Austin	**10-1: Reusable Software for Accurate, Efficient, and Reproducible Water Resources Simulation** Location: **Med Sci 3153** Conveners: Chris Kees, US Army Engineer Research & Development Center and Mark Bakker, Delft University of Technology	**5-4: Advances in Numerical Solvers for Water Resources Applications** Location: **Med Sci 3154** Conveners: Carol Woodward, Lawrence Livermore National Laboratory and Peter Bastian, Universität Heidelberg
10:40am - 11:00am	**CB-5: Morning Coffee Break** Location: **Stone Lobby**			
11:00am - 12:20pm	**9-1: Integrated Hydrologic Models: Advancements and Applications** Location: **Med Sci 2170** Conveners: Reed Maxwell, Colorado School of Mines and Mario Putti, University of Padova	**3-1: Recent Advances in Coastal Ocean Modelling of Waves, Circulation and Transport** Location: **Med Sci 2172** Conveners: Casey Dietrich, North Carolina State University; Clint Dawson, University of Texas at Austin	**10-2: Reusable Software for Accurate, Efficient, and Reproducible Water Resources Simulation** Location: **Med Sci 3153** Conveners: Chris Kees, US Army Engineer Research & Development Center and Mark Bakker, Delft University of Technology	**16-1: Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale** Location: **Med Sci 3154** Convener: Branko Bijeljic, Imperial College; Maša Prodanović, University of Texas at Austin; Matteo Iccardi, University of Warwick
12:20pm - 1:20pm	**L-3: Lunch Break** Location: **Stone Lobby**			
1:20pm - 2:20pm	**Keynote-6: Gabrielle de Lannoy: Assimilation of SMOS and SMAP Observations into the NASA GEOS-5 Land Surface Model to Improve Global Estimates of Surface and Root-Zone Soil Moisture** Location: **Med Sci 3153**			
2:20am - 2:35am	**CB-6: Afternoon Coffee Break** Location: **Stone Lobby**			
2:35pm - 4:15pm	**9-2: Integrated Hydrologic Models: Advancements and Applications** Location: **Med Sci 2170** Conveners: Reed Maxwell, Colorado School of Mines and Mario Putti, University of Padova	**12-1: Modelling and Computational Aspects of Coupled Porous Medium and Free Flow Systems** Location: **Med Sci 2172** Conveners: Iryna Rybak, University of Stuttgart and Marco Discacciati, Loughborough University	**3-2: Recent Advances in Coastal Ocean Modelling of Waves, Circulation and Transport** Location: **Med Sci 3153** Conveners: Casey Dietrich, North Carolina State University; Clint Dawson, University of Texas at Austin	**16-2: Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale** Location: **Med Sci 3154** Convener: Branko Bijeljic, Imperial College; Maša Prodanović, University of Texas at Austin; Matteo Iccardi, University of Warwick
6:00pm - 9:00pm	**D-1: Conference Dinner** Location: **Mill Street Brewery**. Shuttle buses will leave King's Circle at 5:00 pm. Please show your conference badge to the driver as you enter the bus.			

Friday, 24/Jun/2016				
8:30am - 9:30am	**Keynote-7: Harry Vereecken: High Performance Scientific Computing in terrestrial hydrology: linking data and models** Location: **Med Sci 3153**			
9:40am - 10:40am	**17-1: Data Assimilation in Water Resources Modelling** Location: **Med Sci 2170** Co-Conveners: Henrik Madsen, DHI Group; Paulin Coulibaly, McMaster University	**18-1: Multiscale Algorithms and Their Applications: From Upscaling to Scalable Solvers and Multiphysics Modelling** Location: **Med Sci 2172** Conveners: Pavel Tomin (Stanford University), Hadi Hajibeygi (TU Delft), and Ivan Lunati, University of Lausanne	**10-3: Reusable Software for Accurate, Efficient, and Reproducible Water Resources Simulation** Location: **Med Sci 3153** Conveners: Chris Kees, US Army Engineer Research & Development Center and Mark Bakker, Delft University of Technology NOTE: This session may extend to after the coffee break as needed.	**16-3: Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale** Location: **Med Sci 3154** Convener: Branko Bijeljic, Imperial College; Maša Prodanović, University of Texas at Austin; Matteo Iccardi, University of Warwick
10:40am - 11:00am	**CB-7: Morning Coffee Break** Location: **Stone Lobby**			
11:00am - 12:20pm	**17-2: Data Assimilation in Water Resources Modelling** Location: **Med Sci 2170** Co-Conveners: Henrik Madsen, DHI Group; Paulin Coulibaly, McMaster University	**18-2: Multiscale Algorithms and Their Applications: From Upscaling to Scalable Solvers and Multiphysics Modelling** Location: **Med Sci 2172** Conveners: Pavel Tomin (Stanford University), Hadi Hajibeygi (TU Delft), and Ivan Lunati, University of Lausanne	**16-4: Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale** Location: **Med Sci 3154** Convener: Branko Bijeljic, Imperial College; Maša Prodanović, University of Texas at Austin; Matteo Iccardi, University of Warwick	**19-1: Computational Developments in Modelling Climate Change and Water Resources** Location: **Med Sci 2173** Convener: Peter Bastian, Heidelberg University
12:20pm - 1:20pm	**L-4: Lunch Break** Location: **Stone Lobby**			
1:20pm - 2:20pm	**Keynote-8: Richard Peltier: Climate Coupled Hydrology in a Warming World** Location: **Med Sci 3153**			
2:20am - 2:35am	**CB-8: Afternoon Coffee Break** Location: **Stone Lobby**			
2:35pm - 4:15pm	**9-3: Integrated Hydrologic Models: Advancements and Applications** Location: **Med Sci 2170** Conveners: Reed Maxwell, Colorado School of Mines and Mario Putti, University of Padova	**19-2: Computational Developments in Modelling Climate Change and Water Resources** Location: **Med Sci 2172** Convener: Peter Bastian, Heidelberg University	**18-3: Multiscale Algorithms and Their Applications: From Upscaling to Scalable Solvers and Multiphysics Modelling** Location: **Med Sci 3153** Conveners: Pavel Tomin (Stanford University), Hadi Hajibeygi (TU Delft), and Ivan Lunati, University of Lausanne	**16-5: Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale** Location: **Med Sci 3154** Convener: Branko Bijeljic, Imperial College; Maša Prodanović, University of Texas at Austin; Matteo Iccardi, University of Warwick
4:15pm - 4:45pm	**Closing: Closing Session** Location: **Med Sci 3153** Student poster awards will be presented and the location of the next CWMR conference announced.			

Keynotes

David DiCarlo: Measurements of Three-Phase Flow and How Three-Phase Flow is Both More Complicated and Simpler than Two-Phase Flow

Christine Shoemaker: Efficient Surrogate Methods for Global Optimization and Uncertainty Quantification of Computationally Expensive Nonconvex Models of Hydrogeologic Systems

Ruben Juanes: Induced Seismicity in Subsurface Technologies: New Operational Constraints in Need of New Computational Models.

Stéphane Zaleski: The simulation of droplets, bubbles and interfaces

Randall Leveque: Multi-scale Tsunami Modeling and Probabilistic Hazard Assessment.

Gabrielle de Lannoy: Assimilation of SMOS and SMAP Observations into the NASA GEOS-5 Land Surface Model to Improve Global Estimates of Surface and Root-Zone Soil Moisture

Harry Vereecken: High Performance Scientific Computing in terrestrial hydrology: linking data and models

Richard Peltier: Climate Coupled Hydrology in a Warming World

Sessions

Session 1	The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media
Session 2	Mixing and Reaction Across Scales in Hydrological Systems
Session 3	Recent Advances in Coastal Ocean Modelling of Waves, Circulation and Transport
Session 4	Parameter Estimation and Uncertainty Analyses in Water Resource Models
Session 5	Advances in Numerical Solvers for Water Resources Applications
Session 6	Hybrid Multiscale Modelling of Subsurface Flow and Reactive Transport
Session 7	Novel Developments and Data-Integration in Complex Biogeochemical and Hydrological Process Models
Session 8	Hydro-Mechanical and Thermo-Hydro-Mechanical Modelling of Subsurface Processes
Session 9	Integrated Hydrologic Models: Advancements and Applications
Session 10	Reusable Software for Accurate, Efficient, and Reproducible Water Resources Simulation
Session 11	Computational Ecohydrology
Session 12	Modelling and Computational Aspects of Coupled Porous Medium and Free Flow Systems
Session 13	Targeting Evolving Computational Environments to Advance Hydrological Models
Session 14	General Session on Advances in Computational Methods for Subsurface Water Resources
Session 15	Advances in Fluvial Eco-Hydraulics and Morphodynamics
Session 16	Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale
Session 17	Data Assimilation in Water Resources Modelling
Session 18	Data Assimilation in Water Resources Modelling
Session 19	Multiscale Algorithms and Their Applications: From Upscaling to Scalable Solvers and Multiphysics Modelling
Session 20	Computational Developments in Modelling Climate Change and Water Resources
Session 21	Advances in Computational Methods for Surface Hydrological Processes

Keynote 1

Measurements of Three-Phase Flow and How Three- Phase Flow is Both More Complicated and Simpler than Two-Phase Flow

Time: Tuesday, 21/Jun/2016: 8:30am - 9:30am – Location: MacLeod Auditorium

David DiCarlo
University of Texas at Austin; dicarlo@mail.utexas.edu

Measurements of Three-Phase Flow and How Three-Phase Flow is Both More Complicated and Simpler than Two-Phase Flow

David DiCarlo and Masa Prodanovic

University of Texas at Austin

The recent imaging advances (such as X-ray microtomography) have provided datasets that reveal the pore-space microstructure and allow investigation of flow and mechanical phenomena from first principles using numerical approaches. In this talk, I will discuss two related topics.

The first topic is a new direct pore scale modeling method for filtration, as well as its integration with experiments for upscaling of filtration coefficient. The numerical model simulates the flow of suspension through a realistic 3D structure of an imaged, disordered sphere pack, which acts as the filter medium. Particle capture through size exclusion and jamming is modeled via a coupled discrete element method (DEM) and computational fluid dynamics (CFD) approach. The coupled CFD-DEM approach is capable of modeling the majority of particle-particle, particle-wall, and particle-fluid interactions. We adapted the interface between the pore space and the spherical grains to be represented as a triangulated surface and this allows extensions to any imaged media. The experiments were performed in glass bead packs (1mm glass beads) and were flooded with suspensions of different concentrations and fluxes, and were imaged in a CT scanner for quantifying porosity damage before and after each flood. The numerical and

experimental results show that an increase in the suspension flow rate results in a decrease in the filtration coefficient, which suggests that the hydrodynamic drag force plays the key role in hindering the particle capture in random sphere packs. Further, similar simulations of suspension flow through a sandstone sample, which has a tighter pore space, show that filtration coefficient remains almost constant at different suspension flow rates. We further show a sensitivity study on particulate propagation depending on particulate size, concentration, flux and surface forces in rough walled fractures and discuss implications on hydraulic fracturing.

The second topic is a practical one: developing sustainable infrastructure for storing and sharing the wealth of 2D and 3D imaged geometries. While many research groups have porous media microstructure images, they are large, from diverse sources and not easily accessible to wider scientific community. We are developing an open repository, "Digital rocks portal", that organizes images and related measurements of different porous materials, jumpstarts productivity and enables scientific inquiry and engineering decisions founded on data-driven basis. Please visit https://pep.tacc.utexas.edu/ to evaluate beta version of the portal.

Keynote 2

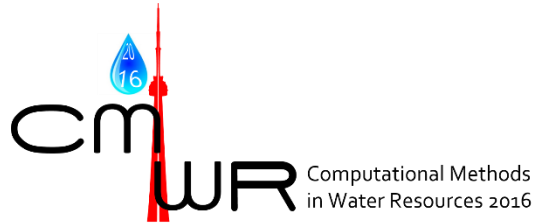### Efficient Surrogate Methods for Global Optimization and Uncertainty Quantification of Computationally Expensive Nonconvex Models of Hydrogeologic Systems

Time: Tuesday, 21/Jun/2016: 1:20pm - 2:20pm – Location: MacLeod Auditorium

Christine A. Shoemaker
Cornell University; CAS12@cornell.edu

Efficient Surrogate Methods for Global Optimization and Uncertainty Quantification of Computationally Expensive Nonconvex Models of Hydrogeologic Systems

Christine Shoemaker

Cornell University

Determining optimal management or parameter calibration of a complex nonconvex hydrogeologic model requires a global optimization and/or an uncertainty quantification method for which relatively few simulations of a computationally expensive simulation model are needed to reach a good solution. I will describe parallel algorithms utilizing iteratively constructed surrogate approximations with continuous and/or integer variables that are available as open source software. The numerical results shown will indicate the software for these surrogate algorithms is very effective at obtaining accurate solutions with relatively few model simulations (and high parallel speed-up) on complex applications including Carbon Sequestration (multi-phase, multi constituent model TOUGH2), Groundwater Remediation (MODFLOW-MT3D), and Phosphorous Transport in watersheds (SWAT). This work has been done jointly with A. Espinet, M. Pang, Y. Wang, Y. Wan, J. Mueller, and Prof. D. Ruppert.
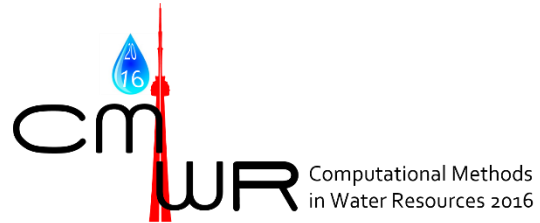
Keynote 3

Induced Seismicity in Subsurface Technologies: New Operational Constraints in Need of New Computational Models.

Time: Wednesday, 22/Jun/2016: 8:30am - 9:30am – Location: MacLeod Auditorium

Ruben Juanes
Massachusetts Institute of Technology; juanes@mit.edu

Induced Seismicity in Subsurface Technologies: New Operational Constraints in Need of New Computational Models.

Ruben Juanes

Massachusetts Institute of Technology

The coupling between subsurface flow and geomechanical deformation is critical in the assessment of the environmental impacts of groundwater use, underground liquid waste disposal, geologic storage of carbon dioxide, and exploitation of shale gas reserves. In particular, seismicity induced by fluid injection and withdrawal has emerged as a central element of the scientific discussion around subsurface technologies that tap into water and energy resources. Here we present a new computational approach to model coupled multiphase flow and geomechanics of faulted reservoirs. We present the application of the coupled flow-geomechanics simulation technology to the post mortem analysis of several earthquake sequences. These early applications suggest that computational modeling of coupled flow and geomechanics, in combination with geologic, seismotectonic, and geodetic constraints, provides a promising approach for assessing and managing risk due to induced seismicity.

Keynote 4

The Simulation of Droplets, Bubbles and Interfaces

Time: Wednesday, 22/Jun/2016: 1:20pm - 2:20pm – *Location:* MacLeod Auditorium

Stéphane Zaleski
University Pierre et Marie Curie; stephane.zaleski@gmail.com

The Simulation of Droplets, Bubbles and Interfaces

Stéphane Zaleski

University Pierre et Marie Curie

Droplets, bubbles and interfaces offer fascinating physical and mathematical problems and are a key part of the microscopic modeling of multiphase flow in porous media and other contexts. The talk will describe how to address these problems numerically, using tools such as the Volume of Fluid method. In particular, I will discuss the problems of contact line motion, the invasion of porous media and turbulent free-surface flows. The issues arising from the upscaling of simulations to more extreme HPC environments will also be discussed.
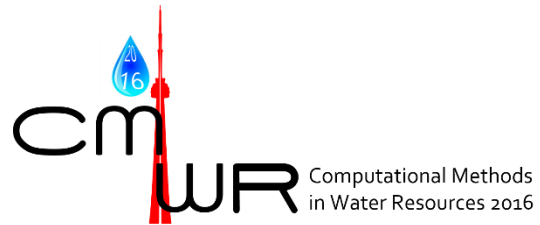
Keynote 5

Multi-scale Tsunami Modeling and Probabilistic Hazard Assessment.

Time: Thursday, 23/Jun/2016: 8:30am - 9:30am – *Location:* MacLeod Auditorium

Randall J. LeVeque
University of Washington; rjl@amath.washington.edu
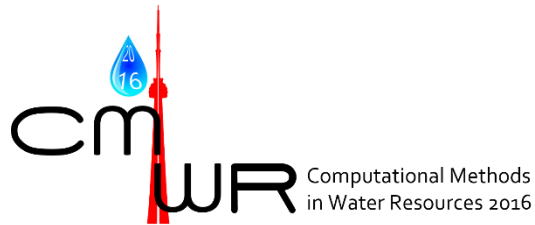
Multi-scale Tsunami Modeling and Probabilistic Hazard Assessment

Randall Leveque

University of Washington

Tsunami modeling generally requires handling a wide range of spatial scales, particularly when modeling far-field events where the propagation across the ocean is followed by fine scale modeling of individual harbors or coastal communities. The GeoClaw software uses adaptive mesh refinement to efficiently solve the shallow water equations for individual events.

Probabilistic hazard assessment requires the study of many potential tsunami sources and perhaps the exploration of a high-dimensional space of possible slip distributions on one or more subduction faults. I will describe recent work toward efficient computation of probabilistic risk maps using a variety of multi-scale techniques.

Keynote 6

Assimilation of SMOS and SMAP Observations into the NASA GEOS-5 Land Surface Model to Improve Global Estimates of Surface and Root-Zone Soil Moisture

Time: Thursday, 23/Jun/2016: 1:20pm - 2:20pm – *Location:* MacLeod Auditorium

Gabrielle J. M. de Lannoy
NASA Goddard Space Flight Center; gabrielle.delannoy@kuleuven.be

Assimilation of SMOS and SMAP Observations into the NASA GEOS-5 Land Surface Model to Improve Global Estimates of Surface and Root-Zone Soil Moisture

Gabrielle de Lannoy

NASA Goddard Space Flight Center

Soil moisture is an important component of the terrestrial water cycle and a key land surface variable in the global weather and climate system. Global estimates of surface soil moisture can be inferred from satellite-based low frequency passive microwave observations, such as collected by, for example, the current Soil Moisture Ocean Salinity (SMOS) mission and the Soil Moisture Active Passive (SMAP) mission. However, the utility of space borne radiometry is constrained by the limited vertical penetration depth, the coarse spatial resolution, the indirect connection to relevant land surface variables and the intermittent nature of the measurements. The assimilation of passive microwave measurements into land surface models has potential to add value to these satellite data by (i) increasing the effective vertical penetration depth though propagation of surface information to the root-zone, (ii) increasing the spatial resolution through dynamic downscaling, (iii) increasing the spatial and temporal coverage by interpolation and extrapolation to unobserved times and locations and (iv) providing enhanced and consistent estimates of various land surface state and flux estimates. The talk will discuss the assimilation of global SMOS and SMAP (separately) brightness temperature observations into the Goddard Earth Observing System version 5 (GEOS-5) Catchment land surface model. Special attention will be devoted to the operational SMAP level 4 soil moisture (L4_SM) product, a data assimilation product specifically aimed at providing globally consistent root-zone soil moisture and other geophysical land surface variables.

Keynote 7

High Performance Scientific Computing in terrestrial hydrology: linking data and models

Time: Friday, 24/Jun/2016: 8:30am - 9:30am – *Location:* MacLeod Auditorium

Harry Vereecken
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High Performance Scientific Computing in terrestrial hydrology: linking data and models

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Forschungszentrum Jülich

Recent advances in computational technologies combined with methodological progress in integrating data and models open completely new perspectives in predicting hydrological fluxes and the real-time management of water resources. In this presentation we will discuss the use of data assimilation techniques combined with high-resolution simulations of the soil-plant-atmosphere system to predict soil moisture dynamics and hydrological fluxes at the catchment to continental scale. Specific attention will be given to the advantages and disadvantages of hyper-resolution versus simpler conceptual models. We will demonstrate the value of combining large scale information on groundwater levels, land surface temperature, remotely sensed soil moisture and leaf area index to improve large scale characterization and prediction of hydrological states and fluxes like evapotranspiration. Combining data assimilation with land-surface atmosphere interaction models and subsurface models such as TerrSysMP may also help to improve real-time management of irrigated agricultural systems and to study how this coupling is controlled by soil and vegetation characteristics. Finally, we will address the need to include small-scale process description of hydrological processes into larger scale land surface models by developing effective parameterizations of e.g. root water uptake processes.

Keynote 8

Climate Coupled Hydrology in a Warming World

Time: Friday, 24/Jun/2016: 1:20pm - 2:20pm – Location: MacLeod Auditorium

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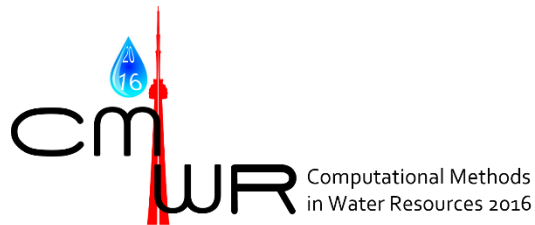# Climate Coupled Hydrology in a Warming World

Richard Peltier

University of Toronto, Canada

One of the least well developed aspects of our understanding of the global warming process concerns its expected impacts upon water resources, especially upon the water table. Although modern global models of the coupled evolution of the atmosphere, oceans , sea ice and land surface processes are able to provide adequate projections of global or continental scale averaged impacts, on sub-continental regional scales these models have proven to be inadequate. Even on the largest scales, however, their skill in representing precipitation is extremely modest. Furthermore the ability of such models to adequately represent the influence of surface features that control hydrological processes, including land forms and land surface processes is limited at best. A methodology that has been developed to overcome the inadequate resolution of the global models is termed "dynamical downscaling" and this methodology has begun to come into its own as computational capacity has increased. Although a good deal may be gained by simply employing a appropriate regional climate model (RCM) in a multiply nested mode to downscale global warming projections from one or more global models to obtain higher resolution projections of impacts for a particular region, the frontier in this area is being defined by further coupling of the highest resolution regional climate model to explicit models of surface and subsurface hydrological processes.

I will describe the results that are being obtained by application of the dynamical downscaling methodology to two distinct regions of Canada whose characteristics present distinct challenges to the methodology. The first of these is the Great Lakes Basin of North America and the Canadian province of Ontario. The second consists of the western provinces of British Columbia and Alberta which are separated by the Rocky Mountains. Upstream of the mountains this region is characterized by extremely high precipitation but downstream by dry conditions. The results of analyses will be presented that primarily employ the Community Earth System Model (CESM) of the US National Centre for Atmospheric Research (NCAR) as the "parent" global coupled model and the Weather Research and Forecasting (WRF) regional climate model to downscale the global warming projections deliver by CESM for both mid-century and end-century conditions, under business as usual trace gas scenarios. In both regions downscaling is performed in 2 steps, the first being to the continental scale at a horizontal resolution of 30 km and the second to a policy relevant scale of 10 km over the target regions. Results will be described that both include and exclude the explicit description of the influence of the lakes (by embedding the European Flake model within WRF) and by forcing an explicit model of surface and subsurface hydrology (Hydrogeosphere) with the surface temperature and precipitation fields delivered by the highest resolution regional climate model.

Of particular interest in work of this kind, aside from the impact of warming on mean temperature and precipitation, is its impact upon extremes, in particular upon the "return times" of events of a given extremity. In this regard we will discuss both extremes in precipitation and extremes in temperature ("heat waves"). As I will demonstrate, the dynamical downscaling methodology is able to deliver important insights into the regional nature of such expected extremes.

1-1: The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media

Time: Tuesday, 21/Jun/2016: 9:40am - 10:40am – *Location: MSB 3153*

Pore-Scale Simulation of Multiphase Flow and Microbial Organic Carbon Transformation in Soils Using Smoothed Particle Hydrodynamics

Nitin Gawande, Bruce Palmer, Timothy Scheibe

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Pore-Scale Simulation of sCO2/Brine Dissolution

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Quick Estimation of Connectivity and Bypassed Volumes after Waterflooding in Geologically Realistic Models of Aquifers/Oil Reservoirs

Paula Alejandra Gago, Ann Muggeridge, Peter King

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Pore-Scale Simulation of Multiphase Flow and Microbial Organic Carbon Transformation in Soils Using Smoothed Particle Hydrodynamics

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Key words: pore-scale, smooth particle hydrodynamics, multi-phase, reactive transport, biogeochemistry

Introduction

Soil carbon processes are known to have a significant impact on the global carbon cycle[1]. Water content and local redox conditions of pore spaces in soil affect emissions of methane (CH_4), carbon dioxide (CO_2), and mono-nitrogen oxides (NO_x) generated from organic matter in soils. The critical processes of formation, transport, and transformation of these gaseous emissions occur in soil pore spaces. We simulated the physical phenomenon of flow of wetting phase (water) and non-wetting phase (gas) at pore-scale using a smoothed particle hydrodynamics (SPH) model[2]. We coupled this flow model with a multi-phase microbiological and chemical reactions model[3] to predict the chemical composition of liquid and gas phases. With the use of this combined model we are able to simulate the processes of formation, transport, and transformation of critical greenhouse gaseous emissions.

Brief Description of Work

Model A three-dimensional spatial domain of soil micro-pore system was discretized into particles of solids, water, and gas phases as shown in Figure 1. Water and gas phase particles are mobile due to the effects of gravity and viscous forces. The solid phase particles are held immobile and free of any deformation. Solid particles represent microporous soil aggregates, are assumed to be fully saturated, and can contain dissolved chemical and microbiological components. The water phase particles also contain dissolved chemical and microbiological components while the gas phase particles are composed of gaseous chemical components. We use chemical potential of components along with diffusion constants for the partitioning of relevant chemical components between different phases. Reaction processes include kinetic microbiological and kinetic and equilibrium chemical reactions.

Simulations and Results The SPH multiphase flow and reactive transport model was executed on an HPC cluster to simulate: (1) the formation of CH4 and CO2 from anaerobic biodegradation of organic matter; (2) transport of these gases in a three phase micro-pore system; and (3) transformation of CH_4 in micro-pores in presence of oxygen.

Figure 1: A three-phase decomposition of soil-pore system.

Using the model described above we are able to simulate processes critical to greenhouse gas emissions from soils.
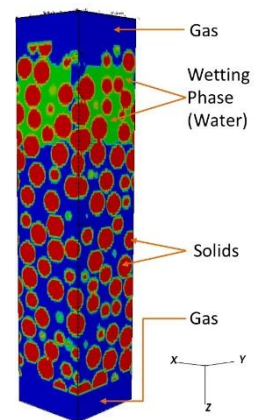
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Pore-Scale Simulation of sCO2/Brine Dissolution

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Stanford University

Key words: pore-scale, multiphase flow, mass transfer, residual trapping

Introduction

There is growing interest in Geological Carbon Sequestration to reduce atmospheric CO2 emission from fossil fuel combustion. In such process, the CO2 under supercritical state (sCO2) is first injected into deep geological formations to drain the brine that occupies the pore space. Then, brine injection or natural groundwater flow displaces the previously stored CO2. During this imbibition process, sCO2 droplets are trapped in the pores. This residual trapping is generally accepted as an important mechanism for immobilizing CO2 and thus, contributing to storage security. The dissolution of sCO2 into the brine raises the question whether trapping is permanent or not. Under such conditions, phenomena like Ostwald ripening might occur and cause a remobilization of the sCO2 clusters.

The goal of this study is to examine the stability of trapped CO2 at the pore scale, using direct simulation in order to improve our understanding of the different mechanisms involved.

Materials and Methods

To simulate immiscible two phase processes such as drainage and imbibition we solve Navier-Stokes equations with the volume of fluid method implemented in the CFD software OpenFOAM [1]. In addition to the multiphase flow, the concentration of CO2 in both phases is tracked following the method proposed by Haroun et al. [2]. In this technique, the mass transfer across interfaces obeys Henry's law and this concentration jump is considered using an additional term in the concentration equation, in the spirit of the continuum surface force that models the surface tension [3].
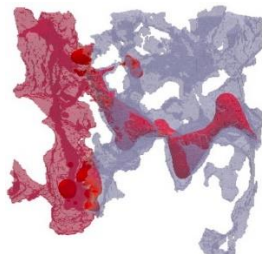

Figure 1: Simulation of a drainage in the pore-scale: a non-wetting fluid displaces a wetting fluid.

This method is also extended to allow a phase change induced by mass transfer at the fluid/fluid interface: when the thermodynamics condition is not respected, a diffusive flux of CO2 across the interface occurs and is responsible for a change of the interface position.

Results and discussion

We can now simulate at the pore-scale the different stages of CO_2 sequestration by direct numerical simulations. Figure 1 illustrates a drainage in the pore space of a carbonate, scanned with microtomography imaging. These simulations allow us to better understand the mechanism of residual trapping.

The concentration of CO_2 in both phases is plotted in Figure 2. There is an accumulation of the component in the residual water due to the mass transfer across fluid/fluid interface. Eventually, this mass transfer by diffusion drives the phase change, and the sCO_2 disappears.

Figure 2: Concentration profile of CO_2

These simulations at the pore-scale provide reference data to upscale the results at Darcy scale and therefore obtain the dependency of effective properties such as the mass transfer coefficient or dispersion tensor with regard to the flow conditions [4].

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Quick Estimation of Connectivity and Bypassed Volumes After Waterflooding in Geologically Realistic Models of Aquifers/Oil Reservoirs

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Key words: EOR, Waterflooding, Percolation

Introduction

Geological heterogeneity affects the flow of water through both aquifers and oil reservoirs. This may result in the bypassing of contaminants or oil. The extent of this bypassing is normally assessed using numerical simulation. The problem with this approach is that the exact pattern of hydraulic conductivity in the subsurface is usually uncertain and yet a very fine grid is needed to resolve all the different length scales of geological heterogeneity that may impact the flow. The solution is usually to perform a Monte Carlo simulation create numerous realizations of the hydraulic conductivity pattern and then perform an expensive, multi-phase simulation of flow in each realization. Each such simulation can take many hours of CPU time which often prohibits the proper assessment of impact of the geological uncertainty on the bypassed volume of contaminants/oil. In this paper we present an algorithm to quickly estimate the bypassed volume of contaminants or oil when water is injected into a geologically heterogeneous aquifer or oil reservoir.

Model

We use a percolation based assessment of the connectivity of hydraulic conductivity pattern. These ideas have been used previously in low net to gross systems. King et al [1] adapted the approach for use in systems with smoothly varying hydraulic conductivity. Such approach was based in the hypothesis that hydraulic conductivity is controlling by high permeability regions setting a permeability threshold to separate the system in good and bad permeabilities. The connected cluster (i.e. the cluster connecting both, the water inlet and oulet) of good sand resulting of the application of such a permeability threshold is then associate to hydraulic pattern. Such a model has been proved useful in system having a high permeability contrast but it usually fails when the permeability distribution of the system presents soft permeability variation and high spatial dependence. We propose to use the local permeability distribution in order to detect the flow pattern.

The algorithm incorporates a dynamic behaviour having into account the pressure drops between the injection point and the outlet and ensure mass conservation trough the system. We assign to each cell grid an occupation probability number depending on the permeability distribution of the surrounding cell grids. Then we define a threshold on the occupation values depending on the specific probability of occupation distribution obtained. Finally we use this occupation threshold to select on our system the most probable hydraulic conductivity pattern by detect the spanning cluster. Many realizations can be quickly performed in order to estimate the impact of the geological uncertainty. This algorithm can enable us also to detect the variation of the hydraulic connecting pattern as a function of the properties of the injected fluid.

Result

The algorithm is tested on a set of 85 2D synthetic models [2] of the Brent group of sandstones (a tidal-deltaic depositional environment). This set can be separate into two groups with a very different kinds of geologies. A group showing channelizing structures of high permeability surrounding by a background of low permeability and presenting a high permeability contrast between channels and background. The second group instead has a soft continuous distribution of permeabilities and strong spatial dependence, having in most of the cases extended regions of low permeabilities near to either the fluid inlet or outlet.

We will show the good agreement between the size and the shape of the regions detected by the present algorithm and the regions selected using the velocity pattern obtained from standard fluid simulation in both kind of geologies.

Finally we will show the differences between the regions detecting using the present model and the regions obtained using a percolation approach based just one permeability threshold.

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1-2: The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media

Time: Tuesday, 21/Jun/2016: 11:00am - 12:20pm – Location: MSB 3153

A Momentum-Based Approach to the Saturation Overshoot

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A Microfluidic and Numerical Modeling Investigation of Two- And Three-Phase Fluid Flow at Geologic Pressures and Temperatures

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Development and Testing of a Hysteresis Modeling Approach for the Two-Phase Flow Capillary Pressure- Saturation-Relative Permeability Relationship: Laboratory-Scale Analyses

Abdullah Cihan[1], Jens Birkholzer[1], Shibo Wang[1], Tetsu Tokunaga[1], Luca Trevisan[2], Tissa Illangasekare[3]

[1]Earth and Environmental Sciences, Lawrence Berkeley National Laboratory, United States of America; [2]Bureau of Economic Geology, Jackson School of Geosciences, University of Texas at Austin; [3]Center for Experimental Study of Subsurface Environmental Processes, Colorado School of Mines; acihan@lbl.gov

Stochastic Modelling of Two-Phase Flow in Heterogeneous Porous Media

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A Momentum-Based Approach to the Saturation Overshoot

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Key words: Saturation overshoot, water infiltration, momentum balance

Multiphase flow in porous materials is a phenomenon encountered in diverse engineering, geophysical, and biological applications. The question whether generalized Darcy's law is appropriate under any conditions has been extensively discussed in the literature. In this context, the problem of gravity-driven water infiltration in dry, homogeneous soils has attracted a particular attention as there is experimental evidence that the vertical saturation profile cannot be described by Richards equation, which is typically used for this class of problem.

At moderate water flow rates, the infiltration profile is non-monotone, exhibiting an overshoot of water saturation and pressure at the wetting front. Several models and numerical techniques have been proposed to reproduce this behavior, emphasizing the apparent shortcomings of traditional formalisms (Richards-like equations based on Darcy's law) and mostly involving the introduction of ad hoc terms.

The most natural way to deal with this observed phenomenon is to introduce a true momentum balance equation, which provides sound theoretical ground for the most salient features observed in the experiments. This solution is simple, reduces to the classical model in the limiting case, and has the advantage that classic numerical schemes introduced for the Navier-Stokes equation can be employed.

First, we introduce a macroscopic momentum balance equation and derive a simple form of the equation that can model the saturation overshoots and reduces to classical model under suitable conditions; then, we discuss the relationship with previously introduced models; finally we discuss the linear stability analysis and show some numerical simulations.

Figure 1: Numerical simulation of water infiltration with a full momentum-balance equation under two different regimes.

Reference

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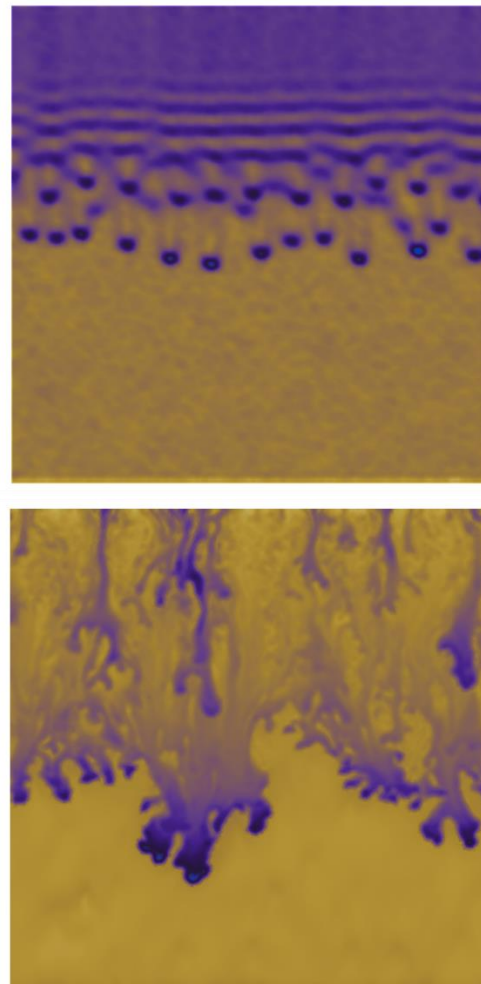[2] Lunati, I. and Ruiz-Baier, R. A momentum-based approach to the saturation overshoot. Submitted (2016).

A Microfluidic and Numerical Modeling Investigation of Two- And Three-Phase Fluid Flow at Geologic Pressures and Temperatures

Mark L. Porter[1], Jeffrey D. Hyman[2], Joaqu´ın Jim´enez-Mart´ınez[1]

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Key words: microfluidics, capillary pressure, specific interfacial area, stochastic pore space generation

Abstract

We describe a unique microfluidic experimental sys- tem for real-time observations of pore-scale fluid flow and transport in geo-material micromodels (e.g., shale, Portland cement, limestone) and engineered material micromodels at pressures (up to 10.34 MPa) and tem- peratures (up to 80 °C) commonly encountered in sub- surface reservoirs [1]. The use of geo-material micro- models allows us to investigate fluid-rock interactions including wettability, chemical reactivity, and matrix effects at conditions representative of natural subsur- face environments that cannot be recreated in engi- neered micromodels.

In this work, we present experimental observations of two- and three-phase flows involving supercritical CO_2 ($scCO_2$), brine, and oil in both shale and silicon micro- models. In these systems, the oil and brine are immis- cible, the $scCO_2$ and brine are partially miscible, with a solubility of $scCO_2$ in brine of approximately 5%, and the $scCO_2$ and oil is miscible, with a solubility of $scCO_2$ in oil of approximately 75%. This creates very interesting and complex fluid flow and transport dy- namics that we quantify using fluorescent microscopy. In particular, we investigate mixing in this three- phase system and show that heterogeneity in the brine sat- uration field enhances mixing between $scCO_2$ and oil, resulting in an increase in oil mobilization [2].

To further investigate these flow processes, we have conducted two- and three-phase flow lattice-Boltzmann (LB) simulations using Taxila LBM [3, 4]. In order to benchmark the LB model our simulations are con- ducted in simplified pore geometries. We compare two- phase flow experiments and simulations in the well known pore doublet–a pore structure consisting of a single channel that branches into two separate chan- nels and then reconnects back into one channel. With this pore structure we are able to compare experiments, simulations and theory. We also show an example LB simulation of three-phase immiscible flow in disordered porous media and preliminary simulations of three- phase flow in which one of the fluid pairs is partially miscible.

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Development and Testing of a Hysteresis Modeling Approach for the Two-Phase Flow Capillary Pressure-Saturation-Relative Permeability Relationship: Laboratory-Scale Analyses

Abdullah Cihan[1], Jens Birkholzer[1], Shibo Wang[1], Tetsu Tokunaga[1], Luca Trevisan[2], Tissa Illangasekare[3],

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Key words: two-phase flow, hysteresis, capillary trapping

Abstract

Understanding and predicting successively occurring drainage and imbibition processes in macroscopic porous media are important for many subsurface energy- and environment-related applications such as geological CO_2 storage (GCS), hydrocarbon extraction, and remediation of groundwater contaminated with non-aqueous phase liquids (NAPLs). Accurate modeling of these processes is needed for predicting and controlling fate and transport of the multiphase fluids in the subsurface. Both distribution and connectivity of void space at the pore scale play a major role for the capillary entrapment of wetting and non-wetting fluids and the hysteretic behavior in macroscopic constitutive models of the traditional two-phase flow theory. This work presents development and testing of an approach for mathematical representation of hysteretic capillary pressure-saturation-relative permeability relationship under capillary-dominated flow conditions based on pore-scale physical properties of the fluids and the porous medium. The approach presented uses distribution functions for void volume and fluid connectivity in the void space to compute the hysteretic constitutive functions and to predict capillary-entrapped fluid phase saturations. Two functions, i.e., the drainage connectivity function and the wetting connectivity function, are introduced to characterize connectivity of fluids in the void space during drainage and imbibition processes. These functions can be estimated through pore-scale simulations in computer-generated porous media or from traditional experimental measurements of primary drainage and main imbibition curves. The model predictions of capillary pressure-saturation curves under successive drainage and imbibition events, residual saturations and relative permeability functions were compared with the core-scale measurements obtained under quasi-steady state or equilibrium conditions in the literature. These comparisons indicated that the new hysteretic constitutive models could be promising to represent two-phase flow during successively occurring drainage and imbibition events in macroscopic porous media. To test the ability of the hysteretic two-phase flow modeling approach in predicting transient two- phase flow processes, the developed hysteretic constitutive models were incorporated into a numerical simulator solving the equations of the traditional two-phase flow theory. Then, the numerical model results were compared against spatial and temporal measurements of fluid distributions from several quasi-two-dimensional flow cell experiments with different dimensions (meter-scale), packed material types, and fluid pairs. All these flow experiments involved an injection stage where a non-wetting fluid is introduced into an initially wetting fluid-saturated porous medium, followed by a post-injection stage where the two fluids are redistributed according to the nature of the forces in the porous medium, mainly gravitational and capillary forces. During this presentation, the results of the model testing with the different sets of the transient flow experiments will be discussed to demonstrate some applications and shortcomings of the developed hysteresis models and the traditional two-phase flow theory.

Stochastic Modelling of Two-Phase Flow in Heterogeneous Porous Media

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Key words: stochastic galerkin, heterogeneous porous media, two-phase flow, finite volume method, mixed finite element method

Introduction

In many applications of natural and technical sciences macroscopic properties strongly depend on the structure of the underlying medium. The most obvious example are heterogeneous aquifers which contain e.g various rock layers or fractures. These heterogeneities may lead to a significant change of the flow behavior in the system. The assumption of an overall representative elementary volume (REV) in order to simplify the descriptive models of such heterogeneous porous media is not justified anymore. To avoid wrong simulation results one typically identifies specific subdomains with homogeneous hydrogeological properties within the heterogeneous porous medium [1]. However the parameter estimation and localization of the subdomains involves detailed information about the aquifer which is often limited. The use of purely deterministic models thus is not sufficient for the appropriate calculation of flow or the evolution of several fluids.

Deterministic Model

We consider two immiscible and incompressible fluid phases in a two dimensional heterogeneous porous medium. Moreover capillarity effects are neglected. In this case the fractional flow formulation reduces to a hyperbolic conservation law coupled with the elliptic flow equation. Each homogeneous subdomain is characterized by different nonlinear fractional flow functions and hydrogeological properties, e.g. intrinsic permeability. Due to the hyperbolic character of the transport equation and the heterogeneities in the medium, standing shock waves occur naturally at the position of the interfaces. Based on the implicit pressure explicit saturation (IMPES) approach we decouple the two types of equations. In the hyperbolic part an explicit finite volume (FVM) scheme is applied [2]. The elliptic part is discretized by mixed finite elements (MFEM) based on the FEM-toolbox Alberta [3].

Stochastic Model

There a different techniques to quantify uncertainties in porous media. Each has intrinsic assets and draw-backs. Collocations like methods are preferential in case of highly complex and high dimensional stochastic problems, but generally suffer from low convergence rates. We consider a hybrid stochastic galerkin (HSG) approach based on a multi-
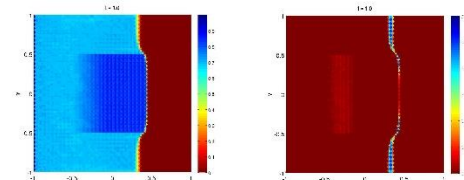

Figure 1: Expecation and variance of saturation
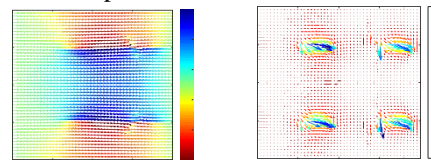

Figure 2: Expecation and variance of velocity

element decomposition in the stochastic space which is particularly well-suited for parallel computations [4, 5]. The unknowns saturation, global pressure and total velocity are expanded in terms of the truncated polynomial chaos expansion (PCE). As the random variable is assumed to be uniformly distributed the multiplication of the system by according Legendre polynomials yield a finite dimensional system which is partially decoupled in the stochastic space. Figure 1 and 2 show expectation and variance of saturation and velocity for a porous medium with heterogeneous lense.

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1-3: The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media

Time: Tuesday, 21/Jun/2016: 2:30pm - 3:30pm – Location: MSB 3153

Applicability of Vertically Integrated Models for Carbon Storage Modeling in Structured Heterogeneous Domains

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Multiscale Vertically-integrated Models with Vertical Dynamics for CO_2 Migration in Heterogeneous Geologic Formations

Bo Guo[1], Karl Bandilla[1], Jan Nordbotten[2], Michael Celia[1], Eirik Keilegavlen[2], Florian Doster[3]

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Applicability of Vertically Integrated Models for Carbon Storage Modeling in Structured Heterogeneous Domains

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Key words: geologic carbon storage modeling, vertically- integrated approaches, model applicability

Numerical modeling is an essential tool for studying the impacts of geologic carbon storage (GCS). Injection of carbon dioxide (CO_2) into the subsurface leads to multi-phase flow (injected CO_2 and resident brine), geomechanical effects due to an increase in formation pressure, and geochemical effects due to co-dissolution of CO2 and brine. However, previous studies have shown that the feedback from geomechanical and geochemical effects on flow properties is usually insignificant, so that multi-phase flow can be modeled independently of geochemical and geomechanical effects. The multi-phase flow is described by a set of three-dimensional governing equations, including mass-balance equation, volumetric flux equations (modified Darcy), and constitutive equations. This is the modeling approach on which commonly used reservoir simulators such as TOUGH2 are based. Due to the large density difference between CO_2 and brine, GCS models can often be further simplified by integrating the three- dimensional governing equations in the vertical direction. The integration leads to a set of two-dimensional equations coupled with reconstruction operators for vertical profiles of saturation and pressure. Vertically-integrated approaches have been shown to give results of comparable quality as three- dimensional reservoir simulators when applied to realistic CO_2 injection sites such as the upper sand wedge at the Sleipner site [1].

In the study reported here, we investigate the applicability of vertically-integrated models for more challenging geologies; in particular we are interested in formations with fluvial deposition environments. We compare the performance of vertically-integrated models to three-dimensional models for a set of hypothetical test cases consisting of high permeability channels (streams) embedded in a low permeability background (floodplains). The domains are randomly generated assuming that stream channels can be represented by sinusoidal waves in the plan-view and by parabolas for the streams' cross-sections. Stream parameters such as width, thickness and wavelength are based on values found at the Ketzin site in Germany [2]. Randomly generated channels are placed into the model domain until a threshold criteria is reached (e.g., 30% of model volume consists of stream channels). Cross-sections of two test cases are shown in Figure 1
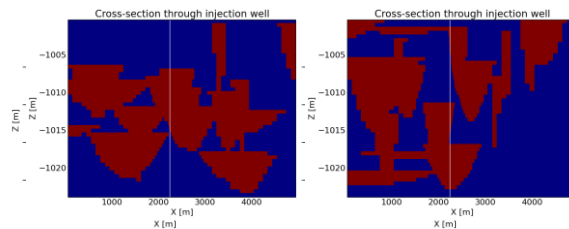

Figure 1: cross-sections through two randomly generated formations with fluvial deposition environment; red represents high-permeability stream deposits; blue represents low-permeability floodplain deposits; the white line represents the location of the CO_2 injection well; vertical exaggeration is about 1:200.

The vertically-integrated approaches are compared to results from the three-dimensional reservoir simulator TOUGH2/ECO2N based on CO_2 saturation profiles, and CO_2 arrival time and pressure response in monitoring wells. Several different vertically- integrated approaches are used, including single- and multi-layer vertical-equilibrium with capillary transition zone approaches and dynamic reconstruction approaches.

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Multiscale Vertically-integrated Models with Vertical Dynamics for CO$_2$ migration in Heterogeneous Geologic Formations

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Key words: Multiscale modeling, vertical integration, dynamic reconstruction, CO2 sequestration

Efficient computational models are desirable for simulation of large-scale geologic CO$_2$ sequestration. Vertically-integrated models, which take advantage of dimension reduction, offer one type of computationally efficient model. The dimension reduction is usually achieved by vertical integration based on the vertical equilibrium (VE) assumption, which assumes that CO$_2$ and brine segregate rapidly in the vertical due to strong buoyancy and quickly reach pressure equilibrium. However, the validity of the VE assumption requires small time scales of fluid segregation, which may not always be fulfilled, especially for heterogeneous geologic formations with low vertical permeability [1]. Recently, Guo et al., (2014) [2] developed a multiscale vertically- integrated model that relaxes the VE assumption by including the vertical two-phase flow dynamics of CO$_2$ and brine as a fine-scale one-dimensional problem in the vertical direction. Although the VE assumption can be relaxed, that model is limited to homogeneous geologic formations. Here, we extend the multiscale algorithm of Guo et al., (2014) [2] for layered heterogeneous formations, which is of more practical interest for saline aquifers in sedimentary basins. We develop a new coarse-scale pressure equation to couple the different coarse-scale (vertically-integrated) layers, while using the fine-scale dynamic reconstruction algorithm in Guo et al., (2014) [2] inside each individual layer. Together, these form a multiscale multilayer dynamic reconstruction algorithm, which we refer to as the MLDR model (see Figure 1).

Comparisons of the MLDR model with a widely used full three-dimensional simulator (TOUGH2) show excellent agreement between these two models (see Figure 2). The MLDR algorithm leads to significant decrease of computational effort, which makes it much more computationally efficient than conventional full three-dimensional models.

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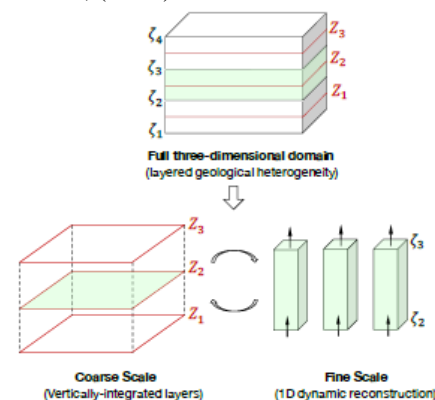
Figure 1: Schematic of the multiscale multilayer dynamic reconstruction algorithm, with three layers as an example. The fine-scale columns belong to the coarse-scale layer, and here we take the columns of the second layer (Z_2) as an example. The arrows in the columns represent CO$_2$ and brine fluxes from layer Z_2 to layer Z_3 and from layer Z_1 to layer Z_2 at the layer boundaries.
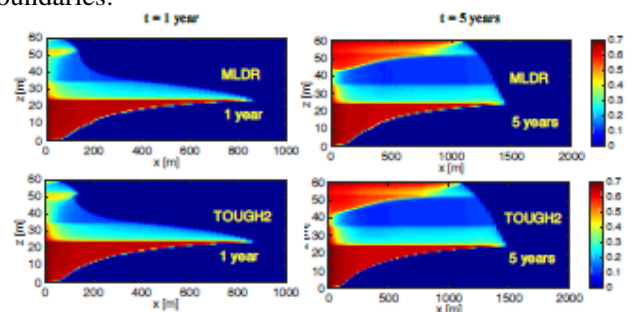

Figure 2: CO2 plume comparison between the MLDR model and TOUGH2 for a four-layer formation with geologic parameters based on Mt Simon formation. The first row shows the CO$_2$ plume from the MLDR model and the second row shows that from TOUGH2.

1-4: The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media

Time: Tuesday, 21/Jun/2016: 3:50pm - 5:30pm – Location: MSB 3153

An Original and Useful Approach to Mesh a Discrete Fracture Network Using a Delaunay Triangulation: Application on Flow and Transport Upscaling From Characterization Scale to Reservoir Scale

André Fourno[1], Benoit Noetinger[1], Christian La Borderie[2]
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The Effect of Fracture-Matrix Interactions on Multiphase Flow in Fractured Reservoirs: Development of A Discrete Fracture Model

Yue Hao, Randolph R. Settgast, Andrew F. B. Tompson, Pengcheng Fu, Joseph P. Morris, Frederick J. Ryerson
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A Lattice Boltzmann Approach to Model Radionuclides Diffusion through Unsaturated Arigillite Micro-Fractures

Alain Genty[1], Soukaina Gueddani[2], Magdalena Dymitrowska[2]
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Pore-Scale Studies of Moisture Transport in Highly Swelling Porous Media

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Numerical Study of Biofilm Growth in Porous Media

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Computational Methods
in Water Resources 2016

An Original and Useful Approach to Mesh a Discrete Fracture Network Using a Delaunay Triangulation: Application on Flow and Transport Upscaling From Characterization Scale to Reservoir Scale

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Key words: fractures, conform mesh, upscaling

Introduction

Modeling mass and heat transfers in fractured media is a challenge. That is due to the geometrical complexity of the discrete fracture network (DFN) and the remaining input data uncertainties. As an illustration, in the field of CO2 sequestration or oil reservoir production, transfers have to be modeled at the scale of reservoirs ($\approx 10km * 10km$) using $\approx 100m * 100m * 10m$ grid cell sizes, [1]. However, fractures are finely characterized on well logs and outcrops (at a scale of few meters). From this characterization a DFN can be built and may contain over 106 fractures. Analogous issues are to be addressed for hydrology and geothermal applications. Direct numerical simulations taking into account the DFN geometry remain still impossible at the reservoir scale. In practice, upscaling approaches are used to determine equivalent transfer parameters at the grid cell scale. The number of fractures belonging to a grid cell and respecting data from characterization scale may be close to 103 fractures. This number is more tractable and direct numerical simulation may be used at this step.

Nevertheless, considering the complexity of the DFN geometry, it still remains to simplify the DFN mesh, considering assumptions about the details of the flow [2, 3, 4]. In order to test the accuracy of these assumptions, reference numerical simulations must be carried- out using a mesh which accounts for the detailed DFN geometry [5].

The goal of this paper is to present an original 3D DFN mesh approach allowing to get high fidelity reference simulations and allowing to test further simplifications required by applications.

DFN mesh and applications

Basic idea In our approach, the basic idea is to broke each DFN fractures into a large number of connected closed outlines. Special focus is put on common outlines boundaries to generate a conforming Delaunay triangulation. The advantages of this mesh are to be conform and to closely respect the geometry of the DFN.

Preliminary results using this approach, implemented in Cast3M, a large number of complex DFN models has been

modeled, Figure 1. Flow is simulated on this mesh, Figure 2, and post-treated to obtain upscaled parameters at the reservoir grid cell scale. Transport simulation is an ongoing work that will be presented during the conference.
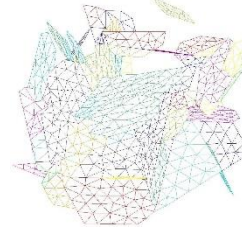

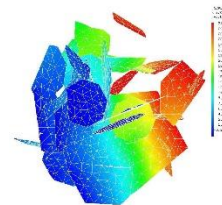*Figure 1:* Mesh of 33 fractures belonging to a 3m grid cell

Figure 2: Simulated pressure field

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The Effect of Fracture-Matrix Interactions on Multiphase Flow in Fractured Reservoirs: Development of a Discrete Fracture Model

Yue Hao, Randolph R. Settgast, Andrew F. B. Tompson, Pengcheng Fu, Joseph P. Morris,
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Multiphase flow and transport phenomena in fractured rocks occur in a variety of subsurface applications, from deep geological CO2 storage to groundwater remediation. Another important example of multiphase flow between fractures and matrix rocks is related to hydrocarbon production from hydraulically fractured shale and other low permeability reservoirs. Production of shale gas/oil is dependent on the immediate release of "trapped" hydrocarbon fluids intercepted by the hydraulically- induced fractures towards production well bores and the somewhat longer transient migration of hydrocarbon fluids from formation matrix rocks to nearby fractures. Understanding and quantifying processes that affect the movement and distribution of fluids between fractures and matrix rocks are critical for prediction of hydrocarbon production, and may provide the key to sustainable productivity. The continuum modeling approaches (e.g. dual continuum or multiple interacting continua models), in which the fracture and matrix systems are treated as separate overlapping continua, have been widely used for simulating multiphase flow in fractured rocks. However, fracture-matrix communication in the continuum models cannot viably describe localized or highly transient conditions in individual fracture and matrix blocks, especially in low permeability rocks.

In this study we develop a discrete fracture model with an explicit representation of both individual fractures and their surrounding rock matrix, therefore providing a more precise description of multiphase flow behaviors at the fracture-matrix interface which the continuum method is difficult to reproduce. A cell-centered multi-point flux approximation (MPFA) finite volume (FV) method is used to handle complex fracture networks and heterogeneous geologic formations with anisotropic permeability. The discrete fracture model is implemented in the GEOS framework, which is a LLNL- developed, massively parallel and multi-physics simulation code, allowing for high fidelity matrix-fracture flow simulations. We apply the developed discrete fracture model to simulate water-oil displacement processes in a low permeability reservoir, and in particular examine the viscous and capillary-driven fluid movements across the fracture-matrix boundary and their effects on hydrocarbon production. Numerical results indicate that the discrete fracture model is able to adequately capture the saturation discontinuity due to capillary heterogeneity across the boundary between fractures and low permeability matrix. In addition the discrete fracture model developed in this study will not only help develop a more accurate understanding of impacts of fracture-matrix interactions on multiphase flow processes, but also provide a useful basis for upscaling multiphase flow and transport from discrete fracture to field scales.

A Lattice Boltzmann Approach to Model Radionuclides Diffusion through Unsaturated Arigillite Micro-Fractures

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[2]Commissariat à l'Energie Atomique et aux Energies Alternatives, France;

Key words: Effective Diffusion, Unsaturated Fractures, Argillaceous Porous Media

Introduction

In the context of radioactive waste management, deep geological repository in indurated argillaceous media is considered as a potential solution. Radionuclides transport through argillaceous media is then of concern and some works focused on the Excavated Damaged Zone (EDZ) surrounding the vaults and the galleries of the repository. Indeed, argillaceous media in the EDZ presents some micro-fractures where radionuclides transport through diffusion can be enhanced and EDZ is considered as a potential preferential pathway and deserve a particular attention.

Micro-fractures can be fully saturated or not depending on their location and on the flows history inside the repository. Saturation level of the fractures can result from desaturation process during the excavation phase or from hydrogen flow where hydrogen is produced from corrosion of the waste metallic canisters after repository closure. In this work, we will focus on radionuclide diffusion through unsaturated micro-fractures.

In order to simulate diffusion process inside micro-fractures geometry, we chose to use a Lattice Boltzmann Model (LBM) that allows i) to easily represent the fracture geometry available from X-ray tomographic images, ii) to simulate water-gas distribution inside the fracture for different saturation levels, and iii) to simulate diffusion inside the resulting connected water pathway.

Lattice Boltzmann Model

The LBM we used in this work is based on a Two-Relaxation-Time (TRT) collision operator. Water-gas distribution was simulated using the LBM described in [1] which follows the Shen-Chen approach through a particular source term. Diffusion simulation in the resulting water connected pathway was conducted using the same procedure than the one described in [2] and allows the computation of the effective diffusion coefficient for the considered fracture.

Results

We conducted diffusion simulations for different saturation in a micro-fracture presenting an average aperture of about 2 µm. Computations were performed starting from an initial Dirac imposed concentration in the center of the fracture. An example of computed concentration distribution after 300 time steps inside the fracture for a saturation value of 0.78 is shown on Figure 1.
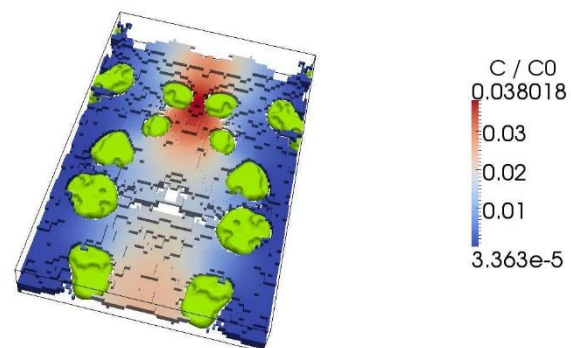

Figure 1: Concentration field inside a micro-fracture filed with gas bubbles (in green) at saturation of 0.78.

Effective diffusion coefficient was computed as a function of fracture saturation from our diffusion simulations. The effective diffusion coefficient behavior was found to be non-standard close to high saturation value.

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Pore-Scale Studies of Moisture Transport in Highly Swelling Porous Media

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Key words: Swelling particles, super absorbent polymer particles, pore-scale finite volume model,

Introduction

Swelling is an important mechanism in numerous biological processes and industrial products, such as biological tissues, fuel cells, and super absorbent polymer (SAP) particles in hygienic products. The commercial design of hygienic products is based on the cost efficient use of super absorbent polymer grains. These grains can absorb water up to hundred times their own volume. Insight is needed in grain- scale processes and their role in the macro-scale description of these media. In particular, information on the grain scale is needed for developing mass transfer equations for macro-scale descriptions. For this purpose, pore-scale models are powerful tools for the pore-scale study of flow and solute transport processes and subsequent extension to the macro scale.

Description of Research

In this research, first, we study the swelling of individual highly absorbing grains under microscope. This allows us to develop relationships for the swelling kinetics of individual grains. Results are used in a grain-scale model of a bed of SAP particles. For grain-scale simulations, we use the open source software Yade-DEM. It is based on an Explicit Discrete Element Method (DEM) for simulating interactions between solid particles, taking into account elastic-frictional contact laws. The pore fluid movement is simulated using a pore-scale finite volume method (PFV). Poro-mechanical coupling is taken into account (Chareyre et al., 2012). By coupling both techniques (DEM and PFV), the mechanical interactions between pore fluid and particles can be simulated. The model is well suited for simulating swelling porous media with a deformable porous skeleton. We perform swelling experiments on a bed of particles and monitor the height of the swelling bed with time (Figure 1). Results of these macro-scale experiments are used to verify our grain-scale modelling. We will present experimental and modelling results on swelling of super absorbent polymer grains, under partially saturated conditions.
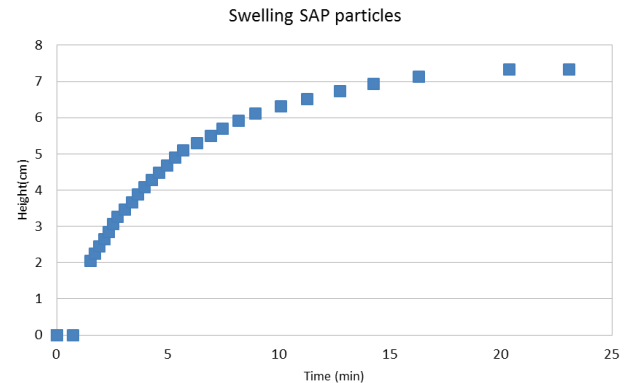

Figure 1: Increase height of a bed of swelling particles with time

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Numerical Study of Biofilm Growth in Porous Media

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Key words: Porous media, solute transport, Biofilm, Cellular Automaton, Lattice Boltzmann, Immersed boundary, NAPL Dissolution, Bioenhanced dissolution of NAPL.

Introduction

Mathematical modeling of transport in porous media of organic chemical species in the presence of a bacterial population growing in the form of biofilms is an important area of research for environmental and industrial applications such as the treatment and the remediation of groundwater contaminated by organic pollutants. Biofilms, which are composed of bacteria and extracellular organic substances, grow on the pore-walls of the porous medium. Biodegradable organic solutes are converted into biomass or other organic compounds by the bacterial metabolism. This evolution of the microbial biomass phase within the porous medium is a complex process due mainly to growth (or decay) and spatial spreading of the cellular phase [1]. Processes such as biofilm sloughing and attachment (or detachment) of cells from the fluid phase may also contribute to the biofilm volume variation. In this context, I focus on the mechanisms that control the development of biofilms in porous media and its impact on the hydrodynamic properties of the porous matrix.

Mathematical Model

To model the pore-scale phenomenon of biofilm

growth we integrate various mechanisms which favor the bacterial development (bacterial proliferation, assimilation of nutrients to synthesize new cellular materials, attachment of cells) or, conversely, which are responsible for slowing down (e.g., detachment of cells, toxicity).

An Immersed Lattice Boltzmann Model (IB-LBM) is developed for flow calculation and non-boundary conforming finite volume methods (volume of fluid and reconstruction methods) are used for reactive solute transport [2].

A quasi-steady approach - based on the disparity of time scales - is classically considered to describe the coupling with mass transport and bacterial growth. If the flow and mass balance equations are rigorously solved at the pore-scale, a sophisticated cellular automaton model is developed to describe the spatial distribution of bacteria.

Several numerical simulations have been performed on complex porous media and a quantitative diagram representing the transitions between the different biofilm growth patterns was proposed.

Finally, the bioenhanced dissolution of NAPL in the presence of biofilms was simulated at the pore scale.

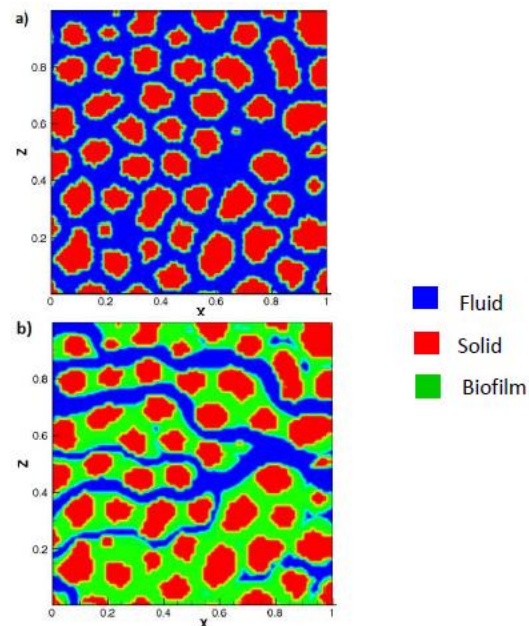The impact of biosurfactants and NAPL toxicity on bacterial growth has been investigated.

Figure 1: a) initial porous medium, b) Simulation of biofilm development at Pe=500, Da=0.1. Appearance of preferential flow paths because of detachment.

References

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1-5: The Pore to Field-Scale Conundrum: Modelling Multiphase Flow and Transport in Porous Media

Time: Wednesday, 22/Jun/2016: 11:00am - 12:20pm – Location: MSB 3153

Complementary constraints on componential multiphase flow problems, should it be implemented locally or globally?

Yonghui Huang[1,2], Haibing Shao[1,3], Martin Thullner[1], Olaf Kolditz[1,2]

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Modelling of Morphology and Petrophysics of Nummulitic Carbonate Rocks

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Impact of the Viscous-Capillary Force Balance on Flow in Layered Porous Media

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A formulation for non-isothermal multiphase multicomponent flow with geochemical reactions

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Numerical simulation of Thermo-Hydro-Chemical processes and multiphase flow in porous media for efficient in-situ remediation of chlorinated solvents

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Complementary Constraints on Componential Multiphase Flow Problems, Should it Be Implemented Locally or Globally?

Yonghui Huang[1,2], Haibing Shao[1,3], Martin Thullner[1], Olaf Kolditz[1,2]

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Key words: multiphase flow, phase transition, complementary condition, thermodynamic equilibrium

Introduction

In applications of CO_2 sequestration, nuclear waste repository, and NAPL contaminated groundwater sites, fully miscible compositional multiphase flow is considered to be the most important physical process. In particular, the behavior of phase appearance and disappearance is critical to the performance of georeservoirs, and it has been a challenge in the scientific community to numerically simulate this strongly coupled process.

The conventional approaches that handle phase transition problem suffer from some specific constrains [1, 2]. For example, two-phase two-component condition is commonly assumed. At location where phase transition happens, saturation may suffer over- and undershoot, and both the special and temporal discretization has to be kept small in order to suppress the numerical oscillation.

Recently, a new approach incorporating the nonlinear complementary constraints has been introduced to handle the nonlinearity from phase transition [1]. The conditions for the (dis)appearance of a given phase can be formulated as Nonlinear Complementary Problems (NCP) which can be then resolved by Semi-smooth Newton scheme. This approach is demonstrated to be efficient and robust in many applications [3].

Method Comparison

This work is devoted to the efficiency comparison of two formulations based on different approaches of implementing nonlinear complementary constraints.

Global-NCP approach. It incorporates the NCP as one "governing equation", and saturation is selected as an extra primary variable. Combined with mass and energy balance equation, the global system is solved by semi-smooth Newton iteration.

Local-NCP approach. The NCP is embedded within constitutive relationships to construct the local problem for all the secondary variables. Semi-smooth Newton iterations are performed on each grid node, while standard Newton iteration is used to solve the global mass and energy balance equation.

The two formulations are compared based on three numerical benchmarks of multi-components two- phase flow process. Complex physical scenario settings are considered, including thermal effects and heterogeneous porous medium with strong gravity.

Conclusions

The two formulations lead to quite similar simulation results with the same level of accuracy. However, from the perspective of computational effort, Local- NCP model is more time-consuming, as it requires more Newton iterations to converge. Furthermore, Local-NCP model requires significantly more assembly time due to the higher non-linearity on each grid node. It can be concluded that by shifting the non-linearity from local to global governing equations lead to a more efficient and stable numerical solution for the componential multiphase problem.

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Modelling of Morphology and Petrophysics of Nummulitic Carbonate Rocks

Zeyun Jiang, Alessandro Mangione, Helen Lewis, Gary Couples

Heriot-Watt University, United Kingdom;

Key words: Nummulites, dolomitisation, diagenetic backstripping, morphological model, petrophysics.

Introduction

Carbonate rocks usually show a complex distribution of heterogeneities at different length scales that are associated with depositional processes and complex diagenetic history. Very often, it is desired to calculate the petrophysical properties at a prior state of diagenesis, which might be used as input in basin modelling, for instance. Here, we describe numerical methods that allow us to understand the possible petrophysical states at key moments in the geological history of a study reservoir.

We focus on a fossiliferous, partly-dolomitised carbonate. Dolomitisation has completely replaced the micrite ("mud") that existed between the fossils enhancing reservoir quality. The Nummulites (fossils) are distributed within the micrite in some characteristic patterns. Dolomitisation has partly or completely dissolved the Nummulites creating local macro-porosity. The pore system of this nummulitic rock thus has two different length scales ([1]). In order to get insight into how the rock morphological structure governs the petrophysical properties, we need to consider how the pore systems are connected within each scale and across these scales. We employ a new methodology ([2]) combining multi-scale pore structures, derived from several imaging methods, into a single pore-scale network. The major petrophysical properties (e.g. porosity, permeability, capillary pressure) can then be calculated, and two-phase drainage/imbibition simulations can be carried out.

To address the variability of the diagenetic processes, we generate three synthetic micrite models, composed solely of micro-pores, that cover the range of porosity and permeability suggested by the literature at the depth at which dolomitisation is believed to occur. We obtain 3D XCT images of the two Nummulites fossil forms, allowing us to generate models (see Figure 1) containing multiple Nummulites via a set of control arguments such as density, orientation, size and types of interaction with neighbouring micro-pores. The latter issue is addressed by creating a connection region between each Nummulites and its neighbouring micrite/dolomite matrix, with pores in both materials being available to be connected or not, based on

some simple geometric measures. Using this approach, we create multiple, realistic models of Nummulitic rocks with a combined two-scale pore structure.

Our flow simulations show that in the micrite models, Nummulites act as baffle to flow. In models using the dolomite matrix, partly-cemented or non-cemented Nummulites have practically no impact, whereas biomouldic porosity created by Nummulites corrosion enhances reservoir quality. This behaviour is confirmed by comparison with a routine core analysis dataset.
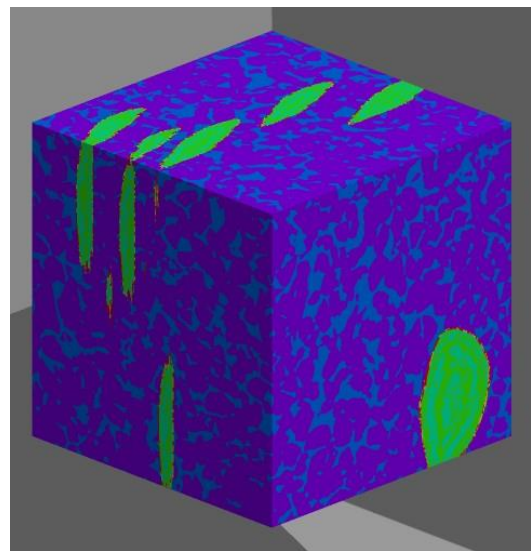

Figure 1: Structure model of Nummulitic rocks

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Impact of the Viscous-Capillary Force Balance on Flow in Layered Porous Media

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Key words: Layered porous media, Dimensionless numbers, Crossflow, Capillary trapping

Motivation Geological heterogeneity occurs over a broad range of length scales, from the pore- to the reservoir-scale, and exerts a first-order influence on multiphase flow relevant to geological carbon storage and hydrocarbon recovery. Most studies that investigate the interaction of multiphase flow and geological heterogeneity focus on a particular reservoir, outcrop or heterogeneity type, using a particular suite of fluid and rock properties and a particular flow scenario. It is usually not possible to extrapolate the results of such studies to new or alternative cases; moreover, they fail to provide simple criteria that can be used to rapidly assess the impact of heterogeneity on flow prior to the development of detailed models. An alternative view is that geological heterogeneities can be captured by a number of key dimensionless geometries observed in numerous depositional environments and over a broad range of length scales. Likewise, flow through a particular type of heterogeneity geometry can be captured by a small set of dimensionless numbers. We investigate here whether the interaction between flow and geological heterogeneity can be captured by a small set of dimensionless heterogeneity models and dimensionless numbers. The aim is not to predict exactly the behaviour of a given system; rather, it is to (i) predict how the system will change as parameters are varied, and (ii) provide a framework to understand the behaviour of complex systems

Focus of this work Here we focus on the impact of viscous and capillary forces on flow parallel and perpendicular to continuous layers of contrasting material properties. Such layers are a ubiquitous geological heterogeneity observed at many length scales, including lamination (millimetre-thick layers), bedding (centimetre- to metre thick layers) and laterally extensive genetic stratigraphic units that may correspond to flow zones in groundwater aquifers. We define a set of dimensionless numbers, some of which are common to flow both parallel and perpendicular to layering, such as the longitudinal permeability ratio σx and the ratio Rs of the storage capacities (moveable pore volumes, MPV) in each layer, and some of which are specific to a given flow direction, such as the dimensionless capillary to viscous ratios Ncv defined differently for layer-parallel and layer-perpendicular flow, and the effective aspect ratio RL that quantifies crossflow for layer-parallel flow. We examine how variations in the dimensionless numbers affect the trapping efficiency, defined as the fraction of the MPV occupied by the injected phase after 1 MPV injected. The results are directly applicable to geological carbon storage.

Results We find that the flow behaviour – expressed here in terms of the trapping efficiency – is clearly controlled by the dimensionless numbers. For example, when flow is perpendicular to layering, we show that heterogeneity only influences flow when capillary forces are significant ($Ncv > 0$). As Ncv is increased, a larger fraction of the non-wetting phase is trapped if the layers have contrasting capillary pressure curves 1. When flow is parallel to layering, both viscous and capillary forces are important. Viscous forces cause the ratio of the fluxes along each layer to be equal to the permeability ratio σx and, in the viscous limit ($Nvc = 0$), heterogeneity reduces storage efficiency if σx j= Rs 2. As capillary forces become more significant (Ncv increases) and if crossflow between layers can occur ($RL > 0$), the storage efficiency also increases in response to capillary crossflow and reaches a maximum at a given Ncv. At lower Ncv, capillary crossflow is reduced and the injected phase preferentially moves through the high permeability layers, yielding reduced storage efficiency. At higher Ncv, the benefit of crossflow is outweighed by along layer diffusion of the injected phase, yielding reduced storage efficiency 3.

Applicability of the results The results allow for a rapid assessment of potential flow regimes and of their consequences in terms of storage efficiency. The results can additionally be used to assist the scaling of laboratory core-flooding experiments
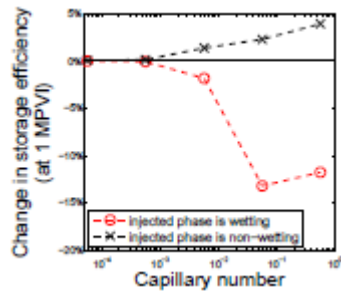
Figure 1: Change in storage efficiency (relative to efficiency obtained without heterogeneity) for flow across an alternation of identical layers vs. the capillary number
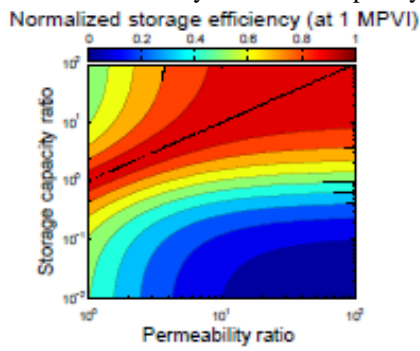

Figure 2: Storage efficiency (normalized w.r.t. efficiency obtained without heterogeneity) for viscous-dominated flow along layers vs. the permeability and storage capacity ratios
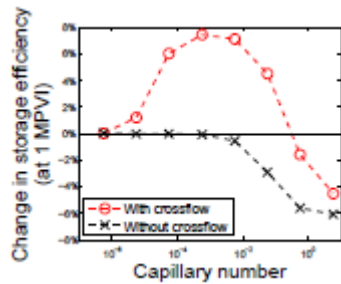

Figure 3: Change in storage efficiency (relative to efficiency obtained without capillary forces) for flow along layers vs. the capillary number.

A Formulation for Non-Isothermal Multiphase Multicomponent Flow with Geochemical Reactions

Fabian Brunner, Peter Knabner, Jens Oberlander

University of Erlangen-Nürnberg

Key words: multiphase flow, model preserving reformulation, fully implicit methods, complementarity problems, parallelcomputations

Introduction

In recent years, the geologic sequestration of carbon dioxide has been widely discussed as a technology to reduce greenhouse gas emissions into the atmosphere. To study the different trapping mechanisms associated with this technique, complex mathematical models are necessary, taking into account the flow of multiple phases consisting of multiple components, the exchange of mass between these phases, capillarity, and geochemical reactions. In this talk, we present a mathematical formulation for efficiently simulating the relevant processes with persistent primary variables using the global implicit approach.

Mathematical model

We study a non-isothermal partially miscible multi- phase multicomponent model in porous media involving general chemical reactions, which may be kinetic reactions or equilibrium reactions. More precisely, we admit homogeneous reactions between the components of the liquid phase and heterogeneous reactions between the liquid and the solid phase, e.g., sorption or mineral reactions. Moreover, the compressibility of the phases and the interphase mass exchange between the gas and the liquid phase is taken into account, which may lead to the appearance or disappearance of one of the phases. Due to the complex physical and chemical interactions, the resulting model is fully coupled and strongly nonlinear, which represents a challenge in the design of numerical solvers.

Variable transformation and choice of primary variables

The mathematical model is transformed using a model- preserving reformulation technique proposed in [2, 1], which eliminates the unknown equilibrium reaction rates and allows an elimination of the algebraic equations resulting from chemical equilibria in terms of a nonlinear, implicitly defined resolution function. Due to this local elimination process, the computational cost is reduced and parallel computations become more efficient. By choosing suitable primary variables and using a complementarity approach [3], interphase mass exchange and the local

appearance and disappearance of the gas phase can be handled. Moreover, our primary variables are persistent and remain valid for an arbitrary mineral assemblage within the domain. In the presence of heterogeneous equilibrium reactions, the inclusion of additional variables can significantly improve the condition number of the resulting linear systems.

Numerical approach and computational results

In our numerical framework, the above model is discretized based on a conservative Finite Element - Finite Volume discretization in space [4] combined with a fully-implicit treatment in time in order to preserve the nonlinear coupling of flow, transport, reactions, and mass transfer across phases. An upwind scheme is implemented to treat advection- dominance. The local nonlinear systems to evaluate the implicit resolution function and the global nonlinear system are both solved using the semi-smooth Newton method. In our numerical results, we show how the above formulation can be applied to simulate mineral trapping in the context of carbon sequestration. Our numerical results indicate that the formulation is well suited to handle vanishing phases and mass exchange due to chemical reactions.

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Numerical Simulation of Thermo-Hydro-Chemical Processes and Multiphase Flow in Porous Media for Efficient In-Situ Remediation of Chlorinated Solvents

Antoine Armandine Les Landes, Anne-Julie Tinet, Constantin Oltean and Michel Buès.

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Chlorinated solvents are widespread groundwater and soil contaminants often released as dense non aqueous phase liquids (DNAPLs). It is likely the most common pollution issues considering the amount of industries, process and activities using such products. These type of contaminants are difficult to remediate, specifically their source zones. In this context, heating can be an effective approach to improve the removal of volatile components. Thermal processes such as steam injection is known in petroleum engineering as one of the most effective methods to enhanced oil recovery from porous medium and has become an effective technique to remediate groundwater aquifers contaminated with VOCs (Volatile Organic Compounds). Due to the complex nature of thermal technics and cost-effective objective, optimization tools, development of predictive models and technical guidance materials are necessary.

Numerical models have become a valuable tool for managing and designing groundwater remediation systems, such as thermal operations. They may be used to understand the major processes controlling chlorinated solvent issue, integrate complex information on site hydrogeology and test different aspects of management and remediation system design. In this study, we present a multiphasic and thermo-hydro- chemical numerical model fully coupled for simulating multiphase flow (three-phase: water, gas and solvents), gas-phase multicomponent transport (air, water vapor and solvent vapor), heat and mass transfer (phase change such as vaporization and condensation) in porous media. This model uses the commercial finite element software COMSOL Multiphysics designed to address a wide range of physical phenomena. Model parameterization is done using in-situ measurements and simulations are realized with a two-dimensional axisymmetric model in porous media to simulate the processes occurring during thermal operation (Figure 1). A parametric study according to in-situ measurements provided design constraints (such as pressure cycling) on remediation system of the contaminated aquifer in order to improve efficiency. The numerical model allows the evaluation of the performance of in situ remediation technique applied. Evaluation is done

in regards to radius of influence (heating, gas saturation…) as well as the remediation efficiency (as function of various parameters: injection rate, air-steam proportion, etc.).

This work comes within a framework of one R&D project designed to develop and improve exploration and in situ remediation technics for chlorinated source zone in aquifer.
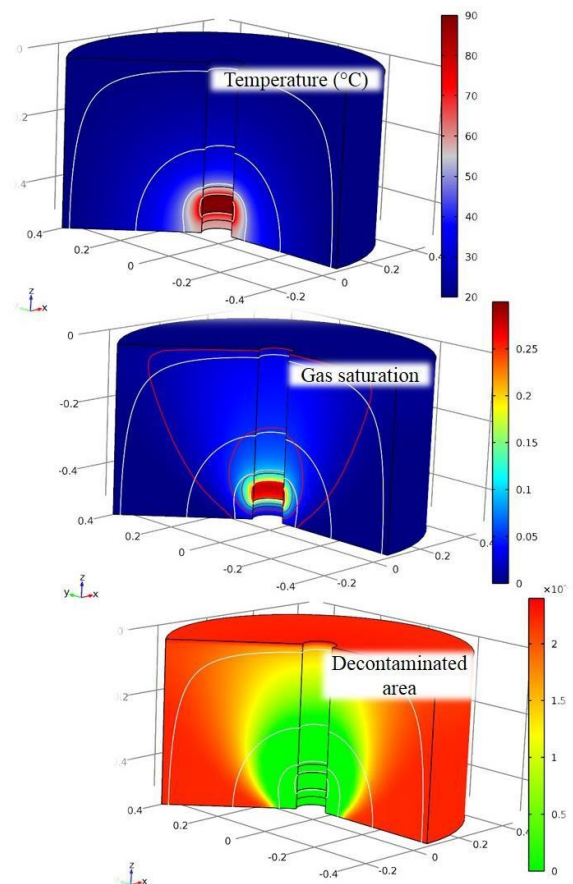

Figure 1. Temperature and gas distributions around the borehole and the associated decontaminated area

2-1: Mixing and Reaction across Scales in Hydrological Systems

Time: Tuesday, 21/Jun/2016: 9:40am - 10:40am – *Location: MSB 3154*

Confronting Experimental Measurements and Models for (Reactive) Transport and Mixing in Two-Dimensional Porous Media

Joaquin Jimenez-Martinez[1,2], Pietro de Anna[3], Régis Turuban[1], Hervé Tabuteau[1], Tanguy Le Borgne[1], Yves Meheust[1] [1]Univ. Rennes 1, France; [2]Los Alamos National Laboratory, Los Alamos, USA; [3]Univ. Lausanne, Switzerland; yves.meheust@univ- rennes1.fr

Competition between Mixing and Deformation and Its Role on Reaction Rates in Subsurface Fluid Flows

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Applicability Conditions for Sequential Homogenization of Reactive Transport in Bi-Disperse Porous Media

Svyatoslav Korneev, Ilenia Battiato
San Diego State University, United States of America; skorneev@mail.sdsu.edu

Confronting Experimental Measurements and Models for (Reactive) Transport and Mixing in Two-Dimensional Porous Media

Joaquin Jimenez-Martinez[1,2], Pietro de Anna[3], Régis Turuban[1], Hervé Tabuteau[1], Tanguy Le Borgne[1], Yves Meheust[1]

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Pore scale characterization of flow velocities and concentration spatial distributions is a key to understanding non-Fickian transport, mixing and reaction in porous media. We use millifluidic setups to investigate such processes in transparent saturated and unsaturated porous media, at the pore scale. The porous media are quasi-two-dimensional, consisting of a Hele-Shaw cell containing cylindrical grains. They are made by soft lithography with full control on a geometry containing thousands of grains. The setup allows for unsaturated flows, be it primary drainage/imbibition, or the injection of two fluids (f. e. water and air) at the same time. A camera positioned above the flow cell records the distributions of fluid phases, at regular times, providing also the position of solid tracers and spatially- resolved images of light emissions inside the flow cell. The pore scale velocity field is measured from the tracking of solid tracers (microspheres), while full pore scale concentration fields are measured accurately in passive transport experiments, using fluorescein and converting the emitted light intensities into solute concentrations. Pressure drops across the medium are also measured. This complete characterization of the system allows confronting the experimental pore scale data to numerical simulations and models that upscale transport and mixing properties. We shall in particular discuss the example of mixing in an unsaturated medium [1,2]. Using two chemo-luminescent liquids, the reaction of which produces photons in addition to the reaction product, we can also study the local production rate of the reaction product as the reactive liquids flow through the system. We shall address this configuration under mixing-limited conditions (very large Damkhöller number) [3], confronting the data to numerical simulation and models based on the lamellar structure of the mixing zone [4].

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Competition between Mixing and Deformation and Its Role on Reaction Rates in Subsurface Fluid Flows

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Washington State University, United States of America;

Key words: Deformation, mixing, reactive transport

Introduction

The rates of mixing limited reactions are dictated by the frequency at which reactants collocate. Fundamentally this process is driven by diffusion but deformation plays a significant role as well. Fluid elements are deformed whenever they are subjected to heterogeneities in the velocity field. Deformation of an incompressible fluid implies that stretching in one direction must be balanced by compression in another. The two processes are intimately linked since mixing effects the overall footprint of a solute, which can then be deformed, but deformation can stretch a solute, increasing the surface area available for diffusion and reaction. However, compressive deformations may decrease surface area, which should decrease reactions, but could also drive up concentrations and accelerate diffusion. Clearly, these processes are more complicated than they initially appear.

This presentation explores the competition between mixing and deformation for a simple reactive transport system. The analysis is based on two simplified models of the velocity field: a linear shear flow, and a parabolic velocity profile, which are compared to a uniform velocity field. These simple velocity fields contain features similar to those that often manifest in realistic flows, but are tractable analytically. The reaction is a generic reversible, bimolecular kinetic reaction, which is described by two conservative components and also simulated numerically using particle methods. The spatio-temporal evolution of the mixing interface is modeled and the mixing, deformation, and reaction rates are analyzed under several different initial conditions for both steady-state and transient velocity functions.

The solute extents and mixing rates are quantified by the dilution index and scalar dissipation rates, respectively. Deformation is quantified by the integrals of the eigenvalues and eigenvectors of the Cauchy-Green tensor [1] and also by the relative elongation of the interface [e.g. 2]. The early time behavior of the system is highly sensitive to the initial conditions. This sensitivity includes alterations to the geometry of the initial condition and transience but the effects are complicated. However, some trends emerge and these help us to being elucidating the conditions under which each process will dominate reaction rates. These results have important implications regarding the most efficient way to upscale the effects of reactions for different kinds of geological environments.

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Applicability Conditions for Sequential Homogenization of Reactive Transport in Bi-Disperse Porous Media

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Key words: reactive transport, homogenization, bi-disperse porous media

Introduction

We investigate the applicability conditions for sequential homogenization of reactive solute transport in bi-disperse porous media. We consider reactive solute transport in a fully saturated porous medium constituted by an array of periodic meso-scale rigid obstacles embedded in a permeable porous matrix (see Fig. 1) with different surface reactivity. The geometric characteristics of the system can be described by two separation of scale parameters ε_I and ε_{II}. The dispersion coefficient and effective reaction rate of the physically and chemically bi-disperse medium can be obtained by sequential homogenization. In contrast with classical one-step homogenization, sequential homogenization is performed through iterations of multiple-scale expansions [3], starting from the smallest scale. Iterations are more computationally efficient, but, in general, less accurate. Beside truncation errors, the iterations intro duce additional errors due to the quasi-periodicity of the porous matrix. Specifically, the error is inversely proportional to the number of non-periodic "unit cells" along the surface of the obstacles. We show that under appropriate conditions, expressed in terms of the Péclet number and the scales separation parameter γ defined as $\varepsilon_I = \varepsilon_{II}^\gamma$, second order accuracy of the sequential upscaling method $O(\varepsilon_{II}^2)$ can be achieved.

Approach and Results

At the pore-scale we consider the Stokes and the advection-diffusion equations to model flow and transport, respectively. The surface reaction enters as a boundary condition in the transport equation. In the first step of sequential homogenization, the "closure problem" [1] is solved for both flow and transport at the pore-scale (i.e. length scale l_I). As a result, we determine the effective permeability K_I and the dispersion tensor D_I^*. In the second step, we solve a "closure problem" for the meso-scale scale (length scale l_{II}) using K_I and D_I^*. We compare the sequential upscaling results with the direct solution of the fully resolved pore-scale problem K and D_* (Fig. 2). The convergence rate of the sequential "closure problem" requires that $\gamma \geq 3$. Finally, we compare direct pore-scale simulations with the homogenized model and show that

reaction rates at each level should satisfy the applicability regimes identified by Battiato & Tartakovsky [2]. The cell-averaged numerical solution was reconstructed by first order conservative total variation diminishing (TVD) reconstruction scheme from the finite volume (FV) methods.
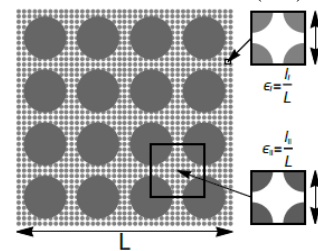

Figure 1: Schematic representation of bi-disperse porous medium. The figure shows full domain and "unit cells" of each length scale.
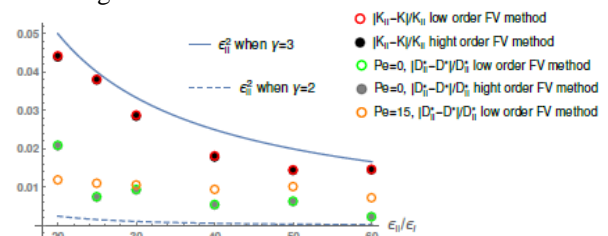

Figure 2: Relative error of the sequential homogenization depending on the ratio between length scales E_{II}/E_I.

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2-2: Mixing and Reaction across Scales in Hydrological Systems

Time: Tuesday, 21/Jun/2016: 11:00am - 12:20pm – Location: MSB 3154

Pore-Scale Modelling of the Combined Effect of Physical and Chemical Heterogeneity on Dynamics of Reactive Flows

Thomas David Serafini Oliveira[1,2]**, Branko Bijeljic**[1]**, Martin J. Blunt**[1]

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Pore-Scale Modeling of Reactive Flows for Applications in Water Purification and Absorption of Pollutants in Soil

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Pore Network Modeling of Reactive Transportand Dissolution in Porous Media

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University of Texas at Austin, United States of America; joeftansey@yahoo.com

Pore-Scale Modelling of the Combined Effect of Physical and Chemical Heterogeneity on Dynamics of Reactive Flows

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Key words: pore-scale modelling, reactive transport, heterogeneity

Abstract

We study the combined impact of physical and chemical heterogeneity in rocks to provide insight into the source of the discrepancy observed between mineral dissolution rates observed in laboratory experiments and in field-scale natural systems. The ultimate purpose of this research is to use pore-scale simulation to compute upscaled properties - such as overall reaction rate - for use in larger-scale models.

We present a methodology to simulate multispecies reactive flow through pore-space images obtained from micro-tomography. We couple the simulation of the transport equations with an advanced geochemical model[1] designed specifically for applications that require sequential equilibrium calculations and which provides novel numerical methods for the solution of multiphase chemical equilibrium and kinetics problems in a well-stirred batch model. Our model assumes that reactions can be classified into fast reactions and slow reactions. The former are assumed to be in equilibrium while the latter are assumed to be controlled by kinetics. This consideration of partial equilibrium simplifies the problem by replacing differential equations with algebraic ones.

We allow for chemical heterogeneity of the solid phase by associating each voxel to a different mineral and reaction rate (Figure 1). A steady-state creeping flow problem is solved (Figure 2) in the imaged pore space using a finite volume method to calculate the velocity field. Then we solve an advection-diffusion-reaction-equation for the concentration in which the source term is calculated by the aforementioned geo-Chemical solver, modelling each liquid voxel as a well-mixed batch, with a solid wall if applicable. Both liquid-solid and liquid-liquid reactions are considered. Dissolution of solid voxels and precipitation in liquid voxels do not reflect instantaneously in geometry changes. Instead, they are accumulated on a voxel basis, and the geometry is updated when dissolved or precipitated mass exceeds a threshold, when the whole voxel is changed into void or solid, accordingly. We present the validation tests for acidic brine injected into rock in different dissolution regimes (worm-hole, face dissolution, and homogeneous dissolution). This serves as a basis for the study of the impact of physical and chemical heterogeneities, including

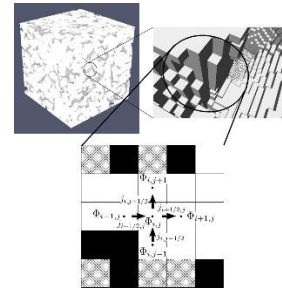pore-by-pore comparison with benchmark experiments [2, 3].

Figure 1: 2D slice of the simulation grid. The property Φ (representing v_i, p and C_i) is stored in the center of the block. The white blocks correspond to liquid voxels. Different minerals are represented by different voxels and reaction rates.
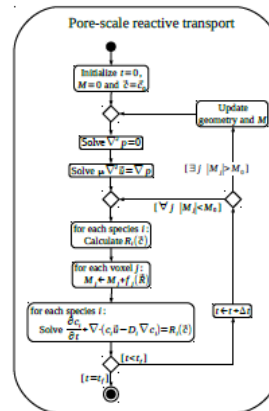

Figure 2: Coupling algorithm for transport and geochemical solver. M_{ij} is the matrix that record how much mass was dissolved from a solid voxel or precipitated in a void voxel. When the corresponding mass for a voxel exceeds a threshold, the geometry is updated.

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Pore-Scale Modeling of Reactive Flows for Applications in Water Purification and Absorption of Pollutants in Soil

Torben Prill[1], Oleg Iliev[1], Katherine Nessler[1], Zahra Lakdawala[2],
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Key words: Multiscale reactive transport in porous media, 3D pore-scale simulation, Surface reactions, water purification, pesticides adorption

Introduction

Reactive flows in porous media are an important process in many areas of water management, including e.g. functionalized membranes for water purifications, adsorption of pollutants in soil, to name just a few. Understanding these processes and their dependence on chemical and morphological parameters poses a number of research challenges.

These processes are usually truly multiscale and developing algorithms for such problems has to be addressed. Important component of these algorithms is the pore scale simulation on images coming from 3D CT. Such simulations can be used either in solving the so called cell problems in the case of homogenization for problems with scale separation, or can be used as fine scale solvers in coupled micro- and macro- scale simulations.

Pore-Scale Simulation

Fraunhofer ITWM has developed algorithms and a software tool, PoreChem, dedicated to simulation of reactive flow on the pore-scale. It enables the investigation of the interplay between convection, diffusion, reaction rate and porous media morphology in real pore scale geometries which are either 3D CT images, or are coming from computer generated geometries. Furthermore, the code can be used in calculating the macroscopic parameters for reactive flows, based on the solution at pore scale of reactive flows. Volumetric and surface reactions can be simulated.

The flow is computed by solving the Navier-Stokes system of equations with a finite volume discretization. Transport and reactions are simulated by solving the reaction-diffusion-advection equation coupled to the surface concentration by Robin boundary conditions. For the reactions, different reaction kinetics, parametrized by reaction isotherms can be taken into account. A fast voxel based solver enables calculations directly on µCT-Images.

Results

To illustrate the capabilities of the developed algorithms and software, we discuss two applications.

First, a study on the effects of pore sizes and morphology

on reactive transport and adsorption of pharmaceuticals in functionalized filter membranes is presented [1,2]. In the membranes, pharmaceuticals are adsorbed on functionalized surfaces (see Figure 1), purifying the water flow in the pore space. The membrane morphology has been modeled by a parametric 3D structure model allowing variations of the geometry, starting from 3D CT image. We show the effect of the pore morphology in different regimes.

Finally, we show a study on the adsorption of MCPA in Goethite. For the study, calculations were made on µCT-Images of soil samples, containing phases with reactive and non-reactive surfaces. Break through curves and concentration distributions were computed with different reaction rates.
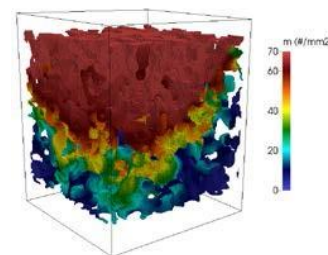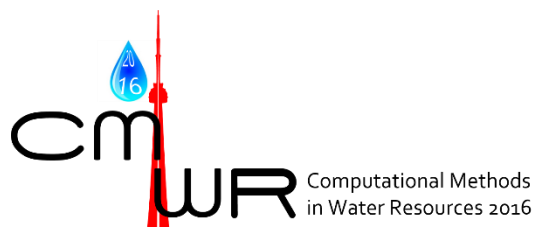

Fig. 1: Deposited mass in functionalized membrane.

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Pore Network Modeling of Reactive Transportand Dissolution in Porous Media

Joseph Tansey, Matthew Balhoff

University of Texas at Austin, United States of America

Abstract

Dissolution of solid grains in a porous medium is important in many applications, such as groundwater transport, carbon storage, mineral systems, formation of geologic features, and enhancement of near-wellbore permeability in carbonate reservoirs. These systems are characterized by a dynamic rate of reactive transport and an increase in permeability as the medium dissolves. Many models for dissolution in porous media are continuum scale descriptions, but the flow, reactive transport, and subsequent increase in porosity and permeability occur at the pore scale. We present a novel, single-phase, 3D, predictive pore network model of dissolution for porous media in the mass transfer-limited regime that is predictive of the experimental optimal injection conditions.While typical pore scale models are limited to small domain sizes on the order of 1 cubic centimeter, we join several domains together using mortar coupling techniques, which allow domains to be solved independently while transport properties are coupled at the interface. Distributed computing is used to simulate matrix dissolution, allowing several hundred pore network models to be simulated as a continuous domain.

2-3: Mixing and Reaction across Scales in Hydrological Systems

Time: Tuesday, 21/Jun/2016: 2:30pm - 3:30pm – Location: MSB 3154

Twisting Groundwater Flow in Anisotropic Geological Media and its Effects on Solute Transport, Mixing, and Reactions

Olaf A. Cirpka[1], Jeremy P. Bennett[1], Claus Haslauer[1], Yu Ye[1], Massimo Rolle[2], Gabriele Chiogna[3]

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Reactive Mixing in Heterogeneous Porous Media Flows: Scalar Gradient Distribution, Spatial Intermittency and Temporal Scaling of Effective Reaction Kinetics

Tanguy Le Borgne[1], Marco Dentz[2], Tim Ginn[3], Emmanuel Villermaux[4]

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On the Kinematics of Tracer Particles in Natural Porous Media

Daniel W. Meyer[1], Branko Bijeljic[2]

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Twisting Groundwater Flow in Anisotropic Geological Media and its Effects on Solute Transport, Mixing, and Reactions

Olaf A. Cirpka[1], Jeremy P. Bennett[1], Claus Haslauer[1], Yu Ye[1], Massimo Rolle[2], Gabriele Chiogna[3]

[1]University of Tübingen, Center for Applied Geoscience, Tübingen Germany; [2]Technical University of Denmark, Department of Environmental Engineering, Lyngby, Denmark ; [3]Technical University of Munich, Faculty of Civil, Geo and Environmental Engineering, Munich, Germany

Key words: fluvial sediments, anisotropy, non-stationarity, helical flow, transverse mixing

Spatially variable orientation of anisotropy can cause helical flow in porous media. In previous studies (Chiogna et al., 2015; Cirpka et al., 2015; see also Figure 1), we analyzed hydraulic conductivity fields with blockwise constant anisotropic correlation structure showing that macroscopically helical flow evolves, and leads to enhanced solute dilution in steady-state advective-dispersive transport. While these studies demonstrated the potential importance of helical flow in heterogeneous porous media, the likelihood of its occurrence remained unclear. In particular, natural sediments do not exhibit extended stripes of materials with diagonally oriented internal anisotropy.

In the present study, we generated realistic looking sedimentary structures mimicking scour fills. The individual geobodies have a spoon-like shape and are filled with anisotropic porous material. Cross-sections show typical cross-bedding. In particular we analyzed how the variability in bulk hydraulic conductivity between the geobodies and the differences in the orientation of anisotropy affect flow and transverse solute mixing. While the variance of log-hydraulic conductivity controls longitudinal spreading and mixing, the variability in the orientation of anisotropy is decisive for folding and mixing perpendicular to the mean flow direction.
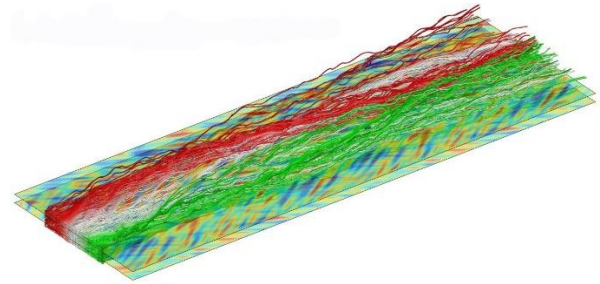

Figure 1: Streamlines in a hydraulic-conductivity with block-wise anisotropic correlation structure.

The importance of non-stationary anisotropy for transverse mixing poses a challenge for the hydraulic characterization of sediments in the context of predicting lengths of quasi steady-state plumes.

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Reactive Mixing in Heterogeneous Porous Media Flows: Scalar Gradient Distribution, Spatial Intermittency and Temporal Scaling of Effective Reaction Kinetics

Tanguy Le Borgne[1], Marco Dentz[2], Tim Ginn[3], Emmanuel Villermaux[4]

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Key words: Mixing, reactive transport, upscaling, porous media

Reactive mixing processes play a central role in a range of porous media systems, including CO2 sequestration operations, reactive geothermal dipoles, or remediation activities. Many of these reactions are limited by fluid mixing processes that bring the reactants into contact. Hence, the temporal dynamics of effective global reactivity is determined by the creation of concentration gradients by fluid stretching and their dissipation by diffusion[4,5].

density functions of concentration values and concentration gradients in heterogeneous Darcy flows over a large range of Peclet numbers and permeability field variances[1,2,3].

In this framework, we show that heterogeneous Darcy fields generate highly intermittent concentration fields, as manifested by the spatial scaling of structure functions. The resulting effective reaction rates display a range of temporal behaviors that depend on the degree of heterogeneity.

In the large Damkohler limit, we derive analytical expressions for these temporal scalings in the different regimes that arise when exploring the Peclet number space3.

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Figure 1: Above: Illustration of a reaction front in a stratified random flow field based on lamellar mixing[3]. (a) Concentration fields show that the interface between displacing and resident waters is deformed by the flow heterogeneity and develops a lamellar structure. (b) Reaction rates along the interface. Interface elongation enhances concentration gradients and thus increases chemical reactivity. Below: Global reaction rates in a mixing front for stratified flow, radial flow, and uniform flow. Reaction rates differ by orders of magnitude depending on the fluid stretching dynamics.

From the analysis of the elongation and aggregation of lamellar structures formed in the transported concentration fields, we derive analytical predictions for the probability

On the Kinematics of Tracer Particles in Natural Porous Media

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Key words: pore-scale dispersion, direct numerical simulation, statistical description, Markov model

Abstract

We present Lagrangian statistics of the fluid-particle motion in natural porous media of different type. Our statistics stem from direct numerical simulations (DNS) of fluid flow in bead packs, Bentheimer sandstone, and Ketton and Estaillades carbonates. Based on the extracted statistics, we devise a universal Lagrangian transport model. Our model provides a low-dimensional parametrization of the flow and transport process that governs advection-dominated dispersion in the listed samples. The model formulation employs a spatio-temporal Markov process for the Lagrangian velocity of fluid particles. Despite the significantly different pore geometry characteristics of the samples, the model provides velocity and transport predictions that display the correct Fickian and non-Fickian asymptotic behavior and that are in good agreement with the set of available DNS data.
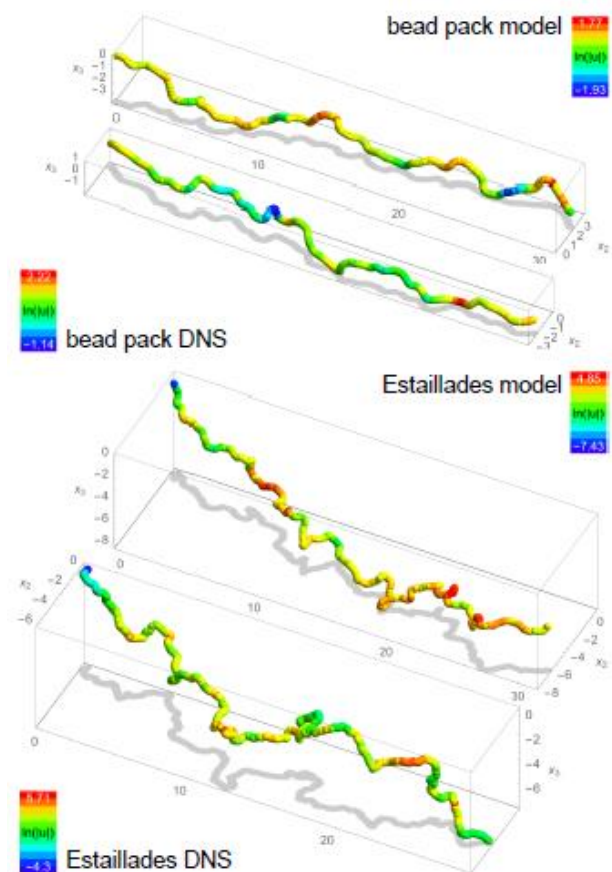
Figure *1:* Exemplary particle path lines tracked (top half) in a mono-disperse bead pack and (bottom half) in Estaillades carbonate. Upper and lower panels correspond to path lines from DNS and our statistical model, respectively. Color represents the logarithm of the normalized velocity magnitude.

2-4: Mixing and Reaction across Scales in Hydrological Systems

Time: Tuesday, 21/Jun/2016: 3:50pm - 5:30pm – Location: MSB 3154

Modeling Single-Phase Fluid-Fluid Reactive Transport at the Pore-Scale

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Generalised Mixed-Cell Mass Balance Solute Transport Modelling in Pore-Scale Disordered Networks: A New Semi-Analytical Approach

Mohammed Adil Sbai[1], Toko Kamtchueng[1,2], Jean-Louis Rouet[2]
[1]BRGM, ISTO UMR 7327, France; [2]University of Orléans, ISTO UMR 7327, France; a.sbai@brgm.fr

Constitutive Relations of Transport in Reacting Porous Media; Evolution in Microscopic Pore Spaces

Amir Raoof[1], Hamid M. Nick[2]
[1]Utrecht University, Netherlands, The; [2]Technical University of Denmark; a.raoof@uu.nl

Mixing dynamics around flow stagnation points

Juan J. Hidalgo, Marco Dentz
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Cumulative Relative Reactivity: A Tool for Catchment-Scale Reactive Transport

Matthias Loschko[1], Olaf Cirpka[1], Thomas Wöhling[2,3], David Rudolph[4]
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Modeling Single-Phase Fluid-Fluid Reactive Transport at the Pore-Scale

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Key words: Fluid/fluid, reactive transport, pore-scale, micro-CT image, mixing, heterogeneity, reaction rate

Abstract

The study of reactive transport in the subsurface is important to understand contaminant transport, nuclear waste disposal, and CO2 sequestration. One of the main complexities in understanding these phenomena stems from the fact that geological porous media are heterogeneous at all scales. The advection- dispersion-reaction equation (ADRE) has been proven to have weaknesses in predicting the behavior of reactive solute in porous media [1-3]. It over- estimates the effective reaction rate as it assumes a complete mixing between reactants. Despite that, a significant body of previous work has focused on studying the validity of the ADRE to predict fluid- fluid reactive transport behavior. These studies either applied averaged equations, which assume a complete mixing of reactants, or used fitting parameters calibrated to experimental data.

We present a pore-scale model capable of simulating fluid/fluid reactive transport on images of porous media from first principles. We use a streamline-based particle tracking method for simulating flow and transport, while for reaction to occur, both reactants must be within a diffusive distance of each other during a time-step. We assign a probability of reaction, as a function of the reaction rate constant and the diffusion length. We validate our model for reaction against analytical solutions for the bimolecular reaction $(A + B \rightarrow C)$ in a free fluid. Then, we simulate transport and reaction in a beadpack to validate the model through predicting the fluid/fluid reaction experimental results provided by [2,3].

Our model accurately predicts the experimental data, as it takes into account the degree of incomplete mixing present at the sub-pore (image voxel) level, in contrast to the ADRE model that over-predicts pore- scale mixing. We also show how our model can predict dynamic changes in the reaction rate accurately accounting for the local geometry, topology and flow field at the pore-scale. We demonstrate the substantial difference between the predicted early-time reaction rate in comparison to the ADRE model (Figure 1). Our model does not use any arbitrary or fitting parameters to describe the physical or chemical behavior.
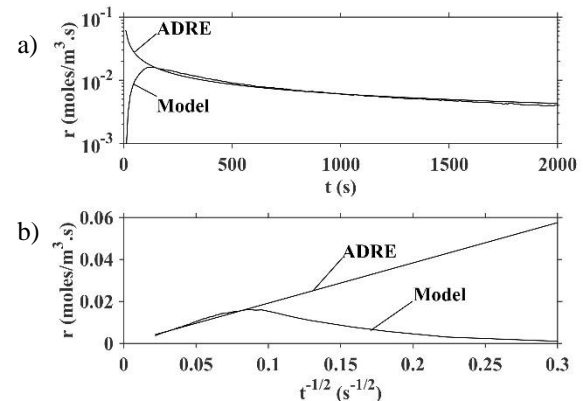

Figure 1: The predicted reaction r for both our model and the ADRE as a function of: a) time t and b) inverse square root of time t-1/2.

We then extend the model to investigate the impact of pore structure heterogeneity on the effective reaction rate in different porous media. We simulate flow, transport, and reaction in three pore-scale images: a beadpack, Bentheimer sandstone, and Doddington sandstone. We study a range of transport and reaction conditions. It is found that the rate of reaction is a subtle combination of the amount of mixing and spreading that cannot be predicted from the dispersion coefficient alone. At low Péclet number, the effective reaction rate is principally controlled by the amount of mixing due to diffusion. On the other hand, at high Péclet number the reaction rate is controlled by a combination of pore-scale mixing due to spreading and the degree of heterogeneity of the pore structure.

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Generalised Mixed-Cell Mass Balance Solute Transport Modelling in Pore-Scale Disordered Networks: A New Semi-Analytical Approach

Mohammed Adil Sbai[1], Toko Kamtchueng[1,2], Jean-Louis Rouet[2]

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Key words: Mass Transport, Pore Network Modeling, Mixed-Cell Method, Semi-Analytical Solution, Laplace Transform

Introduction

Accurately predicting (non-reactive or reactive) solute transport migration, at multiple scales, in subsurface aquifers is identified among urgent societal and scientific challenges in water resources engineering and environmental pollution [1]. In particular, pore- scale models are essential tools to bridge the gap between the pore and REV scales at which observable macroscopic behavior of solute transport processes become apparent. While challenges do persist in this field, we derive cutting-edge pore scale semi- analytical formulation for solute transport modelling in disordered networks. Continuous concentration profiles along pore throats are calculated analytically, a posteriori, from time-dependent numerically simulated concentrations in neighboring pores. A double Laplace transform method is applied to governing advection-diffusion equations in network elements by enforcing mass flux continuity along their interfaces. We show that these solutions involve a time-dependent convolution product kernels or interpolating functions expressed as convergent exponentially decreasing series of locally embedded pore-throat geometrical and flow properties. Explicit dependence of interpolating kernels on the local Péclet numbers leads to a generalized numerical scheme for accurate simulation of solute transport processes in pore networks. Indeed, widely used numerical schemes in the literature [2-7] are equivalent to the asymptotic (long-time) form of our general scheme for extremely small or high Péclet numbers. Therefore, we demonstrate for the first-time that previously adopted numerical schemes for mass balance in pore networks [2-7] may overlook pore scale dynamics for a full range of intermediate Péclet numbers occurring in subsurface aquifers. These findings are illustrated by analysis of simulated concentration distributions in a benchmark pore network extracted from Berea sandstone three- dimensional pore space image. Our findings [8] provide additional insights into the understanding of pore-scale solute transport processes to further improve the predictive capability of existing mixed-cell mass balance network models.

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Constitutive Relations of Transport in Reacting Porous Media; Evolution in Microscopic Pore Spaces

Amir Raoof[1], Hamid M. Nick[2]

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Key words: dissolution reaction, pore scale, transport properties, constitutive relationships

Abstract

Transport of chemicals may cause significant changes in the pore space of a reacting porous media and modify its pore-size distribution properties (Figure 1). Consequently, transport properties, as well as constitutive relationships among them, will be affected. Pore-size distribution affects both single phase properties, such as porosity and permeability, and two-phase flow properties, such as capillary pressure-saturation and relative permeability-saturation curves. Potential applications are geological sequestration of CO_2 and acid-gas injection during enhanced oil recovery.

The main objective of this research is to investigate evolution of transport properties due to changes in pore spaces under reactive transport. The microscopic pore space is modeled using a complex multi-directional pore network, called PoreFlow, allowing for a distribution of pore coordination number, together with distribution of pore sizes [1]. In order to simulate transport of multi-component chemical species, mass balance equations are solved within each element of the network (i.e. pore body and pore throat, both with finite volumes) [2]. We have considered advective and diffusive transport processes within the pore spaces together with multicomponent chemical reactions, including both equilibrium and kinetic reactions [2].

Using dimensionless scaling groups (such as Damköhler number and Péclet-Damköhler number) we characterized the dissolution front behavior, and by averaging over the network domain we calculated the evolution of several different transport properties as well as flux-averaged concentration breakthrough curves. The resulting transport properties (i.e., porosity, permeability, solute dispersion, capillary pressure-saturation, and relative permeability-saturation curves) are utilized within Darcy-scale modeling and examples are presented to show how the choice of constitutive relations can affect the modeling results.
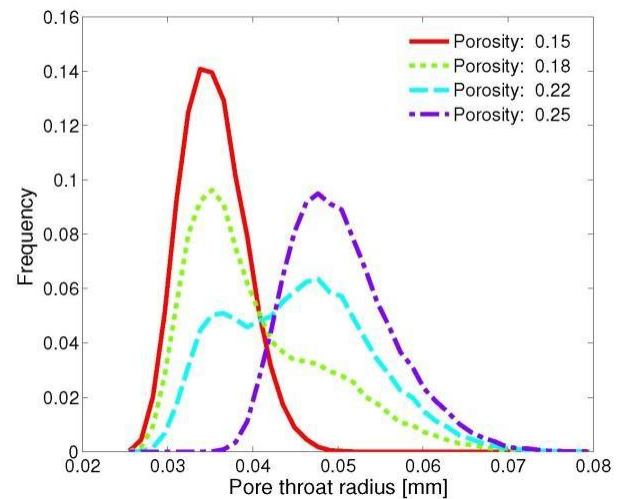
Figure 1: Evolution in pore size distribution due to dissolution reactions. Distribution with porosity value of 0.15 indicates the initial pore size distribution.

Refereces

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Mixing Dynamics around Flow Stagnation Points

Juan J. Hidalgo, Marco Dentz

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Abstract

We study the mixing of two fluids in the presence of convective instabilities. Convection is characterized by the formation of vortices and stagnation points, where the fluid-fluid interface is stretched and compressed enhancing mixing. We analyze the behavior of such structures using a fluid deformation model. We consider velocity fields generated by a double gyre synthetic velocity field and Rayleigh-B´enard and a Rayleigh-Taylor instabilities. The different flow structures can be visualized by the strain rate and the finite time Lyapunov exponents. We show that the mixing enhancement given by the scalar dissipation rate is controlled by the equilibrium between interface compression and diffusion, which depends on the velocity field configuration. Furthermore, we establish a quantitative relation between the mixing rate and the evolution of the potential energy of the fluid when convection is driven by density instabilities.

Cumulative Relative Reactivity: A Tool for Catchment-Scale Reactive Transport

Matthias Loschko[1], Olaf Cirpka[1], Thomas Wöhling[2,3], David Rudolph[4]

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Quantitative understanding of pollutant fluxes from diffuse input and turnover of pollutants at catchment scale requires process-based numerical models that can explain observed time series of heads, fluxes, and concentrations under current conditions and predict future states under changing conditions. The uncertainty of forcing, parameters, and conceptual assumptions as well as the unresolved subscale variability calls for a probabilistic framework, predicting probabilities of reactive-species concentrations rather than single values. Due to the high computational effort, such evaluations cannot be done with a fully coupled, multi-dimensional, spatially explicit reactive-transport model. Conceptual simplifications are needed, keeping spatially explicit calculations whenever required and computationally manageable, but simplifying reactive-transport computations without sacrificing mechanistic understanding.

These simplifications can be achieved with travel- and exposure-time based approaches, where reactive transport is calculated along pathlines, and spatial coordinates are replaced by groundwater travel time. The one-dimensional transport is further simplified by introducing a concentration-independent relative reactivity, which parameterizes the supply of electron donors from the rock matrix. Materials with strong reduction potential, such as peat lenses, exhibit a large relative reactivity, materials clean quartz sand would have a relative reactivity of zero.

With the concept of relative reactivity, the concentrations at a given location and time can be computed from (1) the origin and travel-time of the water parcel, determining the initial concentrations of the compounds when the water parcel was introduced, and (2) the cumulative relative reactivity that the water parcel has experienced while passing through the aquifer. Origin, travel-time, and cumulative relative reactivity are evaluated by particle tracking. For the reactions, ordinary differential equations (ODEs) are solved, in which time is replaced by cumulative relative reactivity. Thus, with a finite set of initial-concentration values, one ODE solution per initial condition, and the information from particle tracking, concentrations of the electron acceptors can be computed at all times and locations, reducing the computational effort by orders of magnitude. The computational effort is strikingly decreased, and Monte Carlo simulations become possible to account for all uncertainties encountered.

The concept of relative reactivity was tested on a synthetic test case with a single reactive zone. The reactive system involves aerobic respiration and denitrification in the saturated zone. The model runs show that the proposed approach enables an efficient way to create a stochastic framework for catchment-scale reactive transport.

2-5: Mixing and Reaction Across Scales in Hydrological Systems

Time: Wednesday, 22/Jun/2016: 11:00am - 12:20pm – Location: MSB 3154

Blending as an effective option to reduce the risk of water acidification from waste rock pile: a stochastic analysis

Daniele Pedretti, Karl Ulrich Mayer, Roger Daniel Beckie
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Coarsening dynamics in partially miscible fluids

Xiaojing Fu[1], Luis Cueto-Felgueroso[1,2], Ruben Juanes[1]
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PDF models for Eulerian simulation of pore-scale mixing and dispersion

Matteo Icardi[1], Juan Hidalgo[2], Marco Dentz[2]
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Blending as an Effective Option to Reduce the Risk of Water Acidification from Waste Rock Pile: A Stochastic Analysis

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Key words: blending, waste rock piles, acid rock drainage, stochastic analysis, risk assessment, cost-benefit analysis

Introduction

Blending has been long considered a valid option to prevent acid generation from waste-rock piles (WRPs). It consists of creating sequences of zones of rock with different neutralizing potential ratio (NPR), defined as the relative proportion of non-acid- generating minerals, such as carbonates, to potentially-acid-generating minerals, such as pyrite. The idea is to force the infiltrating water through alternating net acid-buffering and net acid-producing zones to improve the quality of the exfiltrating water before it reaches the surrounding water bodies [1]. Blending seems to be not yet universally accepted in practical mining applications. One reason is that it is very difficult to predict the resulting composition of the drainage exfiltrating from WRPs (regardless of the degree of blending), as acid rock drainage is controlled by several (strongly) nonlinearly coupled processes which are not easily quantified using traditional experimental approaches.

Goal of the analysis and methodology

We aim to quantify the effectiveness of blending to reduce the risk of water acidification in WRPs. We adopt an efficient stochastic modeling method based on a mixed Lagrangian-Eulerian approach [2] and operate in a Monte Carlo (MC) framework. We generate 100 random distributions of geochemical and hydraulic properties of WRPs using a geostatistical approach. The piles have a bulk NPR=2, and a coefficient of variation CV=0.6. We adopt a simplified model that retains only the essential features needed to study this problem. The system initially contains only pyrite and calcite, but can form gypsum and ferrihydrite as secondary mineral phases. Gas composition is maintained at atmospheric levels throughout the simulation period (1000 years). Scenarios with different blending conditions are simulated by adjusting the characteristic integral scale (I) of the mineralogical heterogeneity along the direction of the tipping faces within the WRPs. Defining Z as the vertical dimension of the WRPs, I=Z indicates homogeneous conditions within the pile (not blended scenario). When *I<Z*, the system is less homogeneous and more mixed (blended scenario).

Results and practical implications

Figure 1 shows the results from the comparison of the non-blended scenario against an illustrative blended scenario set with I/Z=0.3, and in the form of the ensemble mean from 100 random simulations. The results show that the blended WRPs tend to produce a more circumneutral pH drainage than non-blended WRPs, and display acidic behavior for shorter time scales. For instance, WRP is expected to produce pH<5 drainage for about 120 years for the blended case and about 250 years for the non-blended case. These results may have important implications for cost-effective planning waste-rock piles. For instance, if pH=5 is used as a regulatory threshold to trigger remediation (e.g. collection and treatment of the drainage), the time required to run a treatment plant under blended conditions is approximately one half the time required if the pile is not blended, all other conditions being equal. Consequently, the total cost of the remediation operation in case of blended pile could be (on average) half the equivalent costs of operating without blending.
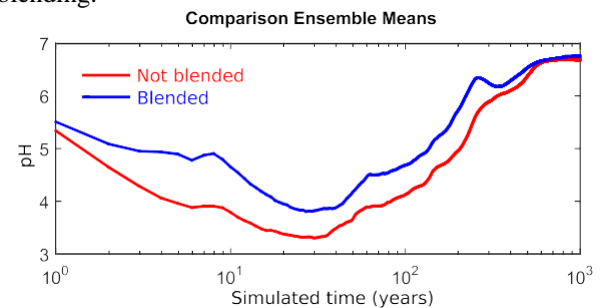

Figure 1: Results from MC simulations

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Coarsening Dynamics in Partially Miscible Fluids

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Key words: two-phase flow, partial miscibility, viscous fingering, Ostwald ripening

Introduction

The miscibility between two fluids can change appreciably with temperature and pressure. Experimental and numerical studies of two-phase flow have focused on fluids that are either fully miscible (e.g. water and glycerol) or perfectly immiscible (e.g. water and oil). In practice, however, the miscibility of two fluids often falls into the case of partial miscibility, where two flu- ids have limited solubility in each other (e.g. CO_2 and water).

Following our recent work for miscible systems [1, 2] and immiscible systems [3, 4], here we propose a phase-field model for fluid-fluid displacements in a porous medium, when the two fluids have limited (but nonzero) solubility in one another. In our model, partial miscibility is characterized through the design of the thermodynamic free energy of the two-fluid system. We express the model in dimensionless form and elucidate the key dimensionless groups that control the behavior of the system. We present high-resolution numerical simulations of the model to study the dynamics of vapor bubble interactions within an initially supersaturated liquid in a Hele-Shaw cell. Without background flow, we confirm that the vapor bubbles coarsen in size due to Ostwald ripening. Under periodic background flow, viscous instability leads to continued break-up and coalescence of the less viscous vapor phase. As a result, we observe a shut-down in Ostwald coarsening and a time-invariant bubble-size distribution. Further, we explain that the interplay between thermodynamic effects and hydrodynamic instability leads to a system that is permanently driven away from thermodynamic equilibrium, in which the liquid phase is always supersaturated.
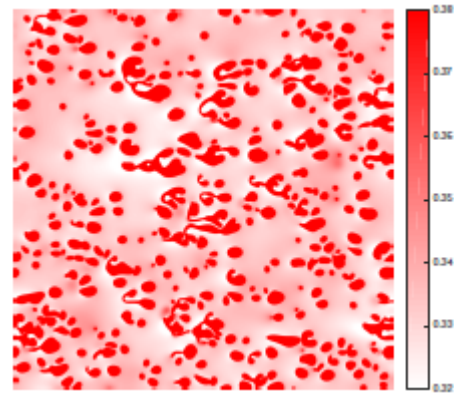

Figure 1: Snapshot of traveling vapor bubbles in a liquid-filled Hele-Shaw cell. The colormap shown here is for the concentration of one component (e.g. CO2) in a two-component, two-phase system (e.g. CO2-water). Due to viscous fingering, vapor bubbles undergo persistent breakup and coalescence. Smaller bubbles is thermodynamically unstable due to Ostwald ripening effects, and will quickly dissolve into the ambient liquid, leading to growth of the larger bubbles. Simultaneously, smaller bubbles are constantly formed as a result of the hydrodynamic instability that breaks up the larger bubbles. The interplay between the two mechanisms result in a liquid phase that is permanently supersaturated.

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PDF Models for Eulerian Simulation of Pore-Scale Mixing and Dispersion

Matteo Icardi[1], Juan Hidalgo[2], Marco Dentz[2]

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Mathematical models based on probability density functions (PDF) have been extensively used in the hydrology and subsurface flow models, to describe the uncertainty in the porous media properties (e.g., permeability modelled as random field). Recently, closer to the spirit of PDF models for turbulent flows, some approaches to use this statistical viewpoint also in pore-scale processes (aka DNS). They can be seen, in fact, as to overcome or better understand the closures performed by classical upscaling methods. In the study of hydrodynamical dispersion, for example, they can replace expensive and noisy Lagrangian simulations at the pore-scale.

In this work we derive a joint position-velocity PDF equation to model the motion of brownian particles in deterministic or stochastic velocity field.

In particular we show i) how this description can be linked to the velocity stochastic models arising in Continuous Time Random Walk (CTRW). A possible general solution method for PDF transport equations based on quadrature-based moment methods is also proposed and tested on random pore-scale geometries. The PDF approach can be used to gain insight on the cases where incomplete mixing and anomalous dispersion occur and to propose alternative closure models.

3-1: Recent Advances in Coastal Ocean Modelling of Waves, Circulation and Transport

Time: Thursday, 23/Jun/2016: 9:40am - 10:40am – Location: MSB 2172

Application of a new parametric wind field model for improving hurricane storm surge predictions of SLOSH

Talea L. Mayo[1], **Ning Lin**[2]

[1]University of Central Florida, United States of America; [2]Princeton University, United States of America;
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Application of a New Parametric Wind Field Model for Improving Hurricane Storm Surge Predictions of SLOSH

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Key words: storm surge, forecasting, coastal ocean modeling, SLOSH, wind field

Introduction

The fidelity of hurricane storm surge forecasts is largely dependent on accurate specification of the storm wind forcing. In both real-time forecasting and long-term risk analysis, parametric wind models are often used to describe the surface wind field. The surface wind field can be estimated as the sum of an axisymmetric wind profile of the storm and a background wind field of the environment. The Sea, Lake, and Over-and Surge from Hurricanes (SLOSH) model [1] is the operational storm surge model of the National Hurricane Center. It uses a radial wind speed profile that is dependent on the maximum windspeed, Vmax, and its radius, Rmax. The same profile is used to nonlinearly scale the translation speed of the storm in order to model the background wind field. Additionally, the SLOSH model currently uses an iterative procedure to solve for Vmax from pressure gradients, as this value was historically not available for real-time forecasting.

Wind Field Modification

Recent advances have shown that the surface wind field may be more accurately characterized by including Coriolis effects in the storm wind profile. Additionally, the background wind field may be more accurately modeled as a constant factor of the translation speed with a counter-clockwise rotation [2].

Furthermore, in modern day forecasting, the true value of Vmax is generally available. We thus remove the iterative procedure used to determine Vmax from the pressure gradients, and allow the model to read this value directly. We hindcast several historical hurricanes to show that storm surges can be more accurately estimated with these modifications (Figure 1).
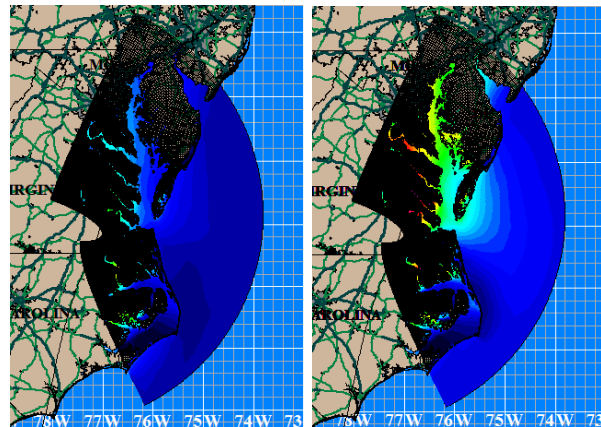

Figure 1: SLOSH hindcast of maximum storm surge during Hurricane Ernesto (2006) before and after wind field modifications

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3-2: Recent Advances in Coastal Ocean Modelling of Waves, Circulation and Transport

Time: Thursday, 23/Jun/2016: 11:00am - 12:20pm – Location: MSB 2172

Influence of Storm Characteristics on Hurricane Surge

Jennifer Proft[1], Clint Dawson[1], J. Nicholas Irza[2], Benjamin Bass[2], Jacob Torres[2], Phil Bedient[2]
[1]The University of Texas at Austin, United States of America; [2]Rice University; jennifer@ices.utexas.edu

Improved Efficiency for Wave and Surge Models via Adaptive Domain Decomposition

Joel Casey Dietrich[1], Ajimon Thomas[1], Clint Dawson[2]
[1]North Carolina State University, United States of America; [2]University of Texas at Austin, United States of America;
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Influence of Storm Characteristics on Hurricane Surge

Jennifer Proft[1], Clint Dawson[1], J. Nicholas Irza[2], Benjamin Bass[2], Jacob Torres[2], Phil Bedient[2] [1]The University of Texas at Austin, United States of America, [2]Rice University

Abstract

The potential wind damage impact of impending hurricanes has traditionally been measured by the Saffir-Simpson scale, a simple model to provide weather forecasters and emergency planners with a Category 1-5 rating. However, reliance on this scale as an indicator of storm surge, the primary destructive force during a hurricane, leads to misconceptions by the public and scientists alike of the impending danger. In this talk, it is shown that the size of a hurricane windfield, the intensity, and a newly proposed potential kinetic energy are the much more influential on resulting storm surge. We present results of a suite of synthetic storms impacting Galveston Bay, TX that demonstrate this phenomena using the highly accurate and robust Advanced Circulation (ADCIRC) numerical model.
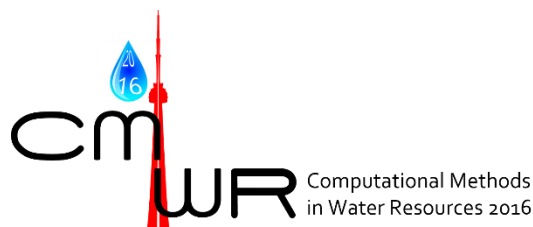
Improved Efficiency for Wave and Surge Models via Adaptive Domain Decomposition

JC Dietrich[1], A Thomas[1], CN Dawson[2]

[1]Dept. of Civil, Construction, and Env. Engineering, North Carolina State Univ.

[2]Inst. for Computational Engineering and Sciences, Univ. of Texas at Austin

Storm-induced waves and flooding can be predicted using computational models such as the ADCIRC+SWAN modeling system, which has been used by DHS and its constituent agencies for mapping of floodplain flood risk and forecasting of storm surge and inundation. This modeling system has been shown to be efficient in parallel computing environments. It is implemented on static meshes and with a static parallelization, and thus it does not evolve as a storm approaches and inundates a coastal region. This implementation can be inefficient when large portions of the mesh remain dry during the simulation. In this project, we are revising the parallel implementation of ADCIRC to utilize the parallel version of METIS. Each core is now responsible for developing input information on its own sub-domain. This upgraded preprocessor is then used to enable dynamic load balancing and assign wet regions to every core. The domain is decomposed initially to balance the sizes of these wet regions, and, as floodplains are inundated and regions become wet, the domains are rebalanced. Thus every core is working on a wet region of similar size. These technologies have improved the efficiency of ADCIRC+SWAN simulations, thus allowing for more model runs in ensemble-based design applications, and for faster simulations in time-sensitive applications such as operational forecasting. These outcomes also increase the accuracy of flood risk products used in building design and the establishment of flood insurance rates, and thus lessen the impact of a disaster

3-3: Recent Advances in Coastal Ocean Modelling of Waves, Circulation and Transport

Time: Thursday, 23/Jun/2016: 2:30pm - 4:10pm – Location: MSB 3153

Formulation and Implementation of the 3D Shallow Water Adaptive Hydraulics (AdH) Software

Corey Jason Trahan[1], Gaurav Savant[2]

[1]Army Corps of Engineers - ERDC/ITL, United States of America; [2]Army Corps of Engineers - ERDC/CHL, United States of America; Corey.J.Trahan@erdc.dren.mil

From creek to ocean: seamless modelling with unstructured grids

Yinglong Joseph Zhang

Virginia Institute of Marine Science, United States of America; yjzhang@vims.edu

Hybrid Discontinuous Galerkin Methods for Shallow Water Wave Models

Clint Dawson, Ali Samii

University of Texas at Austin, United States of America; clint@ices.utexas.edu

Projection-Based Model Reduction for Finite Element Approximation of Shallow Water Flows

Matthew W Farthing[1], Alexander Lozovskiy[2], Christopher Kees[1], Eduardo Gildin[3]

[1]USACE Engineer Research and Development Center; [2]Institute of Scientific Computation, Texas A&M University; [3]Department of Petroleum Engineering, Texas A&M University; matthew.w.farthing@usace.army.mil

Investigation of the flow over a ground sill using OpenFOAM

Katharina Teuber, Tabea Broecker, Waldemar Elsesser, Berken Agaoglu, Reinhard Hinkelmann

Technische Universität Berlin, Germany; katharina.teuber@uwi.tu-berlin.de

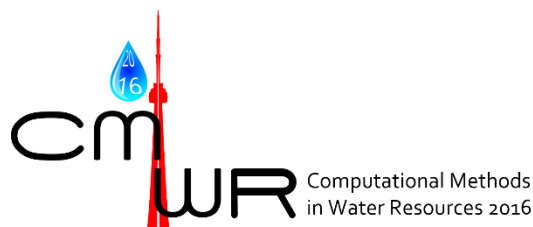# Formulation and Implementation of the 3D Shallow Water Adaptive Hydraulics (AdH) Software

Corey Jason Trahan[1], Gaurav Savant[2]

[1]Army Corps of Engineers - ERDC/ITL, United States of America; [2]Army Corps of Engineers - ERDC/CHL, United States of America

Key words: Shallow water, 3d, adaptive, baroclinic, estuary

Introduction (Abstract)

The Adaptive Hydraulics (AdH) software suite is a state-of-the-art modeling system developed by the Coastal and Hydraulics and Information Technology Laboratories, ERDC, USACE. AdH is a multi- physics and implicit finite element suite focused on both 2d and 3d shallow water models. Some features of AdH include: adaptive mesh control, time- adaption, shallow water 2d wetting and drying, general transport and cohesive/noncohesive sediment transport via the sediment library SEDLIB. The focus of this talk will be on the newly added AdH 3d shallow water, baroclinic model. The 3d shallow water model formulation and implementation will be summarized, and recent applications of the model on Mobile and Galveston Bays will be presented. Also discussed will be the 3d shallow water linkage to SEDLIB, an ERDC sediment transport library.

From Creek to Ocean: Seamless Modelling with Unstructured Grids

Yinglong Joseph Zhang

Virginia Institute of Marine Science, United States of America

Key words: unstructured grids, cross-scale, SCHISM

Introduction

We have made significant progress in simulating baroclinic processes across creek-to-ocean scale. New enabling technology proposed to address this challenge includes: (1) a highly flexible vertical grid system that combines the advantages of geo-potential and terrain-following coordinates [2,3]; (2) a hybrid triangular and quadrangular unstructured grid in the horizontal that results in model polymorphism [1]; (3) reduced numerical dissipation in the eddying regime [1]; (4) an implicit higher-order transport solver (TVD2) that improves both accuracy and efficiency. We show the applications of the new SCHISM model to a few cross-scale problems that encompass both eddying and non-eddying regimes.

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Hybrid Discontinuous Galerkin Methods for Shallow Water Wave Models

Clint Dawson, Ali Samii

University of Texas at Austin, United States of America

Key words: shallow water, wave models, discontinuous Galerkin methods, hybrid methods

Introduction

Discontinuous Galerkin methods have become widely used for modeling flow in shallow water systems. DG methods have several appealing features, including the ability to model both smooth and "rough" flows, ability to locally approximate solutions to high order, local mass conservation, and they are well-suited for parallel computation. The main drawback with DG methods is the large number of degrees of freedom in the solution space, especially when compared to traditional finite element methods. The hybrid DG method introduces unknowns on the finite element skeleton as a means for reducing the total number of degrees of freedom. In this talk, we will discuss the application of the hybrid DG method to shallow water wave models of Green-Naghdi type. These models are meant to capture wave characteristics to higher wave numbers than standard long-wave shallow water approximations. The models are highly nonlinear and contain mixed derivatives of high order. We will discuss the formulation of the method, provide evidence of stability, and discuss numerical results which verify the methodology.

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Projection-Based Model Reduction for Finite Element Approximation of Shallow Water Flows

Matthew Farthing**,** Chris Kees

U.S. Army Engineer Research and Development Center Eduardo Gildin, Texas A&M University

Key words: Shallow Water equations, model reduc- tion, global basis, POD

Introduction

The shallow water equations (SWE) are used to model a wide range of environmental flows from dam breaks and riverine hydrodynamics to hurricane storm surge and atmospheric processes. Despite significant gains in numerical model efficiency stemming from algorithmic and hardware improvements, accurate shallow water modeling can still be very computationally intensive. The resulting expense remains as a barrier to the inclusion of fully resolved two-dimensional shallow water models in many applications, particularly when the analysis involves optimal design, parameter inversion, risk assessment, and/or uncertainty quantification. One approach to alleviate computational burden in such applications is to reduce fidelity in the model dimensionality, physics, and/or numerical resolution. These simplifications are warranted under some conditions but are often invoked without proper support. An alternative to model coarsening or surrogate techniques is to consider formal model reduction techniques that maintain a connection to the underlying, high-fidelity approximation. These methods have proven very efficient for linear systems, but they are still in their infancy for nonlinear and more complex problems.

Among the many available model reduction techniques, we propose global model reduction using Proper Orthogonal Decomposition (POD)-based methods to bridge the gap between physics-based modeling and engineering analysis without resorting to potentially ad hoc simplifications in physical or numerical fidelity [4]. This can be achieved, in the case of POD, by means of performing a series of training simulations as a pre-processing routine. At a high level, our aim is to collect fine-scale snapshots of the states of the system, e.g., depths and velocities in the case of shallow water flows, of good accuracy using a small set of parameter-izations of auxiliary (boundary and initial conditions) or a material or geometric property like roughness coefficients or bathymetry as input during an offline (training) stage [4]. With these snapshots, we then construct a basis consisting of so called empirical modes using Singular Value Decomposition (SVD) or other similar techniques to represent coherent structures of the flow. After truncation, only the most significant modes are kept based on an energy computation, and the reducedsystem is now expected to be cheap to compute. These cheap computations are carried out during the online (analysis) stage in which a reconstruction of the solution is performed based on the linear combination of the basis determined offline [3].

The above process alone does not achieve significant computational gains due to the nonlinearity of the shallow water equations. The need to evaluate these non- linearities and project back to a reduced space introduces a dependence on the fine-scale dimension. As a result, an additional "hyper-reduction" step is required to further reduce the nonlinear dependency [1]. Here, we will consider two alternatives for hyper-reduction that share the same approximation space but differ in their selection criterion, namely Discrete Empirical Interpolation (DEIM) [2] and "gappy POD" [5] approximations. We will also revisit standard POD approximations which rely on Galerkin projection to obtain reduced systems and compare their performance to more recent Petrov-Galerkin techniques [1]. To evaluate these alternative schemes' performance, we will consider their accuracy, robustness, and speed for multiple test problems representative of dam-break and riverine flows.

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Investigation of the Flow over a Ground Sill Using Openfoam

Katharina Teuber, Tabea Broecker, Waldemar Elsesser, Berken Agaoglu, Reinhard Hinkelmann

Technische Universität Berlin, Germany

Key words: two-phase flow, OpenFOAM, interFoam, ground sill, turbulence modelling, CFD

Introduction

Computational Fluid Dynamics (CFD) gains an increasing importance in the field of hydraulic engineer- ing. One application, the open source C + + libraries OpenFOAM will be analysed in the following.

In this contribution, flow over a two-dimensional ground sill is simulated using the volume of fluid (VoF) method and its suitability to describe such complex hydraulic phenomena is investigated. Validation is performed by comparing the results with measurements by [1].

Computational framework

Governing equations; Surface water flow is calculated by using the two-phase flow solver interFoam based on a VoF approach for one- and two-phase flows. Both phases are considered as one fluid with rapidly changing material properties, therefore one set of Navier-Stokes-equations is solved. The phases are defined by an additional transport equation which is used as a marker to describe the distribution of the phases throughout the domain [2].

Turbulence modelling Different turbulence models are applied and the results are compared. Constant turbulent viscosities between $\upsilon = 10^{-3}$ m^2/s and $\upsilon = 10^{-6}$ m^2/s are used as the simplest model. Further, different RANS models such as k-ε, k-ω as well as k-ω SST and LES are analysed.

Results and discussion

Water level drawdown;The water level drawdown can be calculated analytically by using continuity and Bernoulli's equation. Due to additional energy losses caused by the angular structure of the sill as well as losses due to sidewalls when a three-dimensional model is chosen, the drawdown is smaller but reasonably coincides. The drawdown also differs depending on the turbulence model.

Eddy structures; The results of a one-phase validation testcase show a good agreement with the measurements by [1]. Both the one- and two-phase testcases show differences in the eddy structures behind the ground sill (cf. Figure 1 and 2) and the length of the recirculation zone depending on the chosen turbulence model.
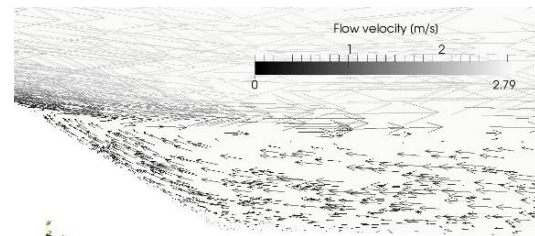

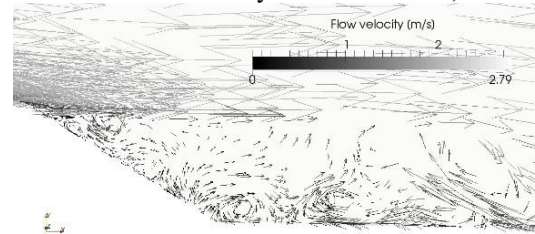*Figure 1:* Velocity distribution in recirculation zone (constant turbulent viscosity $\upsilon = 10^{-3}$ m^2/s)

Figure 2: Velocity distribution in recirculation zone (constant turbulent viscosity $\upsilon = 10^{-3} m^2/s$)

Conclusions

The suitability of OpenFOAM's two-phase solver interFoam to simulate a complex hydraulic testcase has been investigated using two- and three-dimensional model setups. Different turbulence models have been compared and the water level drawdown due to the ground sill has been compared to an analytical solution.

The VoF method implemented is able to reproduce the effects of a complex hydraulic testcase with differences in the accuracy depending on the chosen turbulence model.

Future research will analyse the effects of further hydraulic structures and take the behaviour of the air phase into account.

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4-1: Parameter Estimation and Uncertainty Analyses in Water Resource Models

Time: Tuesday, 21/Jun/2016: 9:40am - 10:40am – Location: MSB 2172

Uniqueness, Scale, and Resolution Issues in Groundwater Model Parameter Identification

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Reproducing the Small-Scale Variability of a Transmissivity Field by Embedding Direct-Inversion Methods in Multiple-Point Geostatistics

Alessandro Comunian[1], Mauro Giudici[1,2,3]

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Multi-Objective vs. Single Objective Calibration of a Hydrologic Model Exploring the Benefit of Hydrologic Signatures

Juliane Mai[1], Mahyar Shafii[2], Matthias Cuntz[1], Bryan Tolson[2]

[1]Helmholtz Centre for Environmental Research- UFZ, Leipzig, Germany; [2]University of Waterloo, Waterloo, Ontario, Canada; juliane.mai@ufz.de

Uniqueness, Scale, and Resolution Issues in Groundwater Model Parameter Identification

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Abstract

This presentation first visits uniqueness, scale, and resolution issues in groundwater flow forward modeling problems. It then points out the fact that non-unique solutions to groundwater flow inverse problems arise from a lack of information necessary to make the problems well defined. It subsequently presents the necessary conditions for a well-defined inverse problem. These conditions are full specifications of (1) flux boundaries and sources/sinks, and (2) head values everywhere in the domain for at least at three times (one of which is $t = 0$), with head change everywhere at those times must being nonzero for transient flow. Numerical experiments are presented to corroborate the fact that, once the necessary conditions are met, the inverse problem has a unique solution. We also demonstrate that measurement noise, instability, and sensitivity are issues related to solution techniques rather than the inverse problems themselves. In addition, we show that a mathematically well-defined inverse problem, based on an equivalent homogeneous or a layered conceptual model, may yield physically incorrect and scenario-dependent parameter values. These issues are attributed to inconsistency between the scale of the head observed and that implied by these models. Such issues can be reduced only if a sufficiently large number of observation wells are used in the equivalent homogeneous domain or each layer. With a large number of wells, we then show that increase in parameterization can lead to a higher-resolution depiction of heterogeneity if an appropriate inverse methodology is used. Furthermore, we illustrate that, using the same number of wells, a highly parameterized model in conjunction with hydraulic tomography can yield better characterization of the aquifer and minimize the scale and scenario-dependent problems. Lastly, benefits of the highly parameterized model and hydraulic tomography are tested according to their ability to improve predictions of aquifer responses induced by independent stresses not used in the inverse modeling efforts.

Reproducing the Small-Scale Variability of a Transmissivity Field by Embedding Direct-Inversion Methods in Multiple-Point Geostatistics

Alessandro Comunian[1], Mauro Giudici[1,2]

[1] Universitá degli Studi di Milano, [2] IDPA, CNR; CINFAI

Key words: inverse problem, multiple-point statis- tics, comparison model method, heterogeneity

Introduction

Parameter estimation represents one of the critical steps in every modeling workflow. Among the techniques proposed to tackle this problem, direct inversion methods are appealing because they are faster than indirect methods by some order of magnitude. Nevertheless, they cannot reproduce the small-scale variability of the parameters fields because they rely upon information, like for example hydraulic head measurements h, that represents only the long-wavelength components of the parameter field.

In this work we apply a direct inversion method, the Comparison Model Method (CMM) [1], which is used to estimate the long-wavelength components of a transmissivity field T. The CMM is used in conjunction with a geostatistical simulation method, multiple- point geostatistics (MPG) [2], which is based on the concept of training image (TI) [3]. The TI is a conceptual model containing the heterogeneity patterns that could be found in a given geological environment (akin to the site under investigation) and that contains all the components of the expected heterogeneity. The long-wavelength T field, estimated with the CMM using the reference h fields estimated on measurements and other information from the conceptual model, is used as an auxiliary variable in the MPG simulation. This allows injecting into the MPG simulation additional site-specific information. The procedure can be iterated to improve the agreement with the measurements.

The T field resulting from this hybrid-inversion pro cedure contains the short-wavelength components that cannot be reproduced by direct inversion methods alone. In addition, multiple realizations of the estimated T field can be obtained using different random seeds.

Both the advantages and the disadvantages of the proposed procedure lie in the usage of a TI image. The TI allows including useful soft information in the inversion procedure, but at the same time represents a strong a priori assumption.

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Multi-Objective v.s. Single Objective Calibration of a Hydrologic Model Exploring the Benefit of Hydrologic Signatures

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Key words: Multi-objective Calibration, Hydrologic Signatures, Sensitivity Analysis

Introduction

Hydrologic models are traditionally calibrated against discharge. Recent studies have shown however, that only a few global model parameters are constrained using the discharge measurements. It is therefore advisable to use additional information to calibrate those models. A signature focused on low flows, for example, could improve the parametrization of baseflow processes, which might be underrepresented when using the complete discharge time series. One common approach is to combine these multiple objectives (MO) into one single objective (SO) function and allow the use of a SO optimization algorithm. Another strategy is to consider the different objectives separately and apply a MO Pareto optimization algorithm. In this study two major research questions will be addressed:

1. How do multi-objective calibrations compare with corresponding single-objective calibrations?
2. How much is the skill of the deduced MO parameter sets deteriorated when transferring them to other catchments for validation and how much can this performance be improved when including signatures in the MO calibration?

Model and Study Area

The hydrologic model employed in this study is a distributed hydrologic model (mHM) with 52 model parameters. It is open source and can be downloaded from www.ufz.de/mhm. The model uses grid cells as a primary hydrologic unit, and accounts for processes like snow accumulation and melting, soil moisture dynamics, infiltration, surface runoff, evapotran- spiration, subsurface storage and discharge generation. The model is applied in three distinct catchments of different hydrological characteristics over Europe.

Single- v.s. Multi-objective Calibration

The SO calibrations are performed using the Dynamically Dimensioned Search (DDS) algorithm [1] with a fixed budget while the MO calibrations are achieved using the Pareto Dynamically Dimensioned Search (PADDS) algorithm [2] allowing for the same budget. The two objectives used here are the Nash Sutcliffe Efficiency (NSE) of the simulated discharge and the NSE of the logarithmic discharge (lnNSE). The results show that the SO DDS results are located close to the edges of the Pareto fronts of the PA-DDS (Fig. 1). They are, however, only insignificantly superior to the MO results. The MO calibrations are hence preferable due to their supply of multiple equivalent solutions from which the user can chose at the end due to the specific needs.
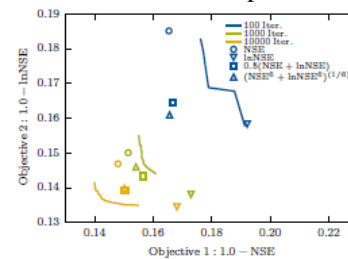

Figure 1: SO vs. MO calibration results (markers and lines respectively) of the German watershed Neckar upstream of Rockenau gauging station using different budgets (indicated by different colors). The SO optimization is regarding the four objectives regarding NSE and/or lnNSE**.**

Performance of MO Parameter Sets

The performance of the inverted parameter sets is assessed by transferring the parameter sets calibrated at one catchment to the others. For the Neckar watershed the skill of the transferred parameter sets is on average 20% below the performance of the on-site calibrated parameter sets. This decrease is notably reduced when including signatures during the calibration following the technique of Shafii and Tolson [3]. A sensitivity analysis is therefore employed to identify basin-specific signatures like limb densities and Flow Duration Curve properties. In total about 10 out of 64 considered signatures are selected per basin.

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4-2: Parameter Estimation and Uncertainty Analyses in Water Resource Models

Time: Tuesday, 21/Jun/2016: 11:00am - 12:20pm – Location: MSB 2172

Assessing the Impact of Model Structure Uncertainty on Coupled 1D-2D Flood Models

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Bayesian Calibration of Groundwater Models with Structural Error

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Good Data, Bad Models? Inverting the Paradigm for Hydrogeologic Inverse Problems

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On the Importance of Geological Data for Three-Dimensional Steady State Hydraulic Tomography at a Highly Heterogeneous Aquifer-Aquitard System

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Assessing the Impact of Model Structure Uncertainty on Coupled 1D-2D Flood Models

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Introduction

Flood inundation modelling in rivers and floodplains is important not only for assessing the risk to life and property but also for understanding the potential impacts of river infrastructure, flood mitigation, and urban development on riparian wetlands. For practical floodplain modelling, there is a trade-off between the complexity of the model description necessary to represent the river and floodplain processes, the accuracy and representativeness of the input and boundary condition data for flood inundation modelling and the accuracy required to achieve reliable floodplain risk assessments. Many flood modelling studies have addressed the uncertainty of parameter estimation, parameter uncertainty and model calibration but very few have examined the impact of model structure error and complexity on model performance and modelling uncertainty. The extent and dynamics of simulated floodplain flows depend on physical characteristics like the size of flood event and the geometry of the river channel, river banks and floodplains. However, the simulated flooding is also controlled by the parametrization of, for example, the river and floodplain hydraulics and model structure elements like the resolution of the numerical model, the numerical approximations applied and the ability of the model to represent and resolve exchanges across the river banks and with the subsurface

Uncertainty Assessment

In this study 1D-2D coupled models of river and floodplain flows are used to investigate the performance of different model structures. While different structures are expected to perform differently, this paper will examine whether there is a trade-off between model complexity and predictive ability. This investigation is carried out for the Lower Murrumbidgee River, Australia. To assess model performance, satellite imagery and aerial photographs are used to evaluate the impact of using different spatial resolutions, and different numerical and process descriptions on the flood dynamics and flood extent, Figure 1.
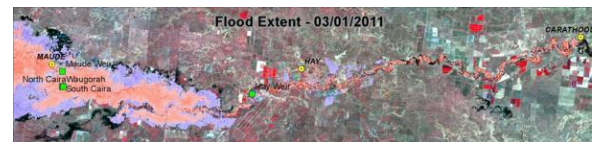

Figure 1: Comparison of simulated flood extent with satellite imagery

The results show that for the upstream section of the reach investigated here, the river-floodplain exchanges and therefore flood extents are very

Sensitive to the local topography, the numerical approximations used to represent the spilling from the river to the floodplain and the numerical approximations used to solve the St. Venant equations within the floodplain. This sensitivity to upstream model structure affects the distribution of flow between the river channel and floodplain, producing large variations in flooding behavior downstream. The long term flood dynamics of wetland flooding downstream depends not only on the upstream behavior but on other processes such as infiltration and evaporation. Further work is needed to perform a systematic analysis of the different sources of uncertainty.

Bayesian Calibration of Groundwater Models with Structural Error

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Key words: uncertainty quantification, groundwater modeling, model structural error, data-driven

Introduction

Numerical groundwater models are being used to inform decisions and policies with enormous social, economical and political implications, such as water resources management, planning for droughts and floods and assessing the risk of subsurface contamination. It is critically important to improve accuracy of these model and quantify their intrinsic uncertainties. However, current state-of-the-art does not properly treat model structural error, which is ubiquitous in groundwater models, for example due to improper interpretation of geological structure and conceptualizations of flow and contaminant transport processes. When calibrating an imperfect model, parameters may be over-adjusted to compensate for model structural error. In addition, parameter compensation may seriously degrade model prediction under a future scenario different from historical conditions reflected by calibration data [1].

Method

We present a Bayesian approach to calibration and prediction of groundwater models with structural error. Our approach integrates the fully Bayesian framework developed by Kennedy and O'Hagan [2] with a data-driven error modeling technique to statistically characterize model discrepancy revealed by the mismatch between model output and observations [3]. By utilizing exploratory data analysis and machine learning techniques such as Bayesian kernel methods, we are able to adequately capture the (often complicated) temporally and spatially varying residual field of groundwater models. What further sets the presented approach apart from existing methods is the capability of the data-driven technique to extrapolate to conditions different from the calibration period. The posterior distributions of model parameters and structural error are jointly explored, thereby allowing for a complete assessment of uncertainty from the two sources.

Results

The Bayesian approach is tested on a groundwater flow model that possesses realistic complexity. The Bayesian inference is facilitated by an efficient multiple-try Markov chain Monte Carlo (MCMC) sampling strategy as well as distributed computing resources. It is found through the case study that explicit treatment of model structural error has substantial impact on the posterior distributions of groundwater model parameters. In addition, using error models reduces predictive bias caused by parameter compensation. Furthermore, we compare the performance of the fully Bayesian approach with a more computationally efficient postprocessor method [4], which constructs complementary data-driven error models that are conditioned on a least-squares calibrated groundwater model.

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Good Data, Bad Models? Inverting the Paradigm for Hydrogeologic Inverse Problems

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Introduction

Bayesian inversion from observation, O, to underlying system state, S, requires one to specify two functions: a prior distribution on system state, p(S), and a likelihood function, l(O|S), linking the plausibility of any observation to the underlying system state. To specify the likelihood, a common strategy is to write O = M(S) + η, where M is an assumed-known model, and η is zero-mean Gaussian "measurement" noise. While appropriate in some disciplines, in transport modeling it is reasonable to expect that the data will not be centered around the model output. Instead, the deviation between observation and underlying state is apt be on account of M being simplified and embedding spatial homogeneity assumptions that do not correspond to reality.

In the transport context, so-called "anomalous" (heavy-tailed) transport is known to be the norm, but the advection-dispersion equation (ADE) does not capture this. Consequently, use of M based on the ADE will bias inference of S, potentially severely (with late breakthrough due to anomalous transport potentially misinterpreted as late release). For practical analysis of uncertainty and risk, it is necessary to understand the impact of such bias.

transport is described by an ADE with spatially homogeneous parameters.

The Study

We analyzed the bias and uncertainty inherent in a problem that is apt to be faced in practical hydrogeology: space-and-time localization of a contaminant source at an unknown location from breakthrough curves at monitoring wells down gradient. We generated multiple realizations of the subsurface with different anomalous transport parameters, selected random well locations, simulated instantaneous contaminant release, and recorded simulated breakthrough curves at the wells. We then attempted to localize the release by fitting ADE-based transport models to our simulated data. A schematic is shown in Figure 1. Using high- performance computing, we generated a large number of realizations of the subsurface and the well field, and were able to qualify the biases inherent in ADE-based interpretation, and to specify error envelopes for predictions as a function of the amount of data available and the anomaly inherent in the transport.

By recognizing that in hydrogeology, prediction error is more due to model infidelity than data infidelity (rather than the converse), we were able to develop likelihood functions and prediction heuristics well suited to reality.
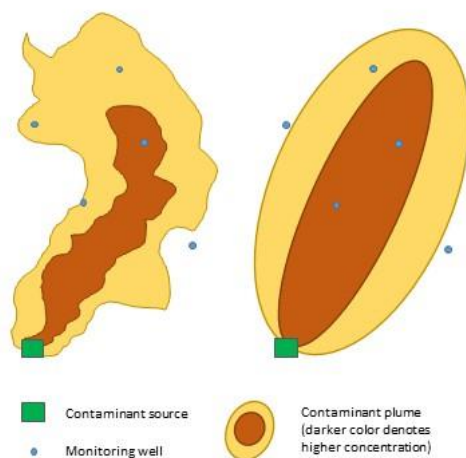

Figure 1: Schematic diagram comparing a "true" contaminant plume developing in a heterogeneous environment (left) with a potential best-fit plume (right) generated by assuming subsurface

On the Importance of Geological Data for Three-Dimensional Steady State Hydraulic Tomography at a Highly Heterogeneous Aquifer-Aquitard System

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Abstract

Hydraulic tomography (HT) is a robust high resolution method for characterizing subsurface heterogeneity of hydraulic parameters. Previous laboratory and field studies of HT have shown higher uncertainties in these estimates beyond where pumping tests and their corresponding drawdown data are available, when effective parameters are utilized as prior information. However, geological data may be readily available through outcrops and borehole logs where hydraulic data are not available. Therefore, we investigate the usefulness of geological data for HT analysis at the North Campus Research Site (NCRS) situated on the University of Waterloo campus by: 1) comparing calibrated geological models of two different resolutions to a geostatistical inverse model in terms of both model calibration and validation as well as correspondence of estimated hydraulic conductivity (K) values with permeameter- estimated K profiles along boreholes; and 2) using calibrated geological models as initial K estimates for the geostatistical inverse model. Results revealed that the simultaneous calibration of geological models to multiple pumping test data yields estimated K values for all layers that correctly reflect the general patterns of vertical K distributions from permeameter tests.

As expected, the geostatistical inverse model with a prior effective K field yields smoothed K distributions beyond areas where hydraulic data are available. In addition, we find that the geostatistical inverse model using a calibrated geological model as prior information performs best for both model calibration and validation. Most importantly, we find that using a calibrated geological model instead of an effective K estimate as prior information for the geostatistical inverse approach is helpful in improving the correspondence between estimated K estimates to permeameter test results along wells, as well as in preserving geological features, where drawdown measurements are lacking. More precise identification of high and low K zones and their connectivities should lead to improved transport predictions. Therefore, our results suggest the joint use of both geological and pumping test data for HT analysis when accurate geological data are available.

4-3: Parameter Estimation and Uncertainty Analyses in Water Resource Models

Time: Tuesday, 21/Jun/2016: 2:30pm - 3:30pm – Location: MSB 2172

Efficient Quantification of Uncertainty in Integrated Surface and Subsurface Hydrologic Simulations

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Let the Data Speak: Polynomial Chaos Expansion Toolbox for Uncertainty Quantification, Sensitivity Analysis and Risk Assessment in Environmental Modeling

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Uncertainty Quantification for Pore-Scale Simulation on Random Samples

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Efficient Quantification of Uncertainty in Integrated Surface and Subsurface Hydrologic Simulations

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Key words: HydroGeoSphere, Integrated Hydrologic Modeling, Probabilistic Collocation Method, Uncertainty Quantification

As a result of today's high performance computing resources, sophisticated numerical models are capable of incorporating many complex processes. As is often the case, the partial or incomplete knowledge of these processes, and the input parameters required to describe them, necessitates the modeler to make various assumptions and approximations, and in doing so, introduces uncertainty into the numerical model. The aim of uncertainty quantification is to measure the variability in model responses of interest propagated by uncertain model inputs. In doing so, uncertainty quantification lends credence to the predications made by numerical models.

In practice, Monte Carlo or Latin Hypercube simulation are the workhorse methods for uncertainty quantification. Although these methods are robust, scale well to higher dimensions, and are trivially parallelizable, they are slow to converge, typically requiring many hundreds to thousands of simulations to obtain an acceptable level of accuracy. In cases where a single simulation may require on the order of days or weeks to finish, such methods are infeasible.

In this work we investigate the probabilistic collocation method (PCM) [7] for quantification of uncertainty in fully-integrated, physics-based hydrologic simulations using the HydroGeoSphere model [4]. Although the effectiveness of PCM at quantifying uncertainty in hydrological applications has already been demonstrated in the literature [1, 2, 3, 5, 6, 8], to the best of our knowledge this is the first time PCM has been used in conjunction with a globally implicit, fully-integrated surface and subsurface flow and solute transport model. In contrast to sampling methods, PCM represents uncertain model input parameters as random variables and represents a model response of interest as a weighted sum of orthogonal polynomials over the random inputs. As our numerical experiments demonstrate, for each model response of interest, PCM computes statistical quantities such as the mean and variance to the same accuracy as Monte Carlo or Latin Hypercube simulation with 10 to 100 times fewer model runs. Consequently, PCM has the potential for significant speedups over traditional sampling methods. In addition, once a PCM object has been constructed, histograms of the probability density and cumulative distribution functions as well as Sobol indices [6] and global sensitivity parameters [5] that measure the model's sensitivity to the uncertain input parameters may be obtained with minimal further computation. We demonstrate the efficiency and accuracy of our approach through extensive and comprehensive numerical experiments involving direct comparison with Latin Hypercube simulation.

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Let the Data Speak: Polynomial Chaos Expansion Toolbox for Uncertainty Quantification, Sensitivity Analysis and Risk Assessment in Environmental Modeling

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Key words: uncertainty, sensitivity, risk, chaos expansion, toolbox

Environmental Modeling

Research over several decades has shown that modeling plays a very important role in reconstructing the complete complex picture of environmental systems. It offers a unique way to predict behaviors of the multifaceted processes at play in such complex systems. Due to the complexity of the surrounding environment, the greatest challenge here is the construction of reliable and feasible models that can adequately describe physical concepts and, at the same time, account for their inherit uncertainty. Many models are extremely complex, incorporating a lot of detailed aspects into the modeling procedure, because our surroundings behave non-trivially on various time and spatial scales. Moreover, many environmental systems are heterogeneous, non-linear and dominated by real-time influences of external driving forces. Thus, environmental simulations demand a lot of computational power. Unfortunately, a complete picture of environmental systems is not available, because many of these systems cannot be observed directly and only can be derived using sparse measurements. Moreover, environmental data is hardly available and expensive to acquire. Overall, this leads to limited observability, and to an inherent uncertainty in all modeling endeavors (see Fig. 1).
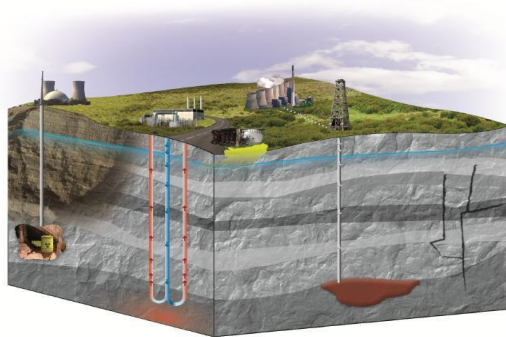

Figure 1: Use of subsurface

Uncertainty quantification

Lacking information about properties of environmental

systems leads to model uncertainties up to a level where quantification of uncertainties may become the dominant question in modeling, simulation and application tasks. Unfortunately, parametric-based uncertainty can change simulation outcomes by several order of magnitude in many typical environmental problems [1]. Current numerical simulation models are often too expensive for straightforward uncertainty quantification (e.g. Monte Carlo). However, application tasks require accurate uncertainty quantification, sensitivity analysis, risk assessment, and model calibration. As feasible and reliable alternative, we suggest to apply a massive stochastic model reduction technique that is based on the theory of polynomial chaos expansion. A recent generalization towards the arbitrary polynomial chaos (aPC) [2] can accommodate for a wide range of data distributions and can be directly applied to various environmental systems. The aPC adapts to arbitrary probability distribution shapes of input parameters and, in addition, can even work with unknown distribution shapes when only raw data is available. Let the data speak it is the key idea behind the aPC development that consists in optimal and straightforward use of available statistical data. The aPC expansion can be seen as non-linear tool that represents the model response to changes in uncertain parameters as multivariate polynomials for each output quantity of interest. The reduced model represented by the multivariate polynomials is vastly faster than the original complex one, and thus provides a promising starting point for follow-up tasks: uncertainty quantification [1,2], global sensitivity analysis [3], probabilistic risk assessment [1,4], robust design [5] and stochastic model calibration [6]. The mentioned tasks have been already successfully performed via aPC for various subsurface problems such as groundwater flow [3], carbon dioxide storage in geological formations [4,7], geothermal energy [8] as well as enhanced oil recovery [9]. We are convinced that such an efficient tool can be helpful for diverse other applications by a wider user community. For that reason, we are offering an open access MATLAB toolbox.

MATLAB Toolbox

The Department of Stochastic Simulation and Safety

Research for Hydrosystems at the University of Stuttgart decided to offer online open access to a MATLAB Toolbox for Uncertainty Quantification, Sensitivity Analysis and Risk Assessment based on the aPC. The main idea of the toolbox is to bridge the gap between the field of stochastic partial differential equations and applied environmental modeling. The toolbox is organized in such way that any used without great knowledge on the theory of polynomial chaos expansion can easily benefit from this theory and can perform the mentioned above tasks for his or her own needs. There are only the three following steps to run the MATLAB Toolbox:

- Step 1. Provide input distributions for the analyzed uncertain parameters (e.g. in form of raw data).
- Step 2. Choose a degree of expansion, which controls the precision of the massive stochastic model reduction.
- Step 3. Connect own physical model as black-box function of its parameters to the toolbox.

Once the mentioned 3 steps are done, the Toolbox automatically performs the necessary mathematical algorithms that provide to the modeler the results for Uncertainty Quantification, Sensitivity Analysis and Risk Assessment based on the provided physical model.

Additionally, in the near future, we plan to include algorithms for Optimal under Uncertainty [5], Stochastic Model Calibration [6] and Advanced Sampling Algorithms [10] that have already been tested successfully on several applications.

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Computational Methods
in Water Resources 2016

Uncertainty Quantification for Pore-Scale Simulation on Random Samples

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An efficient method, based on multilevel Monte Carlo, is proposed to quantify the variabilities associated to the finite sample size. Pore-scale simulations are performed on a hierarchy of levels, characterised by different discretization parameters. Coarse simulations on a large number of statistical samples are then used to reduce the variance in finer simulations. The overall computational cost shows the efficiency of the method and demonstrate the feasibility of uncertainty quantification studies on complex pore-scale geometries. Required conditions are: good convergence properties for the numerical solver, adequate choice of discretisation parameters, and definition of a realistic geostatistical or geometrical model for pore-scale geometry generation. Applications on the robust estimation of diffusivity and permeability are presented and future extensions for more complex flows discussed.

4-4: Parameter Estimation and Uncertainty Analyses in Water Resource Models

Time: Tuesday, 21/Jun/2016: 3:50pm - 5:30pm – Location: MSB 2172

Saltwater Intrusion with Diffuse Front: Wedge Evolution in Heterogeneous vs Homogeneous Media

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Saltwater Intrusion with Diffuse Front: Wedge Evolution in Heterogeneous vs Homogeneous Media

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Key words: saltwater intrusion, heterogeneous media, diffuse front

Introduction

The paper discusses the impact of the aquifer heterogeneity in the assessment of the mixing zone in the saltwater intrusion (SWI) problem. Solutions of SWI problems have been mainly developed for homogeneous aquifers and only few attempts to analyze the effect of the heterogeneity of natural formations on the spatial distribution of the chloride concentration have been developed [e.g. 1,2]. By use of an analytical solution, Dagan and Zeitoun [1] individuated the mean position of the sharp front between freshwater and saltwater and the uncertainty related to the lack of knowledge in the spatial variability of the hydraulic conductivity. They concluded that the variability of the position of the salt-freshwater interface (particularly the location of the toe) is markedly influenced by the permeability variance and integral scale. However their analytical approach does not allow to take into account the presence of a transition zone where variable density flow is coupled with a transport model.

In this work we investigate numerically the combined effects of the hydraulic conductivity heterogeneity and of the pore scale diffusion process to evaluate their mutual relevance in the assessment of the diffuse front median position, compared with that one occurring in an equivalent homogeneous medium. The homogenous case is calibrated on the results of a physical experiment recently developed at the University of Padova, by ensuring the ability of the numerical model to properly reproduce the boundary condition at the outlet face [e.g. 4].

Methodology

The homogeneous solution reproduces the evidences obtained from a physical experiment developed at the University of Padova in a lab canal

5.00 m long and 0.30 m wide, filled by 0.48 m of glass beads with median grain size of 0.6 mm and a uniformity coefficient d60/d10=1.5. The dispersion tensor only was calibrated to replicate the saltwater wedge movement, while the evolution of the outlet face position gives a measure of the reliability of the numerical solution. The latter was

achieved by the Mixed Hybrid Finite Element - Finite Volumes method and time-splitting technique [3] that, managing the outlet condition according to [4], is able to solve the coupled flow and transport problem.

The heterogeneous field maintains the dimension of the homogeneous one, but the spatial distribution of the hydraulic conductivity is assumed lognormally distributed with an exponential correlation function and different anisotropy ratio between vertical and horizontal hydraulic conductivities. The formation heterogeneity in the SWI problem is tackled coupling the numerical solution of the density dependent flow and transport equations with a Monte Carlo technique.

The comparison between the homogeneous and heterogeneous cases for different Peclet values shows that the combined effects of the diffuse front and of the aquifer heterogeneity have a relevant impact on the SWI phenomenon and that the saltwater intrusion in natural formations is not clearly represented by the homogeneous case. Moreover, moving from perfectly stratified formation to the isotropic one the the median position of the saltwater wedge moves back and this effect enhances for smaller Peclet values.

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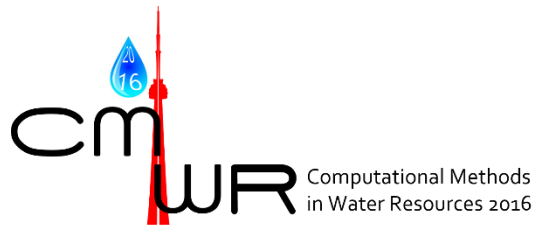
5-1: Advances in Numerical Solvers for Water Resources Applications

Time: Wednesday, 22/Jun/2016: 9:40am - 10:40am – Location: MSB 3153

Matrix-free block-Jacobi smoothers for higher-order DG methods

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New preconditioning strategy for Jacobian-free solvers for variably saturated flows with Richards' equation

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Iterative Solution of Coupled Implicit Subsurface and Overland Flow Simulations

Carol S. Woodward[1], Daniel Osei-Kuffuor[1], Reed M. Maxwell[2], Steven G. Smith[1]

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Matrix-Free Block-Jacobi Smoothers for Higher-Order DG Methods

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Key words: higher order discontinuous Galerkin method, matrix free implementation, sum factorisation, HPC, multigrid, porous media flow

Introduction

Higher order discontinuous Galerkin methods are popular for the simulation of subsurface flow phenomena. Since the resulting mass matrices are block-diagonal, they can be inverted independently in each grid cell and the resulting algorithms are very parallelisable and can solve problems at high spatial solution. However, to fully utilise computational resources, an efficient and algorithmically optimal implementation is necessary. Traditionally a given PDE is solved by assembling a system of sparse equations and solving the resulting matrix equation algebraically, for example with an AMG method. However, on modern multicore chip architectures moving data from memory takes significantly more time than executing floating point operations and this approach becomes very expensive. Let N denote the number of unknowns per element. To apply the operator, in each grid cell a matrix of size N×N has to be loaded from memory and a dense matrix-vector multiplication with low arithmetic intensity is carried out; the overall cost of the method is $O(N^2)$. This cost is reduced by matrix-free implementations where the matrix is recalculated on-the fly. For tensor-product elements in d dimensions sum factorisation techniques reduce the computational complexity from $O(N^2)=O(n^{2d})$ to $O(d \cdot n^{d+1})$, where n is the number of unknowns in one direction.

Matrix-free block-Jacobi smoothers

In preconditioned Krylov-subspace solvers and multi-grid smoothers it is often necessary to invert local matrices of size $n^d \times n^d$ in each grid cell. For example, a block-Jacobi smoother can be written as

$$u \to u + \rho D^{-1}(b - Au) \qquad (1)$$

where $D = \text{blockdiag}(D_{e1}, D_{e2}, \dots)$ is the block diagonal of A and D_{ei} is a dense $n \times n$ matrix in grid of the solver as the order n increases.

To circumvent this problem, we solve the system $D_{ei}x=y$ approximately with an iterative method. Since the application of D_{ei} can be implemented in a matrix-free way, the action of D_{ei}^{-1} ecomes FLOP bound and the cost decreases from $O(n^{2d})$ to $O(n_{iter} \cdot d \cdot n^{d+1})$ where n_{iter} is the number of iterations required to solve the system in each cell. Instead of solving $D_{ei}x=y$ to machine precision, it is also possible to solve to a looser tolerance. This leads to an increase in the number of iterations in the outer Krylov or multigrid solver, but can result in better overall efficiency since n_{iter} is reduced.

Applications

We study the efficiency of this approach for the solution of linear convection-diffusion systems of the form

$$-\nabla \cdot (K\nabla u) + b \cdot \nabla u + c \cdot u = f. \qquad (2)$$

Problems of this type arise, for example, in operator splitting approaches for unstable porous media flow [4,5]. We demonstrate the algorithmic and computational efficiency of the method for two iterative solvers:

1. Krylov methods with block-Jacobi preconditioner

2. Multigrid algorithm with hp coarsening, similar to [3]:on the finest level a matrix-free block- Jacobi smoother is applied to the high-order system, and the low-order system on the coarser levels is solved with the algebraic multigrid solver from the DUNE-ISTL library [1].

All code is implemented in the Distributed and Unified Numerics Environment (DUNE) [2] and the matrix- free computational kernels have been optimised for optimal efficiency on modern chip architectures in the context of the EXADUNE project [4].

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New Preconditioning Strategy for Jacobian-Free Solvers for Variably Saturated Flows with Richards' Equation

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Key words: Richards' equation, Variable saturated flows, Nonlinear solver, the Picard method

Motivation

In a wide variety of environmental applications variably saturated flow in porous media is a critical process which is often modeled by Richards' equation. In Richard's formulation the flow model is considered under the assumption that the gas phase is immobile. This simplification also makes Richards' equation a strongly nonlinear parabolic PDE, creating significant challenges for the performance of nonlinear solvers. The implicit discretization in time of its mixed-form is the standard approach for this type of applications since it enables large time steps and locally conserve mass. This scheme leads to a nonlinear discrete system of equations that must be solved at each time step. The geometric complexity of the subsurface environment requires to handle non-orthogonal and unstructured meshes. To discretize the flow model in these settings advanced discretization methods are essential. These methods offer accurate schemes on general meshes, but close-from formulas for the analytic Jacobian may not exist, e.g slope-limiting methods, nonlinear discretization schemes. For these discrete systems an implementation of the standard Newton-Raphson-type nonlinear solvers becomes very problematic. Therefore, development of Jacobian-Free solvers has attracted a lot of interest in the past decade.

Jacobian-Free methods

Several Jacobian-Free methods have become quite popular in the recent years. Methods, such as the Jacobian-Free Newton-Krylov method, only require the action of the Jacobian matrix on a vector, which is approximated via the numerical computation of the Gateaux derivative. Acceleraed fixed-point methods such as Anderson Mixing and Nonlinear Krylov Acceleration (NKA) methods are design to extend the power of linear iterative schemes to the nonlinear case. In all of these methods the preconditioner plays a crucial role for the efficacy of a nonlinear solver. The standard preconditioning approach is based on a linearized counterpart of the original discrete system. The strong nonlinearity in the coefficients limits the efficacy of that approach and results in the growth of nonlinear iterations.

We propose and analyze a new preconditioning strategy [1] that is based on a stable discretization of the continuum Jacobian. The underlying idea in this work is to reverse the order of the discretization and linearization steps in the development of the nonlinear solver. Specifically, by performing the linearization step first, the analytic Jacobian of the continuum model is derived and then analyzed to establish requirements for accurate and stable discretizetions. This strategy allows us to take full advantage of advanced discretization methods. For example, we may use monotone schemes for the diffusive term in the Jacobian and upwinded schemes for the advective term. This not only leads to an efficient preconditioner but also allows us to control its numerical properties.
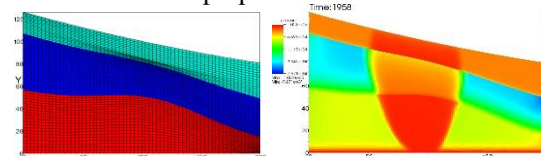

Figure 1: The layered structure of the non-orthogonal computational domain (left) and the pressure profile for tran- sient infiltration simulation (right).

The proposed strategy was tested in simulations of water infiltration into a partially saturated layered medium in steady-state and transient regimes on non-orthogonal subsurface topology with heterogeneous permeabilities and water retention models, Fig. 1. These experiments demonstrate that the new preconditioner improves conve-rgence of the existing Jacobian-Free solvers 3-20 times, see Tables 1-2.

mesh	CPU times (sec)			
	NKA		Picard	
	old	new	old	new
64x64	143.95	43.46	1044.12	36.23
128x128	1226.70	230.38	7259.44	189.01

Table 1: CPU times of the steady-state calculation.

mesh	CPU times (sec)			
	NKA		Picard	
	old	new	old	new
64x64	559.76	334.49	1909.98	299.93
128x128	4997.08	2661.74	15368.60	2034.36

Table 2: CPU times cost of the transient flow calculation

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Iterative Solution of Coupled Implicit Subsurface and Overland Flow Simulations

Carol S. Woodward[1], Daniel Osei-Kuffuor[1], Reed M. Maxwell[2], Steven G. Smith[1]

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Subsurface and overland flow models constitute a significant portion of fresh water resource simulations, and coupling these models can produce insights into efficient management of these renewable resources. However, due to the complex dynamics inherent in the physical models, the numerical formulation of subsurface and overland flow coupling can be challenging to solve. We will discuss an implicit solution approach to the coupled model and overview the formulation and effectiveness of an iterative solution strategy.

5-2: Advances in Numerical Solvers for Water Resources Applications

Time: Wednesday, 22/Jun/2016: 2:30pm - 3:30pm – Location: MSB 3153

An Immersed Boundary Method for the Numerical Simulation of Solid Particles Near Fluid-Fluid Interfaces

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An algebraic multigrid method for coupled linear systems

Daniel Osei-Kuffuor[1], Lu Wang[2], Rob Falgout[3], Ilya Mishev[4]

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An Immersed Boundary Method for the Numerical Simulation of Solid Particles Near Fluid-Fluid Interfaces

O'Brien, M. Bussmann
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Key words: Multiphase flows, immersed boundary methods, sediment, volume-of-fluid

Introduction

The interaction between sediment and a liquid is important in the study of environmental hydrodynamics, as sediments are often significant repositories of groundwater contaminants [1]. The behaviour of multiphase systems comprising of water, air and solid particles when the sediment is essentially a stationary porous media becomes very different when the liquid- phase "entrains" a particle, thereby imparting both its momentum and energy [2]. In addition to the inertial forces of the flow, consideration of surface tension driven effects such as capillary pressure and wetting dynamics (contact lines) is critical in properly modelling groundwater transport. Here, a model is demonstrated for the simulation of particles interacting at fluid-fluid interfaces.

Numerical Methodology

A fully three-dimensional computational framework for solving multiphase flows is being developed. The solution method utilizes a PISO scheme with a fully implicit momentum and pressure correction solver, utilizing the freely available BiCGStab solver in the PETSc library [3].

For modelling the sediment particles, a sharp- interface ghost-cell Immersed Boundary (IB) method is used [4], and is outlined in Fig. 1.
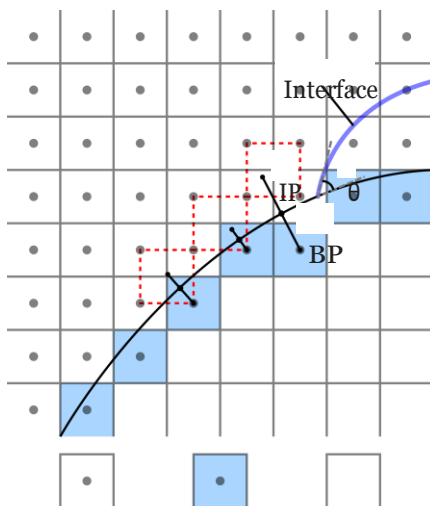
Fluid cell   IB cell   Solid cell

Figure 1: Constructing a symmetry line for the ghost cell Immersed Boundary method, showing also the Image Point (IP) and Boundary Point (BP).

A method has been developed for tracking the contact line as it moves across the surface of the particle boundary. The motivation of this work is that the study of particle wetting dynamics on the smallest possible scale can serve as a starting point for developing models for sediment- laden flows where the assumption of a stationary porous media is no longer valid. Future models will also incorporate interactions between multiple particles, including collision dynamics and a sub-grid viscous/surface tension model for particles in close proximity.

The present work will demonstrate an IB method used to model a particle in motion penetrating a liquid- liquid interface. The model is used to demonstrate the capacity of the IB method for handling multiphase wetting dynamics.

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An algebraic multigrid method for coupled linear systems

Daniel Osei-Kuffuor[1], Lu Wang[2], Rob Falgout[3], Ilya Mishev[4]

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Linear systems with multiple physical unknowns pose a challenge for standard multigrid techniques, particularly when the coupling between the unknowns is strong. We present our efforts to develop a multigrid-preconditioned Krylov solver for coupled and nonsymmetric systems of linear equations. The preconditioner is designed to represent the coupling between the physical variables and account for the underlying physics of the system. We present performance results for the solver on challenging flow and transport applications.

5-3: Advances in Numerical Solvers for Water Resources Applications

Time: Wednesday, 22/Jun/2016: 3:50pm - 5:30pm – Location: MSB 3153

Total Velocity Discretization in Implicit Hybrid Upwinding for Coupled Flow and Transport with Gravity

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Semi-implicit numerical methods for advection dominated problems

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Reactive transport simulations using a global approach

Jocelyne Erhel[1], Tangi Migot[2]
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An efficient numerical solver for reactive multiphase multicomponent flow in porous media

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Comparison of numerical methods for reactive transport modeling in porous media

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Total Velocity Discretization in Implicit Hybrid Upwinding for Coupled Flow and Transport with Gravity

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Key words: conservation laws, three-phase flow, reservoir simulation, implicit finite-volume schemes, coupled flow and transport

Abstract

The systems of algebraic equations arising from implicit (backward-Euler) finite-volume discretization of the conservation laws governing multiphase flow in porous media are quite challenging for nonlinear solvers. In the presence of counter-current flow due to buoyancy, the coupling between flow (pressure) and transport (saturations) is often the cause of nonlinear convergence difficulties when single-point Phase- Potential Upwinding (PPU) is used. To overcome such convergence problems in practice, the time step is reduced and Newton's method is restarted from the solution at the previous converged time step, which can significantly increase the simulation cost.

Here, we generalize the work of Lee, Efendiev and Tchelepi [1] by presenting an Implicit Hybrid Upwinding (IHU) scheme for coupled flow and transport that improves the convergence rate of Newton's method. With IHU, we obtain a monotone and consistent numerical flux that is smoother than that computed with PPU. In the proposed scheme, the total velocity discretization is based on a weighted average of the phase mobilities that adapts to the balance of forces at each control volume interface. We develop an analysis of the scheme that includes the derivation of pressure and saturation estimates, and the proof of solution existence. These results are valid for two- and three-phase flow, and account for a space and time dependent total velocity. Challenging heterogeneous multi-dimensional numerical tests confirm that the new scheme is nonoscillatory and convergent, and illustrate the superior convergence rate of the IHU-based Newton solver for large time steps.

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Semi-Implicit Numerical Methods for Advection Dominated Problems

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Introduction

Many mathematical models used in water resources applications involve advection dominated equations. Consequently, a successful numerical solution of such models must rely on an appropriate solver of advection terms. Interestingly, even in its simplest linear form the advection can cause several troubles for many numerical methods like instabilities, nonphysical oscillations and unpractical requirements on discretization steps. Popular methods to solve advection equations (or hyperbolic systems in general) are numerical schemes based on explicit time discretization. They are available in variants with high accuracy for smooth solutions or in high resolution forms avoiding undesired oscillations. Nevertheless they may require restrictions on the choice of time steps due to stability reasons that can be unpractical especially for nonuniform grids. Moreover undesired restrictions can occur due to time splitting errors [5] for coupled systems or for solutions approaching steady state.

Recently, an interesting option has been proposed for numerical solution of advection in the form of semi- implicit finite volume schemes where the inflow fluxes are discretized implicitly and the outflow fluxes explicitly [2, 3, 4]. One can show that such schemes are unconditionally stable and second order accurate for linear advection with variable velocity [4]. The price to pay is the necessity to solve algebraic systems in each time step, nevertheless the resulting matrix in the case of pure advection has favorable properties, so the system can be solved typically in finite number of iterations using e.g. Gauss-Seidel iterations.

In [4] a special variant of semi-implicit scheme is derived for structured grids, the so called Corner Transport Scheme, that has the properties mentioned in the previous paragraph, and, additionally, it is third order accurate in the case of constant velocity. Several numerical experiments confirm that this scheme is superior to other semi-implicit schemes even for problems with variable velocity, see Figure 1. Up to now we have applied the semi-implicit schemes in level set methods designed for applications having moving interfaces [3]. We plan to apply these methods for groundwater flows with free boundaries [1] and for coupled systems of advection dominated transport and reactions [5], the results will be reported at the conference. In any case we discuss in our talk the advantages and disadvantages of semi-implicit numerical solvers when applied to a large class of water resources applications.

Illustrative numerical experiment

We present for an illustration the standard benchmark of pure linear advection of rotating Gaussian pulse, see Figure 1. We give the results for semi-implicit Corner Transport scheme for which the experimental order of convergence appears to be significantly larger than 2 and which produces very good results on the fine grid even for Courant number larger than 4.
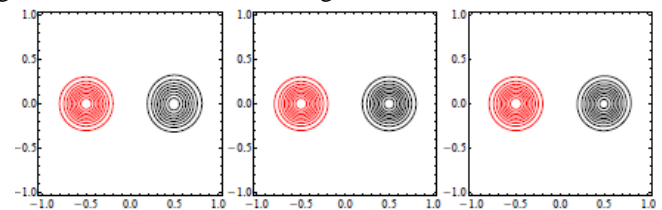

Figure 1: Numerical solutions of benchmark example with one and half rotation of Gaussian pulse where the left (red) contours in each picture denote the initial position of pulse. The left picture represents the numerical solution using semi-implicit Corner Transport scheme [4] with grid of 60^2 nodes after 600 time steps (the minimum of numerical solution being -5.E-3, the maximum .88, the global L1 error in time and space being 1.0E-2), the middle one with 120^2 nodes after 1200 steps (-5.E-5, .98, 1.5E-3), and the right one with 120^2 nodes and 240 steps (-5.E-4, .96, 3.8E-3). The Courant number in the last example is larger than 4, the exact extrema are 0 and 1.

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Reactive Transport Simulations Using a Global Approach

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Key words: reactive transport, nonlinear system, parallelism

Introduction

In many environmental applications, transport of solutes is coupled with chemical reactions, either kinetic or at equilibrium. These reactions involve not only solutes, but also sorbed species and minerals. The mathematical model is a coupled set of nonlinear partial algebraic differential equations. A classical approach is to discretize first in space then in time. Since the problem is rather stiff, explicit time discretization suffers from a drastic CFL-like condition. On the other hand, implicit schemes allow large timesteps during some periods of simulation. Implicit Euler scheme is often used for monotonicity properties. At each timestep, a set of nonlinear algebraic equations must be solved. The Jacobian is computed from the transport operator and the chemical operator. In order to reduce the size of the nonlinear system, unknowns can be eliminated by a substitution approach. Moreover, conservative variables can be decoupled from others. Adaptive mesh refinement, adaptive timestep and adaptive Jacobian updates are also very efficient to reduce the computational time. Finally, computations can combine parallelism through the equations and through the chemical species. We have implemented such a global approach in the software GRT3D. This talk will present the numerical model, the software and some numerical experiments.

Software GRT3D

Space and time discretization The software GRT3D uses free software as much as possible. Flow computations are done with MODFLOW, which provides the velocity for the advection operator. Transport discretization is done with MT3D, which relies on a regular grid and a finite difference method. Then the semi-discrete system is a set of Differential Algebraic Equations, simulated with the software SUNDIALS, using a BDF scheme and a Newton nonlinear solver. The software GRT3D provides the function in the DAE system and its Jacobian. A sparse linear solver, currently UMFPACK, is interfaced with SUNDIALS.

Chemistry system Because a global approach requires a Jacobian, it is not easy to use a chemistry solver. Therefore, we implemented our own software for the chemical part. Currently, kinetic reactions are not implemented, but it should not be too difficult. The main challenge comes from precipitation- dissolution reactions at equilibrium. Indeed, the mathematical model for appearance and disappearance of minerals is a complementarity problem, which is quite difficult to solve. Even if semi-smooth Newton methods are well studied now, in practice convergence can be very low in some cases.

Numerical results

We have defined a simple test case with the two salts KCl and NaCl. The presence of salt depends on the total quantities of potassium and sodium. We use symbolic computations to get the state diagram depicted in Figure 1. Then we study the numerical convergence of Newton method.
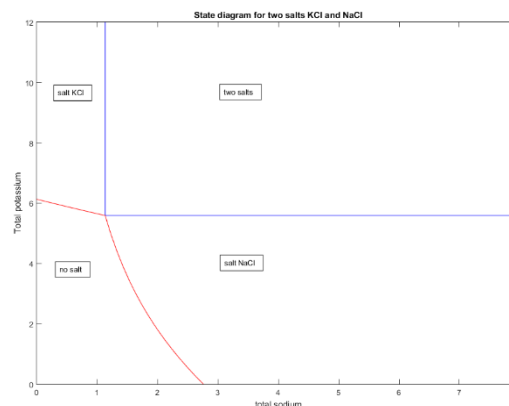

Figure 1: State diagram

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An Efficient Numerical Solver for Reactive Multiphase Multicomponent Flow in Porous Media

Fabian Brunner, Peter Knabner

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Key words: multiphase flow, model preserving reformulation, fully implicit methods, complementarity problems, parallel computations

Introduction

Mathematical formulations and numerical simulations for reactive transport have been widely discussed in the literature in the past decades. While in the 1980s, splitting approaches were preferred for these problems, the availability of increasing computational resources has attracted growing interest in the global implicit approach during the past years. In [2], it was shown that this approach is robust and efficient and that it can well handle the complex chemical interactions associated with these problems. In this talk, we present an efficient numerical frame-work for coupling multiphase multicomponent flow in porous media with general geochemical reactions based on a global implicit approach, which can be used, e.g., to simulate the long-term behaviour of carbon dioxide injected into a deep geological formation with the goal of permanent storage.

Mathematical model

We study a partially miscible multiphase multicomponent model in porous media involving general chemical reactions, which may be kinetic reactions or equilibrium reactions. Moreover, the transfer of mass across the phases is taken into account, which may lead to the appearance or disappearance of one of the phases. Due to the complex physical and chemical interactions, the resulting model is strongly nonlinear, which represents a challenge in the design of numerical solvers.

The numerical solver

The mathematical model is transformed using a model-preserving reformulation technique [1], and the equilibrium reaction rates are resolved on a local level in terms of an implicitly defined resolution function. By choosing persistent primary variables and using a complementarity approach [3], interphase mass exchange and the local appearance and disappearance of the gas phase can be handled. In this talk, we present in detail numerical strategies that are used to obtain an efficient and robust finite element solver for the above model. These strategies include special techniques to evaluate the resolution function numerically using the semi-smooth Newton method, which is accomplished, e.g., by using logarithms of the concentrations as unk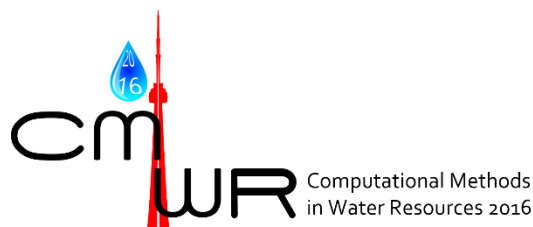nowns and a starting value search to ensure that the variables remain within physicalbounds. Our procedure employs a conservative Finite Element-Finite Volume discretization in space [4] combined with a fully-implicit treatment in time in order to preserve the nonlinear coupling of flow, transport, reactions, and mass transfer across phases. An upwind scheme is implemented to treat advection-dominance. The nonlinear systems of equations that remain to be solved in each time step after the resolution function has been employed are treated using a global implicit approach and the semi-smooth Newton method for linearization. The method is implemented in our in house software Richy, based on the parallel finite element toolbox M++ [5].

Numerical results

The efficiency of the approach is demonstrated for problems related to carbon sequestration and hydrogen migration in deep geological repositories of nuclear waste. In particular, we compare different choices of primary variables and show that the global implicit approach is well suited and efficient for these type of problems. Our numerical results indicate that the formulation can handle vanishing phases and mass exchange due to chemical reactions.

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Comparison of Numerical Methods for Reactive Transport Modeling In Porous Media

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IFPEN, France

Key words: Reactive transport, porous media, numerical schemes, fully implicit, splitting.

Reactive transport numerical models [1] are used to predict temperature and pressure variations, brine and gas phases displacement, and chemical effects of gas-water-rock interactions in porous media. One of the main challenges of these models is to accurately represent the coupling between transport phenomena and mass transfer occurring in sub-surface porous media.

In a previous work [2], we have introduced a new mathematical formulation to handle the phase appearance and disappearance issues associated with multi-component, multi-phase flow combined with stoichiometric mass transfer. In this work, we compare our formulation with an implementation of a splitting scheme between flow, transport and chemical reactions [3] on a larger range of benchmark problems associated with complex chemical equilibria.

Both formulations are implemented in a three-dimensional multi-phase flow code using the HPC numerical framework Arcane [4]. We discuss the gain in robustness, performance and accuracy for the fully implicit method relative to the more traditional splitting algorithm.

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5-4: Advances in Numerical Solvers for Water Resources Applications

Time: Thursday, 23/Jun/2016: 9:40am - 10:40am – Location: MSB 3154

Higher Order Finite Volume Methods for Compositional Flow in Porous Media on Polyhedral Grids

Robert Kloefkorn[1], Anna Kvashchuk[2]

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High performance simulation of a hybrid dimensional compositional multiphase Darcy flow in fractured porous media

Roland Masson[1], Feng Xing[2], Simon Lopez[3]

[1]LJAD University Nice - Sophia Antipolis, INRIA team COFFEE; [2]LJAD University Nice - Sophia Antipolis, INRIA team COFFEE, Institut BRGM; [3]Institut BRGM; feng.xing@unice.fr

Flow simulation in 3D Discrete Fracture Networks

Jean-Raynald de Dreuzy[1], Géraldine Pichot[2], Jocelyne Erhel[2], Patrick Laug[2] [1]CNRS, France; [2]INRIA, France; jr.dreuzy@gmail.com

Higher Order Finite Volume Methods for Compositional Flow in Porous Media on Polyhedral Grids

Robert Kloefkorn[1], Anna Kvashchuk[2]

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Mathematical studies of two-phase (three-phase) compositional flow have been active lately, for example, in [1, 2, 3] and others. From a mathematical point of view it is a very challenging problem. It consists of a system of non-linearly coupled partial differential equations which in addition are of different type (elliptic, hyperbolic). This usually requires different solution methods, as described in [1, 2]. A relevant compositional flow model is, for example, described in [3]. In this paper we will extend the higher order Finite Volume method presented in [4] for application on general polyhedral grids (e.g. Voronoi grids or corner point grids) for the transport part. We will discuss the scheme in terms of accuracy, performance, and scalability. In addition we will discuss time stepping methods and appropriate coupling with a three-phase flow model. Implementations are based on the Open Porous Media (OPM www.opm-project.org) code base.

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High Performance Simulation of a Hybrid Dimensional Compositional Multiphase Darcy Flow in Fractured Porous Media

Roland Masson[1], Feng Xing[2], Simon Lopez[3]

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Key words: Compositional multiphase Darcy flow, Parallel implementation, Code ComPASS

Introduction

Many applications require the simulation of compositional multiphase Darcy flow in heterogeneous porous media, such as high-energy geothermal reservoir modelling, CO2 geological storage, or the study of the gas migration in nuclear waste repositories etc.

The model investigated in this paper accounts for the coupling of the mass balance of each component, the energy conservation, the pore volume conservation and the thermodynamical equilibrium and dynamically manages phase appearance and disappearance.

The model also takes into account the Darcy flow in a discrete fracture network including the mass and energy exchanges between the surrounding matrix and the fractures (see Figure 1). We consider the asymptotic model for which the fractures are represented as interfaces of codimension one immersed in the matrix domain, leading to the so called hybrid dimensional Darcy flow model.

The discretization is an extension of the Vertex Approximate Gradient (VAG) scheme to the case of hybrid dimensional Darcy flow models. The VAG scheme has the advantage to avoid the mixing of the fracture and matrix rock-types at the interfaces between the matrix and the fractures, while keeping the low cost of a nodal discretization on unstructured meshes (see [1], [2]).

This model has been implemented in the framework of code ComPASS (Computing Parallel Architecture to Speed up Simulation) [3], which is a parallel code (MPI) adapted to the finite volume discretization on general polyhedral meshes using various degrees of free- dom such as cells, nodes, faces and edges. The computational efficiency of our model is assessed on a few geothermal test cases ranging from the simulation of a tracer in a faulted reservoir (see Figure 1) to the simulation of a thermal gas liquid Darcy flow in the Boiling high energy geothermal reservoir.
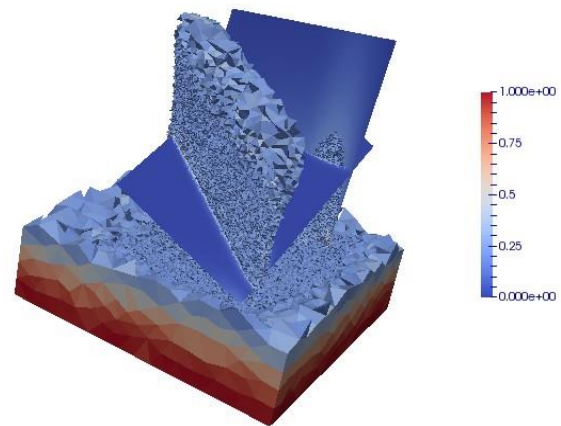

Figure 1: Example of a tracer simulation in a faulted reservoir.

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Flow simulation in 3D Discrete Fracture Networks

Jean-Raynald de Dreuzy[1], Géraldine Pichot[2], Jocelyne Erhel[2], Patrick Laug[2]

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Key words: Diffusion equation, Mixed Hybrid Finite Element Method, Non-conforming mortar methods, Fractured Media

Natural fractured media are characterized by their diversity of structures and organization. Numerous studies in the past decades have evidenced the existence of characteristic structures at multiple scales [1]. At fracture scale, the aperture distribution is widely correlated and heterogeneous. Fractures themselves have widely varying sizes with no obvious dominating or characteristic scale. At network scale, the topology is complex resulting from mutual mechanical interactions as well as from major stresses. The diversity of structures results in widely varying mechanical, hydraulic and transport properties that require some description of the underlying fracture geometries to be predicted.

Modeling mixes dimension in a non-standard way as fracture networks consist in a large number 2D fractures interconnected in the 3D space. It is no longer 2D and not already 3D. Intricate local configurations of fracture intersections cannot be precluded and the multiple scale of the fracture structures require adapted mesh generation and discretization methods. Numerical modeling should not only be specific but also efficient to cope with essentially the statistical characterization of the fracture properties.

We have worked on three alternative strategies. The first one follows the classical methodology of finite element methods [2]. The fracture network is classically meshed with standard mesh generation methods. The flow equation is further discretized using a flow-conservative mixed hybrid finite element. While standard, this method requires an efficient mesh generator that complies with the intricate configurations when not only two but three fractures intersect close together. While these situations might not be relevant physically depending on the fracture generation process, they cannot be avoided in a stochastic framework.

The second strategy relies on the discretization of the fracture boundaries and intersections on a regular 3D grid [2]. Each fracture is then meshed independently with a rerojection in the fracture plane of its boundary and intersections with the other fractures. All elements smaller than the grid size are removed. Any discretization scheme can subsequently be applied. While difficult to implement, this method is quite general.

The third strategy decouples the problem at the fracture scale by (1) generating independent meshes at the fracture scale, (2) using a flow-conservative mixed hybrid finite element methods in the fracture planes, and (3) reconnecting fluxes at fracture intersections with Mortar-like methods [3, 4]. While it requires advanced developments in numerical methods, this method can potentially handle fracture networks by refining the meshes in the most important fractures (Figure 1).
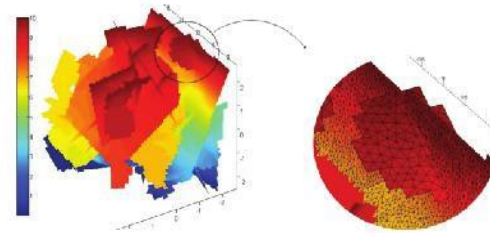

Figure 1: Left: example of fracture network with associated heads computes with a vertical main flow direction. Right: Differential discretization with Mortar-like non-conforming methods [4].

We investigate the respective advantages and drawbacks of these three strategies according not only to their accuracy and efficiency, but also to their implementation complexity and generality.

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6-1: Hybrid Multiscale Modelling of Subsurface Flow and Reactive Transport

Time: Wednesday, 22/Jun/2016: 9:40am - 10:40am – Location: MSB 2170

A multiphysics multiscale framework for modeling mass and heat flow at small scales: carbonate dissolution

Cyprien Soulaine, Hamdi Tchelepi
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Hybrid multiscale simulation of hydrologic-biogeochemical processes in subsurface environments

Xiaofan Yang, Tim Scheibe
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A Multiphysics Multiscale Framework for Modeling Mass and Heat Flow at Small Scales: Carbonate Dissolution

Cyprien Soulaine, Hamdi Tchelepi

Stanford University, United States of America

Key words: hybrid modeling, Darcy-Brinkman formulation, reactive transfer, dissolution

Simulation of dissolution at the pore-scale needs to explicitly represent the pore structure and chemical reactions that occur at the grain boundary. The simula- tion of such a problem is difficult because of the moving boundary induced by the dissolution phenomenon. Since the pioneer works of Békri et al. who proposed pore-scale simulations using a cell-based dissolution rate, the modeling has taken various forms using for instance a level-set approach to transport the reactive fluid/solid interface, or simulations based on a Lattice Boltzmann Method. These works, however, remain restricted to very small domains, no more than a few grains usually. This is a main concern for the simulation of fracture dissolution with application to CO_2 storage, or for the simulation of worm-holing dissolution phenomena involved in acidizing treatment of carbonate formations. In both cases, reactants flow through large channels, penetrate into the block matrix by either diffusion, or convection, and then dissolve minerals at grain surfaces. As a result, the morphology of the large channel evolves changing at the same time the local permeability. In return, the flow properties in the channel are modified. Clearly, these events are multiscale phenomena in both space and time. In order to capture the emerging phenomena at larger scales of practical interest (e.g., cores and ultimately near-well regions), grain-scale full-physics simulation is not feasible and hybrid scale strategy is preferred [1].

For such multiscale phenomena, it may be relevant to introduce a cut-off length so that the flow in the large channels is governed by Navier-Stokes equations while the flow in the surrounding porous medium is modeled by a Darcy's law. The Darcy-Brinkman-Stoke equation offers an appealing framework for hybrid modeling. It assumes that a single equation, first proposed by Brinkman [2], holds for both flow in the channels, so-called 'free flow', and flow in porous media. In this paper, we propose and implement in OpenFOAM [3] a unified framework to solve multiphysics problems of flow, heat, and mass transport in natural porous media based on a Darcy-Brinkman-Stokes formulation. We demonstrate its effectiveness in bridging the gap between the pore and Darcy scales consistently and efficiently. This framework is very promising for the simulate fine scale physics, such as pore-scale where information regarding the solid geometry and the flow below a certain threshold is filtered and modelled. In particular, the model can deal with evolving solid structures due to chemical reaction at the fluid/solid interface, such as dissolution or precipitation (see Figure 1)
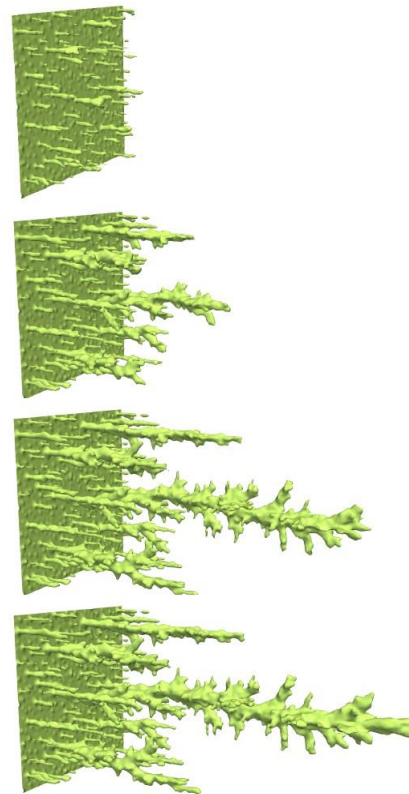

Figure 1: Simulation of wormholes formation due to acidizing treatment of carbonate near well-bore.

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Hybrid Multiscale Simulation of Hydrologic-Biogeochemical Processes in Subsurface Environments

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Key words: multiscale, porous media, reactive transport, hydrologic-biogeochemical processes

Introduction

The multiscale nature of hydrologic-biogeochemical (HBGC) processes in subsurface environments restricts the predictive capability of advanced simulation tools. A hierarchical multiscale approach provides connections between multiple models defined at distinct scales with different mathematical representations of coupled physical, biological and chemical processes, and represents a computationally efficient means of increasing model fidelity. We have been developing a generalized hybrid multiscale approach to facilitate the interoperable combination of model components in a loose coupling workflow on a high-performance computing (HPC) platform [1]. We have applied this approach to two application problems.

Applications

1: Coupling pore- and continuum-scale models to simulate reactive transport We have applied the hybrid multiscale approach to couple pore- and continuum-scale reactive transport simulators in an experimental system (Figure 1). Our loosely-coupled simulation approach provided an efficient way to represent incomplete mixing at the sub-grid scale [2].
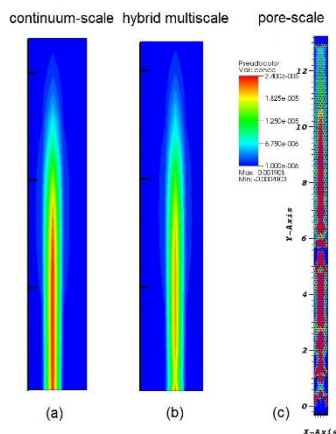
Figure 1: Contour plots of the mixing zone in both macroscopic (a-b) and microscopic (c) points of view.

2: Coupling continuum-models of HBGC at two distinct scales We have extended the application of the hybrid multiscale approach to a local field-scale problem in the groundwater-surface water interaction zone (GSIZ) at DOE's Hanford site (Figure 2). Both model scales (local-scale and field-scale) were represented using the same continuum-scale simulator but with different grid resolution and BGC reaction networks. The hybrid approach facilitates mechanistic modeling of HBGC processes in the thin mud layer coupled to GSIZ over a larger domain of interest [3].
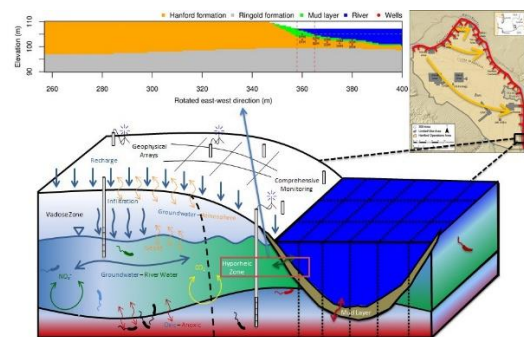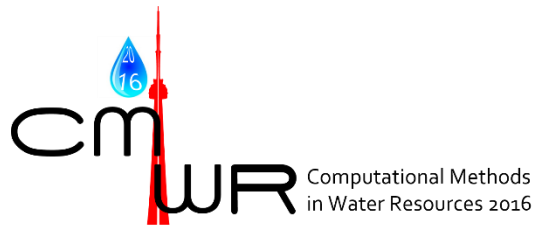

Figure 2: Schematic diagram of multiscale process interactions in the GSIZ. The upper right diagram shows the 300A site in the context of the Hanford Reach of the Columbia River. The main portion shows the local-scale region of interest, and the upper left diagram shows a heterogeneous 2D local-scale model domain where the same continuum- scale simulator was used in both the green zone (mud layer, microscale) and the rest of the domain (macroscale) with different grid resolutions and BGC reaction networks.

References

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6-2: Hybrid Multiscale Modelling of Subsurface Flow and Reactive Transport

Time: Wednesday, 22/Jun/2016: 2:30pm - 3:30pm – Location: MSB 2170

Upscaling reactive flow and transport in an evolving porous medium and its application to soil formation

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Parallelization of MIN3P-THCm: a high performance computational framework for subsurface flow and reactive transport simulation

Danyang Su[1], K. Ulrich Mayer[1], Kerry T.B. MacQuarrie[2]
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Hydraulic-chemical coupling for long-term prediction of mineral reactions in heterogeneous CO2 storage systems

Marco De Lucia, Thomas Kempka, Michael Kühn
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Upscaling Reactive Flow and Transport in an Evolving Porous Medium and Its Application to Soil Formation

Nadja Ray, Andreas Rupp, Peter Knabner; University of Erlangen, Germany

Key words: porous media, soil formation, evolving microstructure, asymptotic expansion, cellular automaton

Introduction

Recently, there has been an increased interest in porous media applications that contain multiple evolving phases. In addition to multi-phase flow, in which the composition and ratio of the liquid and gaseous phases are space and time-dependent, research investigating the evolution of the solid phase has also received greater attention. This evolution causes structural changes in the porous matrix and has largely merited further study. Deriving models that describe such structural changes at a variety of scales is essential to understanding the intimate linking between soil structure, its formation, and its soil functions. With reference to the soil's heterogeneity, we aim to develop a mathematical model at the pore scale, perform its upscaling to transfer our model from the small scale to the macroscale and investigate the resulting model numerically. In doing so, we compare two different models that describe the solid phase's changes: a fully continuous model and a hybrid discretecontinuum model.

Pore-scale modeling: hybrid versus continuum;

At the pore scale, we consider a coupled system of partial differential equations consisting of the incompressible Stokes equations that determine the fluid velocity and the pressure. This coupled system additionally consists of a transport equation for the species' concentrations while taking the processes of convection, diffusion, and potentially even drift into account. In our model, structural changes in the porous medium's composition may occur due to both the growth of biofilm in the pore space and heterogeneous reactions increasing the ratio of the solid phase. Here, we compare the following two model descriptions: In the fully continuous model, we apply a level-set formulation to characterize the underlying evolving geometry. In the hybrid model, we follow the ideas in [1] and assume a discrete distribution of phases that changes based on a cellular automaton method.

Upscaling;

To determine a macroscopic model description based on the pore-scale models above, we use two-scale asymptotic expansion in a level set framework for the fully continuous model, cf. [2]. Generally, a micro-macro model emerges that is comprised of several levels of couplings: Macroscopic equations describing transport and fluid flow at the scale of the porous medium (macro scale) include averaged time- and space-dependent coefficient functions. These functions may explicitly be computed by means of auxiliary cell problems (micro scale). Finally, the pore space in which the cell problems are defined is time- and space dependent. Its geometry is determined by means of the level-set equation, which inherits information from the transport equation's solutions (micro-macro scale). In the hybrid model, averaged time- and space-dependent coefficient functions that enter the transport and flow equations are calculated by means of standard cell problems. These are, however, defined on a geometry prescribed by the cellular automaton method. Here, the growth and spreading of the biomass depends, for instance, on the availability of oxygen from the macroscale transport equation.

Numerics;

For evaluation purposes, we complement our theoretical results with numerical computations. The continuum equations are discretized by means of a mixed finite element method on triangular grids or by means of local discontinuous Galerkin method on rectangular grids, cf. Figure 1. The resulting time- and space-dependent, coupled micro-macro problems require highly sophisticated implementation strategies and massively parallel computing. Ultimately, we evaluate the soil characteristics and the soil's transport properties, such as porosity, diffusion, and permeability tensor.
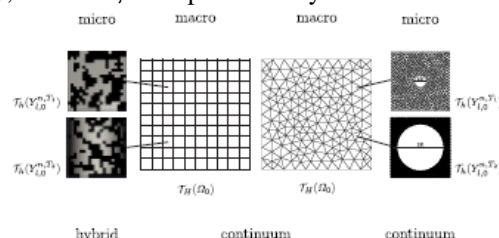

Figure 1: Comparison of hybrid (left) and fully continuous (right) discretization of micro-macro problems

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Parallelization of MIN3P-Thcm: A High Performance Computational Framework for Subsurface Flow and Reactive Transport Simulation

Danyang Su[1], K. Ulrich Mayer[1], Kerry T.B. MacQuarrie[2]

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Key words: MIN3P-THCm, parallelization, reactive transport, subsurface flow, PETSc

Introduction

Reactive transport modeling can be time consuming and memory-intensive, especially for large-scale, long-term simulations with a large number of chemical components and interactions. To meet increasing computational requirements, a parallel version of the reactive transport code MIN3P-THCm [1], ParMIN3P-THCm, has been developed. The parallelized code can run efficiently on machines ranging from desktop PCs to distributed-memory supercomputers. Parallelization of ParMIN3P-THCm was achieved through the domain decomposition method based on the PETSc (Portable Extensible Toolkit for Scientific Computation) library [2], which is also used as the parallel solver package, data structure and message communication tool. The code has been developed from the ground up for parallel scalability and has been tested for up to 768 processors with problem sizes up to 100 million unknowns. The resulting program has shown its strong scalability in modelling large scale reactive transport problems using 768 processors on the WestGrid supercomputer. For isothermal flow and reactive transport problems with uniform density, the total speedup tends to be ideal and near-linear for up to 768 processors when the degrees of freedom per processor is larger than 9000-15000, depending on the relative complexity of the reactive transport and flow problems. For isothermal, uniform density problems, the flow solution usually requires much less time than the reactive transport solution and the total parallel efficiency is around 75%. However, for non-isothermal reactive transport problem including density dependent flow, runtimes significantly increase due to complexities in the flow solution. In some cases, the CPU-time for solution of the flow problem even exceeds that of the reactive transport problem. Difficulties with the solution and scalability of this class of problems have been documented in the literature [3]. To improve the performance, a modified solution method involving both direct and iterative solvers has been implemented, yielding a total parallel efficiency of around 50%. The performance analysis of ParMIN3P-THCm has shown that 2D reactive transport simulations requiring weeks of CPU time, when executed sequentially, can be completed within hours. The new code also allows for refinement of model discretization in both space and time and will facilitate 3D simulations that were impractical to carry out with the sequential version of MIN3P- THCm.
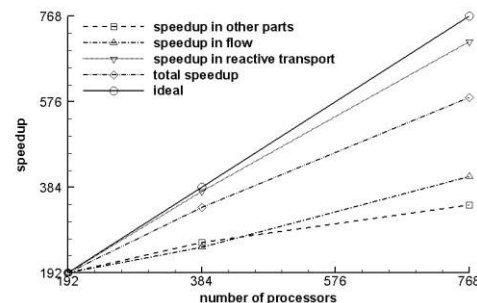

Figure 1: Parallel speedup for general subsurface flow and reactive transport problems

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Hydraulic-Chemical Coupling for Long-Term Prediction Of Mineral Reactions In Heterogeneous CO_2 Storage Systems

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GFZ German Research Centre for Geosciences, Germany

Key words: mineralization, CO_2 storage, simplified coupling

Introduction

Long-term, reservoir-scale, multi-phase reactive transport simulations in heterogeneous settings are computationally extremely challenging, often forcing set up of oversimplified models if compared to purely hydrodynamic simulations. Typically, 1D or 2D models are preferred wherever symmetry allows for it. Only coarse spatial discretizations are adopted for 3D models. As a result, most studies of reactive transport only consider very simple geometries and homogeneous media, thus disregarding spatial heterogeneities at reservoir scale, which in turn are routinely considered by the usually much more detailed geologic models and pure hydrodynamic reservoir simulations.

For estimation of the long-term, reservoir-scale mineralization at the Ketzin pilot site [1], a simplified scheme for coupling chemistry and hydrodynamics was introduced [2]. The purpose of the novel method is not to upscale the simulation grid or apply multi- grid methods, but rather to take advantage of some of the characteristics of the modelled processes, by introducing an approximation in the coupling itself.

Results and Conclusions

The simplified one-way coupling [2] has been validated by means of comparison with fully coupled reactive transport simulations in a typical CO_2 underground storage setting in a saline aquifer, exploring one homogeneous and one heterogeneous case in terms of porosity and permeability [3]. It is demonstrated that for such case studies the chemical reactions in each element of the simulation grid are with good approximation self-similar, which means on the one hand that one single 0D geochemical model can be used as proxy for the reactions occurring in all elements of the simulation grid, and on the other hand that the hydrodynamic transport of solutes plays a secondary role in comparison to the presence or not of the injected CO_2, which is the true driving force of the chemical reactions (Figure 1). Given the advantage of performing coupled simulations on finely discretized grids with no simplifications and upscaling of heterogeneous features of the reservoirs, the uncertainty due to the simplified coupling appears justified. Furthermore, removing the computational burden for reactive transport simulations makes the simplified approach particularly adapted to sensitivity analyses, which are much needed given the uncertainty inherent to geochemical modelling.
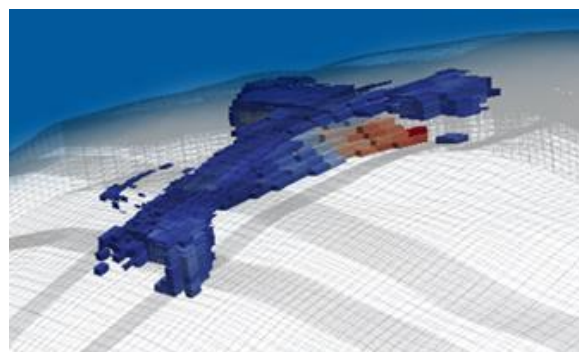

Figure 1: Numerically simulated reaction of mineralization for CO_2 at the Ketzin site

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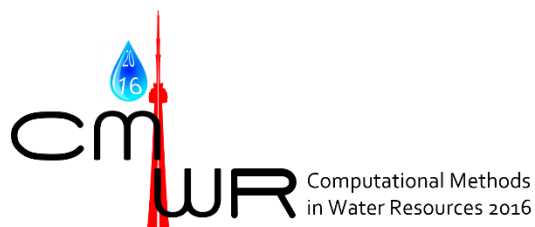
7-1: Novel Developments and Data-Integration in Complex Biogeochemical and Hydrological Process Models

Time: Wednesday, 22/Jun/2016: 9:40am - 10:40am – Location: MSB 3154

Development of a Stochastic Genome-Informed Trait Based Model for Biogeochemical Processes

Eric King[1], Sergi Molins[1], Ulas Karaoz[1], Karthik Anantharaman[2], Nick Bouskill[1], Harry Beller[1], Jillian Banfield[1,2], Carl Steefel[1], Eoin Brodie[1,2]

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Coupling Reactive Transport, Geochemistry, and Geomechanics to Model Changes in Cement Fracture Permeability Due to Exposure to CO_2-Rich Brine

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Development of A Stochastic Genome-Informed Trait Based Model For Biogeochemical Processes

Eric King[1], Sergi Molins[1], Ulas Karaoz[1], Karthik Anantharaman[2], Nick Bouskill[1], Harry Beller[1], Jillian Banfield[1,2], Carl Steefel[1], Eoin Brodie[1,2]

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Abstract

Characterizing and predicting the microbial and chemical compositions of subsurface aquatic systems necessitates an understanding of the metabolism and physiology of organisms that are often uncultured or studied *in situ* under conditions not relevant for one's environment of interest. Cultivation-independent approaches are therefore important and have greatly enhanced our ability to characterize functional microbial diversity. With the capability to reconstruct thousands of genomes from microbial populations using metagenomic techniques, one needs to develop an understanding of how these metabolic blueprints influence the fitness of organisms and to develop methods that incorporate this information into predictive models.

Here, we discuss the development of a genome-informed stochastic trait-based model within a reactive transport framework that describes microbial activity and simulates couple guilds of hypothetical microorganisms. Each group within a functional guild is parameterized from metagenomic data with a unique combination of traits governing organism fitness under dynamic environmental conditions. We simulate the thermodynamics of coupled electron donor and acceptor reactions to predict the energy available for cellular maintenance, respiration, biomass development, and enzyme production.

While 'omics analyses help characterize the metabolic potential of microbial communities, it is currently computationally (among other reasons) prohibitive to explicitly include the thousands of recovered organisms into biogeochemical models. However, one can derive potential metabolic pathways from the genomes (e.g. nitrate reduction; top left, Fig. 1) along with trait-linkages (e.g. organisms that perform 1 or more steps in denitrification) to build probability distributions of

traits. These distributions are used to assemble groups of microbes that couple one or more of these pathways (bottom right, Fig. 1) and whose fitness is impacted by additional physiological traits.
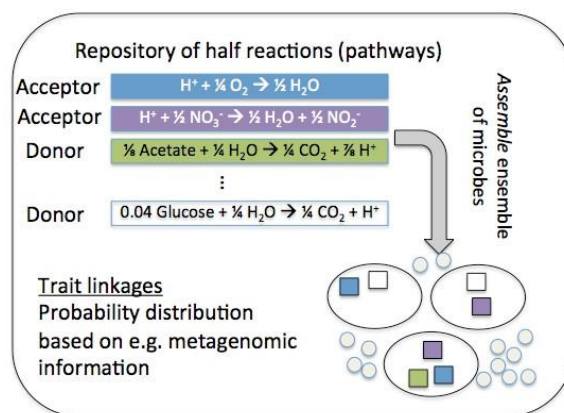

Figure 1: Generalized scheme to construct a microbial community from genome derived metabolic pathways.

From the initial ensemble of microbes, only a subset will persist based on the interaction of their physiological and metabolic traits with environmental conditions, competing organisms, etc. Here, we analyze the predicted niches of these hypothetical microbes and assess the ability of a stochastically assembled community of organisms to predict subsurface biogeochemical dynamics.
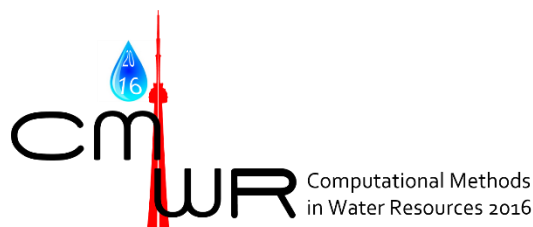
Coupling Reactive Transport, Geochemistry, And Geomechanics to Model Changes in Cement Fracture Permeability Due To Exposure to CO^2-Rich Brine

Jaisree Iyer, Stuart D. C. Walsh, Yue Hao, Joseph P. Morris, Pratanu Roy, Susan A. Carroll

Lawrence Livermore National Laboratory, United States of America

Wellbore integrity is one of the primary concerns associated with the long term storage of carbon dioxide in the subsurface. As wells can serve as conduits between the atmosphere and the storage site, they are often sealed with cement to prevent leakage of fluids. Fractures in the cement or at the cement-caprock interface present potential leakage pathways for stored CO_2. In addition, exposure of cement to acidic CO_2-rich brine results in chemical reactions that include the dissolution of portlandite and precipitation of calcite within the cement. Experiments have demonstrated that these reactions lead to the formation of distinct reaction zones within the cement, having different chemical and mechanical properties. Depending on the conditions, experiments have also shown that the chemical interaction between cement and CO_2-rich brine can result in precipitation of calcite inside the fracture. The extent of these reactions and their effect on the permeability of the fracture strongly depends on the chemistry of the reactions, the transport of the brine in the fracture and the cement, and stresses acting upon them. In this study, we present a model that couples reactive transport, geochemistry, and geomechanics to evaluate the impact of exposure of cement to CO_2-rich brine on fracture permeability. The model incorporates the effects of the rate of reaction and the rate of diffusion to predict the growth of reaction zones in the cement and calcite precipitate in the fracture. This allows for the evaluation of conditions under which cement fractures can be sealed off due to precipitation of calcite in the fracture. For example, for a given fracture geometry, as the flow rate of brine is reduced, the growth of the reactions zones inside the cement diminishes, and the amount of calcite precipitate in the fracture increases. Reduction in fracture aperture is also affected by the deformation of the cement due to stress. Since the different reaction zones in the cement have different mechanical properties, coupling geomechanics with the chemical model quantifies the combined effect of stress and geochemistry in the alteration of fracture permeability.

7-2: Novel Developments and Data-Integration in Complex Biogeochemical and Hydrological Process Models

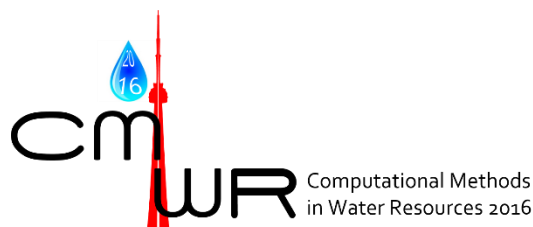*Time: Wednesday, 22/Jun/2016: 2:30pm - 3:30pm – Location: MSB 3154*

Uncertainty Quantification for Discrimination of Nuclear Events as Violations of the Comprehensive Nuclear Test Ban Treaty

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How Much Detail is Detailed Enough? Assessing the Importance of Flow Field Complexity in Predicting Fractured Rock Property Evolution Induced by Mineral Dissolution

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Blind Source Separation for Contaminant Source Characterization

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Computational Methods
in Water Resources 2016

Uncertainty Quantification for Discrimination of Nuclear Events as Violations of the Comprehensive Nuclear Test Ban Treaty

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Since the Comprehensive Nuclear Test Ban Treaty of 1996, nations have been interested in scientific methods to detect recent conduct of Underground Nuclear Explosions (UNEs). A UNE quickly releases a variety of radioisotopes which then decay through connected radionuclide chains.

A particular species of interest is xenon, namely the four isotopes ^{131m}Xe, ^{133m}Xe, ^{133}Xe, and ^{135}Xe. Due to their half lives, some of these isotopes can remain present underground for more than 10 days. This convenient timescale, combined with strong modern detection capabilities, make the xenon family a desirable candidate for UNE detection. These xenon ratios as a func- tion of time have been studied in the past. However, the initial yields from UNEs have been treated as fixed values. In reality, these independent yields are uncertain to a large degree. This study aims to quantify the uncertainty in xenon ratios as a result of these uncertain initial conditions to better bound the values that xenon ratios can assume. We have successfully used a combination of analytical and sampling based statistical methods to reliably bound xenon isotopic ratios. We have also conducted a sensitivity analysis and found that xenon isotopic ratios are primarily sensitive to only a few of many uncertain initial conditions.

How Much Detail is Detailed Enough? Assessing the Importance of Flow Field Complexity in Predicting Fractured Rock Property Evolution Induced by Mineral Dissolution

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Key words: flow field, fractured rock, reactive transport, mineral dissolution, matrix diffusion

Introduction

To reduce the computational cost, reactive transport studies for fractured rock often assume relatively simplified velocity distributions (uniform or parabolic) in the transverse flow direction (perpendicular to the main flow). The objective of this work is to understand and identify conditions where complex, Navier-Stokes type of flow field is needed for predicting fractured rock property evolution, in particular the effective matrix diffusion coefficients and solute transport characteristics, induced by dissolution of multiple minerals with varying reactivity.

Results and discussion

We compared numerical experiments of multi-component reactive transport using three types of flow velocity fields, including velocity profile from solving the Navier-Stokes equations (NS), parabolic velocity profile (P), and uniform velocity profile (U). Numerical experiments were carried out based on a series of 2D fracture slices from CT scanning data of a real fractured rock composed of carbonate, clay, and quartz. Variations in injection flow rates and mineral dissolution rates led to a myriad of Damköhler (Da) values, a measure of the relative magnitude of advection / geochemical reactions. Results show that the difference induced by using the P and U flow fields compared to the NS fields increase with decreasing Da values. There exists a critical Da value above which uniform velocity profile can predict the evolution of fractured rock accurately. Below the critical Da value, NS flow field needs to be used for accurate prediction. The insights gained here will help understand and provide guidelines on the conditions under which simplified flow velocity field is applicable in understanding reactive transport processes in fractured rock.

Blind Source Separation for Contaminant Source Characterization

Velimir Vesselinov, Boian Alaxandrov, Dan O'Malley

Los Alamos National Laboratory, United States of America

Introduction; Contamination of groundwater water-supply resources poses significant social and environmental problems. The remediation of these problems is a huge challenge due to many factors including severe uncertainties and unknowns associated with the contaminant source characterization. Frequently, at the contamination sites, the groundwater is a mixture of waters with different origins (sources) that are commingled in the aquifer; several of these groundwater recharge sources might include contaminants. Typically, all these sources will have different geochemical signatures due to differences in their origins and flowpaths through the subsurface before infiltrating in the aquifer. The identification of the contamination/infiltration sources causing the observed geochemical concentrations in the aquifer can be very challenging at sites where complex physical and chemical processes occur. Source identification can be complicated because (1) some of these sources may have similar geochemical signatures, (2) some of the sources may geochemically interfere with each other, and (3) groundwater transport through the subsurface (from the entry point at the ground surface to the observation point in the aquifer) may be impacted by various physical and chemical processes (e.g., diffusion, dispersion, sorption, retardation, precipit-ation, etc.). To address all these issues, the source characterization may require calibration of a numerical model simulating these complexities against the observed geochemical data. However, this inverse task can be very challenging and computationally demanding. Here, we propose an alternative approach based on a novel model-free machine-learning algorithm.

Blind Source Separation (BSS); BSS methods are based on unsupervised (objective and adaptive) machine-learning algorithms. A classical BSS conundrum is the "cocktail-party" problem [1]: several microphones are recording the sounds in a room (e.g., music, convers-ations, noise, etc.), and each microphone is recording a mixture of all the available sounds. The BSS goal is to "unmix" and reconstruct the original sound sources from the recorded mixtures. For our groundwater contamination problem, the BSS goal is to retrieve the original geochemical concentrations of the contamination /infiltration sources, $S_{p \times k}$, based only on the observed geochemical concentrations in groundwater samples, $D_{p \times m}$, collected at a set of monitoring wells, where p is the number of the wells, k is the number of unknown sources, and m is the number of geochemical components observed at the wells. We initially know only the matrix D of the concentrations observed at the monitoring wells; D is formed by mixing of k original groundwater sources of unknown geochemical composition S. These original sources are blended by an unknown mixing matrix (representative of some unknown groundwater mixing model), $W_{k \times m}$ and pro- duce the observations: $D_{p \times m} = S_{p \times k} W_{k \times m} + \varepsilon_{p \times m}$, where $E_{p \times m}$ denotes a noise or errors in the measure- ments (also unknown). Since both S and W are unknown (we do not know even the exact size of these matrices, because we do not know k), the main difficulty is that our groundwater-contamination BSS problem is illposed. To address this, we have developed a novel BSS method coupling Non-negative Matrix Factorization (NMF) with k-means clustering algorithm, and called this new framework NMFk [1]. Here, we demonstrate that NMFk can be used to solve various synthetic and real-world contaminant-source identification problems using the open-source code MADS [2].
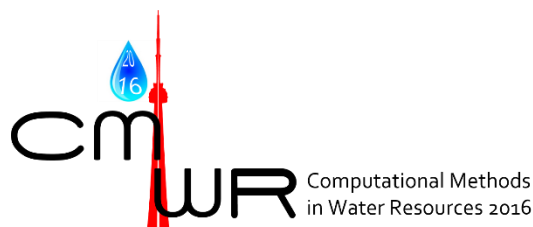
Results & Conclusions; NMFk is applied for analysis[4] and deconstruction of groundwater geochemistry observed in the regional aquifer beneath the Los Alamos National Labora- tory (LANL) site for characterization of contaminant sources. Our preliminary results suggest that 5 orig- inal groundwater sources with different geochemical composition are mixed in the aquifer; potentially 3 of them are associated with contaminant (Cr^{6+}, ClO_4^- and ^3H) releases (Table 1). The source concentrations estimated by NMFk are consistent with more complicated inverse analyses using numerical models. The results are also consistent with Principal Component Analysis of the same data.

#	Cr^{6+} $\mu g/L$	ClO_4^- $\mu g/L$	SO_4^{2-} mg/L	NO_3^- mg/L	Cl^- mg/L	^3H pCi/L
1	2000	0	140	14	100	18
2	0.33	0.88	17	0	0.033	210
3	0.39	80	3.1	21	0.15	0
4	0.36	0	30	6.8	53	0.11
5	0.014	0	11	33	0	0

Table 1: NKFk identified 5 original groundwater sources with different geochemical composition; the key components associated with each type are in orange; the first three types represent contaminant sources.

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7-3: Novel Developments and Data-Integration in Complex Biogeochemical and Hydrological Process Models

Time: Wednesday, 22/Jun/2016: 3:50pm - 5:30pm – Location: MSB 3154

Multi-Component Reactive Transport Modeling of Potential Bacteria-Mediated Nitrous Oxide Sinks in Subsurface Environments

Eugene Ma, Jiao Zhao, Radhakrishnan Mahadevan
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Predictive Modeling of Changes in Riverine Nutrient Fluxes due to Damming

Philippe Van Cappellen, Taylor Maavara
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Process-based Modelling of the Formation and Consolidation of Soil Microaggregates

Alexander Prechtel[1], Nadja Ray[1], Andreas Rupp[1], Kai Uwe Totsche[2]
[1]Friedrich-Alexander University of Erlangen-Nürnberg, Germany; [2]Friedrich-Schiller University of Jena, Germany;
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Development of RT-Flux-PIHM: Understanding Hydrogeochemical Processes at the Watershed Scale

Chen Bao[1], Li Li[1], Yuning Shi[1], Pamela Sullivan[2], Chris Duffy[1], Susan Brantley[1]
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Electron Transfer in Marine Sediments: New Insights and Model Descriptions For Methane-Oxidizing Microbial Consortia

Christof Meile[1], Xiaojia He[1], Jurjen Rooze[1], Yimeng Shi[1], Grayson Chadwick[2], Victoria Orphan[2], Shawn McGlynn[3], Chris Kempes[4]
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Numerical Modelling of Flow, Transport and Biofilm Development in a Single Rock Fracture

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Multi-Component Reactive Transport Modeling of Potential Bacteria-Mediated Nitrous Oxide Sinks in Subsurface Environments

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Key words: global warming, greenhouse gas, nitrous oxide reductase, microbial community

Introduction

Nitrous oxide (N_2O) is a powerful greenhouse gas with 300-fold greater potential for global warming effects than that of carbon dioxide. While many sources of non-biological emissions of N_2O arising from industry have been significantly lowered to address climate change issues, soil-derived N_2O emissions arising from agricultural and biological processes remain less understood.

Nitrate (NO_3^-) in the biosphere can be reduced to nitrogen gas (N_2) through the denitrification pathway by a wide range of bacterial and archaeal taxa, producing a series of incomplete reduced intermediates such as NO_2^-, NO and N_2O, among which N_2O can be either an intermediate for consumption by the microbial community or end product for emissions to the global atmosphere.

Genome analysis has indicated that diverse microbial taxa, such as *A. dehalogenans*, possesses an effective nitrous oxide reductase [1] that enables these bacterial species to take up the potent greenhouse gas (N_2O) that would otherwise be emitted to the atmosphere. The recent finding [2] that such microbial taxa thrives in sediments where chemodenitrification occurs further suggests that bacteria-mediated nitrous oxide sinks may link to the geochemical process in subsurface environments, leading to a decline in N_2O emissions from manipulated soils.

This work aims to investigate the contribution of bacteria-mediated nitrous oxide sinks in subsurface environments to the reduction of soil-derived N_2O emissions by a multi-component reactive transport modeling (RTM) approach.

Methods

A microcosm model was established to study the relationship between *A. dehalogenans* (AD) and other dissimilatory bacteria that have been identified in OR-IFAC sediments based on metagenomic analysis [3], such as *Geobacter* and *Rhodoferax* representing the iron reducers and *Desulfovibrio* representing the sulfate reducers. This microcosm model was then coupled to hydrological and geochemical processes involving chemodenitrification that produces N_2O and Fe^{3+} from NO_2^- and Fe^{2+} present in subsurface environments as a result of both biotic and abiotic reactions.

Results

A community model consisting of AD and other iron and sulfate reducers was established and calibrated against the data observed for a real microcosm experiment. Such community model was extended to couple the chemodenitrification to the growth of AD and other bacterial species. The simulations suggest that AD may play an important role in the evolution of a microcosm under denitrifiying conditions, since the intermediate NO_2^- could react with the biogenic Fe^{2+} to produce N_2O (that can be further taken up by AD), and Fe^{3+} (that can be further reduced by AD and other iron reducers). Finally, this microcosm model that captures the nitrate reduction in anaerobic environments can be coupled to hydrological and geochemical processes by a RTM approach to supplement existing models of N_2O emission leading to improved models for global warming and climate change.

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Predictive Modeling of Changes in Riverine Nutrient Fluxes due to Damming

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University of Waterloo, Canada

Key words: river damming; nutrient fluxes and speciation; reservoir dynamics; projections; eutrophication

Introduction

The damming of rivers represents one of the major anthropogenic disturbances of the natural cycles of water and nutrient elements on the continents. The associated changes in the environmental flows of nutrients have far-reaching ecohydrological consequences, from individual ecosystems to the global biosphere. While dam reservoirs usually act as sinks of macronutrients in river systems, their effects on riverine fluxes and chemical speciation differ markedly from one nutrient element to another. Dams thus fundamentally alter nutrient limitation patterns, trophic conditions and water quality in river ecosystems and receiving water bodies, including lakes, floodplains, wetlands and coastal marine areas. Regional and global assessments of the changes in riverine nutrient fluxes caused by the construction of dams have so far relied on empirical correction factors with limited predictive capability. Here, we develop a knowledge-based upscaling framework, which integrates available data on elemental budgets for individual reservoirs, mechanistic models of nutrient cycling in surface water bodies, and a stochastic analysis of model outcomes [1,2]. The approach enables us to simulate temporal changes in nutrient elimination by damming in all the major river basins of the world. The approach is illustrated by calculating the spatially explicit retention of phosphorus (P) in dam reservoirs for the period 1970- 2030 [2].

Methods

Biogeochemical reservoir modeling: At the core of the upscaling approach is a mass balance model that represents the key biogeochemical processes controlling P cycling in dam reservoirs. The model separates total phosphorus (TP) into total dissolved P (TDP); particulate organic P (POP); exchangeable P (EP); and unreactive particulate P (UPP). Reactive P (RP) is defined as the sum of TDP, EP and POP; it represents the potentially bioavailable fraction of TP. Global predictive relationships for the retention of TP and RP in reservoirs are derived from a Monte Carlo analysis of the model, which accounts for parameter variability within expected ranges. The relationships are applied to the reservoirs of the Global Reservoirs and Dams (GRanD) database [3], in order to estimate the sequestration of TP and RP by dams in each of the major river basins of the world.

Implications: With the proposed approach, we reconstruct global TP and RP retentions by dams in 1970 and 2000, and make projections for 2030. For the latter, we combine nutrient P loading trends developed for the four Millennium Ecosystem Assessment (MEA) scenarios [4] plus a recent survey of dams under construction or projected to be completed by 2030 [5]. A key question we address is the extent to which damming can offset the rising anthropogenic P export by rivers to the coastal zone. The modeling results illustrate the evolving role of damming in the continental P cycle and, in particular, the ongoing geographical shift in P retention associated with the recent surge in dam construction, which is mainly concentrated in South America, central Asia, Africa and Southeast Asia.

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Process-based Modelling of the Formation and Consolidation of Soil Microaggregates

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Key words: deterministic aggregation model, mech- anistic multiscale approach, biogeochemical process model

Introduction

Soil microaggregates have sizes in the range of $20 - 250$ µm and are considered to be the fundamental building blocks for aggregate structure in almost all soils. Their building units (< 20 µm) are mineral-organic associations, minerals, organic compounds. Aggregate forming agents are responsible for the cohesion of the building units: those comprise inorganic cementing agents (e.g. Fe- and Al-oxides, calcium carbonate) and or- ganic gluing agents (e.g. polysaccharides, extra cellular polymeric substances).

Those aggregates are essentially linked with all processes that control interaction, transport and turnover of soil constituents, thus they are intimately linked to the major energy and biogeochemical cycles. They are formed by a complex interplay of physical, chemical and biological aggregation mechanisms, the quantitative role of which is still poorly understood. A mechanistic representation of small-scale processes is identified as one of the priorities to improve soil organic matter dynamics models [1].

Experimental Techniques

A major problem for the quantification of processes related to aggregate formation and consolidation lies in the fact that the isolation and separation of aggre- gates, e.g. by ultrasound, results in physical damage and chemical alteration of the building blocks [2]. Only recently, new experimental techniques allow to characterize their properties down to the nanoscale. Different techniques as, e.g., field flow fractionation, atomic force microscopy, or nanoscale secondary ion mass spectrometry, will be combined in the research group MadSoil [3]. This combination will be the basis for the derivation of new deterministic, process-based mechanisms describing microaggregate formation and turnover.

Modelling Aggregate Formation

A common modelling approach deals with different hi-erarchies of soil organic matter pools, resulting in an ODE system describing the temporal evolution of the constituents [4, 5]. The transfer between the compartments / constituents however is modelled by linear turnover rates for the sake of simplicity - also due to a lack of a mechanistic understanding of the underly- ing processes. Corresponding parameters may be well fitted to a data set, but with little predictive capacity. We briefly discuss the problem of equifinality of such highly parametrized models. Our goal is to gain insight in process mechanisms and derive new mechanistic models on the basis of the aforementionend new experimental techniques. Therefore we establish deterministic partial differen- tial equation models operating on a micro and a macro scale. Thus we can take various small scale soil processes into account as, e.g., molecular diffusion, convection, drift emerging from electric forces, or homo- geneous multicomponent reactions of chemical species in the aqueous phase. Also heterogeneous reactions are considered that change geometry or porosity of the solid particles. The growth of biofilms including con- sumption of nutrients, varying glueing properties, or its influence on the void space also can be included. These small scale processes are implemented in a flexible cellular automaton setting with a coupling to the macroscopic equations by time- and space-dependent averaged coefficient functions, obtained by the technique of homogenization.

The deterministic model approach allows to study the process mechanisms and should further provide a to link to soil functions, as e.g. the hydraulic conductivity, or habitat functions for microbial populations.

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Development of RT-Flux-PIHM: Understanding Hydrogeochemical Processes at the Watershed Scale

Chen Bao[1], Li Li[1], Yuning Shi[1], Pamela Sullivan[2], C hristopher Duffy[1], Susan Brantley[1]

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Key words: watershed hydrogeochemistry, reactive transport

Introduction

We developed a code RT-Flux-PIHM integrating hydrology, land-surface interactions, and reactive transport processes. RT-Flux-PIHM explicitly simulates the terrestrial water cycle, the surface energy balance, and transport and geochemical reactions, including mineral dissolution, precipitation, and ion exchange, and aqueous complexation at the watershed scale (Figure 1). The code offers modeling capabilities interfacing subsurface biogeochemistry, surface hydrology, and hydrogeology [1].

Results and discussion

The model was applied at the Susquehanna Shale Hills watershed, a National Science Foundation (NSF) Critical Zone Observatory (SSHCZO). The model reproduced the field observations of the spatiotemporal patterns of solute concentrations in pore water and in the stream discharge.

Chloride (Cl) dynamics. Simulation results show that the non-reactive chloride concentration is controlled by inputs from rain and the hydrological connectivity of the watershed. The watershed is well connected in the wet seasons (spring and winter), which allows fast flushing of chloride. In contrast, the less connected watershed in the summer sees the "trapping" of chloride in less connected area. Large rainfall events connect the whole watershed and wash out the pockets of high Cl concentrations. However, by the time the water emits at the stream mouth it is diluted significantly. The seasonal change in hydrological connectivity at the watershed scale regulates the chloride concentration in the stream.

Magnesium (Mg) dynamics. The concentrations of the reactive species Mg, however, are regulated by the interplay between clay dissolution and groundwater influx as sources, discharge as the sink, and ion exchange as the storage buffer. Faster clay dissolution in the wet season with abundant water is accompanied by more diluted groundwater influxes and discharge. In the dry summer, the slower clay dissolution is accompanied by less diluted groundwater influxes and lower discharge. Cation exchange buffers the Mg concentration by storing Mg on exchange sites an order of magnitude more than in pore water. Large rainfall events flush out significant amount of stored Mg from the exchange sites while also diluting the waters,

leading to similar Mg concentrations in the stream waters in large and small rainfall events. In general, the multiple processes work together to generate the relatively consistent concentrations for both solutes. The development of RT-Flux-PIHM enables integrated understanding of the hydrogeochemical dynamics at the watershed scale while at the same time offer capabilities to distinguish the role of each process.
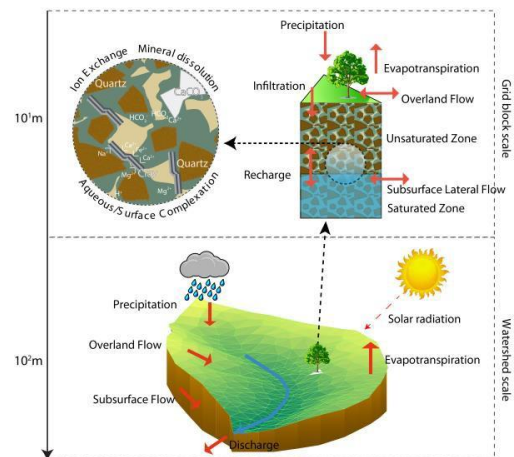

Figure 1. Processes included in RT-Flux-PIHM. Flux-PIHM simulates the hydrological and land surface dynamics (e.g., precipitation, canopy interception, overland flow, subsurface flow, and surface energy balance). The RT module takes the water output from Flux-PIHM and simulates reactive transport, allowing hydrological and biogeochemical coupling at the watershed scale. Geochemical processes include mineral dissolution and precipitation, ion exchange, surface complexation, and aqueous complexation

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Electron Transfer in Marine Sediments: New Insights and Model Descriptions for Methane-Oxidizing Microbial Consortia

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Key words: Direct Interspecies Electron Transfer, Marine Sediments, Anaerobic Methane Oxidation

Introduction

Recent findings suggest that direct extracellular electron transport (DEET) is a common characteristic of microorganisms, allowing for redox interactions across scales that far exceed the local environment of an individual cell. Proteinaceous pilus-like filaments ('nanowires') have been demonstrated to possess electrical conductivity [1], conductive biofilms have been suggested to be a further expansion of pili from microbial cells, extending to 40-50 µm [2] and long- range electron transfer at the cm scale has been found to be involved in sulfur oxidation [3, 4].

The novel insight gained into the functioning of and interactions between microbial groups prompts the development of new model descriptions ranging from microscopic [5] to macroscopic [6] scales. Here we present our developments on the model descriptions in anaerobic marine sediments.

Anaerobic methane oxidation

Anaerobic oxidation of methane in near-surface sediment is mediated by a consortium of anaerobic methanotrophic archaea (ANME) and sulfate reducing bacteria (SRB) [7]. These microorganisms have been thought to exchange chemicals, such that the SRB maintain a chemical environment that is energetically favorable for the ANME to oxidize methane [8]. However, recently the transfer of electrons by extracellular multiheme cytochromes has been suggested as a mechanism for syntrophic exchange in the consortium. Both genes indicative of DEET and structures 10 nm thick and > 1 mm long were reported, suggesting that these structures permit electron transport [9, 10]. Thus, our modeling efforts aimed to develop model descriptions of this consortium accounting for DEET and compare and contrast it with traditional descriptions of electron transport between the microbial partners through diffusional exchange of electron donors. Two model descriptions, one in which electron transport is related to a gradient in reduced electron carrying molecules on a nanowire, the other in which it is driven by an electric field,

were implemented. Our simulations show that the efficient electron transport through nanowires enables methane-oxidizing archaea to circumvent the energetic constraints they face as the accumulation of reaction products lowers the energy yield.

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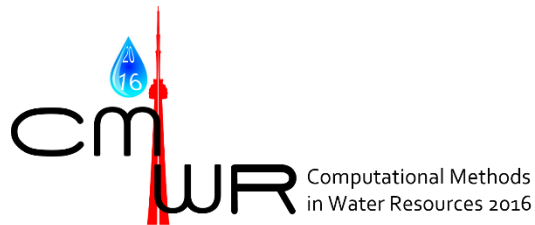
Numerical Modelling of Flow, Transport and Biofilm Development in a Single Rock Fracture

Scott Briggs, Brent Sleep

University of Toronto, Canada

Abstract

In fractured media, formation of biofilms can be used as a remediation technique to degrade undesired contaminants or to act as bio-barriers impeding transport of contaminants. Using micrometer scale discrete numerical algorithms, the behaviour of biofilms in a single fracture was examined to improve the understanding of the role of fracture geometry and flow rates on development. The small-scale approach allows for a unique view on the biofilm growth process where local substrate-to-bacteria reactions drive growth. This discrete model can capture local effects, as a biofilm will only grow when a substrate particle is physically adjacent to a bacteria cell in the numerical grid.

Discrete modeling approaches to the motion of fluid, and substrate transport in a single fracture were taken using Lattice Boltzmann Methods (LBM) and Random Walk (RW) methods respectively. Biofilm development was modelled using a discrete Cellular Automata (CA) approach where each node represents a group of bacteria and their evolution is controlled by local rule based consumption of substrate. Shear was applied to bacterial colonies based on local fracture velocities resulting in removal of biomass at a local scale. Numerical modelling is implemented using General Purpose Graphics Processing Units (GPGPUs) and developed to solve parallel implementations of LBM, RW and CA. The LBM and RW implementation are well suited to efficient parallel computation due to their simplified next-neighbour communication as global knowledge of the system is not required. Performance of the CA, however, is complicated by branching code paths caused by randomized growth patterns that are not well suited to the simplified hardware design of individual cores in GPGPUs.

8-1: Hydro-Mechanical and Thermo-Hydro-Mechanical Modelling of Subsurface Processes

Time: Wednesday, 22/Jun/2016: 9:40am - 10:40am – Location: MSB 2172

Coupling Stress and Reactive Transport in Fractures: Effects of Mineralogy on the Evolution of Contacting Asperities and Fracture Permeability

Kasparas Spokas, Catherine A. Peters

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Efficient solution algorithms for Mixed Finite Element coupled poromechanical models

Massimiliano Ferronato[1], Nicola Castelletto[2], Joshua A. White[3]

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Coupling Stress and Reactive Transport in Fractures: Effects of Mineralogy on the Evolution of Contacting Asperities and Fracture Permeability

Kasparas Spokas, Catherine A. Peters

Princeton University, United States of America

Abstract:

Permeability of rock fractures can increase significantly if reactive flow results in mineral dissolution, especially if positive feedback between flow and reaction results in channelization. While a nascent understanding of this process is emerging, very little is understood about how changes in fracture apertures due to mineral dissolution affects the fracture's geomechanical equilibrium and permeability evolution during reactive flow. Understanding the coupling of geochemical and geomechanical processes is critical to predicting the potential for migration of environmentally-relevant fluids and to identifying important leakage pathways in the subsurface.

This study couples a two-dimensional reactive transport model [1] with a geomechanical equilibrium model [2] to simulate reaction, flow and elastic deformation in a fractured carbonate rock under subsurface confining pressures. The simulations aim to understand the effects of the spatial distribution of reactive and non-reactive minerals on fracture evolution in shales and other caprock candidate formations. Initial fracture aperture geometries are simulated to match the statistical characteristics of the distributions and spatial patterns of apertures in experimentally-fractured rocks. Mineral maps that identify reactive versus non-reactive minerals have been inferred from experimental analyses, including synchrotron- based XRF maps (Figure 1).

This work explores the unique numerical challenges that arise from coupling geochemical and geomechanical processes given their inherently different temporal dynamics. Moreover, this work also addresses the need for hybrid and adaptive spatial grid size that results from the positive feedback phenomenon between reaction and flow that results in the channelization of fractures.

This work has relevance for geologic carbon sequestration, natural gas storage, hydraulic fracturing, geothermal energy and deep well injection of hazardous waste.
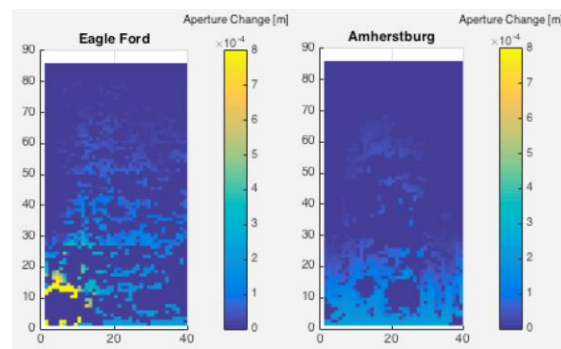

Figure 1: Change in aperture from mineral dissolution after six hours of fluid flow through fractures from two formations: Eagle Ford and Amherstburg.

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Efficient Solution Algorithms for Mixed Finite Element Coupled Poromechanical Models

Massimiliano Ferronato[1], Nicola Castelletto[2], Joshua A. White[3]

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Key words: poromechanics, preconditioners, iterative methods

Introduction

The numerical solution to coupled poromechanics is still a challenging task because of several issues: (1) pore pressure instability, (2) large number of unknowns, and (3) ill-conditioning of the discrete problem. Mixed Finite Element formulations [1] can help alleviate the numerical oscillations in the pressure solution and provide a mass-conservative approach, but typically give rise to very large and ill-conditioned systems of algebraic equations. In the present work a class of efficient block preconditioners is developed with the aim of accelerating the convergence of Krylov subspace methods in complex real-world applications. The main idea relies on building cheap and effective approximations of the two-level Schur complement using a physics-based approach. A purely algebraic formulation is also advanced, thus allowing for the extension to different kinds of coupled problems. The solution algorithm is tested in some numerical applications, proving an efficient and scalable approach.

Numerical model

The Mixed Finite Element integration of the coupled poromechanical equations gives rise to the following system of differential-algebraic equations:

$$\begin{bmatrix} K & 0 & -Q \\ 0 & A & -B \\ 0 & B^T & 0 \end{bmatrix}\begin{bmatrix} u \\ q \\ p \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ Q^T & 0 & P \end{bmatrix}\begin{bmatrix} \dot{u} \\ \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} f^u \\ f^q \\ f^p \end{bmatrix} \quad (1)$$

where K is the structural block, Q and B are the displacement-pressure and pressure-velocity coupling blocks, P is the flow capacity block, A the mass block for the velocity space, and u, p, and q are the vectors of displacements, pressures and velocities, respectively. The integration in time of system (1) by a standard Finite Difference θ-method yields the repeated solution of a sequence of linear algebraic systems in the form κ d = f, with the non-symmetric indefinite 3×3 block matrix:

$$\kappa = \begin{bmatrix} K & 0 & -Q \\ 0 & A & -B \\ Q^T & \gamma B^T & 0 \end{bmatrix} \quad (2)$$

In equation (2) $\gamma = \theta\Delta t$ with Δt the time integration step. The algebraic system is solved monolithically using a non-symmetric preconditioned Krylov subspace method, such as Bi-CGStab. The preconditioner has the following block structure:

$$M^{-1} = \begin{bmatrix} M_K^{-1} & 0 & 0 \\ 0 & M_A^{-1} & 0 \\ -M_S^{-1}Q^T M_K^{-1} & -\gamma M_S^{-1}B^T M_A^{-1} & M_S^{-1} \end{bmatrix} \quad (3)$$

where M_K^{-1}, M_A^{-1} and M_S^{-1} are approximations of K[-1], A[-1] and S[-1] respectively, S being the two-level Schur complement of κ:

$$S = P + Q^T K^{-1} Q + \gamma B^T A^{-1} B \quad (4)$$

The issue of approximating $B^T A^{-1} B$ has been already addressed in the context of the Mixed Finite Element solution of Darcy's flow [2] by defining the diagonal matrix A˜ with entries:

$$\tilde{a}_i = \sqrt{\sum_{j=1}^{nq} |A_{ij}|^2}, \quad i = 1, \dots, n_q \quad (5)$$

The contribution $B^T A^{-1} B$ is then approximated by:

$$S_A = B^T \tilde{A}^{-1} B \quad (6)$$

that has proved to be optimal in the sense that the number of iterations to converge for a conjugate gradient algorithm does not depend on the grid size h [2]. A sparse approximation of the contribution $Q^T K^{-1} Q$ can be obtained using physics-based considerations. Recalling the classical theory of uncoupled groundwater hydrology [3], it follows naturally to approximate $Q^T K^{-1} Q$ with:

$$[S_K]_{ij} = \int_\Omega \frac{b^2}{\overline{K}} N_i^p . N_j^p d\Omega \quad i, j = 1, \dots, n_p \quad (7)$$

Where $\overline{K}$ is is the bulk modulus and b the Biot coefficient. In the context of the current choice for the basis function Np, the matrix SK turns out to be diagonal with non-negative entries.

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8-2: Hydro-Mechanical and Thermo-Hydro-Mechanical Modelling of Subsurface Processes

Time: Wednesday, 22/Jun/2016: 11:00am - 12:20pm – Location: MSB 2172

Studying Long-Term Geochemical Alterations and Geochemically-Induced Stress Changes in Bentonite Using Coupled THMC Models

Liange Zheng, **Jonny Rutqvist, Jens Birkholzer**
Lawrence Berkeley National Laboratory, United States of America; lzheng@lbl.gov

An Assumed Enhanced Strain Method for Modeling Hydraulic Fracture Propagation With Full Poromechanical Coupling

Joshua Alexander White
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Studying Long-Term Geochemical Alterations and Geochemically-Induced Stress Changes in Bentonite Using Coupled THMC Models

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Key words: illitization, THMC modeling, bentonite

Abstract

Geological repositories for disposal of high-level nuclear waste generally rely on a multi-barrier system to isolate radioactive waste from the biosphere. The multi-barrier system typically consists of host rock and the engineered barrier system (EBS) which comprises the waste canister and in many design concepts a bentonite backfill. Illitization, the transformation of smectite to illite, could compromise some beneficiary features of bentonite backfill as an important part of the EBS. It is a major determining factor to establish the maximum design temperature of the repositories because illitization could be greatly enhanced at temperatures higher than 100 ℃ and thus significantly lower the sorption and swelling capacity of this material. However, existing experimental and modeling studies on the occurrence of illitization and related performance impacts are not conclusive, partially because illitization, as one chain of a complex reaction network, is affected by many geochemical factors, and partially because the relevant couplings between the thermal, hydrological, chemical, and mechanical (THMC) processes have not been fully represented in the models. Here we present fully coupled THMC simulations of a generic nuclear waste repository in a clay formation with bentonite-backfilled EBS.

The simulations were conducted with TOUGHREACT-FLAC3D, which sequentially couples the finite-difference geomechanical code FLAC3D [1] with the finite-volume, multiphase flow and reactive transport code, TOUGHREACT [2]. TOUGHREACT calculates the primary variables for THC processes including temperature, liquid pressure or gas pressure, water saturation, ion concentrations and concentration of exchangeable cations and abundance of swelling clay minerals. These primary variables are then passed to FLAC3D via a coupling module to conduct stress and strain analysis. An extended linear elastic swelling model [3] was used in this study to account for swelling as a result of changes in saturation and pore-water composition and the abundance of swelling clay.

Two scenarios were simulated for comparison: a case in which the temperature in the bentonite near the waste canister can reach about 200 ℃ and a case in which the temperature in the bentonite near the waste canister peaks at about 100 ℃. Our model results indicate that illitization is enhanced at higher temperature. Other chemical alterations include the dissolution of K-feldspar and calcite, and the precipitation of quartz, chlorite, and kaolinite. However, the quantity of illitization is affected by many chemical factors and therefore varies a great deal. The most important chemical factors are the concentration of K in the pore water as well as the abundance and dissolution rate of K-feldspar. The geochemical interaction between EBS bentonite and the clay formation has a strong effect on long term illitization in bentonite.

We also compared the chemical changes and the resulting swelling stress change for two types of bentonite: Kunigel-VI and FEBEX bentonite. Less degree of illitization was observed for FEBEX bentonite. Chemical changes lead to a reduction in swelling stress, which is more pronounced for Kunigel-VI bentonite than for FEBEX bentonite.

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An Assumed Enhanced Strain Method for Modeling Hydraulic Fracture Propagation with Full Poromechanical Coupling

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Key words: Hydraulic Fracturing, Poromechanics, Embedded Discontinuities, Finite Element Methods, Finite Volume Methods

Abstract

When modeling hydraulic fractures, it is often necessary to include tightly coupled interactions between fuid-flled fractures and the porous host rock. Further, the numerical scheme must accurately discretize processes taking place both in the rock volume and along growing fracture surfaces. This work describes an effective scheme for handling these challenging numerical issues. Solid deformation and uid pressure in the host rock are modeled using a mixed fnite-element/fnite-volume scheme. The continuum formulation is enriched with an assumed enhanced strain (AES) method to represent discontinuities in the displacement feld due to fractures. Fractures can be arbitrarily oriented and located with respect to the underlying mesh, and no re-meshing is necessary during fracture propagation. Flow along the fracture is modeled using a locally conservative Fnite volume scheme. Leak-off coupling allows for uid exchange between the porous matrix and the fracture. Special attention is paid to accurately representing tip conditions on coarse meshes to ensure accurate prediction of tip propagation velocities. We also describe an efcient preconditioning process that leads to rapid convergence of the resulting discrete system. The scheme is validated using analytical solutions for fractures propagating under viscosity, toughness, and leak off dominated conditions.
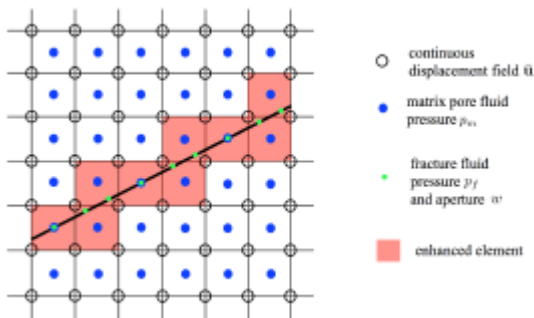

Figure 1: Computational mesh with an embedded fracture. Host rock displacements are modeling using a fnite element scheme, while pore pressures use a cell-centered finite volume discretization. The continuum formulation is enriched with additional degrees of freedom to represent the displacement discontinuity and uid pressure at the fracture surface
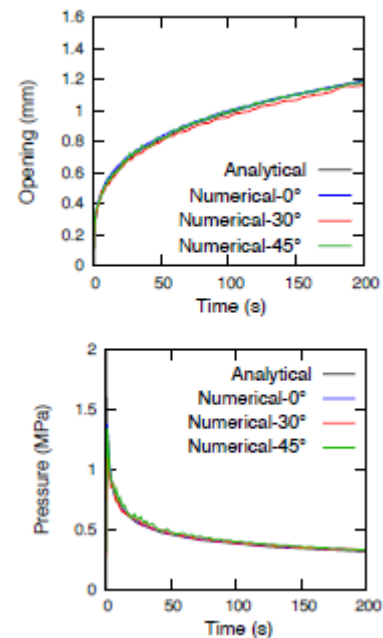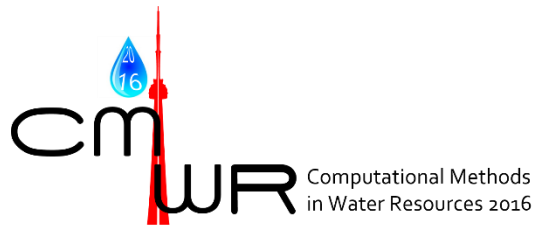

Figure 2: Comparison of numerical and analytical results for a hydraulic fracture propagating under plane-strain conditions in a viscosity-dominated regime. Numerical solutions are presented for a fracture rotated at different angles with respect to the underlying mesh.

8-3: Hydro-Mechanical and Thermo-Hydro-Mechanical Modelling of Subsurface Processes

Time: Wednesday, 22/Jun/2016: 3:50pm - 5:30pm – Location: MSB 2170

On the Analysis of Multirate Iterative and Explicit Coupling Schemes for Coupling Flow with Geomechanics: from Rigorous Mathematical Analysis to Validated Numerical Results

Tameem Almani[1], Kundan Kumar[2], Gurpreet Singh[1], Mary Wheeler[1]

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Inverse Modeling in Coupled Fluid-Flow and Geomechanics: Assimilating Earthquake Time, Location and Magnitude

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Ice-sheet Impacts of Crustal Flexure on the Formation of Abnormal Pore Fluid Pressures in the Geosphere

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On the Analysis of Multirate Iterative and Explicit Coupling Schemes for Coupling Flow with Geomechanics: from Rigorous Mathematical Analysis to Validated Numerical Results

Tameem Almani[1], Kundan Kumar[2], Gurpreet Singh[1], Mary Wheeler[1]

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Key words: Poroelasticity, Fractures, Iterative and explicit coupling, Multirate schemes, Banach contraction mapping, Stability

Introduction

The coupling between subsurface flow and reservoir geomechanics plays a critical role in obtaining accurate results for both environmental and petroleum engineering applications [2]. Due to its physical nature, the geomechanics problem can cope with a much coarser time step compared to the flow problem. Multirate coupling schemes exploit the different time scales for the mechanics and flow problems by taking multiple finer time steps for flow within one coarse mechanics time step. In this work, we first formulate multirate iterative and explicit coupling schemes for coupling flow with geomechanics in poroelastic and fractured poroelastic media. Second, we analyze convergence properties of the devised multirate coupling schemes. Third, we validate the accuracy and efficiency of those schemes numerically.

Single Rave vs Multirate Coupling

In multirate coupling schemes, we solve for q flow finer time steps (Δt), within one coarser geomechanics time step ($q\Delta t$). Both multirate iterative and explicit coupling schemes will be analyzed in this work.

Theoretical Results

For iterative coupling schemes, our analysis is based on studying the equations satisfied by the difference of iterates, and is an extension of the work in [1] and [3]. By a Banach contraction argument, we prove that the corresponding iterative scheme is a fixed-point contraction. In addition, the analysis provides the values of adjustable coefficients used in the proposed schemes. For explicit coupling schemes, we consider stability rather than convergence. We show that, for both single rate and multirate explicit coupling schemes, our computed solution remain well-behaved as long as the initial date are well-behaved.

Numerical Results

The proposed multirate iterative coupling scheme is implemented in the Integrated Parallel Accurate Reservoir Simulator (IPARS). The Multipoint Flux Mixed Finite Element Method (MfMFE) is used for flow discretization, while Conformal Galerkin is used for linear elasticity discretization. We validate our scheme against the Frio field model. Numerical results are shown in Figures 1, and 2.
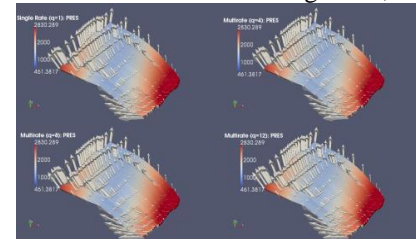

Figure 1: Single rate (q=1) vs multirate (q= 4, 8, and 12) coupling results after 96.0 simulation days. Contours represent pressure filed, arrows represent mechanical displacement field.
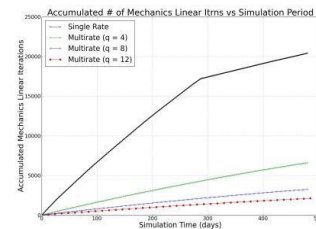

Figure 2: Multirate couplings (q=4), (q=8), and (q=12) result in 67.7%, 84.1%, and 89.6% reduction in total number mechanics linear iterations respectively.

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Inverse Modeling in Coupled Fluid-Flow and Geomechanics: Assimilating Earthquake Time, Location and Magnitude

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Key words: coupled flow and geomechanics, induced seismicity, inverse problem

Introduction

Induced seismicity has emerged as a new constraint in the deployment of subsurface technologies such as groundwater extraction, geologic wastewater disposal, geologic carbon sequestration, geothermal energy, and shale oil and shale gas production [1].

In the past few years, several coupled fluid-flow and mechanical deformation computational models have been proposed to explain the potential relationship between observed seismic activity and subsurface operations impacting the stability of underground geologic structures. These computational models can play a key role in the post mortem analysis and viability assessment of underground fluid extraction/injection [e.g., 2].

A fundamental challenge in all these studies is the inherent uncertainty associated with the forward simulation, which stems from the always-difficult description of complex geological structures in the subsurface. Proper quantification of this uncertainty is required to obtain robust evaluations from induced seismicity studies. In this work, we propose a new methodology to reduce this uncertainty by directly incorporating earthquake-based observations (time, location and magnitude) into the coupled model.

Challenges in inverse modeling

A key challenge in inversion approaches for coupled flow and geomechanics models is that characterizing the posterior distribution—whether through sampling or variational approximation—inevitably requires repeated evaluations of the forward model; thousands, hundreds of thousands, or even millions. The computational cost associated with this large number of model runs is typically prohibitive for the complex nonlinear models required in coupled flow and geomechanics. The difficulties in reconstructing the posterior distribution stem from the fact that (1) sampling is typically inefficient due to the large dimensionality of the inversion parameters, and (2) the posterior often has a complex structure that typically contains strong correlations, skewness and other non-Gaussian features, and even multiple modes.

Proposed approach and results

To overcome some of these challenges, here we propose the application of an uncertainty analysis and data assimilation technique that builds on advanced data-driven methods. The distinct feature of our proposed approach is to incorporate observed seismicity responses into an existing coupled flow and geomechanics mode. These responses include earthquake time, location and magnitude, which are primary descriptors of induced seismicity. These data allow us to constrain model uncertainties in fault angle, rock permeability, fault transmissibility and fault coefficients of friction.

A synthetic 2D, two-way coupled model is used to validate our approach. Results from our nonintrusive Bayesian inverse-modeling approach illustrate the ability to directly incorporate the earthquake observations into the coupled fluid flow and geomechanics description. We show that the posterior distribution correctly combines information from the synthetic earthquake observations with a priori knowledge about the unknown parameters. In particular, we show that we can correctly identify the fault plane and field permeability distributions that explain seismicity triggering. In future work we will extend the methodology to 3D field studies with real seismic observations.

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Ice-sheet Impacts of Crustal Flexure on the Formation of Abnormal Pore Fluid Pressures in the Geosphere

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Key words: poroelastic coupling, crustal flexure, ice-sheets

Introduction

The growth and retreat of ice-sheets can impose significant mechanical and hydraulic loads onto a geosphere, resulting in the isostatic depression and rebound of the Earth's surface, and the possible formation of abnormal subsurface pore fluid pressures. One-dimensional hydro-mechanical coupling, assuming zero lateral strains, can be used to investigate vertical stresses imposed by an ice-sheet on a geosphere, and can be implemented simply as a source/sink term in the groundwater flow equation [1]. The Earth's lithosphere can be represented as an elastic plate. Bending of the lithosphere during and after glaciation will generate flexural stresses in addition to the vertical stresses imposed by an ice-sheet. In some cases, the flexural stresses can be greater than the vertical stresses [2]. These additional flexural stresses can affect insitu pore fluid pressures and requires a fully coupled poroelastic analysis.

Analysis

A two-dimensional, axisymmetric, triangular finite element computational model with 3 degrees-of- freedom per node was developed to investigate the role of crustal flexure on the formation of abnormal insitu pressures. The model was verified against analytical solutions for one-dimensional, two- dimensional and axisymmetric domains. An equivalent elastic thickness of 100 km was used to represent the Earth's lithosphere, similar to Johnson et al. [2]. An elastic lithosphere, relaxed asthenosphere (ELRA) is applied in which the base of the lithosphere was represented using a spring/dashpot boundary condition [3]. The linear elastic spring represents a buoyant restoring force while the dashpot represents the viscous response of the asthenosphere to a time varying load. The ice-sheet is represented using a parabolic profile.

Numerical analyses of approximately 120,000 years were conducted using an axisymmetric domain. Sensitivity cases included varying permeability with depth, differing sizes of continental-scale ice-sheets, differing relaxation times for the viscoelastic boundary conditions, and differing hydraulic conditions at the base of an ice-sheet representing both dry- and wet-bottomed ice-sheets.

The degree of importance of crustal flexure to the generation of abnormal pressures is related to the choice of geosphere parameters, such as permeability, ice-sheet size, and hydraulic boundary conditions. Large ice-sheets tend to generate reduced abnormal pressures compared to smaller ice-sheets. Crustal flexure can lead to the formation of greater over- and under-pressures as compared to vertical stresses alone, however, low rock matrix permeabilities are needed for abnormal pressures to persist in the geosphere thousands of years after glacial retreat.

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9-1: Integrated Hydrologic Models: Advancements and Applications

Time: Thursday, 23/Jun/2016: 11:00am - 12:20pm – Location: MSB 2170

Applications of Watershed-Scale Integrated Modelling in a Canadian Context

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Assessing Continental Scale Groundwater Surface Water Interactions with an Integrated Hydrologic Model

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Integrated Hydrological Model of the California Basin

Jason H. Davison[1], Hyoun-Tae Hwang[2], Edward A. Sudicky[1], Derek V. Mallia[3], John C. Lin[3]
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Impacts of Water Table Configuration on Atmospheric Response over the San Joaquin River Basin

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Applications of Watershed-Scale Integrated Modelling in a Canadian Context

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Earthfx Incorporated, Canada

Integrated modelling has emerged as a powerful tool to assess and understand the interactions between surface water and groundwater processes. The trend towards integrated modelling is being driven by engineering and water management challenges such as water budgeting, resource extraction, water supply takings, and cumulative impact assessments that must now consider complex issues such as ecological flow needs under both drought and high-flow conditions. The USGS GSFLOW integrated surface water and groundwater model is an open source code [1] based on the PRMS hydrologic model [2] and the MODFLOW-NWT groundwater model [3]. Earthfx has completed 10 integrated modelling studies with the GSFLOW code over the past 5 years. Nine of the studies were completed in Ontario and Alberta under varying geologic and hydrologic conditions, and levels of urbanization. These projects have demonstrated the practical value of an integrated approach when undertaking watershed-scale studies.

Recent modelling projects have included: (1) a detailed assessment the hydrologic and hydrogeologic changes of a proposed large scale urban development; (2) a sustainability study of municipal wellfields which support over 1 million residents; (3) evaluation of ecologically significant groundwater recharge areas (ESGRAs) and the groundwater flow paths to sensitive receptors; (4) a water budget of a municipal wellfield affected by operations of a nearby reservoir; (5) an assessment of hydrologic and hydrogeologic conditions under future climate change; (6) a cumulative assessment of industrial water takings in a northern Alberta watershed; (7) an analysis of irrigation demands on the drought response of an ecologically sensitive watershed; and, (8) application of integrated modelling to support the planning and permitting of a large scale mining operation. In every study, the enhanced understanding of groundwater systems and its interaction with streams and wetlands provided by the integrated model produced unique insights and altered the current understanding of the study area.

Experience has shown that spatial scale is a critical factor when undertaking integrated studies. The models provided the most meaningful results when applied to watersheds or multiple subwatersheds. At this scale, it was possible to have the fine spatial detail needed to represent the specific environmental features (e.g. low-order streams, lakes, wetlands) and potential alterations (e.g. surface or groundwater water takings, urbanization, and pits and quarries) that were of interest to the watershed managers. This allowed model results, for example in terms of change in low flow duration or wetland hydroperiod) to be translated into practical water management actions.

A second advantage of this new approach is that cumulative effects assessments can move beyond simple current and future condition "snapshot" comparisons. With a fully integrated model, multi-year comparative simulations can be used to assess the entire hydrologic water budget in a continuous manner, providing significant insight into system response to development plans under both seasonal and longer term climatic patterns.

Practical problems such as model stability and long run times are still issues that must be addressed from the computational end. However, the models have produced results that demonstrate the value of an integrated modelling approach to understanding watershed function and the movement of water over varying spatial and temporal scales. Integrated modelling represents the tool of choice for understanding and solving today's complex water management challenges.

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Assessing Continental Scale Groundwater Surface Water Interactions with an Integrated Hydrologic Model

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Key words: integrated modeling, groundwater surface water interactions

Abstract

Despite growing focus on groundwater surface water interactions, there remain open questions regarding the dynamic behavior of integrated systems. Understanding large-scale response to anthropogenic stressors and climate variability is considered a grand challenge in hydrology that will require novel tools and analytical techniques. We address this challenge using a physics based modeling approach that allows us to simulate dynamically evolving hydrologic interactions from the groundwater to the land surface. Here we present results from a high-resolution (1km^2 lateral resolution) simulation of the majority of the contiguous US (roughly 6.3 million km^2). Previous work demonstrated the feasibility of this approach for a steady state simulation of the same domain [1], and illustrated the utility of model outputs for evaluating spatial patterns in groundwater behavior across many spatial scales [2, 3].

Expanding on the steady state simulation, we developed transient simulations using ParFlow-CLM. This modeling framework simulates three dimensional variably saturated groundwater flow with fully integrated overland flow and coupled water energy balance at the land surface. While computationally expensive, this physics based approach allows for integrated simulation of the surface and subsurface systems, and hydrologic connections that can evolve as the system is stressed. Extensive model validation of a simulation using historical atmospheric forcings shows that this approach does a good job of capturing both groundwater and surface water dynamics across many spatial scales. However, uncertainty in model parameters and extensive human development of hydrologic systems do limit the predictive capabilities of the model.

Here, we use the transient simulations of the continental US to evaluate spatiotemporal patterns in groundwater surface water exchanges across large heterogeneous systems. Model results are used to identify spatial areas with strong feedbacks between the surface and subsurface and to classify the physical characteristics of these regions. Additionally, we evaluate temporal variability in surface-subsurface exchanges in order to quantify the buffering capacity of groundwater to surface systems. Our findings illustrate the importance of incorporating subsurface dynamics into physical hydrology models to accurately capture larges scale system variability and sensitivity to stress.

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Integrated Hydrological Model of the California Basin

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Key words: Hydrology, Groundwater, Surface Water, California, HydroGeoSphere, Weather Research and Forecasting, Water Resources

Introduction

The United States relies on groundwater resources for irrigation, industrial processes, thermal cooling, and human consumption. The unsustainable use of fossil groundwater has resulted in a drastic decrease in water table elevations and has changed natural groundwater flow patterns. Groundwater resources in arid climates are a finite resource, and current excessive groundwater use will impact food security for future generations.

The recent drought in California has pressured farmers to excessively mine groundwater resources. California currently lacks adequate regulation, which has resulted in dire environmental impacts, including extreme land subsidence (2 inches per month), decreased surface water storage (6.6 million acre feet), and loss of agricultural yields ($2.2 billion) [1, 2, 3].

Methods

In order to quantify the risk of water resources, we implemented HydroGeoSphere (HGS), an integrated 3-D control-volume finite element surface and variably-saturated subsurface model, for the entire state of California. The California basin shown in Figure 1 is a 14-layer model with 400,000 nodes. The geological model is based on the STATSGO2 soil data, USGS HYDRO1K topographic data, USGS water use data.
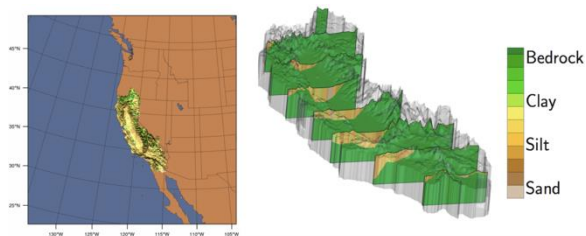

Figure 1: California Soil Model.

Initially, the HGS model was spun-up with historic precipitation and PET data (provided by CMIP5). Once the model reached steady state, groundwater pumping was turned on, and the HGS model run to present-day conditions.

Next, we coupled the HGS California basin to the Weather Research and Forecasting (WRF) model, a 3D mesoscale nonhydrostatic atmospheric model, shown in Figure 2. HGS replaces the land surface components of WRF by providing the actual evapotranspiration (AET) and soil saturation from the porous media to the atmosphere. In exchange, WRF provides HGS with the potential evapotranspiration (PET) and precipitation fluxes. The two-way coupling technique uniquely accepts independent model meshing and projections and links domains based on their geographic coordinates (i.e., latitude and longitude).
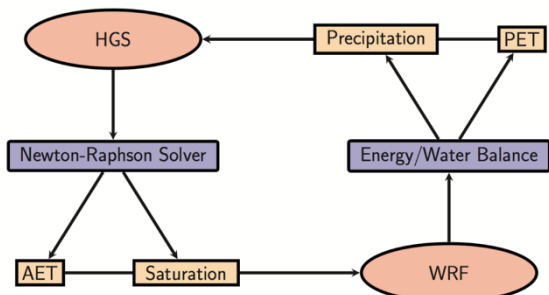

Figure 2: HGS---WRF Model Linkage.

Our methods replicated Central Valley field measured evapotranspiration rates and showed a strong correlation between the depth to water table and turbulent heat fluxes. Our approach to explore the water resources issues due to drought in California is unique because we incorporate the atmosphere, surface, and variably-saturated subsurface into one system.

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Impacts of Water Table Configuration on Atmospheric Response over the San Joaquin River Basin

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Key words: groundwater, atmospheric boundary layer, ParFlow, integrated hydrologic model

Introduction

Soil moisture is known to be a key determinant of the strength of coupling between the land surface and atmospheric responses like precipitation, e.g [1]. Because lateral and vertical subsurface flow links groundwater and soil moisture, the configuration of the water table logically implicates groundwater as a potential driver of land-atmosphere interaction [2,3]. Groundwater extraction and irrigation alter subsurface hydrology (by lowering water tables and wetting the land surface asynchronously with seasonal cycles) and are thus expected to influence subsurface-land surface-atmospheric interactions. Recent modeling studies have examined, for example, the impact of irrigation-wetted soils on regional atmospheric moisture fluxes and precipitation patterns [4], but do not address the role of deeper groundwater on precipitation and other atmospheric responses. Therefore, in this study we seek to better understand the role of subsurface flow under conditions of groundwater extraction and irrigation on resulting atmospheric states. We use an ensemble of coupled ParFlow-WRF (PF.WRF) simulations over the San Joaquin River Basin in California to identify the type and character of land-atmosphere interactions for a set of scenarios that incorporate the effects of irrigation- driven groundwater extraction. We run the coupled models at 1 km lateral resolution using a convection- resolving WRF configuration. Ensemble members include a selection of common boundary layer schemes, variable land surface model configurations, and initial condition perturbations. The coupled PF.WRF model is run for a two-week period in mid-summer that includes local and regional precipitation events. Variability in atmospheric response, particularly in boundary layer height, precipitation patterns, and mountain-valley circulation, under high water table (characteristic of predevelopment conditions) and lowered water table (resulting from historic groundwater extraction) conditions are evaluated in the context of the uncertainty resulting from choice of model physics and atmospheric perturbations.

Changes to the hydrologic system associated with lowered water table elevation appear linked to the atmosphere via changes in boundary layer height. Precipitation response is sensitive to initial condition perturbations, suggesting the water table configuration may be a less significant factor in controlling precipitation processes for this particular domain and time period.

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9-2: Integrated Hydrologic Models: Advancements and Applications

Time: Thursday, 23/Jun/2016: 2:30pm - 4:10pm – Location: MSB 2170

Evaluating the Impact of Landscape Evolution on Soil Carbon and Nutrient Dynamics

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Implementation and Testing Of Reactive Transport Processes for a Coupled (Groundwater/Surface Water) Physically Based Model

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Mass Conservative Velocity Reconstruction for Coupled Flow and Transport Simulations

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Evaluating the Impact of Landscape Evolution on Soil Carbon and Nutrient Dynamics

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Abstract

The intensively managed landscapes (IML) of the agricultural Midwestern US have gone through rapid transformations over the past 200 years due to anthropogenic activities. Land use conversion and modification of soil-moisture regimes have led to the unintended consequences of high nutrient loading in the rivers and receiving water bodies. These shifts on the landscape are central to understanding the cycles of water, energy, carbon and nutrient under environmental changes. However, the magnitude of anthropogenic activities and environmental changes on ecohydrologic and nutrient dynamics have been notoriously difficult to characterize over large areas. Part of the problem is that the underlying vegetation acclamatory processes that affect plant photosynthesis, transpiration, and thus nutrient uptake under elevated CO_2 conditions are not captured in current multi-dimensional biogeochemical models. In addition, large-scale simulations of ecohydrologic and nutrient processes at the emerging lidar-data resolution are numerically expensive due to the density of the computational grid and the iterative nature of the algorithms for solving nonlinearity. Here, we develop a scalable, hybrid CPU-GPU parallel modeling system that links a vertically resolved model of canopy-root-soil biophysical processes with a distributed physically-based integrated surface – subsurface flow and nutrient model to investigate the impacts of environmental changes on large-scale nutrient dynamics. In this coupled model, while canopy processes in the aboveground systems are simulated in parallel in CPU using MPI, hydrologic processes on the land surface and in the belowground systems are simulated using GPU parallel computing. The results show that the micro-topographic and manmade tile drains play an important role in governing the ecohydrologic and nutrient dynamics.

Implementation and Testing of Reactive Transport Processes for a Coupled (Groundwater/Surface Water) Physically Based Model

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Keywords: hydrology, modelling, contaminants, adsorption, degradation

In the context of the European Water Framework Directive (WFD, 2000/60/EC), which aims to achieve a good ecological and chemical status for all natural aquatic environments, tools to help understand and quantify pesticide transfers in agricultural watersheds are necessary. Physically based, spatially distributed models can be particularly useful for representing in detail processes and interactions between the soil surface and subsurface. The present study aims to add reactive transport to one such coupled surface water/groundwater model, CATHY, in order to represent pesticide transfers. Contaminant reactions implemented in CATHY for this study are adsorption (linear and general Freundlich isotherm) and degradation (first order kinetics). The advection part of the model is solved according to the finite volume method, while the diffusive part is solved with the finite element method. Reactions were computed on nodes, after diffusion, using a sequential noniterative approach. This version of CATHY was tested on experimental data from MASHYNS, a hillslope physical model (2 m long, 1 m deep, and 0.5 m wide). On this experimental hillslope, all input and output fluxes are controlled, for water as well as for contaminants, and state variables are monitored. It is fully instrumented with tensiometers, and the soil texture is well characterized and homogeneous. The new CATHY model is progressively tested and validated: first, on water flow under steady and non-steady state conditions, then on nonreactive solute transport with various initial conditions, and finally on pesticide (reactive) transport. Such a dataset makes it easy to define the parameter set for this completely controlled and homogeneous porous medium and to focus on the model's capacity to properly represent the physical behaviour of reactive pollutants in variably saturated media. This is a first step before moving to real and more complicated hillslopes.

Mass Conservative Velocity Reconstruction for Coupled Flow and Transport Simulations

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Accurate evaluation of mass-conservative velocity fields from the numerical solution of Richards' equation is a central component in the simulation of surface- subsurface flow and transport processes. Especially when large-time results are sought, as for example when investigating residence time distributions in a catchment, mass conservation of the tracer transport solver is fundamental to obtain reliable estimates. In this study we present some modeling results obtained with a linear (P1) Galerkin finite element (FE) model for the discretization of Richards' equation and a second order TVD finite volume scheme for the solution of the companion advective transport equation. The local Larson-Niklasson (LN) post-processing procedure is employed to reconstruct mass conservative velocities from the Galerkin solution. This approach, originally proposed for a-posteriori error estimation, modifies the standard FE velocities imposing local conservation on element patches. The resulting reconstructed flow field is characterized by continuous fluxes on element edges that can be used efficiently to drive the finite volume based advection solver. Moreover, continuity of edge fluxes ensures a local conservation principle, allowing the efficient and accurate simulation of long-term transport processes. The accuracy of the LN reconstruction procedure has been shown to be similar to that of the inherently conservative mixed finite element (MFE) approach but with a much lower computational cost, especially for large three-dimensional problems. We test the overall procedure by assessing the ability of the transport model to conserve mass. To this aim, we compare the results obtained by using the velocity field directly derived from the P1 Galerkin solution and the velocity field reconstructed by the LN local post- processing technique in a number of realistic test cases. As a benchmark, we show a comparison also with the results obtained using the MFE velocity field, which is taken as the reference solution. The first sample problems consider simple scenarios involving saturated steady flow and unsteady transport in a homogeneous and heterogeneous simplified aquifer especially designed to test the conservation properties in a case of transient and highly curved streamlines. More realistic and complex scenarios involve the second test case that considers infiltration into an initially dry soil and subsequent seepage towards an open outlet. This complex unsteady and unsaturated flow scenario, involving alternate solute and water injections, a seepage face outflow boundary, and heterogeneous soil, is designed to stress the LN algorithm and unveil its full ability to recover conservative vector fields. From the simpler to the more complex cases, we show that a locally mass conservative velocity field is necessary to obtain accurate transport results. Typical discrepancies in the case of P1 Galerkin velocities are manifest as outgoing solute flux from no flow boundaries, solute permanently trapped in zones of low hydraulic conductivity, and appearance of artificial sources or sinks. These errors often lead to oscillations of numerical concentration that eventually cause the solution to blow up. These inaccuracies do not appear when the LN post-processed velocities are used, showing the importance of using a conservative velocity field to obtain simulations with good mass balance properties.

9-3: Integrated Hydrologic Models: Advancements and Applications

Time: Friday, 24/Jun/2016: 2:30pm - 4:10pm – Location: MSB 2170

Modelling Feedbacks between Vegetation and Soil Moisture in Mountain Grasslands

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Importance of Incorporating Peatlands and Winter Processes into Integrated Surface-subsurface Models of the Athabasca River Basin

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Modelling Free Surface Aquifers to Analyze the Interaction between Groundwater and Sinuous Streams

Nicola Balbarini[1], Wietse Boon[2], Poul Løgstrup Bjerg[1], Jan Martin Nordbotten[2], Philip John Binning[1]
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Wetlands and Flood Mitigation in Ontario: Natural Adaptation to a Changing Climate

Mason Marchildon
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Modeling Urban Flood Dynamics Using High-Resolution Topography and Bathymetry

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Modelling Feedbacks between Vegetation and Soil Moisture in Mountain Grasslands

Giacomo Bertoldi[1], Claudia Notarnicola[2], Johannes Brenner[1], Felix Greifeneder[2], Mariapina Castelli[2], Georg Niedrist[1,3], Ulrike Tappeiner[1,3]

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Key words: soil moisture, mountain grasslands, GEOtop model, vegetation

Soil moisture content (SMC) is a key variable for water budget and controls both physical processes, as runoff generation, and biological processes, as vegetation development. On the other hand, vegetation and land management influence soil evolution and therefore SMC dynamic. Moreover, in mountain areas complex topography adds an additional control on water fluxes and climate. For those reasons, understanding the controls on the spatio-temporal variability of SMC is essential to predict how perturbations in vegetation and climate affects mountain hydrology.

In this contribution we want to model the impact of different land management (meadows versus pastures) on the spatial and temporal dynamic of surface and root-zone SMC, and its relationships with climate and topography. We focus on water-limited alpine grasslands in the LTER area Mazia Valley in the European Alps. The infrastructure includes a dense network of more than 20 stations measuring soil moisture, biomass production observations and two eddy-covariance stations over meadow and pasture. Moreover, more than ten high-resolution SAR (Sentinel1 and RADARSAT2) images were acquired [1], in combination with ground surveys to monitor SMC spatial distribution (Figure 1). In order to understand the different physical controls, SMC has been modelled using the GEOtop hydrological model [2,3], coupled with a dynamic vegetation model [4]. Model simulations allow quantifying the role of local topographic and vegetation properties on soil- vegetation coevolution processes and to distinguish the different controls on soil moisture dynamics related to soil type, topography, land management and microclimate.

Results show that meadows and pastures have different behaviors. Meadows are in general wetter and in flatter locations. This leads to higher vegetation productivity, development of soils with higher water holding capacity and to a positive feedback on SMC. In contrast, pastures are drier, in steeper locations with lower vegetation density and more compact soils due animal trampling, with a negative feedback on SMC. This strong co-evolution of land cover and SMC leads to persistent spatial patterns controlled by topography and management.
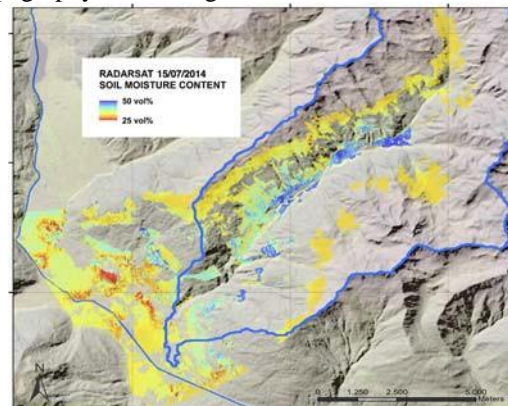

Figure 1: Map of soil moisture estimated with Radarsat SAR image of 15 July 2014 in the Mazia Valley, South Tyrol, Italy.

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Importance of Incorporating Peatlands and Winter Processes into Integrated Surface-Subsurface Models of the Athabasca River Basin

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Key words: Integrated surface-subsurface model, HydroGeoSphere, Athabasca River Basin, Peatland, Winter process

Anthropogenic water stresses including climate and land-use change, agriculture and oil sands mining activities in the Athabasca River Basin (ARB) can have significant impacts on the capacity and sustainability of the existing surface and groundwater resources within the Basin. An appropriate representation of the key surface and subsurface hydrological processes, including those relevant to peatlands and winter processes (snow accumulation and melting) is critical to improve the calibration and predictive ability of models to compute stream flow, groundwater levels and recharge rates throughout the seasons.

The main objective of this study is to demonstrate the importance of the inclusion of peatland and cold-season hydrologic processes in integrated surface/subsurface models, with particular emphasis on the ARB. HydroGeoSphere (HGS), a fully-integrated surface-subsurface flow and solute transport simulator is used here for this purpose (Aquanty Inc, 2013; Hwang et al., 2014). The high- resolution 3D HGS model of the ARB is constructed based on data from the Geological Atlas of the Western Canada Sedimentary Basin (Alberta Geological Survey) and the University of Maryland (UMD) global land cover classification dataset. Historical climate data maintained by the Climate Research Unit of the University of East Anglia was used to drive HGS for calibration against long-term average and transient surface flow and groundwater levels during the historic instrumental period.

Based on the simulation results, it is shown that the peatland distributions and the seasonality of climatic conditions exhibit strong controls on the behaviour of the hydrologic system. In particular, the peatlands in the ARB exhibit a large influence on temporal groundwater storage and releases and evapotranspiration rates, and accounting for cold- season hydrologic processes improves the representation of the timing of peak stream flows.

peatland coverage (%)
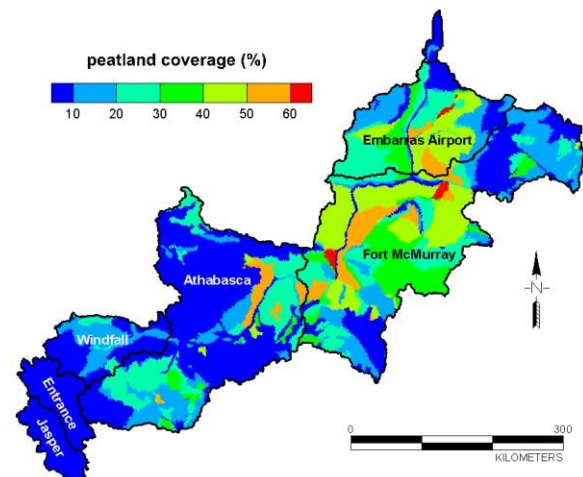
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Modelling Free Surface Aquifers to Analyze the Interaction between Groundwater and Sinuous Streams

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Key words: Groundwater-stream interaction, meandering streams, coordinate transformation, free surface aquifers

Several mathematical methods for modelling free surface aquifers are available. Aquifer-stream interaction is an important application of these models, and are challenging to simulate because stream interaction is described by a highly variable head boundary, which can cause numerical instabilities and errors. In addition, when streams are sinuous, groundwater flow is truly 3-dimensional, with strong vertical flows and sharp changes in horizontal direction. Here 3 different approaches to simulating free surface aquifers are compared for simulating groundwater-stream interaction. The aim of the models was to investigate the effect of meander bends on the spatial and temporal variability of aquifer-stream interaction, and to develop a new 3D conceptual model of groundwater-stream interaction.

Three mathematical methods were tested, representing the three main methods available for modeling 3D unconfined aquifers: a saturated- unsaturated flow model, moving mesh, and a new coordinate transformation. The saturated/unsaturated model couples the saturated groundwater flow equation with a solution of Richards equation. The moving mesh solves the saturated groundwater equation with a free surface and deformable numerical finite element mesh. Finally, the new coordinate transform method employs a coordinate transform so that the saturated groundwater flow equation is solved on a fixed finite element mesh with a stationary free surface.

This paper describes in detail the new coordinate transform method. It employs a transformation of the vertical coordinate, so that the top surface remains stationary. The transformation introduces non-linearities into the saturated groundwater flow equation, with the hydraulic conductivity becoming a function of the head at the top boundary. Mathematical analysis is then applied to show well posedness, and provide stability and linear convergence results. Numerical results confirm the mathematical analysis.

The three methods were compared for a simplified 2-dimensional test case with highly variable stream flow boundaries. Results showed that all methods can properly simulate the groundwater head under steady-state and transient conditions. The coordinate transformation method was the least computationally demanding method, requiring 6 times less simulation time than the saturated-unsaturated and moving mesh flow models. The methods were then compared for a more challenging 3-dimensional problem. Results showed that the coordinate transformation method required 41 times less computational effort than the moving mesh.

The coordinate transformation method was then applied to simulate a field site located at Grindsted stream, Denmark. In order to investigate the importance of stream geometry for the problem, two scenarios were implemented: straight stream and a meandering stream. The model was compared to field data to verify results.

The model was shown to properly simulate groundwater head variability measured at piezometers and discharge to the stream as measured by heat flux, point velocity probes and flux meters. The results from the straight stream scenario and the meandering stream scenario showed that meander bends strongly affect groundwater-discharge to the stream: the discharge is focused at the outward pointing side of the meander bends. Similarly, the groundwater flow paths toward the stream are affected by the stream meanders. Shallow groundwater enters the meander from the outward-pointing side of the bend, while deep groundwater flows beneath the stream and enters the stream from the opposite side. On the basis of these results, a new three-dimensional conceptual model of groundwater-stream interaction is proposed. The new conceptual model demonstrates that conventional two-dimensional symmetric groundwater streamflow conceptual models do not apply for real meandering streams.
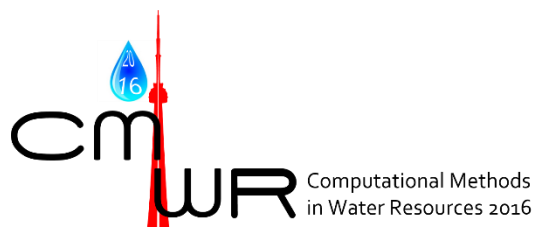
Wetlands and Flood Mitigation in Ontario: Natural adaptation to a changing climate

Mason Marchildon

YPDT-CAMC, Canada

Abstract

Wetlands are often recognized for their flood control value, but little research exists specific to Ontario, where extreme weather in the form of flooding poses ever-greater threats to urban areas. Ducks Unlimited Canada, in partnership with Credit Valley Conservation, has undertaken new research to better understand the role of wetlands in storing and slowing flood waters in an urban/rural watershed. This research employs advanced hydrologic modelling to address the questions of where and how wetlands are most effective at retaining water; what consequences further wetland loss may have on flooding; and what potential wetland restoration could have to improve flood storage within a watershed. The modelling was accomplished using fully-integrated, three-dimensional variably saturated HydroGeoSphere model of the entire Credit valley watershed at a high temporal resolution. Model uncertainty was assessed through Monte Carlo Sampling and cluster computing. This presentation will feature findings from the research, and how this may help inform adaptation actions.

Modeling Urban Flood Dynamics Using High-Resolution Topography and Bathymetry

M. Chase Dwelle, Jongho Kim, Valeriy Ivanov
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Key words: runoff, tRIBS, numerical methods

Abstract

Flooding is the leading natural disaster and poses pub- lic health and economic risks to develope and de- veloping cities. In order to better assess these risks, models of flooding need to rely on modern, up-to-date information about urban environments. Approaches based on grids are computationally expensive because of the restriction of the Courant-Friedrichs-Levy condition. The latter introduces a resolution dependency into hydrodynamic models, severely affecting a number of states such as velocity and water depth and may therefore impact management and design decisions, becoming a serious handicap in real-time situations.

This research links watershed processes to the urban environment by applying an upscaling method that relies on fine-scale information of elevation, roughness, land cover, and soil moisture. The benefit of this approach is that it reduces resolution dependency, allowing for the calculation of hydrodynamic variables at subgrid scales. This approach alleviates the need for grid refinement in complex geometries and surface conditions of the urban interface, improving the computational efficiency for simulating and predicting flooding events.

This improvement allows for the efficient investigation of sensitivities of runoff—which exhibits a non-unique response—while still preserving high-resolution information in the computational domain.

A subgrid hydrodynamic algorithm [1, 2] coupled with the tRIBS hydrologic model suite [3, 4] is used. The approach is verified using appropriate experimental domains for cases of urban flooding. We will discuss the advantages and disadvantes of the approach as well as the implications of the approach for real-time simulations and risk analysis.

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10-1: Reusable Software for Accurate, Efficient, and Reproducible Water Resources Simulation

Time: Thursday, 23/Jun/2016: 9:40am - 10:40am – Location: MSB 3153

Efficient Numerical Implementation of a Groundwater Flow Model of the Unstrut Catchment in Opengeosys

Dmitri Naumov[1,2]**, Thomas Fischer**[1]**, Marc Walther**[1,3]**, Sabine Sattler**[4]**, Olaf Kolditz**[1,3]

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Interoperable Designs and Community Approaches to Software Productivity in Environmental Applications

David Moulton[3]**, Ethan Coon**[3]**, Jeff Johnson**[2]**, Sergi Molins**[2]**, Glenn Hammond**[5]**, Carl Steefel**[2]**, Scott Painter**[4]**, Mike Heroux**[5]**, Lois Curfman McInnes**[1]**, Hans Johansen**[2]**, David Bernholdt**[4]

[1]Argonne National Laboratory, United States of America; [2]Lawrence Berkeley National Laboratory, United States of America; [3]Los Alamos National Laboratory, United States of America; [4]Oak Ridge National Laboratory, United States of America; [5]Sandia National Laboratory, United States of America; moulton@lanl.gov

Using C++ and Object Oriented Design Techniques to Develop the PEST++ Software Suite

David E. Welter

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Efficient Numerical Implementation of a Groundwater Flow Model of the Unstrut Catchment in Opengeosys

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Key words: OpenGeoSys, Hydrology, Simulation, Thermo-hydro-mechanical/chemical (THMC) processes, Groundwater modeling, Unstrut catchment

Introduction

OpenGeoSys (OGS) is a scientific open-source initiative for numerical simulation of thermo-hydro-mechanical /chemical (THMC) processes in porous and fractured media. It has been continuously developed since the mid-eighties with the goal to provide a flexible numerical framework for solving coupled multi-field problems. OGS is targeting mainly applications in environmental geoscience, e.g. in the fields of contaminant hydrology, water resources management, waste deposits, or geothermal energy systems. Recently it has also been successfully applied to new topics in energy storage. OGS is actively participating in several international benchmarking initiatives, e.g. DECOVALEX (waste management), CO2BENCH (CO_2 storage and sequestration), SeSBENCH (reactive transport processes) and HM- Intercomp (coupled hydrosystems). Despite the broad applicability of OGS in geo-, hydro- and energy-sciences, several shortcomings became obvious concerning the computational efficiency as well as the code structure became too complex for further efficient development due to inter- dependencies. OGS-5 version was designed in an object-oriented FEM manner, but in many multi-field applications, however, an even greater flexibility for tailored numerical schemes is essential. Therefore, a new concept was designed to overcome existing bottlenecks.

Development

OGS-6 has a module-oriented architecture based on thematic libraries (Mesh, Numerics) on the large scale and uses object-oriented approach for the small scale interfaces. With recent developments of the C++ language (ISO C++11 standard [2], concepts [3]) the expressiveness of the code increased and made it more developer-friendly. The new C++ standard also makes the template metaprogramming technique code used for compile-time optimizations more compact. Using existing algorithms provided by the Standard Template Library and Boost library, linear algebra solver libraries like Eigen [4], LIS [5], or PETSc [6] it was possible to increase the code efficiency. This allowed for solution of large problems (currently up to 107 elements) as a single thread process. The continuous testing procedure of the benchmarks [1] as it is established for OGS-5 is maintained while development.

Example: Unstrut catchment

The Unstrut catchment is located in large parts in Thuringia, Germany.[7, 8] Starting with a GoCAD geological model a FEM-suitable mesh was constructed. Ground-water flow simulations on a large scale were executed on a single computer node showing validity of the code and its efficiency.
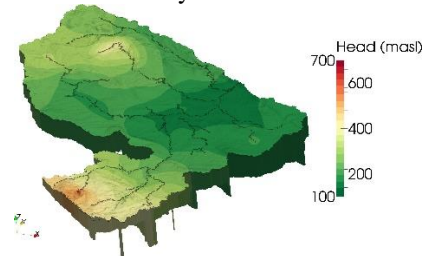

Figure 1: Hydraulic head in the Unstrut catchment, Thuringia, Germany. Flow from higher to lower regions following natural way to catchment outlet.

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Interoperable Designs and Community Approaches to Software Productivity in Environmental Applications

David Moulton[3], Ethan Coon[3], Jeff Johnson[2], Sergi Molins[2], Glenn Hammond[5], Carl Steefel[2],
Scott Painter[4], Mike Heroux[5], Lois Curfman McInnes[1], Hans Johansen[2], David Bernholdt[4]

[1]Argonne National Laboratory, [2]Lawrence Berkeley National Laboratory, [3]Los Alamos National Laboratory,
[4]Oak Ridge National Laboratory, [5]Sandia National Laboratory

Key words: interoperable, open-source, IDEAS,Alquimia, Amanzi/ATS, PFLOTRAN

Motivation; The increasing need to understand and predict climate impacts and feedbacks in terrestrial systems is creating challenges in multiscale and multiphysics modeling. Managing the complexity of these process-rich integrated hydrologic models requires exible software designs that enable exploration of model features and model coupling. Compounding these challenges in modeling are disruptive changes in computer architectures, with the demand for signifcant increases in parallelism creating uncertainty in programming models. This conuence of interdisciplinary challenges is driving the Interoperable Design of Extreme-Scale Application Software (IDEAS) project to explore new community-based approaches to software development. Specifcally, IDEAS is developing the concept of an extreme-scale software development kit (xSDK) that combines improvements in the interoperability of scientifc libraries with advances in software development methodologies and a shift to interoperable model components that can be shared across application teams, to enhance the productivity of developers and users.

Frameworks and Interfaces; To realize the benefits of this approach, we are exploring a flexible and extensible multiphysics framework for these applications that specifies interfaces for coupled processes and automates weak and strong coupling strategies. This framework, dubbed Arcos, supports both model and algorithm development for environmental applications by allowing components to be readily customized, swapped, added, or removed from a simulation. It is used by the open source flow and reactive transport simulator Amanzi, and its derivative work the Advanced Terrestrial Simulator (ATS). In addition, the Arcos design naturally supports process specific interface libraries. For example, reactive transport plays a critical role in environmental pplications, but uncertainty regarding the representation and solution of the underlying reactive systems has led to the development of several similar reactive transport codes with specialized features in their

reaction networks. To share these capabilities across codes efficiently, the biogeochemical engine has been isolated as a component and a generic biogeochemistry interface library, dubbed Alquimia, has been developed. This generic interface makes it easy for a developer to use a specialized feature from another biogeochemistry component, assess its relative importance, and determine if a native implementation in the host code is worth pursuing. Similarly, Alquimia makes the development of new biogeochemical features more efficient because it allows benchmarking comparisons to isolate the new process. For these reasons, Alquimia is targeted as the first Domain Component library in the xSDK. Alquimia was initially developed assuming transport and reaction were weakly coupled (Figure 1), and support for fully-implicit coupling is being added.
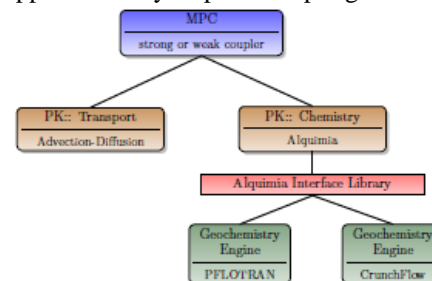

Figure 1: Schematic of the Alquimia interface library providing uniform access to PFLOTRAN and CrunchFlow geochemistry in the flow and reactive transport simulator, Amanzi. This schematic shows the weak or sequential coupling used with operator-splitting, a fully-implicit coupling through Alquimia is under development.

Use Cases; To guide this work in IDEAS, use cases are selected that address scientific questions for existing application projects, and exercise components of established and new codes. In this talk, we will highlight progress on Arcos and Alquimia in the context of the IDEAS use case that is focused on the hydrological and biogeochemical cycling in the Colorado River System.

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Using C++ and Object Oriented Design Techniques to Develop the PEST++ Software Suite

David E. Welter

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Key words: object oriented, inverse modeling, reusable software
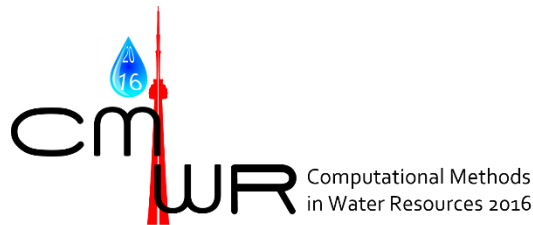
Introduction

PEST++ [4] is an object oriented refactorization of the popular PEST inverse model [1,2,3] which leverages C++ and modern programming techniques to develop an extensible framework for the numerical methods in PEST and builds a foundation to support future development in the areas of inverse modeling, uncertainty analysis, global sensitivity and optimization. Using C++ has facilitated developing an efficient code base with minimal system specific dependencies which runs under Windows, Linux and Mac-OS.

Inverse modeling, uncertainty analysis, global sensitivity and optimization require that the forward model be run many times using different sets of parameters. For highly parameterized models, this may necessitate running the forward model hundreds if not thousands of times so the ability to parallelize these runs can greatly improve efficiency. The original design of PEST has struggled to implement new methodologies to perform model runs efficiently and implementing a new a methodology typically necessitates creating an additional executable. Thus there are many adaptations of PEST. PEST utilizes a serial run manger, Parallel PEST uses a file based parallel run manger, while BEO PEST and GENIE PEST use TCP/IP based parallel run managers. To help promote reusable code, PEST++ has adopted an abstract run manager class which defines a common interface between the PEST++ inverse model and the run managers. The current version of PEST++ provides support for a serial run manger, the YAMR (Yet Another run ManageR) which is an extension of the TCP/IP run manager used in BEO-PEST and the GENIE run manger. Thus a single PEST++ executable replaces many adaptations of PEST. The file base run manger from parallel PEST has not been included in PEST++ as it has been superseded by the TCP/IP based parallel run managers. To further promote reuse of the run manager code, C++, C, FORTRAN, and python interfaces have been created to help third party applications leverage the power of PEST++ run manager. The PEST++ and GSA++ [4] codes use the C++ interface to the run manger to implement inverse modeling and global sensitivity analysis software. Both of these applications are written in

C++ and use object oriented programming techniques. While the current version of PEST++ focuses on supporting the functionality of PEST, it has been designed to be extensible and there are plan to add global and hybrid methods. The GSA++ code currently supports the Method of Morris and Sobol's method and is expected to grow as additional methods are added. While the PEST++ provides for code reuse between applications in the PEST++ suite, third party applications such as PESTPP-PSO also use the PEST++ run manger to manage their forward model runs. PEST-PSO was written in FOTRAN and combines the particle swarm and Pareto methods to provide a global estimate of the Pareto front. By using the PEST++ run manager, PEST-PSO development was able to focus on implementing the numerical method without being burdened by developing its own run management software.

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10-2: Reusable Software for Accurate, Efficient, and Reproducible Water Resources Simulation

Time: Thursday, 23/Jun/2016: 11:00am - 12:20pm – Location: MSB 3153

Benchmarks and Reusable Interfaces for Efficient Reactive Multicomponent Flow Solvers

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A Flexible Framework for Process-Based Hydraulic and Water Quality Modeling of BMP Performance

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Application of PA-DDS in Solving Bi-Objective Water Distribution Systems Benchmark Design Problems

Mohammadamin Jahanpour[1], Juliane Mai[2], Thouheed Abdul Gaffoor[1], Bryan Tolson[1]

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Development of the Operational WRF-Hydro Meteorological Forcing Engine for U.S. National Water Forecasting Capabilities

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Benchmarks and Reusable Interfaces for Efficient Reactive Multicomponent Flow Solvers

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Key words: decoupling algorithm, global implicit approach, object–oriented software design

Introduction

We consider problems with coupled multiphase (includeing phase appearance/disappearance) multicomponent flow for general reaction networks (including kinetic and equilibrium reactions as well as dissolution and precipitation of minerals) with a large number of biochemical species. Applications of those problems include but are not limited to water resources. We discuss algorithms for the numerical solution of those problems as they are implemented in the software package Richy (see below) in terms of accuracy, reliability and efficiency. Finally we discuss possibilities to design highly flexible and reusable interfaces for those algorithms.

Richy Richy is a software package for coupled systems of nonlinear partial differential equations on multiple scales developed at the chair of applied mathematics 1 of the university of Erlangen-Nürnberg. It is based on M++ [1] and uses distributed memory parallelization.

Algorithms under Consideration

The algorithms implemented in Richy are generalizations of the algorithm presented in [2]. In a first step, linear combinations of the governing equations are performed. The resulting system has less coupled partial differential equations and can therefore be solved with a decreased computational complexity. In the context of multiple scales, this algorithm is applied scale by scale with a special treatment of the inter–scale dependencies. The decoupled linear equations are solved in the second step. Finally, the remaining coupled problems are solved using Newton's method with local implicit elimination for the equilibrium conditions. The algorithms have been implemented using different spatial discretizations (e.g. Lagrange elements and hybrid mixed finite elements) on unstructured meshes in 1 to 3 dimensions. Implicit time stepping schemes are used for discretization in time. Richy has been compared with other software packages in terms of accuracy and efficiency for several problems in the MoMaS benchmark [3]. While the results of the simulations were reproducible with all other software packages, the efficiency of Richy was the best. We remark that the main aspects ensuring the efficiency of our implementations is the combination of the decoupled structure and a global implicit approach (i.e. Newton's method). Modifications for this benchmark that test problems with narrow mixing zones will be suggested.

Flexible and Reusable Interfaces

The above mentioned algorithms are implemented for unstructured meshes and can therefore be applied to arbitrary geometries. In each time step, any space dependent but species independent quantity (e.g. porosity or fluid velocity) can easily be passed as space dependent functions. Regarding the inter–species and inter–scale dependencies, more sophisticated software design approaches have to be used in order to obtain highly flexible and reusable interfaces. In particular, we want to retain the accuracy and reliability of our algorithms, as well as the efficiency resulting from the decoupled structure of our problem and the use of global implicit approaches. Furthermore our algorithms shall be able to exploit the benefits of distributed memory architectures. The global implicit approach implies the use of interfaces that do not only provide reaction rate information, but also derivative information. While this is straight forward for kinetic reactions without inter-scale dependencies, a perfect interface for the opposite case (i.e. reactions that are either controlled by equilibrium and/or have inter–scale dependencies) has not yet been found. Nevertheless, there are promising object– oriented approaches that might be used to push the above mentioned algorithms towards a highly flexible and reusable implementation.

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A Flexible Framework for Process-Based Hydraulic and Water Quality Modeling of BMP Performance

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Key words: Green Infrastructure, Reactive Transport, Water Quality

Introduction

Models that allow for design considerations of green infrastructure (GI) practices to control stormwater runoff and associated contaminants have received considerable attention in recent years. While popular, generally, the GI models are relatively simplistic. However, GI model predictions are being relied upon by many municipalities and State/Local agencies to make decisions about grey vs. green infrastructure improvement planning. Adding complexity to GI modeling frameworks may preclude their use in simpler urban planning situations. Therefore, the goal here was to develop a sophisticated, yet flexible tool that could be used by design engineers and researchers to capture and explore the effect of design factors and properties of the media used in the performance of GI systems at a relatively small scale. We deemed it essential to have a flexible GI modeling tool that is capable of simulating GI system components and specific biophysical processes affecting contaminants such as reactions, and particle-associated transport accurately while maintaining a high degree of flexibly to account for the myriad of GI alternatives. The mathematical framework for a stand-alone GI performance assessment tool has been developed and will be demonstrated. The process-based model framework developed here can be used to model a diverse range of GI practices such as green roof, retention pond, bioretention, infiltration trench, permeable pavement and other custom-designed combinatory systems. We demonstrate the utility of this GI modeling framework to simulate flow and transport four different GI systems.

Framework Description

The tool accommodates three layers of processes including hydraulic, particle/colloid transport and dissolved and particle-associated reactive transport of multiple chemical species. Water quality systems are represented as a series of interconnected fully mixed blocks representing different media including surface water bodies, saturated and unsaturated porous media and aggregate storage layers. The blocks are connected using features referred to as connectors. There is a great deal of flexibility in specifying the head-storage relationships for the blocks and head- flow relationships for the connectors giving the tool flexibility in representing a wide range of systems with different levels of complexity. Processes such as atmospheric exchange (e.g. aeration), build-up and wash-off of contaminants, vapor transfer and evaporation can also be introduced via catalogs pre- defined models or through user-provided expressions.

Numerical Method

An adaptive time step Newton-Raphson algorithm is designed to solve hydraulic, particle transport and reactive transport. The algorithm is designed to provide an optimal computational efficiency using an innovative approach that only updates the Jacobian matrix at times necessary. Special treatment is considered to deal with the problem of dry domains occurring when for example surface water blocks or storage zones become fully dry.

Example applications

Four demonstration applications covering a diverse range of systems will be presented. The example applications include a evaluating hydraulic performance of a complex bioretention system, hydraulic analysis of porous pavement system, flow colloid-facilitated transport, reactive transport and groundwater recharge underneath an infiltration pond and finally reactive transport and bed-sediment interactions in a wetland system will be presented.

Application of PA-DDS in Solving Bi-Objective Water Distribution Systems Benchmark Design Problems

Mohammadamin Jahanpour[1], Juliane Mai[2], Thouheed Abdul Gaffoor[1], Bryan Tolson[1]
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Key words: PA-DDS, Water Distribution Systems, Multi-objective Design

Introduction

Multi objective evolutionary algorithms (MOEAs) are extensively employed to optimally design water distribution systems (WDS) regarding multiple design objectives. Wang et al. [1] recently reported estimates of optimal Pareto fronts for twelve WDS benchmark problems of different complexity using the five different MOEAs AMALGAM, Borg, E-NSGA-II, E-MOEA, and NSGA-II. They solved the twelve problems regarding design cost and network resilience and presented the optimal and best-known Pareto fronts for three small and nine large problems, respectively. These reference Pareto fronts enable rigorous tests of the capability of newly proposed algorithms. Each MOEA employed in Wang's study requires the adjustment of four to eleven algorithm specified parameters. Knowing that the performance of those MOEAs is very sensitive to these settings, one needs to spend a considerable amount of time and effort to fine-tune the algorithmic parameters.

Materials & Methods

In this study, the Pareto archived dynamically dimensioned search (PA-DDS) [2] is employed to solve Wang's twelve benchmark design problems. The PA-DDS algorithm is a parsimonious multi-objective optimization algorithm with only one adjustable parameter to determine the perturbation size r (default value of 0.2). The user's effort of tuning algorithm parameters is hence diminished. The PA-DDS method has already been successfully applied to solve WDS design problems [2]. The key point of the PA-DDS algorithm is the generation of new candidate solutions based on the current archived non-dominated solutions. Several different metrics controlling this candidate generation are available for PA-DDS, i.e. random sampling, crowding distance, hypervolume contribution, and convex hull contribution [3]. Different budgets for objective function evaluations to solve each benchmark problem are tested. The maximal budget per problem, however, is the one used in Wang's study.

Results & Discussion

Without parameter tuning, i.e. using the default of 0.2 for the algorithmic parameter r, the performance of PA-DDS is compared with the optimal and/or best- known Pareto fronts obtained by pooling the results of the five MOEAs [1]. The PA-DDS optimization algorithm is capable to approach Wang's best-known Pareto front for almost all case studies using even less objective function evaluations (Fig. 1). The comparison of the different selection metrics yields that the method of hypervolume contribution is directing the evolutionary search more reliable compared to the other metrics.
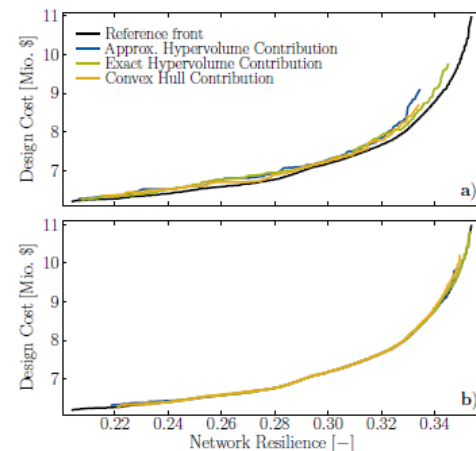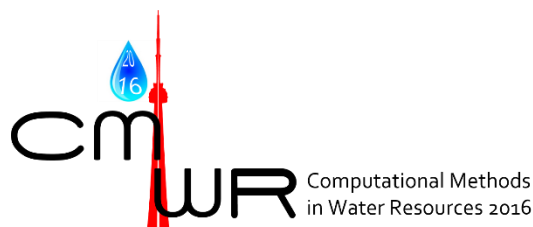

Figure 1: Performance of PA-DDS with different metrics to generate new candidate solutions (colored lines) compared to the reference Pareto front reported by Wang et al. [1] (black line) for the Hanoi network with its 34 decision variables and 6 pipe diameter options. The budgets used for PA-DDS are (a) 10 000 and (b) 100 000 model evaluations while the budget in Wang's study has been 600 000 for each of the used algorithms.

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Development of the Operational WRF-Hydro Meteorological Forcing Engine for U.S. National Water Forecasting Capabilities

Wei Yu, Dave Gochis, Linlin Pan, Logan Karsten, Minna Winn, Dave Albo

NCAR, United States of America;

The WRF-Hydro modeling system is a community-based model coupling framework designed to link multi-scale process models of the atmosphere and terrestrial hydrology. The system provides the capability to perform simulations and predictions of terrestrial water cycle processes on a wide range of spatial and temporal scales. The fully-distributed, WRF-Hydro modeling system is currently scheduled for operational implementation as a nationwide streamflow forecast system for the U.S. National Water Center (NWC) during the spring of 2016. This presentation will describe the meteorological forcing engine developed for the NWC Initial Operating Capability (IOC), where the WRF-Hydro modeling system is driven by multiple meteorological forcing products coming from multiple temporal and spatial scales. The forcing engine has been designed and created for use in real time operations and to ac commodate the different time and space scales of input data. The forcing engine encompasses the regridding, downscaling, layering and, where relevant, bias correction of operational meteorological inputs.

These input products include the Multi-Radar Multi-Sensor (MRMS) precipitation estimate product (used as the real-time precipitation estimate product for analysis and for hydrological model spin-up), the High Resolution Rapid Refresh (HRRR) and Rapid Refresh (RAP) models for short term hydrologic forecasts, NCEP Global Forecast System product for medium term hydrologic forecasts, and NCEP Climate Forecast System product for long term ensemble hydrologic forecasts. The overarching engineering goal of the meteorological forcing engine development effort is to provide a comprehensive software package, which emphasizes real time performance and flexibility for different applications in both real time and research, as well as to foster improvements in scientific results from the WRF-Hydro modeling system.

10-3: Reusable Software for Accurate, Efficient, and Reproducible Water Resources Simulation

Time: Friday, 24/Jun/2016: 9:40am - 10:40am – Location: MSB 3153

Automated Systemtesting in Scientific Numerical Software Frameworks Using the Example of Dune

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An Open-Source Method for Flow and Flood Inundation Estimation at Regional Scales

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BET: Software for Measure-Theoretic Stochastic Problems

Steven Mattis[1], Lindley Graham[2]

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A Python Framework for Laplace-Transform Solutions

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Development of a Program Data Structure Enabling the Flexible Integration of Effects into a Basis Flow   Model

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Verification and Validation of 3D Models for Wave and Current Interactions with Rigid and Erodible Structures

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Automated Systemtesting in Scientific Numerical Software Frameworks Using the Example of Dune

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Key words: System testing, automated software testing, numerical software, Dune, dune-pdelab, DuMux

Quality of scientific software

Many current publications for numerical methods and computational science contain results obtained with research code developed by the scientists themselves at universities and research institutes. Development time is often limited and sustainable software development not the focus. However, software reliability and reproducibility of results are of utmost importance in scientific research. Several attempts have been made to formally define software quality, see e.g [4]. Within the context of scientific software, the authors identify code documentation and maintainability, implementation correctness, performance, and numerical correctness as important software quality features with respect to every day usability, development and scientific value. Thereof, at least implementation correctness and numerical correctness, and with limitations, performance can be tested in an automated way, taking workload off users and developers. Automated, publicly visible software testing contributes greatly to the reliability of the scientific software.

Towards systemtesting in scientific software

Especially in larger open-source numerical software frameworks developed at universities, such as deal.II, FEniCS, and Dune, regular (and automated) unit testing is already successfully improving development process, maintainability and reliability of the software. Such software often provides a wide number of features that can be diversely combined and are continuously extended. The available combinations to build a running program soon become vast. The interaction cannot be captured by unit testing and heavily relies on user feedback via mailing lists, issue trackers, and message boards. Often however, the developer himself can overlook the possible uses of a software component in the context of a running program. Following this thought, we present an easy-to-use interface for developers to configure systemtests, i.e. tests that aim at testing the software's components within a realistic user setup and emulate the diverse combination possibilities. This interface is developed using the example of the Distributed and Unified Numerics Environment (Dune [3]) but the ideas are kept sufficiently general to allow for portability to other frameworks.

Systemtesting using the example of Dune

Dune is a modular open-source numeric environment providing basic features for developing numerical applications. Dune-pdelab [2] is a discretization module for fast prototyping of finite element and finite volume applications. DuMux [1] is an open-source simulator for flow and transport in porous media simulator built on Dune.

We introduce dune-testtools, a new Dune-module providing testing tools and the necessary features for systemtesting in application-focused modules like dune-pdelab and DuMux. An easy interface is introduced using an extended INI-file syntax that allows developers to write systemtests featuring dynamic and static feature variation. Our testtools make use of a CMake-based build system and tests with CTest [5]. Results of a systemtest can be evaluated with specific testtools extending the usual return-code based evaluation. Furthermore, we present the necessary infrastructure to use those testing tools in an automated setup using BuildBot (http://buildbot.net/). Finally, we suggest an open-source work-flow for testing in scien- tific software development.

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An Open-Source Method for Flow and Flood Inundation Estimation at Regional Scales

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Key words: Flood Inundation, Open-Source, AutoRAPID

Abstract

Flooding is a leading cause of fatalities and destruction among natural disasters, with its effects being felt in both rich and poor countries of the world. In areas with ample data and financial resources, predictive and protective measures can greatly reduce the harmful effects of floods. However, in areas with limited data and financial resources the effects of flooding can be devastating and with little warning. This presentation will introduce an open-source model to simulate (hindcast and forecast) hyper-resolution flow and flood inundation estimates using near-global, freely available data.

The method routes gridded runoff data from land- surface models (LSMs) through a one-dimensional river routing model called Routing Application for Parallel computatIon of Discharge (RAPID) [1]. Peak flow in each river segment is then used to estimate flood inundation using a simple flood delineation model called AutoRoute [2]. This combined approach (referred to as AutoRAPID) has been used to simulate flow and flood inundation over a 230,000 km2 area in the United States [3], and can be applied in more data austere regions as well. The conceptual diagram of the AutoRAPID model is shown in Figure 1.
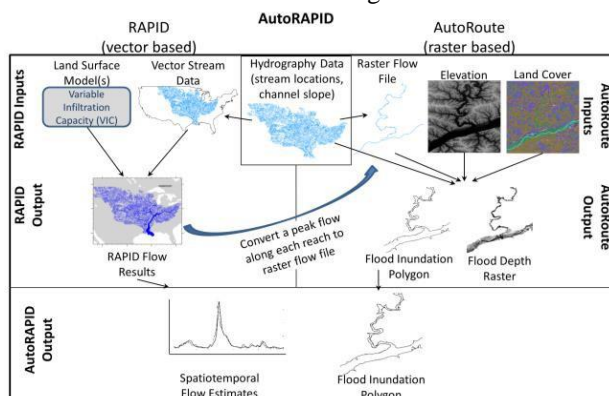
Figure 1: Conceptual diagram of AutoRAPID model framework, data requirements, and data outputs.

The following state data is required: hydrography (stream location and channel slope), elevation, and land cover data. Forcing data is limited to hindcast or forecast gridded runoff data from LSMs and outflow estimates from dams and reservoirs (if available). The outputs of the AutoRAPID model are spatiotemporal flow estimates in any river reach, and peak-flow flood inundation maps.

Several sources of elevation and land cover data are available, often freely obtained from the Unites States Geological Survey (USGS) or the National Aeronautics and Space Administration (NASA). Hydrography data is freely obtained from the USGS or can be derived using elevation data and geographic information system (GIS) models. Regional and global LSMs produce both historical and forecasted runoff data in a gridded format at spatial resolutions typically ranging from 10 to 100km. Although some sources of LSM runoff data require purchase, many are free to the public.

Using predominately open-source models and data available in the public domain, a test case will be presented where river flow and flood inundation are hindcasted as well as forecasted. Comparisons to observation data will be provided where available.

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BET: Software for Measure-Theoretic Stochastic Problems

Steven Mattis[1], Lindley Graham[2]

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Key words: uncertainty quantification, open source software, measure theory

Introduction

BET [1] is an open source python package for solving measure-theoretic stochastic problems [2]. The name BET stands for the Butler, Estep, and Tavener method for measure-theoretic stochastic inversion, the frame- work for which the software has been built. The package contains modules and methods for approximately solving the physics-based measure-theoretic stochastic inverse problem and processing the solution for analysis, decision-making, or predictions. The method involves sampling in a domain of uncertain parameters, calculating quantities of interest related to those parameters, and using known probabilistic information about measured data to predict the probability in the domain of parameters. This software has been applied successfully for stochastic inversion for a variety of geo-physical problems including shallow water flow, multi-phase subsurface flow, and groundwater contaminant transport [3].

There are four main submodules in the package. The first provides methods for sampling the parameter domain. The second provides methods for constructing the discrete stochastic inverse problem and calculating probabilities. The third contains methods for performing sensitivity studies. The fourth contains methods of post-processing, plotting, and saving data.

Packages

1.   Sampling subpackage: Provides methods for basic and goal-oriented adaptive sampling.
2.   CalculateP subpackage: This subpackage provides classes and methods for calculating the probability measures.

Modules:

- **SimpleFunP** module provides methods for creating simple function approximations of basic probability densities, ρD.
- **VoronoiHistogram** module provides methods used by simpleFunP to calculate the generating points, edges, and volumes for the regular Voronoi tessellation of a rectangular domain.
- **CalculateP** module provides methods for approximating induced probability densities, $\rho\Lambda$.

3.   Sensitivity subpackage: This subpackage contains classes and methods for calculating sensitivities and choosing optimal quantities of interest.
4.   PostProcess subpackage: This subpackage contains classes and methods for post-processing results from calculations.

Modules:

- **PlotP** module provides methods for approximating, visualizing, and plotting 1-D and 2-D marginal probability densities.
- **PlotDomains** module provides methods used to plot two-dimensional domains and/or two-dimensional slices/projections of domains.
- **PostTools** module provides methods for sorting probability data, identifying regions of high probability, and saving data in a variety of formats.
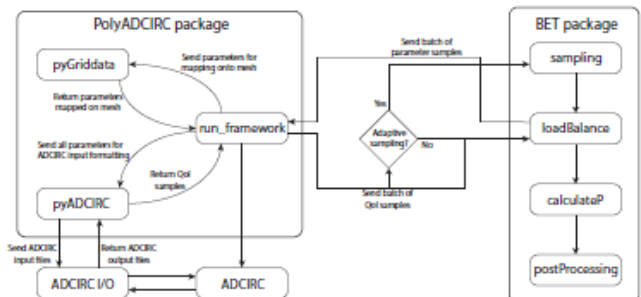

Figure 1: Package Layout

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A Python Framework for Laplace-Transform Solutions

Mark Bakker

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Key words: Laplace transform, Python, semi analytic, Jupyter

Abstract

The Laplace-Transform method is a powerful method for the solution of flow problems, especially groundwater flow problems. Solutions can be obtained analytically in the Laplace domain for a variety of settings. Analytic back-transformation from the Laplace domain to the time domain is much more difficult and often not possible in closed form. Luckily, numerical algorithms exist to perform the back-transformation. Such solutions are referred to as semi-analytic and commonly give very accurate results. In this presentation, examples will be given using the back-transformation algorithm of De Hoog et al. [2].

A framework has been developed in Python to program semi-analytic Laplace transform solutions. Examples will be given for a number of groundwater flow problems varying from simple one-dimensional solutions to complex multi-layer analytic element simulations with the open-source code TTim [1]. All examples are presented as Jupyter Notebooks. The algorithm of De Hoog et al. [2] has been implemented in a variety of ways, from pure Python to Cython, Numba and a FORTRAN extension.

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Development of a Program Data Structure Enabling the Flexible Integration of Effects into a Basis Flow Model

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Motivation

The assessment of the long-term safety of a deep underground repository for radioactive waste requires a comprehensive understanding of the system and capable numerical tools. RepoTREND is a final repository simulator being developed by GRS for simulating the

- release of contaminants and
- their transport through the near-field and far-field to the biosphere including
- the estimation of the radiological consequences for man and environment.

It shall be applicable to different concepts of the final repository in different host formations.

For such simulation, additional to the underlying basic processes, such as the two-phase flow in porous media, a number of other effects have to be taken into account. These effects may transform system parameters that are fixed in the basic processes into variables. As a result the basic equations and global equation system change. For instance, the rock convergence dynamically changes the pore volume in some region. The convergence process is controlled by a number of additional factors, and the change of the pore volume is described by a nonlinear differential equation that has to be integrated into the global equation system. During a simulation of the processes in a repository for radioactive waste different effects as well as different combinations of these effects have to be considered. The relevance of effects depends on the environment parameters and may change during the simulation time.

One of the challenges in developing the structure for such simulator program is to enable a flexible choice of effects and their combination during a simulation and an easy way to extend the program by new effects.

On the other hand, it is intended to avoid accounting for all effects throughout every calculation or developing a special, non-reusable code for every application.

The paper presents a concept for realizing these requirements.

Starting Point

The basic process models a fluid flow in a medium described by equation(s) of the form:

$$(\text{Accumulation term}) - (\text{Flow term}) - (\text{Source term}) = 0$$

with basic variables X_i and constant equation parameters.

Further, an effect is defined as a process affecting the system in such a way that one/some parameters of the basic equations get variable (additional variables Y_i). Modelling an effect may lead to additional terms in the equations and to additional differential equations for Y_i which have to be introduced into the global equation system. It is important to mention that the structure of a block row of the global Jacobian-matrix is not changed by the introduction of an effect.

Data Structure Concept Idea

The concept of flexible introduction of effects into the simulation consists of several steps:

- Define a family of Effects. An Effect-class encapsulates the related parameters und effect specific routines for pre-/post processing for a time/iteration step.
- Define a family of Equations. An Equation-class encapsulates numerical calculation algorithms for one differential equation.
- Define a family of Situation-objects that capture a current system state (relevant effects, basic model) and encapsulates the interaction of relevant Effects and Equations. Make these Situation-objects interchangeable according to a changed system state. Situation-objects enable the loose coupling of data structure. By using Situation-objects the explicit dependency between objects can be avoided. This concept enables the interaction of objects to be varied and modified independently of the objects themselves.

This concept ensures:

- the implementation of new effects in an easy way according to the predefined pattern,
- flexibility, transparency and reusability in extending and developing the program.

Verification and Validation of 3D Models for Wave and Current Interactions with Rigid and Erodible Structures

Christopher E. Kees[1], Matthew W. Farthing[1], Aggelos Dimakopoulos[2], Tristan de Lataillade[2]

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Key words: Finite Element Method, Level Set Method, Multiphase Flow, Arbitrary Lagrangian Eulerian Method

Introduction

An open source test set of verification and validation problems suitable for testing 3D computational models of air/water and air/water/solid interactions is presented. Solid dynamics include floating rigid structures, such as vessels and moored platforms, as well as granular structures that permit flow, wave transmission, erosion, and deposition.

The last decade has seen an expansion in the development and application of 3D free surface flow models in the context of environmental simulation. These models are based primarily on the combination of effective algorithms, namely level set and volume-of-fluid methods, with high-performance, parallel computing. These models are still computationally expensive and suitable primarily when high-fidelity modeling near structures is required. Validation of the models on lab and field data as well as verification and model inter-comparison are critical for making the models useful to the wider engineering community.

This work considers models of three-phase flow in domains containing air, water, and granular phases as well as impermeable moving rigid bodies. The models are implemented in the open source Proteus toolkit for computational methods and simulation. The target applications of these models are porous coastal and riverine structures. The applications require the ability to simulate wave breaking and structure over-topping, particularly fully three-dimensional, non-hydrostatic flows that drive these phenomena.

The structure of the test set and illustrative examples will be given along with details of the level set, finite element, and operator splitting methods upon which the models rely.Particular attention will be given to important qualitative features of the numerical methods including phase conservation, wave energy dissipation, and computational efficiency in regimes of interest.

11-1: Computational Ecohydrology

Time: Tuesday, 21/Jun/2016: 9:40am - 10:40am – *Location: MSB 2170*

Development of an Integrated Eco-Hydrological Model of a Restored Riparian Wetland

Birgitte von Christierson[1], Michael Butts[1], Laura A. Nieuwenhoven[1], Flemming T. Hansen[1], Jannick K. Jensen[2], Jane B. Poulsen[3], Bertel Nilsson[4]

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Hydrological Modeling of Ephemeral Catchments with Different Land Uses

Matteo Camporese[1], Joshua F. Dean[2], Edoardo Daly[3]

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Modeling Drought-Related Disturbance in Water-Limited Environments

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Development of an Integrated Eco-Hydrological Model of a Restored Riparian Wetland

Birgitte von Christierson[1], Michael Butts[1], Laura A. Nieuwenhoven[1], Flemming T. Hansen[1], Jannick K. Jensen[2], Jane B. Poulsen[3], Bertel Nilsson[4]

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Key words: wetland restoration, integrated modelling, flooding, hydroperiod, water quality, diffuse pollution

Introduction

The restoration of rivers and riparian wetlands is increasingly used as a means in river basin management strategies across Europe for achieving 'good ecological status' of water bodies as required by the EU Water Framework Directive (WFD). In Denmark diffuse pollution from agriculture is recognized as one of the most important challenges in improving ecological conditions and the restoration of wetlands continues to be an important measure in Danish river basin plans for reducing nutrient loads.

Riparian zones intercept surface as well as subsurface flows, significantly reducing nutrient loadings through processes such as sedimentation and regeneration, denitrification/nitrification and to a smaller degree plant uptake, decay and mineralisation. The hydrology of the wetland, the dynamics of the hydrological processes such as flooding and the interaction between surface water and groundwater are key factors in determining their effectiveness in reducing nutrient loadings. Whilst most studies indicate improved river water quality as a result of wetland restoration, the influence of extensive alterations on the hydraulic interaction between streams, their floodplains and subsurface and the effect on nutrient processes have received limited attention. In this paper we present an integrated eco-hydrological modelling tool that represents the flow, transport and water quality processes in riparian wetlands.

Pilot study

To evaluate the performance of this tool and to assess the importance of the various eco-hydrological processes for wetland unctioning, this model has been used to examine the flow processes and nitrate dynamics within a restored riparian wetland on the Odense River in Denmark. The ability of the model to capture both the surface and subsurface processes has been verified using measurements of flows and water levels in the river and wetland system, including groundwater levels in profiles across the wetland during both dry and wet periods. Water quality simulation of the nitrate processes in the groundwater has been validated against in-situ measurements of nitrate concentrations in the subsurface and the model has been used for investigating nitrate reductions within the integrated system.
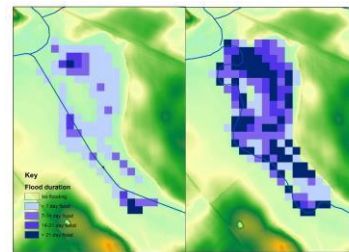

Figure 1: Modelled hydroperiod before (left) and after (right) river and wetland restoration

The model has been used to compare the flow and nitrate dynamics before and after restoration. The initial results indicate that flooding behavior from the stream is critical for nitrate removal in the wetland with nitrate removal in the floodplain compartment accounting for 85-90% of total nitrate removal. Cutting drains is also of significance with respect to restoring natural groundwater flow conditions but less so in terms of nitrate removal in the subsurface for this particular wetland. The results demonstrate the applicability of this modelling tool for evaluating the benefits of wetland restoration and for wetland design with regards to improving the water quality in streams.

Hydrological Modeling of Ephemeral Catchments with Different Land Uses

Matteo Camporese[1], Joshua F. Dean[2], Edoardo Daly[3]

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Key words: land use change, evapotranspiration, integrated modeling

Introduction

Land use, particularly tree cover, has a strong influence on evapotranspiration (ET) and thus a large effect on catchment hydrology. However, the dearth of medium to long term experimental observations limits the understanding of the interplay between catchment geology, land use, and climate in driving catchment water balance. Here we use four years (2011-2014) of rainfall, streamflow, and groundwater level measurements to estimate the water balance components in two small, adjacent, ephemeral catchments in a semi-arid region of south-eastern Australia; one catchment was predominantly covered with a eucalypt plantation established in July 2008 and the other was dedicated to grazing pasture.

Model Application

The integrated hydrological model CATHY (CATchment HYdrology[1]) was calibrated against the data in the two catchments using streamflow and groundwater level observations in 2011; the data in the following years (2011-2014) were used for the model validation. The model was able to adequately reproduce the periods of flow in both catchments in all years (Figures 1 and 2). Streamflow and groundwater levels were better reproduced in the pasture than in the plantation. This can partly be attributed to the root growth of the trees, which is difficult to estimate; the declining water storage in the eucalypt catchment could only be obtained when including a simple model of root growth dynamics. Other sources of uncertainty could be due to i) an imperfect description of the subsurface boundary conditions at the outlet and ii) lack of information regarding the spatial variability of suburface parameters such as the hydraulic conductivity. The water balances estimated from both data and model showed a significant increase in ET in the eucalypt plantation catchment at the expense of groundwater storage (Figures 1 and 2): ET accounted for 95-104% of rainfall in the pasture catchment and 104- 119% in the eucalypt catchment across the four years studied. However, the observed streamflow decline in the plantation was significantly less than predicted by the model, with streamflow discharge ranging from 1 to 4% of rainfall in both catchments for the entire study period (Figures 1 and 2).

Overall, the observed data and model simulations suggest the response of ephemeral catchments to land use change is driven by complex interactions between climate, geology and vegetation; long-term, data-rich, highly parameterized modeling studies are required to further separate these factors.
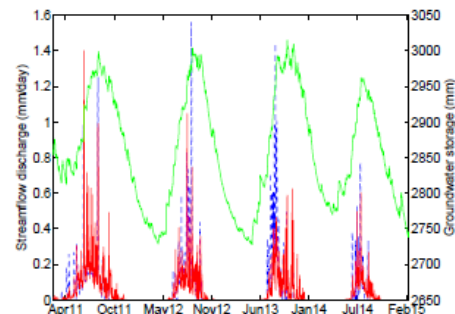

Figure 1: Observed (blue dashed line) and simulated (red solid line) streamflow discharge in the pasture catchment, along with the simulated groundwater storage (green solid line).
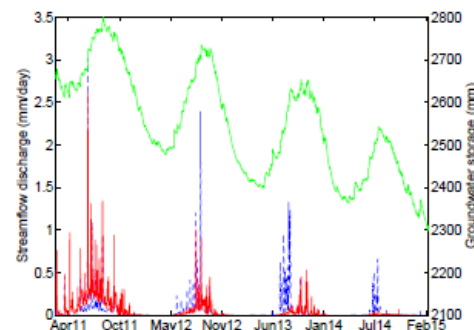

Figure 2: Observed (blue dashed line) and simulated (red solid line) streamflow discharge in the eucalypt catchment, along with the simulated groundwater storage (green solid line).

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Modeling Drought-Related Disturbance in Water-Limited Environments

Naomi (Christina) Tague, Max Mortiz

University of California Santa Barbara, United States of America

Fire, dieback, productivity declines and insect related forest mortality are abrupt disturbances related to drought that result in substantial changes to ecosystem structure and function. Drought related disturbance, particularly fire, are also an underlying motivation for human-driven changes to forests through fuel treatments. In drought- prone environments spatial-temporal patterns of water availability are likely to be an important control on disturbance vulnerability. At the same time, the hydrologic consequences of changes to forest structure for water quality and quantity are important from a water resource management perspective.

Droughts, disturbance and forest management treatments, however, are infrequent events which leads to challenges when interpreting field based analysis of the site- specific controls on hydrologic responses. Coupled ecohydrology models provide an important tool for estimating both hydrologic consequences of biomass reduction, through management or disturbance, and how these change impact subsequent drought vulnerability. Models can account for temporal variation in meteorology in the year following disturbance and during post-disturbance recovery rates. What is often overlooked, however, is the importance of subsurface characteristics. While spatial information on soil properties are available, the information is rarely sufficient to characterize subsurface drainage and moisture storage characteristics; consequently most hydrologic models still require calibration of subsurface drainage properties to match observed streamflow or water flux data. Similarly, a particular challenge for ecological modeling is estimating rooting depths. When assessing the impact of density reduction on forest water use, there is a second potentially important source of uncertainty related to incomplete knowledge how neighboring plants share water in the subsurface. When trees or understory vegetation are removed, the remaining trees may be able to make use of the water that was previously used by removed vegetation.

This paper uses a coupled eco-hydrologic model to show that both vulnerability to drought and hydrologic responses to vegetation loss are strongly influenced by both local and watershed scale subsurface geologic controls. We use sensitivity analysis to demonstrate the conditions under which sharing of water stored in the subsurface can lead to increases rather than decreases in forest water use under scenarios where forest density has been reduced. Results highlight the tight coupling between geology and climate that influence eco-hydrology of vegetation in drought-prone environments and show how different assumptions about subsurface storage and drainage behavior may have implications for how we think about forest management and disturbance vulnerability. Results emphasize the utility of new geophysical data collection at observatories (such as the Critical Zone Observatory Network) to support watershed scale models and to improve eco-hydrologic information that we provide forest managers.

11-2: Computational Ecohydrology

Time: Tuesday, 21/Jun/2016: 11:00am - 12:20pm – Location: MSB 2170

Soil Moisture Spatio-Temporal Variability: Insights from Mechanistic Ecohydrological Modeling

Simone Fatichi[1], Gabriel G. Katul[2], Valeriy Y. Ivanov[3], Christoforos Pappas[4], Athanasios Paschalis[5], Jongho Kim[3], Paolo Burlando[1]

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Non-Linear Continuous Time Random Walks for the Evolution of Point Water-Vegetation Dynamics

Marco Dentz[1], Luis Cueto-Felgueroso[2], Ruben Juanes[3]

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Evaluating the Impact of Root Hydraulic Traits at the Forest Scale

Elizabeth Agee[1], M. Chase Dwelle[1], Valeriy Ivanov[1], Lingli He[1], Gautam Bisht[2], Valentin Couvreur[3]

[1]University of Michigan, United States of America; [2]Lawrence Berkeley National Laboratory, United States of America; [3]Universite Catholique de Louvain, Belgium; lizagee@umich.edu

Integrating a Model of Plant Hydraulics with Coordination and Trade-Offs among Plant Trait Spectra in Tropical Forests

Bradley Christoffersen[1], Chonggang Xu[1], Manuel Gloor[2], Maurizio Mencuccini[3,4], Brendan Choat[5], Rosie Fisher[6], Patrick Meir[3,7], Nate McDowell[1]

[1]Los Alamos National Laboratory, United States of America; [2]University of Leeds, United Kingdom; [3]University of Edinburgh, United Kingdom; [4]ICREA at CREAF, Spain; [5]University of Western Sydney, Australia; [6]National Center for Atmospheric Research, United States of America; [7]Australian National University, Australia; bradleychristo@gmail.com

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[1]ETH Zurich, Zurich, Switzerland; [2]Duke University, Durham, NC, USA; [3]University of Michigan, Ann Arbor, MI, USA; [4]Université de Montréal, Montréal, Canada; [5]University of Southampton, Southampton, UK

Key words: hillslope hydrology, soil heterogeneity, evapotranspiration

Introduction

Soil moisture is a key variable affecting water and energy exchanges at the land surface as well as ecological processes. Soil moisture is highly variable in space and time up to the point of showing a hysteretic behavior in the soil moisture spatial coefficient of variation $C_V(\theta)$ versus mean soil moisture $\bar{\theta}$ diagram. Studies that investigate the relative importance of climate, soil properties and vegetation on soil moisture spatio-temporal dynamics are therefore warranted. An analytical expression that separates biotic and abiotic controls on the temporal dynamics of $Cv(\theta)$ was derived and the different terms explored via numerical simulations using a mechanistic ecohydrological model, Tethys-Chloris, a tool that integrates essential hydrological and plant physiological processes [1].

Continuous soil moisture spatio-temporal dynamics at an exemplary hillslope domain were computed for six sites characterized by different climate and vegetation cover and for three configurations of soil hydraulic properties. It was shown that abiotic controls largely exceed their biotic counterparts in wet climates. Biotic controls on $Cv(\theta)$ were found to be more pronounced in Mediterranean climates. The relation between $Cv(\theta)$ and spatial mean soil moisture $\bar{\theta}$ was found to be unique in wet locations, regardless of the soil properties. For the case of homogeneous soil texture, hysteretic cycles between $Cv(\theta)$ and $\bar{\theta}$ were observed in all Mediterranean climate locations considered in the analysis and to a lesser extent in a deciduous temperate forest. Heterogeneity in soil properties increased $Cv(\theta)$ to values commensurate with field observations and weakened signatures of hysteresis at all of the studied locations [2]. This finding highlights the role of site-specific heterogeneities in hiding or even eliminating the signature of climatic and biotic controls on $Cv(\theta)$, thereby offering a new perspective on causes of confounding results reported across field experiments.

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[2] S. Fatichi, G. G. Katul, V. Y. Ivanov, C. Pappas, A. Paschalis, A. Consolo, J. Kim, P. Burlando (2015). Abiotic and biotic controls of soil moisture spatio-temporal variability and the occurrence of hysteresis. *Water Resources Research* 51(5), 3505-3524 doi:10.1002/2014WR016102

Non-Linear Continuous Time Random Walks for the Evolution of Point Water-Vegetation Dynamics

Marco Dentz[1], Luis Cueto-Felgueroso[2], Ruben Juanes[3]

[1]IDAEA-CSIC, Barcelona, Spain; [2]UPM, Madrid, Spain; [3]MIT, Cambridge, USA;

Abstract

We present an approach that casts the non-linear point water-vegetation dynamics under stochastic rainfall forcing as a continuous-time random walk (CTRW) characterized by an arbitrary inter-storm waiting time. We derive an evolution equation for the joint probability density function (PDF) of soil-moisture and biomass. The deterministic dynamic system is characterized by two attractors for a vegetated and non-vegetated state, respectively. The stochastic dynamic system exhibits regime shifts in the steady-state PDF as a consequence of changes in the rainfall structure, which can reverse the relative strengths of the system attractors, even for the same mean precipitation. Through an effective potential, we quantify the impact of rainfall variability on ecosystem resilience. From this we conclude that variability in the interstorm waiting times may reduce the resilience of water-stressed ecosystems, even if the mean annual precipi- tation remains constant.

Evaluating the Impact of Root Hydraulic Traits at the Forest Scale

Elizabeth Agee[1], M. Chase Dwelle[1], Valeriy Ivanov[1], Lingli He[1], Gautam Bisht[2], Valentin Couvreur[3]

[1]University of Michigan, United States of America; [2]Lawrence Berkeley National Laboratory, United States of America; [3]Universite Catholique de Louvain, Belgium

Key words: root water uptake, plant hydraulic traits

Introduction

Root hydraulic traits, in particular root hydraulic conductivity, remain a large source of uncertainty in root water uptake models. Measurement of the parameters is difficult and results can vary within a species as a function of age or environmental factors (i.e., water or nutrient availability). Despite these complexities, we theorize that for a community, a region of optimality exists for root hydraulic traits under water stressed conditions. Using recent advances in root water uptake modeling, we examine the impact of root hydraulic traits at the forest scale.

Model Description and Application

Land-surface models use simplified representations of root water uptake based on biomass distributions and empirical functions that constrain water uptake during unfavorable soil moisture conditions. The largely one-dimensional representation of root water uptake fails to capture the observed 'hydraulic plasticity', i.e., adjustment of hydraulic gradients through water uptake, which allows plants to regulate root hydraulic conductivity and zones of active uptake. Traditional models of three-dimensional root water uptake that explicitly find water fluxes at the level of individual root are impractical for ecosystem scale modeling. Recent developments have sought to bridge the gap between physically based microscopic models and computationally feasible macroscopic approaches. The application of these novel approaches allow for deeper investigation of how plant hydraulic traits are expressed in community level dynamics.

Using methodology from Couvreur et al. [1], we resolve root hydraulic architectures created with the RootBox model [2] into macroscopic parameters representative of species specific hydraulic traits (i.e., xylem and soil-root conductivity). Using a modified version of the PFLOTRAN model [3], which represents the three-dimensional physics of variably saturated flow in soil, we model a one-hectare temperate forest stand under simulated drought conditions. Employing an ensemble of plant hydraulic characteristics, we aim at quantifying an optimal range of hydraulic characteristics under which the stand can maintain transpiration during water stress.
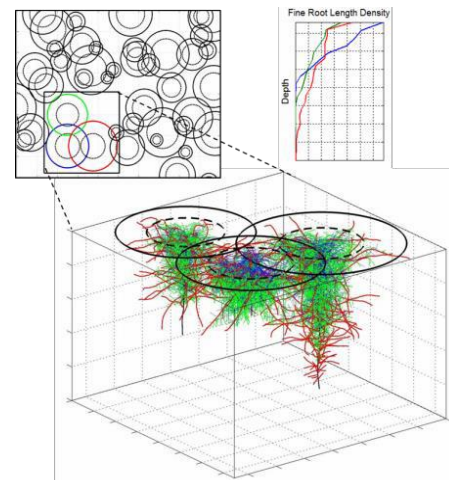

Figure 1: Root hydraulic architectures created in RootBox [2] show variability in size, structure, and overlap, that can occur in root systems with similar bulk properties like root length density.

References

[1] V. Couvreur, J. Vanderborght, & M. Javaux. A simple three-dimensional macroscopic root water uptake model based on the hydraulic architecture approach. *Hydrol. Earth Syst. Sci.*, 8, 2957-2971, (2012).

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Integrating a Model of Plant Hydraulics with Coordination and Trade-Offs among Plant Trait Spectra in Tropical Forests

Bradley Christoffersen[1], Chonggang Xu[1], Manuel Gloor[2], Maurizio Mencuccini[3,4], Brendan Choat[5], Rosie Fisher[6], Patrick Meir[3,7], Nate McDowell[1]

[1]Los Alamos National Laboratory, United States of America; [2]University of Leeds, United Kingdom; [3]University of Edinburgh, United Kingdom; [4]ICREA at CREAF, Spain; [5]University of Western Sydney, Australia; [6]National Center for Atmospheric Research, United States of America; [7]Australian National University, Australia

Key words: trait-based modeling, plant hydraulics, size scaling

Introduction

Forest ecosystem models poorly predict tropical forest response to drought. Heuristic water stress functions are uninformed by the large diversity of tree size and hydraulic traits observed in tropical forests. We developed a dynamic model of plant hydraulics within an individual- and trait-based forest simulator TFS [1] and the cohort-based land surface model CLM(ED) [2]. We synthesized literature and databases to parameterize all hydraulic traits as a function of leaf and stem economics trait spectra, and then assessed the evidence for and capability of our model framework to represent coordination and trade-offs among hydraulic traits.

Key Findings

We found statistically significant relationships in all hydraulic traits with leaf or stem economics. Leaf drought tolerance and xylem vulnerability to embolism were coordinated. Evidence for a trade-off between xylem safety and efficiency was weak, being restricted to tropical dry forests. We used these relationships to parameterize the necessary hydraulic components of the model (Fig. 1).
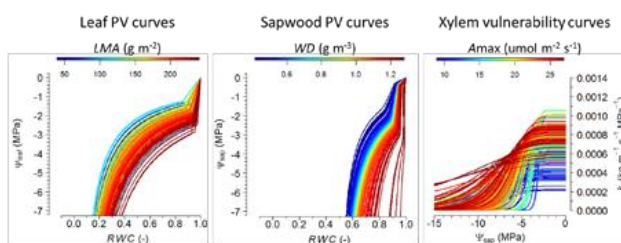
Figure 1: Hydraulics model parameterized by the plant traits leaf mass per area (LMA), wood density (WD), and photosynthetic capacity (Amax)

The model successfully captured individual variation in leaf water potential due to increasing tree size, with model representation of hydraulic architecture exerting strong control on the fidelity of model predictions (Fig. 2).
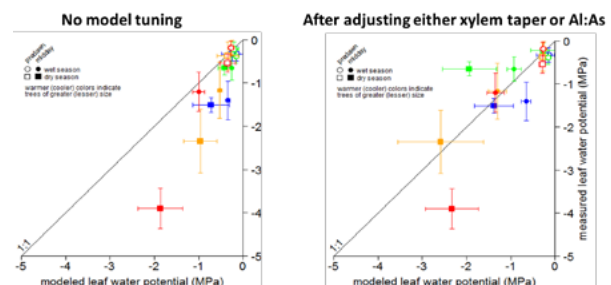

Figure 2: Simulated vs. observed individual-level variation in leaf water potential, Caxiuana, Brazil

Implications

By using a limited set of leaf and stem economics traits as input, our model framework is capable of representing observed patterns of hydraulic trait coordination, while remaining flexible with respect to the xylem safety-efficiency tradeoff. Our framework does not prescribe this tradeoff in moist and wet tropical forests where leaf and stem economics axes remained orthogonal. This suggests broad application of the model to forests pantropically. Remaining uncertainties and limitations of the trait paradigm for plant hydraulics modeling are highlighted.

References

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11-3: Computational Ecohydrology

Time: Tuesday, 21/Jun/2016: 2:30pm - 3:30pm – Location: MSB 2170

Simulating Hydraulic Redistribution and its Effects on Land Surface Fluxes in a California Oak Savanna

Gretchen R. Miller[1], **Si Gou**[1,2], **Cody Saville**[1]

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Computational Methods
in Water Resources 2016

Simulating Hydraulic Redistribution and its Effects on Land Surface Fluxes in a California Oak Savanna

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Key words: hydraulic redistribution, soil-plant-atmosphere continuum, plant water uptake, stand scale, phreatophyte

Introduction

Subsurface redistribution of water by plant roots may significantly impact land surface fluxes in arid and semi-arid regions. However, very few models incorporate hydraulic lift in a mechanistic manner, particularly when the saturated zone is the main source of redistributed water. No models account for recharge enhancement through the reverse process, hydraulic descent. The objective of this work was to assess the impact of new model developments aimed at better simulating these ecohydrological processes.

Methods

PARFLOW.CLM was used to create a stand-scale model of the Tonzi Ranch AmeriFlux site; an oak savanna in the Sierra Nevada foothills of California, USA. New plant uptake functions were incorporated into the model code, which allowed for more realistic mechanistic modeling of hydraulic redistribution in plants in direct contact with the saturated zone [1]. The model, when forced with site specific meteorological data, has performed well in comparison to 8 years of biometeorological data, including trace gas fluxes from eddy-covariance, soil moisture, leaf water potential, and diurnal groundwater fluctuation data [2].

Results

The model predicted that blue oaks (Quercus douglasii) at the site undergo hydraulic redistribution, both lift and descent. Hydraulic lift occurred during nights in the oaks' active season, which coincides with the site's dry season. The process brings water from the 10-m deep saturated zone to surface soil layers (Figure 1a) and can contribute up to 50% of the water required for the next day's tree transpiration. Hydraulic descent typically occurs after rains at the start of the wet season, when soil moisture becomes higher in the top layers than in the bottom ones. The model predicts that this process can move up to 1.9 mm/d from the surface soil to deeper soil layers, short-circuiting normal infiltration patterns (Figure 1b). Timing of hydraulic descent was also consistent with previous observations of reverse sapflow in these trees. Overall, the model indicates

that hydraulic redistribution has non-trivial effects on the stand's evapotranspiration rates during the dry season and groundwater recharge during the wet season.
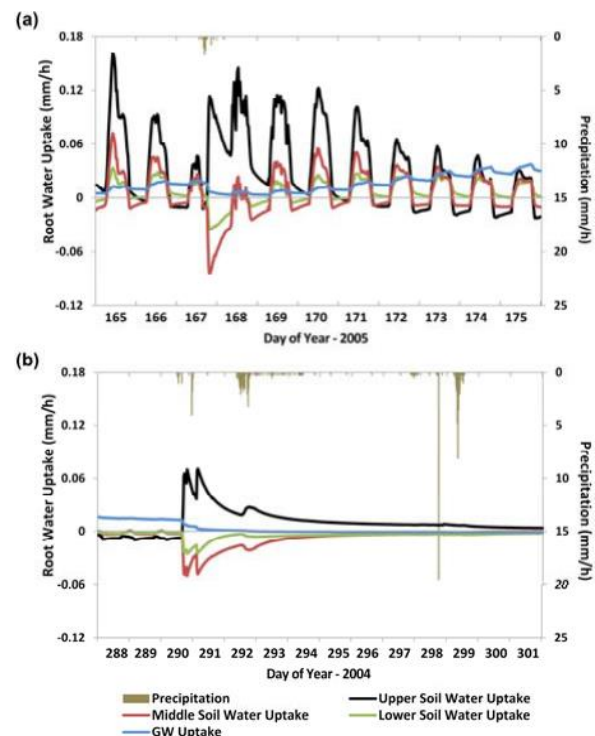

Figure 1: Root uptake rates for selected time periods during the 2005 growing season (a) and 2004 dormant period (b). Positive values indicate that roots in that layer are extracting water while negative values indicate that roots are releasing water.

References

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12-1: Modelling and Computational Aspects of Coupled Porous Medium and Free Flow Systems

Time: Thursday, 23/Jun/2016: 2:30pm - 4:10pm – Location: MSB 2172

Coupled Fluid Flow and Heat Transport in 3D Faulted Hydrothermal Systems: The Tiberias Basin Example

Fabien Magri[1,2], Nimrod Inbar[3], Christian Siebert[4], Tino Rödiger[4], Peter Möller[5], Eliyahu Rosenthal[3], Norihiro Watanabe[1] [1]Helmholtz Centre for Environmental Research – UFZ, Department of Environmental Informatics, Leipzig, Germany; [2]Freie Universität Berlin, Hydrogeology, Berlin, Germany; [3]Tel Aviv University, The Department of Geophysics and Planetary Sciences, Tel Aviv, Israel; [4]Helmholtz Centre for Environmental Research – UFZ, Catchment Hydrology, Halle, Germany; [5]Helmholtz Centre Potsdam, GFZ German Research Centre for Geosciences, Potsdam, Germany; fabien.magri@ufz.de

Coupling Compositional Gas Liquid Darcy and Free Gas Flows At Porous and Free Flow Domains Interface

Roland Masson[1], Laurent Trenty[2], Yumeng Zhang[1]
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SPH Modeling of Multi-Phase Flow over a Porous Layer

Hossein Basser, Edoardo Daly, Chunhui Lu, Ha Bui
Monash University, Australia; Hossein.Basser@monash.edu

Coupling Non-Isothermal, Two-Component Darcy and Navier-Stokes Flow to Investigate Evaporation of Soil Water

Christoph Grüninger, Thomas Fetzer, Bernd Flemisch, Rainer Helmig
University of Stuttgart, Germany; christoph.grueninger@iws.uni-stuttgart.de

Coupled Fluid Flow and Heat Transport in 3D Faulted Hydrothermal Systems: The Tiberias Basin Example

Fabien Magri[1,2], Nimrod Inbar[3], Christian Siebert[4], Tino Rödiger[4], Peter Möller[5], Eliyahu Rosenthal[3], Norihiro Watanabe[1,2]

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Key words: fault, convection, simulation, spring

Temperature variations encountered in hydrothermal systems strongly couple fluid flow and energy transport processes. The resulting convective flows are often invoked to explain environmental anomalies, such as hot springs or ore deposits. In the specific case of faulted systems, this dynamic feature is very complex to study as fault and fractures can either favor or hinder groundwater flow. However, it has been shown that thermal convection in faults can also occur for subcritical Rayleigh conditions. This type of convection develops after a certain period and is referred to as "delayed convection" [1]. The delay in the onset of convection is due to the natural coupling between the damage zone and the surrounding units that adds a thermal buffer for heat transfer along the fault walls. Few numerical studies investigated those delayed thermal convection phenomena in fractured zones, despite it has the potential to transport energy and dissolved metals over large spatial scales.

Here 3D finite element simulations of thermally driven flow in faults are presented in order to investigate the impact of delayed convection on deep fluid processes at basin-scale. The Tiberias Basin (TB), in the Jordan Dead Sea Transform Valley, serves as study area. The TB is characterized by upsurge of deep-seated hot brines along the faulted shores of Lake Tiberias and high temperature gradients, which can locally reach 46 °C/km, as in the Lower Yarmouk Gorge (LYG). 3D simulations show buoyant flow ascend in permeable faults, which hydraulic conductivity is estimated to vary between

30 m/yr and 140 m/yr. Delayed convection starts respectively at 46x103 and 200x103 years and generate temperature anomalies in agreement with observations (Fig. 1). It turned out that delayed convective cells are transient. Cellular patterns that initially develop in permeable units surrounding the faults can trigger convection also within the fault plane. The combination of these two convective modes leads to helicoidal-like flow patterns. This complex hydraulic behavior can explain the location of springs along different fault traces of the TB. Besides being of importance for understanding the hydrogeological processes of the TB, the presented simulations provide a scenario illustrating fault- induced 3D cells that could develop in any geothermal system.
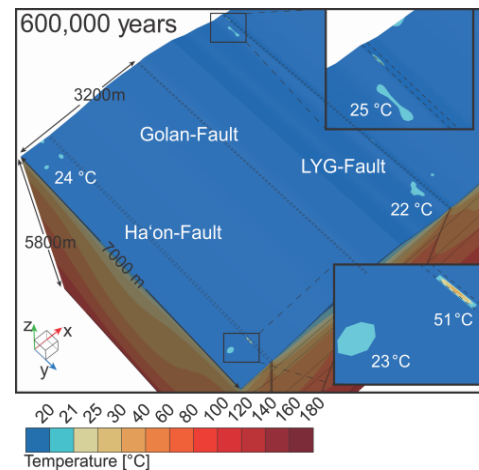

Figure 1: Calculated temperature in the LYG

Reference

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Coupling Compositional Gas Liquid Darcy and Free Gas Flows at Porous and Free Flow Domains Interface

Roland Masson[1], Laurent Trenty[2], Yumeng Zhang[1]

[1]LJAD University Nice Sophia Antipolis and INRIA, France; [2]Andra, Chatenay Malabry, France

Key words: Coupling Darcy and free flows, reduced model, drying

Introduction

This paper deals with the coupling at the interface between a liquid gas compositional Darcy flow and a compositional free gas flow (see Figure 1). This type of model appears in a wide range of applications. It includes for example, in industrial drying applications, the production of building materials, food processing, and wood and paper production, or also, in environmental applications, land-atmospheric interaction and soil evaporation and evapotranspiration.

If many works have been performed to model and discretize the coupling of single phase Darcy and free flows, there is very little work so far on the coupling of a two phase gas liquid compositional Darcy flow with a single phase compositional gas free flow. Such a coupled model has been recently proposed in [1] using matching conditions at the interface between the porous medium and the free flow regions.

Starting from the model proposed in [1], this paper proposes an efficient algorithm to solve the coupled system based on a splitting between the strongly and weakly coupled equations and unknowns of the full system. This approach can be used either as a fixed point algorithm leading to the fully coupled solution at convergence or simply as a sequential algorithm which is shown to provide a sufficient accuracy compared with the fully coupled solution. Our choice of the splitting of the full system is based on the physical understanding of the strong and weak couplings in the system. On the one hand, the water molar fraction in the free flow region is strongly coupled to the liquid pressure and liquid flux at the porous and free flow domains interface due to the liquid gas thermodynamical equilibrium. On the other hand, the gas velocity perturbation in the free flow domain, which is induced by the coupling with the porous medium, is small compared with the forced convection velocity.

The second objective of this paper is to develop a reduced model in the case of large longitudinal dimension of the free flow domain compared with its diameter allowing to reduce the model in the free flow domain to a 1D free flow. In the spirit of Convective Mass Transfer Coefficients CMTCs (see the review [2] and the references there in for a discussion about

CMTCs), the model includes on the free flow side a gas molar fraction at the interface and a normal diffusion flux between the interface and the free flow domain modelling the gas molar fraction boundary layer (see [3]). In this paper, an approximation of the gas molar fraction boundary layer thickness in the free flow domain is proposed based on a low frequency approximation of a Steklov Poincaré type operator related to the convection diffusion equation in the free flow domain for the water molar fraction.

The splitting algorithm and the reduced model are assessed and compared in the case of the modelling of the mass exchanges at the interface between the storage and the ventilation galleries in radioactive waste deposits.
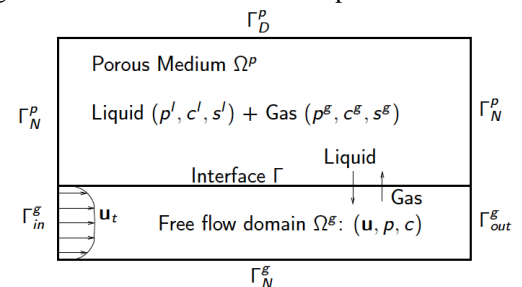

Figure 1: Sketch of the model with the porous medium Ω^p, the free flow domain Ω^g and the interface Γ.

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SPH Modeling of Multi-Phase Flow over a Porous Layer

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Key words: Smoothed Particle Hydrodynamics, multi-phase flow, porous media

Introduction

Multi-phase flow over porous media is ubiquitous in nature and engineering applications. For example, the interaction between stream-flow and river beds affects flow structure, solute and head transfer, and river ecosystems [1]. Flow over porous media is important in engineering applications, such as irrigation, seawater intrusion, and spillage of contaminants.

The modeling of flow in many of these applications requires the description of complex geometries, free surfaces, and deformable boundaries. In this work, we use a Smoothed Particle Hydrodynamics model to simulate multiphase flow over a porous layer.

Model description and application

We simulated the experiments of Thomas et al. [2], who examined the motion of a gravity current over a porous layer. The experiments aimed to investigate the behaviour of plane inertial gravity currents running over realistic permeable layers. In the experiments, dense salt water was released from behind a lock into a tank filled up with fresh water. The ratio between the densities of salt and fresh water varied from 1.002 to 1.074. The gravity current generated by the salt water was moving over and through a porous layer composed of glass spheres. The experimental tank was 3 m long, 0.2 m wide, and 0.6 m deep. An empty space was left between the porous layer and the tank's wall to let the drained fresh water moves upward through the opening (see Figure 1). In the simulations, three phases were simulated to reproduce the salt water, fresh water, and porous layer. Simulating the interaction between the three phases and the motion of the interface between the fluids are key factors in multi-phase flow modeling that require precise care.

We solved the Navier-Stokes equations to simulate the motion of the fluids, and assumed fluids to be incompressible. The equations were solved using the SPH approximation with an explicit scheme consisting of prediction and correction steps. In the first step, intermediate velocity and position of the particles were computed by applying viscous, external, and drag forces. The viscous force was calculated using a hybrid strain-based equation [3]. The interaction of the soil and the fluid particles was treated as a drag force which was exerted by the porous layer on the fluids, and it was calculated based on Darcy's law [4]. In the second step, the pressure force was solved using the Poisson equation to update the particles' velocity and position [3]. In addition, at the interface between the two fluids, a repulsive force was added to stabilize the interface [5]. Rigid boundaries were simulated using Monaghan and Libersky's virtual particles [6].

This model can be applied in modeling practical applications such as seawater intrusion in groundwater. Furthermore, it can be further developed to model more challenging problems such as interaction of fluids with greater differences in densities.
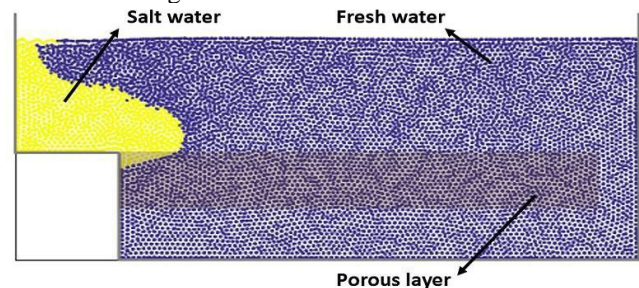

Figure 1: Gravity current of salt water (higher density) within fresh water (lower density) over and through a porous layer.

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Coupling Non-Isothermal, Two-Component Darcy and Navier-Stokes Flow to Investigate Evaporation of Soil Water

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Key words: porous medium, free flow, coupling, evaporation, drying, linear solver

Introduction

In order to solve diverse environmental and technical problems, flow in porous media must be coupled to free flow. We focus on the modeling and interpretation of evaporation from porous media under the influence of atmospheric driving forces, such as wind and radiation. We present an REV-scale model concept which allows the monolithic coupling of a laminar one-phase free flow and a two-phase porous-medium flow under non-isothermal, compositional flow conditions.

Model concept

Our concept is based on the one presented in [1]. We have a sharp interface between the domains and ap- ply coupling conditions to exchange the fluxes. We use a cell-centered finite-volume scheme for the Darcy domain and a staggered-grid scheme for the Navier-Stokes domain. Our scheme is capable to simulate turbulent effects and can be extended to three-dimensional problems.
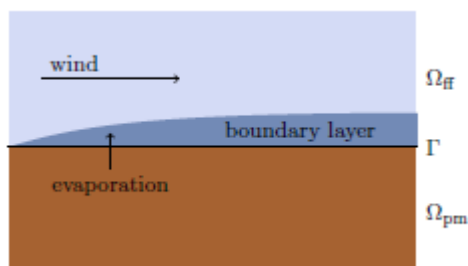
Figure 1: Setting and division of the domain in subdomains for free flow Ω_{ff} and porous medium flow Ω_{pm} with the coupling interface Γ in between

Linear solver

The resulting linearized equations are solved together in one large system. This monolithic concept of our coupling ties both compartments together, which leads to long simulation runs. The discretization of the Navier-Stokes method leads to a saddle-point problem which is part of the system. Because the physical processes indicate the use of upwinding, our problem is not symmetric. The overall linear system cannot be solved by the common iterative linear solver algorithms with acceptable effort. Direct linear solvers do not scale well for larger systems or for three-dimensional problems.

In the course of this work, we present a linear solver that utilizes the structure of the linear system. Building blocks are the Schur complement as used in [2], iterative block methods, and saddle point solvers. This results in smaller matrices which can be individually preconditioned and solved.

Aim

With the resulting software we will be able to simu- late realistic lab experiments. That will help to push the understanding of evaporation processes a bit further. With the gained robustness we hope to extend the laminar flow to turbulent flow and use Reynolds averaging with an algebraic turbulence model or k-ε model. This would open the door to field scale simulations. Additional effects like solar radiation or salt precipitation could be modeled and studied.

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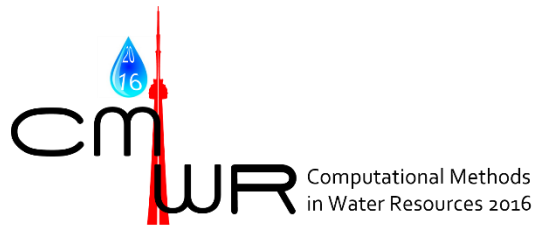
13-1: Targeting Evolving Computational Environments to Advance Hydrological Models

Time: Tuesday, 21/Jun/2016: 3:50pm - 5:30pm – Location: MSB 2170

Building Next-Generation Atmosphere and Land-Ice Models Using the Kokkos Trilinos Library

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Computational and Algorithmic Considerations for Hydrological Models Running on Modern Computers

Matthew Ross Norman
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Hybrid GPU+CPU Modeling of Ecohydrological and Biogeochemical Processes in Intensively Managed Landscapes

Praveen Kumar, Phong V. V. Le, Dong K. Woo
University of Illinois at Urbana-Champaign, United States of America; kumar1@illinois.edu

Multi-GPU Simulation of Tsunamis Generated by Earthquakes Using Nested Meshes

Marc De La Asunción, Manuel J. Castro, José M. González, Jorge Macías Universidad de Málaga, Spain; marcah@uma.es

Building Next-Generation Atmosphere and Land-Ice Models
Using the Kokkos Trilinos Library

Irina Tezaur, Irina Demeshko, Andrew Salinger, William Spotz

Sandia National Laboratories, United States of America

Key words: performance portability, many-core programming, Albany finite element code, ice sheet model, atmosphere model, Kokkos Trilinos library.

Performance portability to new and emerging architecture machines (e.g., multi-core, many-core and GPU systems) is becoming a requirement in many applications, climate modeling in particular. Parallel code must execute correctly and with good performance on machines with drastically different architectures, operating systems, and software libraries. Porting large, complex codes to multicore /manycore architectures is far from trivial, however. A program or algorithm optimized for one coprocessor may not run as well on the next generation of processors or on a device from a different vendor. Similarly, a program or algorithm optimized for GPU execution is often very different from one optimized for CPU execution. Often, codes and algorithms must be rewritten substantially to take advantage of emerging architecture, which requires a tremendous investment of time and resources.

Performance portability of a finite element code can be achieved using the Kokkos [1] library and programming model of Trilinos [2]. Kokkos is a library- based programming model, which has been developed at Sandia National Laboratories to provide scientific and engineering codes with user-accessible, many- core, performance portable capabilities. Kokkos enables computational kernels to be performance portable across many-core architectures by decoupling computational kernels from device-specific data access performance requirements (e.g., NVIDIA coalesced memory access) through an intuitive multidi- mensional array API. The library is designed to maximize the amount of user code that can be compiled for diverse devices and obtain similar performance as a variant of the code that is written specifically for that device. There are two primary abstractions in Kokkos: (1) The Kokkos polymorphic multidimentional array: Kokkos::View, and (2) Kokkos parallel dispatch functions: Kokkos::parallel_for, Kok- kos ::parallel_reduce and Kokkos::parallel_scan. The integration of these abstractions enables user code to satisfy multiple architecture-specific memory access pattern performance constraints, all without requiring modifications to the source code.

This talk will detail our effort in developing a performance portable implementation of the finite element- based Albany code [3], which houses a number of climate applications. Performance results for two different climate simulation modules within Albany will be presented: the Aeras atmosphere solver [4] and the FELIX land-ice dynamical core [5]. Figure 1 shows a sample result (finite element assembly CPU times) for an atmosphere simulation performed using the Aeras solver. The figure suggests success of the Kokkos programming model: a single implementation is able to achieve performance portability across three different architectures (Serial, OpenMP and CUDA). Speedups of 9x and 17x are achieved using OpenMP and CUDA, respectively, relative to the Serial run. As expected, better performance is obtained on the GPU for a larger workset size (threading index), due to the high cost in data transfer between the host and the GPU. Additional results, including weak scaling studies for large-scale problems on Titan with OpenMP and CUDA, will be shown in the talk.
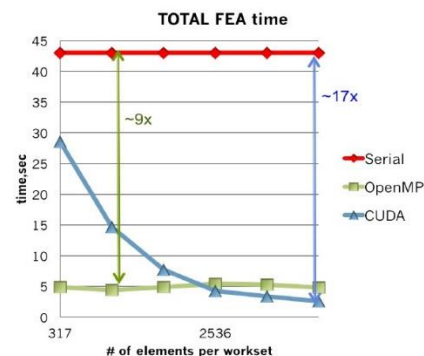

Figure 1: Finite element assembly (FEA) CPU times as a function of the number of elements per workset (threading index) for an Aeras shallow water test case.

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Computational and Algorithmic Considerations for Hydrological Models Running on Modern Computers

Matthew Ross Norman

Oak Ridge National Laboratory, United States of America

Key words: HPC, Algorithms, Accelerators

Introduction

Hydrological processes encompass some of the most important socioeconomic impacts of weather and climate change, largely through extreme events. Much of society's infrastructure depends on the water cycle, such as power plants needing large water sources for cooling. In order to model hydrological processes end to end, many modeling components are needed in the atmosphere, land, ocean, and cryosphere. Each of these components must simulate extremely complex, coupled, and often stiff physical phenomena across a multitude of spatial and temporal scales. The overall goal of an effective code to model the hydrological cycle is to produce simulations that are as useful as possible with as few resources as possible.

Each of these model components is constructed from some mathematical representation of the underlying physics and a subsequent algorithmic approach to advancing the solution in time. Then, the algorithm is coded in a manner most amenable to the computer architecture at hand. Often times, when thinking about hydrological modeling and computing, we tend to separate these concerns as if they were roughly orthogonal. One group develops the mathematical formulations and algorithmic approaches, and another handles computational concerns. The goal of this talk is to demonstrate that reality is quite the opposite. To be effective on modern hardware, all aspects of the hydrological code must be reconsidered because they interact strongly.

Interactions between Mathematical Formulation and Computational Efficiency

The mathematical formulation has a dominant influence on the overall effectiveness of a codebase on a given architecture. If the physics are very stiff, a time-implicit method stably passes over less impactful physics (such as acoustic propagation or viscosity) and efficiently targets the most important physics. However, implicit methods often incur significant non-local (MPI) data transfer overheads due to global sparse linear solves, meaning they are not typically effective for less stiff problems (like atmospheric dynamics, for instance). Also, for time-explicit implementations, the spatial operator choice has more influence on the time step size than does the temporal operator. Galerkin methods, for instance, exhibit nearly quadratic time step reduction with increasing order of accuracy, while Finite-Volume methods suffer no time step reduction with increasing order of accuracy. Yet, Galerkin methods are also substantially cheaper in serial than FV. Other formulations time step behavior in the middle.

Also critical on modern computing is the ability to perform as many useful computations on a given block of data as possible, a concept known as compute intensity. This is because modern computers incur increasing penalties for moving data and perform relatively cheap local computations. Thus, our mathematical formulations need to be higher- and higher-order in accuracy. The reason is that computational expense increases at an asymptotically higher rate than data movement for higher-order- accurate methods. However, this must not come at the cost of significantly lower time steps or less robust data (e.g., oscillations or erroneous negative values).
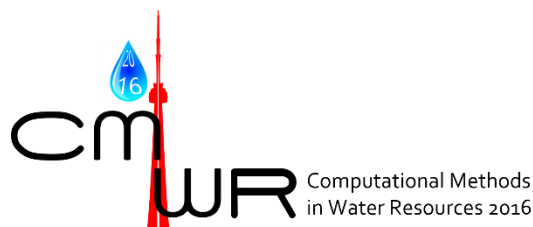
Implementation Concerns

There are also implementation concerns to consider. Looping is likely the dominate issue. Inner loops should be as "SIMD" (Single Instruction Multiple Data) as possible, performing the same operations on different data, in order to properly utilize accelerators like GPUs and MICs. Also, cache space must be respected by "blocking off" looping structures into chunks that are roughly the same sizes as various levels of cache space. Developers must be aware of the impact of branching logic (e.g., "if / then / else") as well. On certain architectures, this must be in outer loops, while on others, it can be inside inner loops without performance degradataion.

In sum, modern hydrological cycle simulations must consider the constraints of modern architecture during all aspects of development and not just a final "performance tuning" phase.

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Hybrid GPU+CPU Modeling of Ecohydrological and Biogeochemical Processes in Intensively Managed Landscapes

Praveen Kumar, Phong V. V. Le, Dong K. Woo

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Abstract

The intensively managed landscapes (IML) of the agricultural Midwestern US have gone through rapid transformations over the past 200 years due to anthropogenic activities. Land use conversion and modification of soil-moisture regimes have led to the unintended consequences of high nutrient loading in the rivers and receiving water bodies. These shifts on the landscape are central to understanding the cycles of water, energy, carbon and nutrient under environmental changes. However, the magnitude of anthropogenic activities and environmental changes on ecohydrologic and nutrient dynamics have been notoriously difficult to characterize over large areas. Part of the problem is that the underlying vegetation acclamatory processes that affect plant photosynthesis, transpiration, and thus nutrient uptake under elevated CO_2 conditions are not captured in current multi-dimensional biogeochemical models. In addition, large-scale simulations of ecohydrologic and nutrient processes at the emerging lidar-data resolution are numerically expensive due to the density of the computational grid and the iterative nature of the algorithms for solving nonlinearity. Here, we develop a scalable, hybrid CPU-GPU parallel modeling system that links a vertically resolved model of canopy-root-soil biophysical processes with a distributed physically-based integrated surface – subsurface flow and nutrient model to investigate the impacts of environmental changes on large-scale nutrient dynamics. In this coupled model, while canopy processes in the aboveground systems are simulated in parallel in CPU using MPI, hydrologic processes on the land surface and in the belowground systems are simulated using GPU parallel computing. The results show that the micro-topographic and manmade tile drains play an important role in governing the ecohydrologic and nutrient dynamics.

Multi-GPU Simulation of Tsunamis Generated by Earthquakes Using Nested Meshes

Marc De La Asunción, Manuel J. Castro, José M. González, Jorge Macías

Universidad de Málaga, Spain

Introduction

In this work we present a faster than real time (FTRT) simulator of tsunamis generated by earthquakes. This achievement has been possible thanks to the great advances of GPU computational power during the last years. The Tsunami-HySEA model performs in the same code the three phases of an earthquake generated tsunami: deformation of the seafloor, propagation of the tsunami and inundation of coastal areas. Further- more, it supports nested meshes with different spatial resolutions and execution in a multi-GPU cluster using load balancing algorithms. The Italian Tsunami Early Warning System at INGV (Istituto Nazionale di Geofisica e Vulcanologia) has adopted Tsunami- HySEA for its National System.

Numerical Scheme

Tsunami-HySEA uses nonlinear shallow water equations in spherical coordinates. Specifically, it implements a two-step scheme similar to leap-frog for the propagation step, and a second order TVD- WAF flux-limiter scheme described in [1] for the inundation step. The combination of both schemes guarantees the mass conservation and prevents the generation of spurious high frequency oscillations near discontinuities generated by leap-frog type schemes. In order to interpolate the ghost cells of the sub-meshes we take into account the variations of the values of the coarse cells that happen during the simulation. In a similar way, to propagate the values of the fine cells to a coarser submesh we take into account the variations of the mean values of the fine cells. A flux correction step at the boundaries of the submeshes is also needed to ensure mass conservation [2]. The Okada model [3] is used to obtain the seafloor deformation caused by the earthquake.

Implementation

Tsunami-HySEA, along with the Okada model, have been implemented using CUDA and MPI. We apply a row domain decomposition to get the different sub- domains, and overlapping techniques are employed to increase the efficiency by overlapping kernel executions with communications. CUDA streams are used to compute in parallel different submeshes in a same level. Also, load balancing algorithms are used so that all the processes have a similar computational load, taking into account the wet and dry areas of the domain and the nested submeshes. In addition, the implementation supports multiple deformations at any time instant.
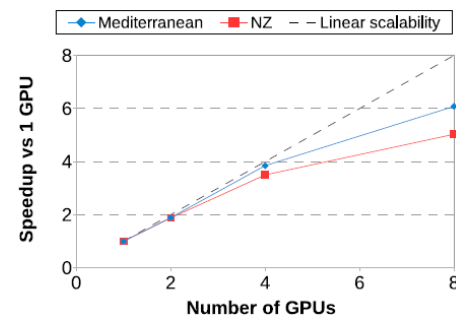

Figure 1: Strong scalability using up to 8 GPUs

Numerical Results

We consider two problems with real topographies and bathymetries: a tsunami in the Mediterranean Sea using one level with a mesh of 7 millions of volumes, and a tsunami near New Zealand using three levels with three nested meshes summing a total of 15.1 millions of volumes. We run all the simulations in a cluster formed by 4 nodes with Intel Xeon E5-2620 processors and 2 GeForce GTX Titan Black in each node. Figure 1 shows the strong scalability obtained for both problems. Using 8 GPUs a speedup of 6 and 5 has been reached with respect to one GPU for the Mediterranean and New Zealand problems, respectively. Also, using one GTX Titan Black we have been able to process up to 184 millions of volumes per second in the Mediterranean Sea simulation.

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14-1: General Session on Advances in Computational Methods for Subsurface Water Resources

Time: Wednesday, 22/Jun/2016: 2:30pm - 3:30pm – Location: MSB 2172

Anomalous Porous-Medium Mass Transport across a Sharp Material Interface

James Montague, George Pinder

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The Application of High-Resolution Schemes in Groundwater Flow and Transport Modeling on Unstructured Polyhedral Grids

Ivan Kapyrin, Fedor Grigoriev

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Anomalous Porous-Medium Mass Transport across a Sharp Material Interface

James Montague, George Pinder

University of Vermont, United States of America

Key words: MRI, sharp interfaces, porous flow and transport, osmosis

Introduction

Low permeability lenses within courser grained porous media create a tailing of concentration breakthrough curves [1]. In experiments described in a companion talk, transport across the fine-grain coarse-grain boundary was shown to create a maximum value in concentration at the boundary that is above the maximum concentration of the host fluid. Similar phenomena have been observed by others [2].

We hypothesize that the boundary between the fine grained and course grained material acts as an osmotic membrane. The mixing of the two grain sizes directly around the membrane creates a thin layer of very low mass transport. Osmotic boundaries provide the theoretical foundation for a discontinuous concentration and is dependent on the osmotic efficiency of the material [3].

Numerical Model

The Navier-Stokes equations are employed to solve for pressure and velocity with a Darcy-Forcheimer drag term applied to the velocity equation. The computed velocity is then initially incorporated into the standard convection-diffusion equation modified to take into account the osmotic efficiency, σ, of the material. Taking into account the osmotic effect provides equations 1 and 2 for the mass flux of the fluid, j_{tot} and the mass flux of the solute, j_s. The second half of equation 1, below, represents the osmotic flow.

$$j_{tot} = -\frac{k}{\mu}\left[\nabla P - \sigma \nu RT \rho \nabla\left(\frac{c_s}{\rho}\right)\right] \quad (1)$$

$$j_s = (1 - \sigma)c_s j_{tot} - D(1 - \sigma)\nabla c_s \quad (2)$$

Here, k is the permeability, μ is the dynamic viscosity, D is the diffusion tensor, P is the fluid pressure, ν is the van't Hoff factor, R is the gas constant, T is the temperature, ρ is the fluid density, and c_s is the solute concentration. Equation 2 represents the osmotic transport of the solute from diffusion and convection. A value of 0 for σ reduces equations 1 and 2 to the standard flow and transport equations in porous media.

We employ this set of constitutive relationships to explain the concentration jump shown in the left pane of figure 2.

A conservative finite volume scheme is applied in the open source modelling software OpenFOAM to test the above hypothesis.
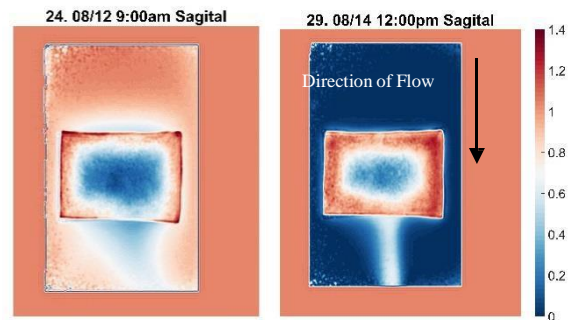

Figure 1: MR image of the concentration of Magnevist [mg/mL] before and after flushing with distilled water.
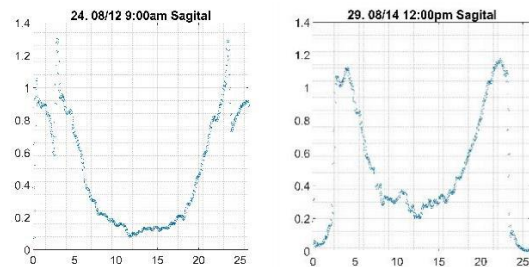

Figure 2: Line scans of concentration versus distance (cm) across the column at roughly the mid-point of the fine grained material

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The Application of High-Resolution Schemes in Groundwater Flow and Transport Modeling On Unstructured Polyhedral Grids

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Key words: high-resolution schemes, polyhedral grids, unsaturated flow

Abstract

High-resolution schemes [1,2] are nowadays widely used in hydrogeological software for the advection operator discretization. These methods allow to achieve a monotone solution while introducing little numerical diffusion and featuring high-order accuracy in smooth regions of the solution.

Here we discuss a high-resolution scheme for unstructured grids, which is based on the linear reconstruction of the scalar solution (either concentration for transport problems or hydraulic head for flow problems) on the grid cells.

Let $\overline{C}_i(\vec{x}) = C_i + \vec{g}.(\vec{x} - \vec{x}_i)$

Be the linear reconstruction of concentration on the cell E_i, x_i is the barycenter of cell E_i and $\vec{g}$ is the gradient vector, which is the unknown. The process of gradient computation is based on the following principles:

1. Minimization of the squared sum of deviations of $\overline{C}_i(\vec{x})$ defined by (1) in neighbouring cells' baricenters from the computed values of concentration in these cells.

2. Limitation of the face values of $\overline{C}_i(\vec{x})$ by the maximum and minimum values on the neighboring cells.

The problem appears to be a linear least squares (LLS) optimization problem with linear inequality constraints. The class of arbitrary polyhedral grids doesn't allow for simplification, and the problem is solved using the active set method.

The scheme is compared to a simpler and numerically cheaper scheme introduced in [3], in which first the unconstrained LLS problem is solved and second the resulting gradient vector is scaled in order to satisfy the inequality constraints. The first scheme exhibits less numerical diffusion.

Front smearing is not only a challenge for transport problems, but for unsaturated flow problems as well: modeling wetting of dry soils one has to refine the mesh to obtain a sufficiently accurate saturation profile. The idea of aforementioned piecewise-linear solution reconstruction may be applied to hydraulic head when calculating the upwind saturation values and relative permeability.
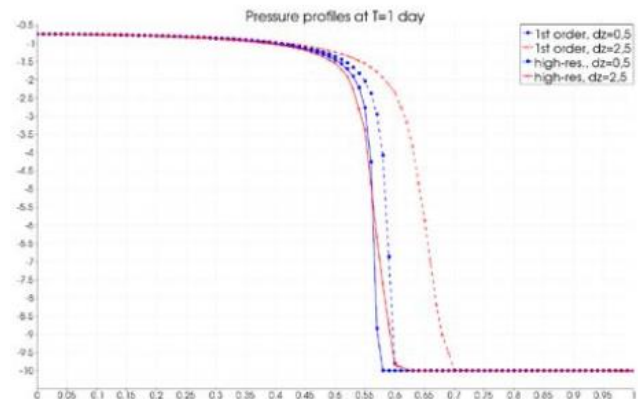

Figure 1: Pressure profiles for the Celia test at T=1 day obtained using high-resolution and simple saturation upwinding

On figure 1 an example of high-resolution saturation upwinding is presented for the Celia test case [4]. In comparison with the traditional upwinding of piecewise-constant saturation the application of piecewise-linear head reconstruction allows to obtain a better saturation front resolution using coarser grids.

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14-2: General Session on Advances in Computational Methods for Subsurface Water Resources

Time: Wednesday, 22/Jun/2016: 3:50pm - 5:30pm – Location: MSB 2173

A New Finite Volume Method for the Transport Equation

Xin Kou, George F.Pinder

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Preserving Physical and Mathematical Properties under Reduced-Order Modeling for Flow and Transport in Porous Media

Maruti Mudunuru[1], Kalyana Nakshatrala[2], Satish Karra[1]

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Approximation of Underground Flows Using a Composite Mixed Finite Element Method on Deformed Hexahedral Meshes

Nabil Birgle[1], Jérôme Jaffré[2], Jean Roberts[2]

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Field Application of Source Search Algorithm at a DNAPL-Contaminated Site in Nanjing, China

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Factors Impacting Stable Isotope Fractionation Related to Aqueous Phase Diffusion in the Subsurface

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dfnWorks: A High-Performance Computing Suite for Subsurface Flow and Transport Modeling Using Discrete Fracture Network

Nataliia Makedonska[1], Satish Karra[1], Jeffrey D. Hyman[1], Hari S. Viswanathan[1], Carl W. Gable[1], Scott L. Painter[2]

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A New Finite Volume Method for the Transport Equation

Xin Kou, George F.Pinder

The University of Vermont, United States of America

Key words: asymmetric weighting function, finite volume method, Fourier analysis, error analysis

In the present work we develop a new finite volume method using an asymmetric weighting function to solve the one-dimensional convection-diffusion transport equation:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} - D\frac{\partial^2 c}{\partial x^2} = 0, \quad (x,t) \in (0,1)\times(0,T], \quad (1)$$

with boundary conditions

$$c(0,t) = 1, \quad \frac{\partial c}{\partial x}|_{x=1} = 0, \quad t \in (0,T], \quad (2)$$

and initial condition

$$c(x,0) = 0, \quad x \in (0,1). \quad (3)$$

We start with discretizing the space interval $(0,1)$ into the finite element grid T^h and the finite volume grid V^h, where

$$T^h := \{x_0, x_1, x_2, \ldots, x_n\}, \quad x_i = ih, \quad h = 1/n, \quad (4)$$

$$V^h := \{x_0, x_{1/2}, x_{3/2} \ldots, x_n\}, \quad x_{i/2} = ih/2. \quad (5)$$

The asymmetric weighting function is defined on each volume:

$$\widetilde{w}_i(x) = \begin{cases} 1 - \frac{2p}{h}(x - x_i) & x_{i-1/2} \leq x \leq x_{i+1/2} \\ 0 & elsewhere \end{cases} \quad (6)$$

Suppose that the approximated solution can be written in the form

$$\hat{c}(x,t) = \sum_{j=0}^{n} C_j(t)l_j(x), \quad (7)$$

where the $C_j(t)$ are undermined, time-dependent coefficients and the $l_j(x)$ are the chapeau basis functions and defined for the node i as

$$l_i(x) = \begin{cases} \frac{x - x_{i-1}}{h} & x_{i-1} \leq x \leq x_i \\ \frac{x_{i+1} - x}{h} & x_i \leq x \leq x_{i+1} \end{cases} \quad (8)$$

Defining the residual as:

$$R(x,t) = \frac{\partial \hat{c}}{\partial t} + u\frac{\partial \hat{c}}{\partial x} - D\frac{\partial^2 \hat{c}}{\partial x^2} \quad (9)$$
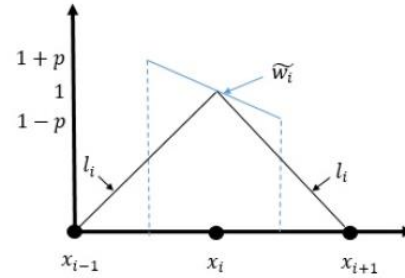

Figure 1: Asymmetric weighting function $\widetilde{w}_i(x)$

Our finite volume method requires that the residual R(x, t) be orthogonal to each weighting function (6):

$$\int_0^L R(x,t)w_i(x)dx = 0, \quad i = 0,1,\cdots,n. \quad (10)$$

(10) reduces to a finite system of differential equations:

$$[B]\{\frac{dC}{dt}\} + [A]\{C\} + \{f\} = 0. \quad (11)$$

Consider a grid $\{0, \kappa, 2\kappa, \ldots, m\kappa\}$ on the time interval, where κ is the time step. We then can approx imate the time derivative dC/dt by using a finite difference approximation with a weighting parameter ϵ, we get

$$(B)\frac{C^{(k+1)} - C^{(k)}}{k} + \epsilon[A]C^{(k+1)} + (1 - \epsilon)[A]C^{(k)} + \{f\}$$
$$= 0 \quad (12)$$

where $C^{(k)} = (C^{(k)}, C^{(k)}, \cdots, C^{(k)})^T$ is the solution $\{C\}$ estimated at the time level k. (12) has a unique solution for k = 1, 2, . . . , m.

This method is superior to the finite element and finite difference methods in generating oscillation-free solutions. We also perform the Fourier analysis to explain the observed behavior of the numerical solutions.

Last but not least, we derive an error estimate of the semi-discrete scheme (only the spatial variable is discretized), and we show that the convergence of our finite volume method is of O(h).

Preserving Physical and Mathematical Properties under Reduced-Order Modeling for Flow and Transport in Porous Media

Maruti Mudunuru[1], Kalyana Nakshatrala[2], Satish Karra[1]

[1]Los Alamos National Laboratory, United States of America; [2]University of Houston, Houston, Texas, United States of America

Numerical simulations of the associated porous media models are one of the few available means in studying a wide range of complex phenomena occurring in subsurface systems. The growing requirement for improved accuracy warrants the incorporation of more details in the modeling phase. However, due to the inherent nature of the porous media models and ever increasing need to simulate many different possible realizations often leads to unmanageable demand on computational resources. Model reduction and parametric model reduction methods aim to reduce this computational burden. This is achieved by generating reduced order models that are faster and cheaper to simulate. Nevertheless, a robust and accurate computational framework is needed to represent the original system behavior. Unfortunately, the current numerical formulations are plagued with deficiencies and are not reliable for predictive simulations. For instance, many existing and popular numerical formulations such as SUPG, GLS, Two-Point Flux methods, and MPFA produce unphysical values for temperature and concentration of chemical species. This has dire consequences in constructing reduced order models (ROMs). Moreover, important physical and mathematical properties such as monotone property, local species balance, and global species balance are not inherited from the continuous setting. This talk aims to present a physics-compatible model reduction framework to overcome such difficulties. The computational framework is constructed by drawing together recent advancements based on a robust locally conservative non-negative numerical formulation [1, 2] and reduced order modeling methods for PDEs [3]. The goal is to generate low-cost but accurate ROMs that characterize system response for different values of the input data and model parameters. Representative numerical examples from contaminant transport are presented to illustrate the importance of the proposed framework to accurately describe and simulate reactive transport in porous media. Finally, we highlight the important role played by the proposed model reduction framework in subsequent predictions of future contaminant evolution and corresponding decision analysis for remediation process.

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Approximation of Underground Flows Using a Composite Mixed Finite Element Method on Deformed Hexahedral Meshes

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Key words: flow in porous media, composite finite element, mixed finite element, hexahedral mesh

In hydrogeology as well as in many other domains of application for flow in porous media, locally conservative cell-centered approximation methods are preferred for modeling flow and transport in porous media. In many cases we wish that the discretization of the domain keeps the natural layering of the geological medium while minimizing the number of degrees of freedom of the calculated solution. This leads us to study numerical methods for meshes made of general hexahedra and deformed cubes with curved faces. On the other hand we would like to keep the standard setting of degrees of freedom of cell-centered methods that is one degree of freedom per cell for pressure and one degree of freedom per face for the face normal flux of the Darcy velocity, in order to facilitate the implementation in an existing code.

Numerical models based on mixed finite elements are a good candidate for such methods: they calculate the Darcy velocity and the pressure simultaneously to the same order of accuracy. The classical mixed finite element method of Raviart-Thomas-Nédélec work well on tetrahedral meshes or on meshes made of hexahedra which are transforms of a cube by a linear transformation. But they do not give satisfactory results with general hexahedral meshes.

To overcome this difficulty, a new composite mixed finite element method was developed in [1] in which a hexahedron is divided into 5 tetrahedra. In this method the Darcy velocity is calculated in the Raviart-Thomas- Nédélec space of lowest order inside each tetrahedron of the subdivision but has only one degree of freedom per face of the hexahedral mesh, and the pressure has one degree of freedom per hexahedral cell. However this method could not be extended to the case of deformed cubes with curved faces. Since the curved faces would be split into 2 triangular sub-faces, the choice of this division may introduce a gap between two neighbouring cells.

To handle meshes having curved faces and to obtain better symmetry properties, we develop a new composite method [2] in which an hexahedron is split into 24 tetrahedra as shown in Fig. 1, by adding an additional node at the barycenter of its vertices. The faces of the hexahedron are then split into 4 triangular subfaces. The method has still the same number of degrees of freedom as before, one per face of the deformed cube for the Darcy velocity and one for each deformed cube for the pressure. Numerical results will be shown confirming theoretical convergence results and for experiments relevant to flow in the subsurface around a nuclear waste storagesite.
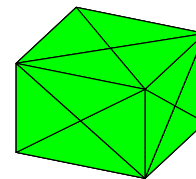

Figure 1: Hexahedron split into 24 tetrahedra.

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Field Application of Source Search Algorithm at a DNAPL-Contaminated Site in Nanjing, China

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Key words: DNAPL, source search, field application

Introduction

Various mathematical methods have been proposed to locate the source zone using plume data. Given DNAPL's complex transport paths in the subsurface and the fact that its source is generally small and filamentous, it is difficult to identify the source efficiently using borings or geophysical methods. However, the dissolved plume can be quite large and easy to locate. An algorithm developed by Dokou and Pinder [1], which highlighted an optimal sampling strategy and a realistic representation of the site's stochastic permeability field, with minor modifications, is applied to a DNAPLs-contaminated site in Nanjing to define the source locations.

Methodology

The overall strategy uses Monte Carlo stochastic groundwater flow and transport modeling, Kalman filtering as well as fuzzy set technique. Approximate source locations are first assumed and initial weights that reflect the degree of truth regarding the source locations are assigned based on field information. The stochastic groundwater flow and mass transport model are developed, and the concentration mean and the varience-covarience matrix are calculated using the Monte-Carlo technique. A Kalman filter is then used to update the composite plume and the variance- covariance matrix using the data from the optimal sampling locations, which are selected based on the proximity to the assumed source locations and the reduction in overall uncertainty field. The convergence on optimal source characteristics should be finally reached.

Field application

The field site, located in Northeastern Nanjing, was a chemical plant producing the optical brightener agent PF from 1999 to 2010. Investigations in 2012 and 2013 at the Nanjing site confirmed contamination in groundwater. Trichlorobenzene (TCB) is identified as the major contaminants of concern with the highest concentration of 7.3 mg/L and found mainly in the northeastern part of the site in unconfined aquifer, where the former wastewater basins and PF workshops are located.
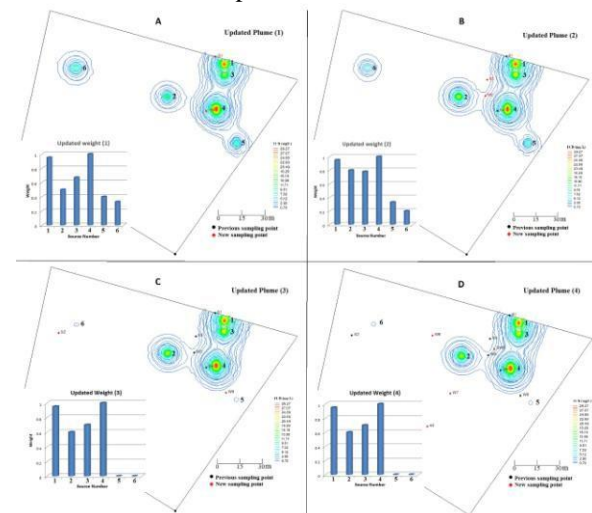

Figure 1: The updated composite plumes and the correspondingly updated weights

Sources #1 and #4 (Figure 1) are identified as the true sources. Source #1 is located in the previous waste water basin, and source #4 is located in the former PF workshop, both of which can release DNAPL into the subsurface. The algorithm ruled sources #5 and #6 out as true sources, which are located in the former liquid alkali tank and boiler room. Sources #2 and #3 are very likely the true sources with moderate weight values and considering they have similar operational histories as sources #1 and #4.

Conclusions

For the Nanjing Site example, the search algorithm successfully identifies sources #1 and #4 as the true sources, sources #5 and #6 as the false sources, and sources #2 and #3 as very likely true sources after collecting 9 samples. The results obtained from the algorithm can guide us in further field study. Additional sampling around source #2 and source #3 are needed at Nanjing Site to confirm that they are primary source areas.

References

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Factors Impacting Stable Isotope Fractionation Related to Aqueous Phase Diffusion in the Subsurface

Bruce S. Xu[1], Brent E. Sleep[1], Barbara Sherwood Lollar[2], Elodie Passeport[1]

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Key words: stable isotope fractionation, diffusion, sampling

Introduction

Use of compound specific isotope analysis (CSIA) for assessment of intrinsic biodegradation is now an accepted practice. However, due to differences in molecular weights of isotopologues, aqueous phase diffusion may also lead to isotopic fractionation and potentially confound the CSIA application. In this study, three-dimensional (3D) simulations were conducted to investigate the key factors impacting the aqueous phase diffusion-related isotope fractionation (DRIF) in the subsurface at the field scale. These factors include the ratio of source concentration to method detection limit for CSIA technique (C0/MDL), the ratio of mechanical dispersion coefficient to effective diffusion coefficient (Dmech/Deff), the sampling methods, and the thickness of aquifer (in an aquifer-aquitard system).

Modeling Approach

The numerical model MT3DMS was coupled with fundamental isotope equations to model the DRIF effects at a hypothetical field under a range of hydrogeological conditions. In sampling simulations, a low pumping flow rate (250 mL/min) was used for purging and sampling. The vertical distribution of flux into the well was determined following the paper [1], in which the actual monitoring zones (i.e., where the sample water comes from) for different types of well were identified.

Results and Conclusions

In the simulations of benzene transport in a 3D aquifer, even for a relatively high ratio of C0/MDL, the different diffusion coefficients of the light and heavy isotopologues did not lead to observable DRIF in the entire system when the transverse vertical mechanical dispersion coefficient (Dmech,TV) was one order of magnitude larger than the effective diffusion coefficient. In the aquifer-aquitard system, benzene diffused into the aquitard at the beginning and back into the aquifer after the source was depleted. However, there was no observable DRIF predicted within the aquifer associated with diffusion into the aquitard or during back diffusion when the thickness of the aquifer was meters large. Sampling well simulations demonstrated that

any exaggerated DRIF effects achieved by using very small soil dispersivities would be largely reduced when the typical screen lengths were used for groundwater sampling (Figure 1). The simulation results in this study suggest that for a subsurface aquifer or an aquifer-aquitard system with aquifer thickness on the order of meters, if Dmech,TV/Deff ≥ 10 or if a conventional sampling approach is applied, DRIF effects would not be significant considering a metric of $\pm 2‰$ for detection of DRIF.
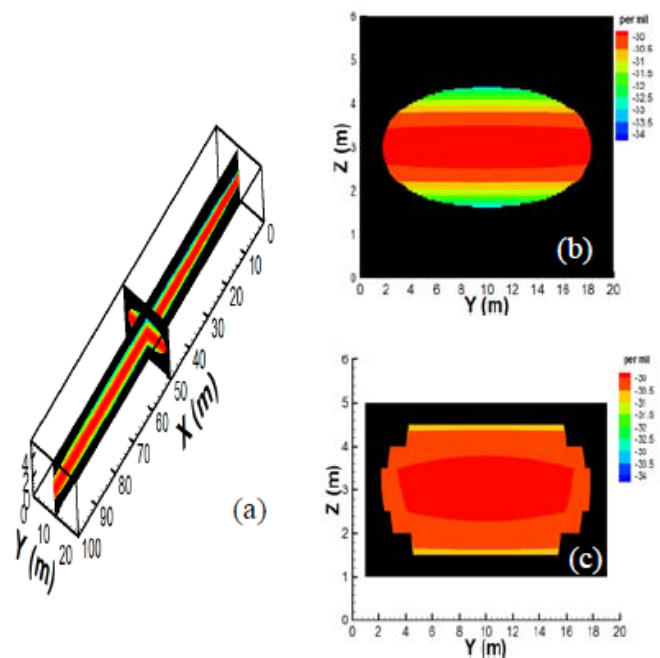

Figure 1: δ^{13}C of benzene after 600 days non-reactive transport (a) in a 3-D simulation domain; (b) at the cross-section at 50 m from the source; (c) predicted by the simulation of partially penetrating sampling well with a screen length of 1.5 m.

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dfnWorks: A High-Performance Computing Suite for Subsurface Flow and Transport Modeling Using Discrete Fracture Network

Nataliia Makedonska[1], Satish Karra[1], Jeffrey D. Hyman[1], Hari S. Viswanathan[1], Carl W. Gable[1], Scott L. Painter[2]

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Key words: Discrete Fracture Network, Subsurface Flow and Transport, Unconventional hydrocarbon extraction

Flow and solute transport modeling using discrete fracture network (DFN) is an important approach for understanding the subsurface flow and transport in impermeable rock, where fractures provide dominant flow and transport pathways. It is challenging to obtain accurate transport results in three-dimensional DFNs because of the high computational burden and difficulty in constructing a high-quality unstructured computational mesh on simulated fractures. A recently developed computational suite, dfnWorks [1], generates discrete fracture networks of planar polygons; constructs a high quality conforming Delaunay triangulation of the intersecting fractures in DFNs; assigns fracture properties, such as aperture and permeability, using geostatistics; sets boundary and initial conditions; solves pressure and flow in single or multi-phase fluids using the parallel finite volume approach, PFLOTRAN [2], which is locally mass conserving and thus eliminates mass balance problems during solving for transport; simulates particle transport using Lagrangian particle tracking approach. dfnWorks enables accurate flow and particle tracking modeling on kilometer-scale DFNs with tens of thousands of fractures and millions of computational cells.

dfnWorks toolkit has been successfully applied for studying contaminant transport in nuclear waste repository [3], CO2 sequestration and extraction of unconventional hydrocarbons [4]. In this talk, the details of dfnWorks along with its application to hydrocarbon extraction from unconventional oil & gas, will be discussed. Numerical experiments on a realistic fractured shale system (Figure 1) are presented to identify how in-fracture heterogeneity of aperture and transmissivity affect the production curves. The contributions of main gas transport mechanisms, such as advection, desorption, and matrix diffusion to the production curve shape will be discussed.
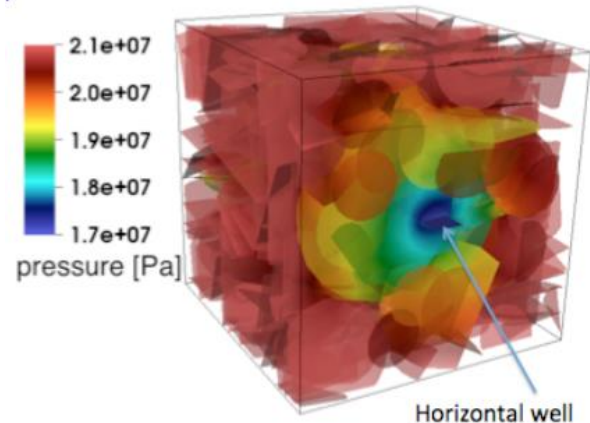

Figure 1: Discrete fracture network generated based on fracture statistics from a naturally fractured shale site. Horizontal well is located in the center of the simulation domain. Color represents obtained pressure solution.

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15-1: Advances in Fluvial Eco-Hydraulics and Morphodynamics

Time: Wednesday, 22/Jun/2016: 11:00am - 12:20pm – Location: MSB 2170

The Coupling of Fine Particle and Bedload Transport using Data Integration and Process Modeling

James Robert Hunt[1], Jungsu Park[1,2]
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Hydrologic Control of Channel Morphology and Organization in Gravel-Bed Streams: Field Studies and Flume Experiments

Gordon E. Grant[1], Laura Hempel[2], Sarah Lewis[2]
[1]USDA Forest Service, United States of America; [2]Oregon State University, United States of America; Gordon.Grant@oregonstate.edu

Vegetation against Erosion Downstream of a Hydraulic Structure

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The Coupling of Fine Particle and Bedload Transport using Data Integration and Process Modeling

James Robert Hunt[1], Jungsu Park[1,2]

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Key words: filtration, erosion, particle loading

Introduction

Fine particles in the silt and clay size range are important determinants of surface water quality and they control the transport of chemical and microbiological contaminants. Empirical power law models can represent particle transport in streams but that approach does not permit generalization from one climatic condition to the next or from one watershed to another. An alternative, more mechanistic modeling approach is needed that is based on monitoring data but seeks to represent critical processes at an appropriate level.

Analysis

Within California there are 38 USGS gauging station locations that we classified as minimally developed and each contained more than three years of flow and daily suspended particle concentration data. Thirty of those 38 sites demonstrated a transition to increased particle loading at higher flow rates, and all of these sites were gravel-bedded. The transition flow rate approximately corresponded to the flow rate that a Shields analysis predicted the initiation of bedload transport. The remaining eight gauging locations without a transition had stream beds composed of sand, cobbles, boulders, or bedrock. The results led to a conceptual model that fine particles accumulated within the sediment bed during lower flow periods and these particles eroded during flood events that mobilized bed sediments.

The data and the conceptual model guided the development of a quantitative model that couples continuous fine particle deposition with episodic particle release by flood events. The particle deposition model assumes first order dependence on suspended particle concentration. The particle release model was based on the empirical data reported by Haschenberger [1] during scour and fill during individual flood events. The model has parameters that were identified from watershed data (transition flow rate, maximum mass of particles present in the sediment bed, flow rate required to remove all particles, and a background particle concentration dependence on flow rate). Two additional fitting parameters were associated with particle filtration and bed erosion.

Model calibration was undertaken at two sites along the Russian River, California utilizing at least 18 months of continuous flow and suspended solids monitoring data. Unique values of the filtration and erosion model parameters were identified during calibration and a limited sensitivity analysis was possible at these two locations. The calibrated model could predict particle release over a time interval not used in calibration utilizing only measured flow rate. Figure 1 demonstrates the level of partial validation achieved for the two Russian River sites where the model provided a reasonable prediction for fine particle release during larger flood events. The challenge was to balance uncertainties across the various critical processes [2].
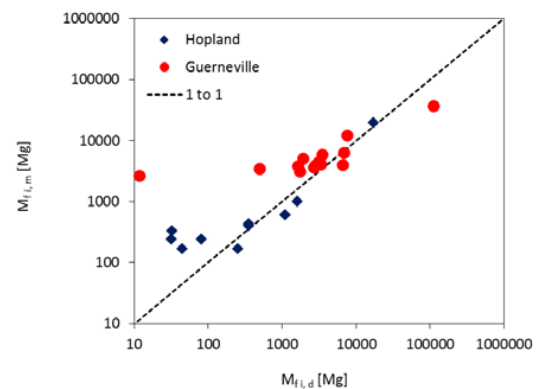

Figure 1: Comparison of mass of fine particles calculated from data during flood events ($M_{fi,d}$) with the mass predicted by the model ($M_{fi,m}$) during the validation period for the two sites along the Russian River, California.

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Hydrologic Control of Channel Morphology and Organization in Gravel-Bed Streams: Field Studies and Flume Experiments

Gordon E. Grant[1], Laura Hempel[2], Sarah Lewis[2]

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A fundamental research question in fluvial geomorphology is to understand how channel form reflects the hydrologic regime of the channel. Historically, the prevailing view has been that channel dimensions adjust to a so-termed "dominant discharge", which is often approximated as the bankfull flow, or the flow that just fills the channel. While there is strong evidence that many channels appear to have physical dimensions that correspond to this flow, which typically has a return period of 1-2 years, referencing the geomorphic effectiveness of the entire hydrologic regime by a single discharge or geometry is problematic. In particular, many decades of research have shown that different flows play different geomorphic roles in the channel: some flows entrain fine grain sediment, some entrain the full size distribution of bed sediment, some destabilize or build bars, some erode the banks, some float woody debris and so forth. There is no overarching principle that requires that these flows have the same frequency and magnitude, opening the door to the question of how different flow regimes shape the active channel and its full suite of processes.

To address this issue, we have used a combination of physical experiments, field studies, and numerical models to explore how hydrographs having different shapes, durations, and frequencies of bedload transport result in different degrees of channel organization, which we define in terms of the regularity, spacing, and architecture of bedforms and channel dimensions. Field studies reveal that streams having very constant hydrographs, i.e., spring-fed streams, have very different morphologies than streams with more peaked hydrographs. The former typically have rectangular cross-sections and lack well defined bar-pool morphology. Streams with moderately flashy hydrographs have better formed and regularly spaced bars and pools and asymmetrical cross-sections. At the most extreme end,

channels with sharply peaked, short duration hydrographs, such as streams in Mediterranean climates, also lack well developed bars and pools. Similar distinctions apply to the architecture of wood accumulations in channels across a range of hydrograph shapes. Flume experiments support these observations and reveal the close coupling between timescales of sediment transport responsible for these differences. Taken together, this work points to the importance of the duration of sediment transporting events as a fundamental control on channel morphhology, and offers the prospect of better understanding how changing hydrologic regimes, either through climate, land use, or dams, will translate into geomorphic changes.

Vegetation against Erosion Downstream of a Hydraulic Structure

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Key words: Rivers, scouring, flow characteristics, vegetation

Introduction

Due to the introduction of man-made sediment barriers along a river, the amount of sediment load entering in the downstream river reach is different from that going out and erosion processes occur downstream of the barrier itself. Most studies have been devoted to formulation of empirical equations to estimate the maximum (or equilibrium) scour depth and length (among others [1, 2, 3],) for a specific scour problem. This information is important to identify adequate protective measures against scouring process. But, in order to evaluate the advantages of a specific protective technique, it is important to investigate the effects of the technique itself on flow velocity field and sediment transport processes. The design of the protective measures needs the knowledge of flow velocity field and of geometrical characteristics of scour transient profiles. On the other side, the uncertainty regarding the interpretation of sediment transport phenomena during the transients determines some limitations in mathematical modeling of scouring process. Quantitative estimate of the bed profile deformation and of its temporal evolution is essential in order to define structural protective measures or to consider possible alternative or complementary components in risk analysis projects.
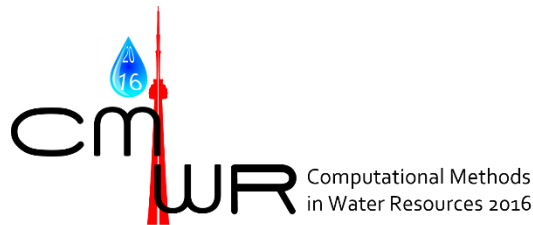
Vegetation has been recently used as a bioengineering technique against erosion. In the attempt to respond to the aforementioned question, an experimental program has been conducted, at the Dipartimento di Ingegneria Civile, Ambientale, Aereospaziale, dei Materiali (DICAM) - Palermo's University (Italy), to analyze scour caused by a horizontal jet downstream of a rigid bed. Experimental campaigns were specifically designed to investigate turbulence flow characteristics inside the scour hole and to verify the effect of countermeasures around the hydraulic structure on flow turbulent structure. In the present work attention is restricted at assessing the effectiveness of carpet of flexible vegetation planted downstream of the barrier. The experiments were conducted to examine the flow velocity field, including turbulent characteristics both within the scour hole (in absence of vegetation) and

downstream the hydraulic structure when the vegetated carpet is installed.

The present work shows the effects of vegetation on sediment transport process. The volume of sediments transported at different time steps is determined by applying a numerical model previously developed [4] and the model parameters are calibrated by using the experimental data.

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16-1: Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale

Time: Thursday, 23/Jun/2016: 11:00am - 12:20pm – Location: MSB 3154

Experimental Investigation of Immiscible Two-Phase Flows in Micromodels for the Validation of Modeling Tools

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Magnetic Resonance Imaging of the Effect of Sharp Material Interfaces on Transport in Porous Media

James Montague[1], George Pinder[1], Richard Watts[2], Jay Gonyea[2], Scott Hipko[2]

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Simulation of Reactive Transport using CTRW and NMR Validation

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Micro-PIV Measurements of Multiphase Flow of Water and Supercritical CO_2 in 2D Heterogeneous Porous Micromodels

Yaofa Li[1,2], Gianluca Blois[1,2], Farzan Kazemifar[1,2], **Kenneth Christensen**[1,2]

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Experimental Investigation of Immiscible Two-Phase Flows in Micromodels for the Validation of Modeling Tools

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Key words: Multiphase Flow, Micromodel, Micro- PIV, Pore-scale flow

A fundamental understanding of multiphase flow displacement mechanisms in porous media is relevant to hydrocarbon recovery or to the process of CO_2 sequestration in hydrocarbon reservoirs and saline aquifers. Detailed observations reveal that the macroscopically continuous and seemingly smooth motion of fluid displacement fronts results in reality from numerous interfacial jumps at the pore-scale. Such fast jumps have been known for more than 80 years as Haines jumps or rheon [1]. These jumps result from local competition between capillary and viscous forces. Recently, we observed and quantified such behavior in micro- models that represent natural complex porous media [2]. Using micro-Particle Image Velocimetry (micro- PIV), we are able to measure accuratly the velocity distributions in porous media with a typical pore size of 5- 40 µm and with a vector grid of 2µm. Moreover, we observed dissipative events, such as eddies within the aqueous phase, in the micro-PIV results, Figure 1. These recirculating phenomena may have implications for multicomponent mass transport by enhancing mixing, or accelerating surface reactions such as dissolution mechanisms. These observations of complex interface dynamics at the pore scale motivate further measure- ment of multiphase fluid movement at the pore scale and requisite modeling.
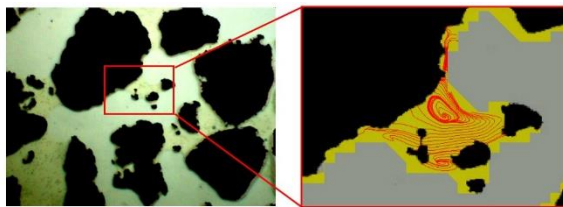

Figure 1: Two-phase flow experiment in a sandstone micro- model. Left: Oil (bright green) is displacing water (green), grains are dark. Right: plotted streamline.

In this work we performed measurements for immiscible two-phase flow in micromodels. The micromodels are representative of complex porous media or simplified geometry. Our aim is to understand, characterize and quantify phenomena such as interfacial jumps and dissipative recirculations during two-phase flow. Our simplified micromodels are composed of alignments of pores of different sizes (Figure 2) or of eddy pockets. They allow for a quantitative comparison between experimental results and numerical simulations. Using image processing techniques we track the displacement of the moving interface between both fluids, Figure 2. In addition, velocity distribution are measured with micro-PIV technique. These measurements provide high resolution reference data to validate modeling tools that are still in development for two-phase flows.
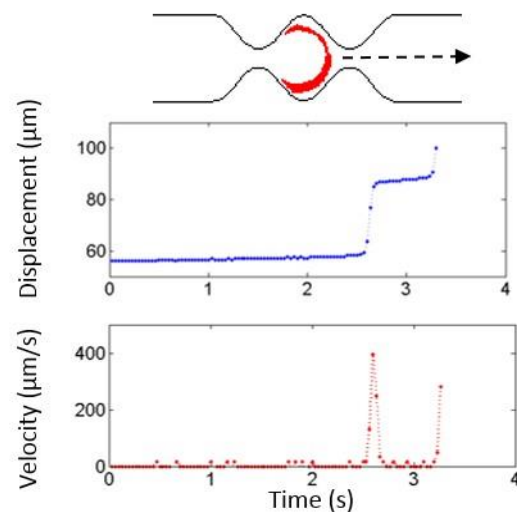
t

Figure 2: Top: interface (red) between two immiscible fluids flowing in a microchannel (dark edges) detected by image processing, graphs: measurements of the displacement and velocity of the interface.

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Magnetic Resonance Imaging of the Effect of Sharp Material Interfaces on Transport in Porous Media

James A. Montague[1], George F. Pinder[1], Richard Watts[2], Jay V. Gonyea[2], Scott Hipko[2]

[1]University of Vermont, School of Engineering; [2]University of Vermont, College of Medicine;

Key words: MRI, sharp interfaces, porous flow and transport

Introduction

Low permeability lenses within courser grained porous media create a tailing of concentration breakthrough curves [1]. Understanding the physics that drive the tailing phenomena is critical for dealing with the remediation challenges that it poses.

Lab Experiments in which ideal conditions exist, i.e. the values of permeability are known exactly, the initial conditions for flow and concentration are set, and all boundary conditions are accounted for, often monitor concentration using point sensors. This means that, while most values are known perfectly at these points, the concentration cannot be known at every location. This becomes especially important at the interface between fine and course grained materials. Ideally, we would like to know the exact concentration on a scale similar to or less than that of our numerical model to ease direct comparisons. Magnetic resonance imaging (MRI) allows for voxel level detail of the concentration plume, where voxels are on the order of millimeters and thus satisfy this scaling requirement [2].

Lab Experiment

A physical model has been developed for use in a MRI, meaning that it is made entirely out of non- magnetic materials. A cylinder of fine grained crushed silica (SIL-CO-SIL) is placed within the center of the cylindrical column and surrounded by a uniform courser silica sand (AFS Testing Sand 50- 70). The column is initially fully saturated with distilled water. At the start of the experiment contrast agent, in the form of Magnevist, is pumped into one end of the column. Images are taken regularly to track the concentration of Magnevist within the column. Effective diffusion coefficients can be determined from the inverse problem for the materials used.

The time series of MRI images are used to investigate the boundary between the fine and course grained silica through the use of numerical models. Figure 1 shows the concentration of Magnevist three weeks after filling the course sand with contrast agent before and after flushing the column with distilled water. MR imagery reveals an unanticipated build-up of concentration at the interface between the two silicas (Figure 2). Modeling efforts are now directed at reproducing the observed results to predict and understand the asymmetric mass transport behavior across this boundary [3].
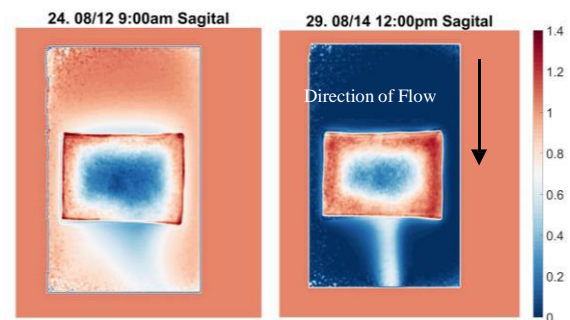

Figure 1: MR image of the concentration of Magnevist [mg/mL] before and after flushing with distilled water.
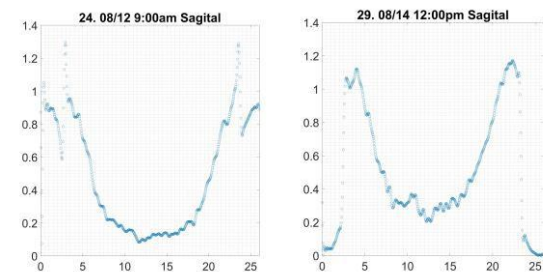

Figure 2: Line scans of concentration versus distance (cm) across the column at roughly the mid-point of the fine grained material

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Simulation of Reactive Transport using CTRW and NMR Validation

Bagus P. Muljadi[1], Martin J. Blunt[1], Branko Bijeljic[1], Adam Colbourne[2], Andy J. Sederman[2],
Mick D. Mantle[2], Lynn F. Gladden[2]

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Key words: Continuous Time Random Walk, Nuclear Magnetic
Resonance, Propagators, Reactive Transport

Introduction

A continuous time random walk method [2] for modeling
reactive single-phase transport is presented and calibrated
with NMR experiments of dissolutions of car- bonates.
Transport is modeled as a continuous time random walk:
particles make a series of hops between nodes—in a node-
link lattice—with a probability $\psi(t)$ that a particle will first
arrive at a node from a nearest neighbor in a time t to t+dt.
We compute the probability density function of particle
displacements (propagator) and calibrate it with the
propagators from NMR experiments wherein HCl is flowed
through several carbonate cores. Upon calibration, the
transit time function ψ_p is then used to calculate transport at
the core scale and a ψ_c is found that accounts for cm-scale
transitions.

Transport Model

At the micron scale, we fit a truncated power law

$$\psi_p(t) = Ae^{-t/t2}\,(1 + t/t1)^{-1+\beta} \qquad (1)$$

for the distribution of transition times between pores, and t_1
$= l/v$, l is the link length and v is the fluid velocity within
that link. $t_2 = l^2/Dm$ is the cut-off diffusion time, where
Dm is molecular diffusion coefficient. The mediums
heterogeneity is now characterised by the exponent β. For β
> 2 the system displays Gaussian behavior, while
anomalous behaviour is observed for $0 < \beta < 2$. Fig. 1
depicts the simulation of particles plume through rock cores
using different values of β.

Transport model is validated with the NMR
experiments—Fig. 2 shows the comparison of propagators
predicted using our method with the experiments of
Scheven [1] for beadpack and Bentheimer sandstone.
Reactive transport is modeled by taking into account the
change in porosity, permeability and velocity field which
leads to β varying with time. The method is calibrated with
NMR experiments of acid dissolution in Ketton and
Estaillades carbonates providing the change in propagators

and porosity profiles.

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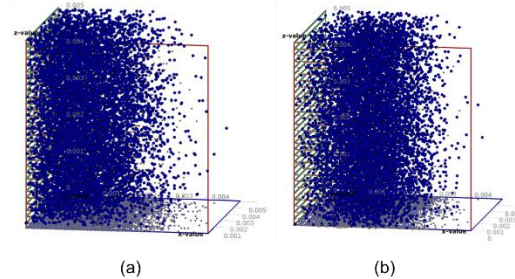2006;44:RG2003. doi:10.1029/2005WR004578.

Figure 1: Tracer plumes through a lattice with (a) $\beta =$
0.55 showing an anomalous behaviour; and (b) $\beta = 1.67$
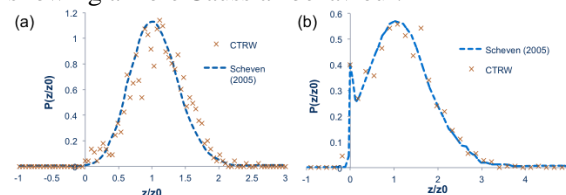showing a more Gaussian behaviour.

Figure 2: Predicted propagators and comparison with
experiments using (a) $\beta = 1.95$ and a beadpack; and (b)
$\beta = 1.76$ and Bentheimer sandstone. Crosses denote our
simulation results, and dashed lines denote the propagators
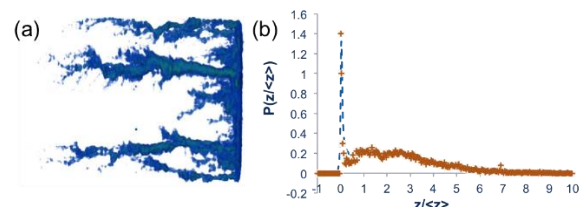from Scheven et al. [1] measured at 1 second of observation
time.

Figure 3: Experiment result of *HCl* flowing through a
Ketton core. (a) The porosity difference after dissolution;
and (b) The computed propagator ($\beta = 0.55$) and the
comparison with the propagator obtained from NMR
experiment.

Micro-PIV Measurements of Multiphase Flow of Water and Supercritical CO2 in 2D Heterogeneous Porous Micromodels

Yaofa Li[1], Gianluca Blois[1], Farzan Kazemifar[1], Kenneth Christensen[1,2]

[1]University of Notre Dame, United States of America; [2]International Institute for Carbon-Neutral Energy Research, Kyushu University, Japan;

Key words: Micro-PIV, CO2 sequestration, Pore scale, Multiphase flow, Porous media

Introduction

Carbon capture and sequestration (CCS) is a viable technique for reducing carbon emissions from large CO_2 sources [1]. An important stage in the CCS process is the injection of supercritical CO_2 into saline aquifers, which are porous formations saturated with brine, and thus CO_2 must displace the resident brine during and post injection. Our fundamental understanding of the coupled flow dynamics of CO_2 and brine in geologic media is still limited. This is particularly true at the pore scale, despite pore-scale processes representing a critical component of accurately predicting large-scale migration of injected CO_2. To this end, the pore-scale flow dynamics of liquid/supercritical CO_2 infiltration into water- saturated 2D *heterogeneous* porous micro-models, inspired by the structure of real reservoir rock, is studied at reservoir conditions (`80 bar, 24 °C).

Experimental Methods:

The micromodels used in these experiments were fabricated from silicon, with the porous matrix formed from the reprint of the pore structure of real sandstone as shown in Figure 1 [2].
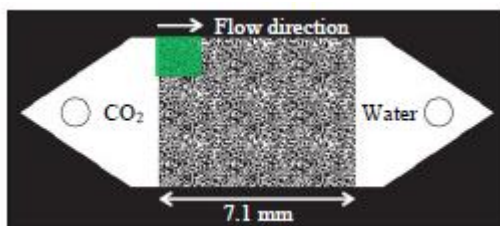

Figure 1: Schematic diagram of the micromodel with the green region indicating the imaging field of view.

The coupled flow of water and CO_2 through the micromodel is accurately controlled by two high- pressure syringe pumps. Fluorescent microscopy and the micro-PIV method are employed by seeding the water phase with fluorescent particles and tagging the CO_2 phase with a fluorescent dye of a different spectral emission. Doing so allows for simultaneous measurement of the spatially-resolved instantaneous water velocity field and quantification of the instantaneous spatial configuration of both phases [3].

Initial Results:

The initial results provide a clear picture of the flow physics during the migration of the CO_2 front, the evolution of individual menisci and the growth of dendritic structures, so-called fingers [3]. During the CO_2 infiltration process, CO_2 suddenly breaks through the resident water, forming fingers which grow in directions both along and normal to the bulk pressure gradient, and even against the bulk pressure gradient, indicating capillary fingering (Fig. 2). The complex phase configuration highlights the importance of local pressure gradients in CO_2 front migration.
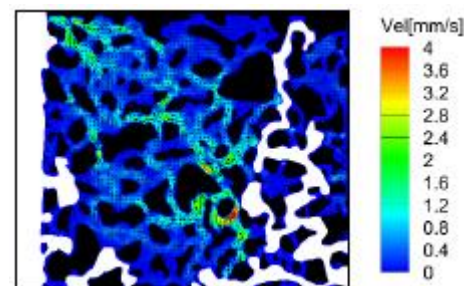

Figure 2: Sample result (80bar, 24 °C, 0.005 ml/min), showing water velocities as color contours; CO_2 and silicon grains as white and dark, respectively.

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16-2: Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale

Time: Thursday, 23/Jun/2016: 2:30pm - 4:10pm – Location: MSB 3154

Generalized Network Modelling – Validation on a Pore-By-Pore Basis

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Pore-scale Modeling of Non-Newtonian Fluid Flow in Porous Media

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Two-Phase Displacements in Rough Fractures: Beyond Darcy's Law

Amir Alizadeh Pahlavan, Luis Cueto-Felgueroso, Gareth McKinley, Ruben Juanes

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Local Analysis of Single-Phase Flow Through Complex Porous Media Using Flow Propagators

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Generalized Network Modelling – Validation on a Pore-By-Pore Basis

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Key words: generalized, dynamic, network modelling, two-phase flow

Summary

We present and validate a generalized network modelling workflow for two-phase flow through porous media. In order to avoid the uncertainties introduced due to the over-simplification of flow domain in conventional network models [1], parameters of the generalized network are computed from direct single-phase flow simulations and from medial-surface analysis of the pore space. The model is validated using experimental capillary pressure and relative permeability curves as well as using direct simulation and micro-CT imaging of two-phase flow experiments on a pore-by-pore basis.

Network extraction from micro-CT scans

In the network extraction step, the pore space is discretized by first segmenting it into individual pores and then subdividing each pore into sub-elements called half-throats. Each half-throat connection is further subdivided into corners by analyzing its medial axis. To minimize the approximation errors, the corner conductivities are calculated using direct single-phase flow simulation. The parameters approximating the corners - corner angle, volume and connectivities - are computed as a tabulated function for each corner and used in flow simulations.

Two-phase flow simulation

We have implemented a dynamic two-phase simulator to model flow through the generalized network and to predict capillary pressure and relative permeability curves. The flow simulator incorporates the main mechanisms of pore-scale displacement, such as corner and oil-layer flow, snap-off and Haines jumps, while taking the effect of viscous pressure into account. The interface location and curvatures are computed analytically using the M-SP theory. The phase volumes and conductivities are computed from the tabulated data extracted during network extraction while adding the effect of contact angle and coupling terms using empirical equations.

Validation

In addition to validating our model predictions of capillary pressure and relative permeability curves with experimental data from literature, the model is validated on a pore-by-pore basis. Direct simulations on a simple star-shaped geometry (Figure 1) and on small sections of a Ketton carbonate sample (Figure 2) are used to validate the piston-like and snap-off entry pressures as well as phase distributions. We also compare our results with experimentally obtained high resolution images of residual sc CO2 ganglia after a water-flood experiment in Ketton (Figure 2b).
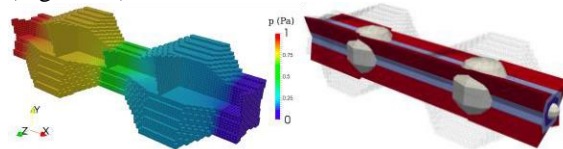

Figure 1. Voxelized representation of a star-shaped geometry and its generalized network model. This geometry is used to validate our model against direct simulations and theoretical solutions for interface curvature.
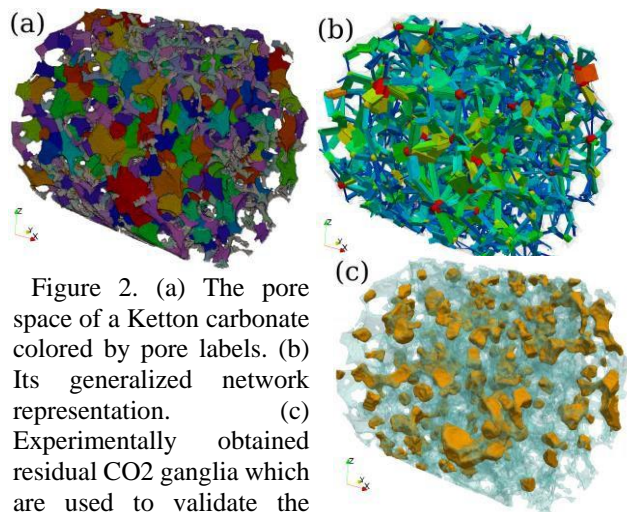

Figure 2. (a) The pore space of a Ketton carbonate colored by pore labels. (b) Its generalized network representation. (c) Experimentally obtained residual CO2 ganglia which are used to validate the network model.

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Pore-scale Modeling of Non-Newtonian Fluid Flow in Porous Media

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;

Key words: Lattice Boltzmann method, Non-Newtonian fluid

Systems involving the flow of non-Newtonian fluids in porous media arise in a number of settings, including hydraulic fracturing, enhanced oil recovery, contaminant remediation, and biological systems. Development of accurate macroscale models of such systems requires an understanding of the relationship between the fluid and medium properties at the microscale and averaged macroscale properties. This study examines the flow of aqueous solutions of guar gum, a major component of hydraulic fracturing fluids that exhibits Cross model rheological behavior.

To simulate flow of such fluids in porous medium systems, a lattice Boltzmann method (LBM) incorporating non-Newtonian behavior was developed. The model was validated with a semianalytical solution for the flow of Cross model fluids between parallel plates, then used to simulate onedimensional column flow experiments. The computational results were used in conjunction with the experimental data to investigate the relationships between fluid and media properties, microscale physics, and macroscale parameters.

Two-Phase Displacements in Rough Fractures: Beyond Darcy's Law

Amir Alizadeh Pahlavan[1], Luis Cueto-Felgueroso[1,2], Gareth McKinley[1], Ruben Juanes[1]

[1]Massachusetts Institute of Technology, [2]Universidad Politécnica de Madrid

Key words: immiscible displacement, wetting, disorder, porous media, phase-field modeling

Abstract

Immiscible flow in a disordered medium is an ubiquitous phenomenon, from spreading of an ink droplet on a piece of paper to infiltration of water in soil, with applications ranging from CO_2 sequestration to water desalination. Wetting is inherently a multiscale phenomenon; the complex interplay between porous and fractured media and immiscible flows lead to a wealth of fascinating displacement patterns that continue to challenge our descriptions across scales. While much is known about stable imbibition (when a more viscous and wetting fluid displaces a less viscous nonwetting fluid) into disordered media and their corresponding universality classes [1], unstable flows (when a less viscous fluid displaces a more viscous fluid) are still poorly understood. In this work, we use a roughened Hele-Shaw cell (two rough glass plates separated by a thin gap) to study viscously unstable displacements under different wetting conditions. The disorder introduced into the system leads to multiple effects, from spatial heterogeneity in the permeability field and capillary pressure distribution, to contact-line pinning and hysteresis. The ability to account for all these effects and simultaneously visualize the flow with high fidelity makes this system and ideal candidate to study immiscible flow in disordered media. We saturate the circular cell with a high-viscosity silicone oil and displace it with water injected at the center of the cell. We tune the wetting properties of the cells independently using chemical vapor deposition to explore both drainage (a less wetting fluid displacing a more wetting fluid) and imbibition (a more wetting fluid displacing a less wetting fluid). At low capillary numbers (ratio of viscous to capillary forces) in smooth cells, drainage leads to a rather stable displacement front, whereas imbibition leads to a more unstable pattern; this observation is consistent with those of [2], but is currently unexplained and is at odds with the trend observed in glass-bead-filled Hele-Shaw cells [3], in which drainage results in fingers of the size of the pore while imbibition leads to macroscopic fingering patterns. Introducing roughness results in preferential flow paths in drainage due to the permeability and capillary pressure heterogeneity, and leads to contact-line pinning in imbibition, and drastically affects the patterns. At higher capillary numbers, viscous forces become more dominant and suppress the influence of disorder; in this regime, roughness only modulates the patterns. Based on these observations and inspired by Lenormand's phase diagram [4, 5], we propose a phase diagram, whose axis include wettability, capillary number, and effective roughness of the medium. To explain the experimental observations, we build on our earlier modeling efforts on wetting and immiscible displacements [6, 7], and propose a phase-filed model that generalizes Darcy's law by incorporating the chemical potential of the two phases through a thermodynamically consistent free energy. Our model naturally incorporates contact-line dynamics, and captures the essential features of the immiscible flow in a rough fracture.
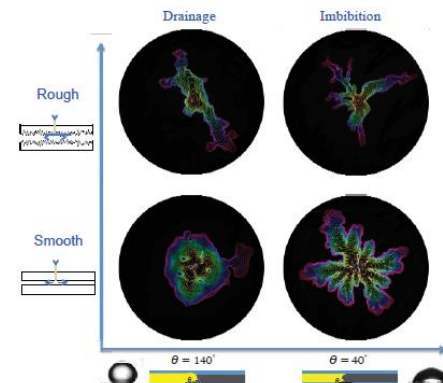
Figure 1: Experimental time-lapse images representing the influence of roughness (top: rough Hele-Shaw cell; bottom: smooth Hele-Shaw cell) and wetting properties (left: drainage; right: imbibition) on viscously unstable fluid-fluid displacement in a radial Hele-Shaw cell (viscosity contrast $M \approx 350$ and capillary number $Ca \approx 0.01$).

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Local Analysis of Single-Phase Flow through Complex Porous Media Using Flow Propagators

Y. Zheng, I. Shikhov, M.N. d'Eurydice, and Christoph Hermann Arns

UNSW Australia, Australia

Introduction

Flow propagators have been frequently used in porous media characterization and to characterize fluid flow within. Scheven et al. [1], Codd et al. [2] and others measured flow propagators in various media and discussed how dispersion or other effects like relaxation and internal gradients affect its shape by changing flow behaviour. In addition, numerical simulations were used by many researchers to match their measurements [3]. However, these works mainly focused on homogeneous media like beads pack and clean sandstones. Heterogeneous cores were also studied by a few groups, but their interpretations lacked quantitative analysis of how pore geometries affect fluid transport which shapes the flow propagators.

In this work we consider the flow propagator as tool to partition disordered materials in terms of the local environment. In particular, we are interested in the connectivity of local regions as well as their individual properties.

Methods

We introduce the concept of a local propagator, which refers to a propagator measured over a short encoding interval such that regions of different character do not significantly couple. In this regime it is assumed that the averaged propagator measured via NMR is the weighted sum of the propagators of the individual regions. At longer dispersion times the local propagators will show effects of mixing before eventually coupling fully.

Here we use bead packs to represent different sample regions. For the analysis we define two different regions of the sample, namely micro- and macro-porous regions. These regions are realised experimentally by 0.5mm diameter beads and 1.5mm diameter beads, respectively. The simulations are carried out with embedded region labels. Dispersion is then modeled using a random walk on top of a velocity field derived with a lattice Boltzmann method [3, 4]. The region labels are used to track individual random walks overtime.

Results

We compare the average propagator accessible via NMR to the simulation results for a range of different dispersion times and Peclet numbers and find good agreement. Given this, we then use the numerical simulations to compose the average propagator into four categories, namely two "pure" propagators which include only averages over the microporous and macro- porous regions, as well as "mixed" propagators capturing the cases of random walks crossing region labels. The measured average propagators are thus decomposed into their respective mixed compartments as function of mixing time. We quantify the effect of this mixing with respect to both the sphere packs considered as well as random media and relate the mixing modes to the level of disorder of the microstructures considered.

Acknowledgement

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16-3: Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale

Time: Friday, 24/Jun/2016: 9:40am - 10:40am – Location: MSB 3154

Modeling Polymer Stabilized Nano-scale Zero Valent Iron Transport Experiments in Variable Aperture Single Fractures

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Mineral Dissolution Rates in Physically and Geochemically Heterogeneous Media

Hang Wen, Li Li, Fatemeh Salehikhoo
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Modeling Polymer Stabilized Nano-scale Zero Valent Iron Transport Experiments in Variable Aperture Single Fractures

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Key words: nano-scale zero valent iron, variable-aperture fractures, modeling transport, polymer stabilization

Introduction

Nano-scale zero valent iron (nZVI) is very small in size (10 to 100 nm) and has high specific surface area (15 to 40 m^2/g). Due to high specific surface area and high redox potential (-0.44V) nZVI can react with a wide variety of groundwater contaminants. Therefore, during the last decade nZVI has received significant attention for application in subsurface remediation, particularly for sites contaminated with chlorinated compounds and heavy metals [1]. However, due to agglomeration to larger size, delivery of nZVI into the contaminated subsurface zones becomes challenging. Polymer coating can stabilize nZVI and can enhance the mobility of the iron particles in the subsurface. The objective of this study was to develop the understanding of polymer stabilized nZVI transport in fractured rock through modeling of lab scale transport experiments.

Materials and Methods

Rock and Glass Fractures: The glass-replica fracture (0.28 m x 0.21 m) was prepared by creating molds with melted glass on two opposing sides of a fractured slate rock. Similar size fractured dolomite rock block was prepared by artificially inducing fracture along a stylolite. Fracture aperture distribution was measured by a 3D optical scanning technique using ATOS II. **Tests:** Transport experiments were conducted in the glass-replica and dolomite fracture under water saturated condition to identify the effects of water specific discharge and carboxymethyl cellulose polymer (CMC) concentration on nZVI transport. Lissamine Green B (LGB) dye was used as a nonreactive tracer. The LGB dye and nZVI movements in the glass fracture were monitored using time-lapsed images captured using a light source and a dark box. **Modeling Transport:** LGB, CMC, and nZVI transport was modeled using a 3D multiphase flow and transport model, Compsim [2] considering LGB and CMC as solutes, and nZVI as a colloid. Variable viscosity was considered in modeling CMC transport. The permeability field of the fractures were calculated from the measured aperture field data.

Results and Discussion

Lower LGB recovery in the rock fracture compared to the glass fracture indicated the effects of diffusion into the rock matrix. CMC recovery was high (> 95%) in both fractures, indicating lower attachment and lower diffusion in the fractures. However, CMC caused change in the hydraulics in the fractures and caused preferential flow paths for the flushing water [*Figure 1*]. This also caused increased tailing in LGB transport. Mass recovery of nZVI was significantly lower (< 60%) due to attachment on the fracture surfaces and surface cavities. Higher specific discharge resulted in higher nZVI and LGB recovery and peak concentrations. The modeling results of LGB, CMC, and nZVI breakthrough curves and the movements in the glass fracture matched well with the experimental observations. nZVI attachment coefficient was estimated in the modeling. This estimated attachment coefficient can be used to predict CMC stabilized nZVI movement in variable aperture single fractures.
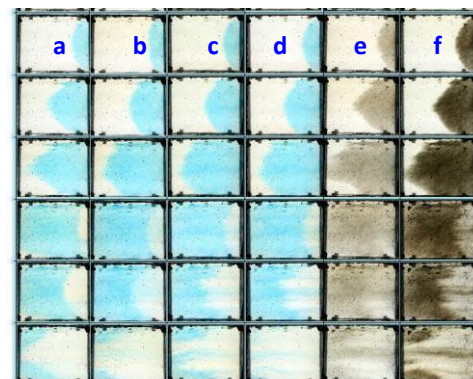

Figure 1: Visualization of LGB (a), CMC-LGB (b, c & d), and CMC-nZVI (e & f) movements in glass fracture at different times in transport experiments.

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Mineral Dissolution Rates in Physically and Geochemically Heterogeneous Media

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Key words: mineral dissolution; heterogeneity; geostatistic; reactive transport, residence time

Introduction

Mineral dissolution plays a critical role in earth system formation and functioning. Mineral dissolution rates measured in field studies have been reported to be orders of magnitude lower than those measured under well-mixed batch reactors. Our column experiments have shown that spatial patterns of magnesite control preferential flow paths and the effectively-dissolving mineral surface area, therefore contributing to the rate discrepancy[1-3]. Our work on chromium sorption experiments has demonstrated that connectivity of porous media, largely determined by the spatial distribution of clay, governs the rate and capacity of chromium sorption[4].

Results and discussion

To extend our experimental work, here we applied reactive transport modeling to understand the dependence of magnesite dissolution rates on spatial heterogeneities. Multiple realizations of heterogeneous hydraulic conductivity distributions were generated using the Gaussian sequential simulation method. The realizations differ in hydraulic conductivity variance, correlation length in the longitudinal direction, and length scale of the simulation domain. We found that large variance and correlation lengths results in smaller magnesite dissolution rates. Sensitivity analysis indicated that this dependence is highly related to the length scale and flow velocity, which can be organized into a dimensionless residence time ($\tau_D = \tau_r/\tau_t$, the ratio of fluid residence time in the magnesite zones τ_r versus overall residence time through the domain τ_t). There exists a critical τ_D below which the heterogeneity effects are negligible due to reaching equilibrium. Above the critical value, magnesite dissolution rates increase with increasing τ_D values. From the output of 1000 simulations with different characteristics of spatial heterogeneities under different flow velocity and domain length conditions, we derived a general equation that quantifies the rates in heterogeneous media in the form of

$$R_{magnesite}(mol/m^2/s) = R_{homo} \cdot \beta = R_{homo}\left[1 - \exp\left[-\frac{n \cdot \tau_t}{\tau_r}\right]\right]^m,$$

Where R_{homo} is the dissolution rate at the equivalent homogeneous domain; β is the rate ratio between the rates in the heterogeneous and equivalent homogeneous porous media, essentially a scaling factor of spatial heterogeneity, and n and m are constants related to the flow velocity and hydraulic conductivity variance.
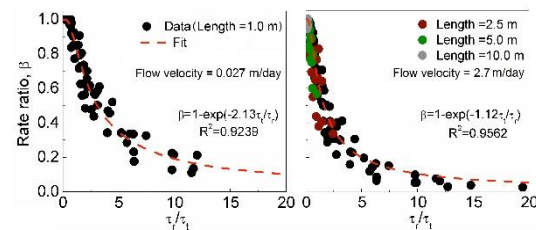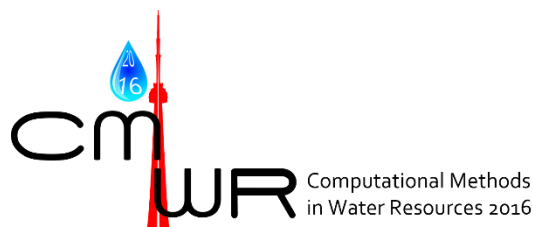

Figure 1. Ratio of the magnesite dissolution rates in heterogeneous media (variance = 6 but different correlation length) versus the equivalent homogeneous media, β, as a function of τ_D (τ_r/τ_t). Other realizations (e.g. variance = 0.5 and 2) have similar trends, following the general equation.

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16-4: Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale

Time: Friday, 24/Jun/2016: 11:00am - 12:20pm – Location: MSB 3154

DNAPL Modeling with Permeabilities Obtained by Geostatistical Inverse Modeling: How Much Detail Is Enough?

Amalia Kokkinaki, Jonghyun Lee, Peter K Kitanidis, Brent E Sleep, Hongkyu Yoon, Charles J Werth, Albert J Valocchi, Stanford University, United States of Americ; amaliak@stanford.edu

Modeling Contaminant Plumes in Fractured Limestone in 3-D: Comparison of Modeling Approaches

Klaus Mosthaf, Mette M. Broholm, Poul L. Bjerg, Annika S. Fjordbøge, Philip J. Binning

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A Benchmark Laboratory Experiment for Saltwater Intrusion in Coastal Aquifers

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A Novel Optical Method for Quantifying Geological Properties of Oil Shale across Scales

Yashar Mehmani[1], Alan Burnham[1], Michael Vanden Berg[2], Francois Gelin[3], Hamdi Tchelepi[1]

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DNAPL Modeling with Permeabilities Obtained by Geostatistical Inverse Modeling: How Much Detail is Enough?

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Key words: DNAPL modeling, dissolution, inversion, uncertainty

Abstract

Prediction of DNAPL fate, in terms of source depletion and dissolved plume generation, is highly uncertain and is believed to strongly depend on accurate knowledge of domain heterogeneity and source zone architecture. Given inherent and unavoidable limitations on how much detail can be obtained by characterization efforts, it would be useful to know how much detail is needed to obtain meaningful DNAPL predictions for management and remediation efforts. With this knowledge, we can set appropriate expectations for characterization, and better design data collection for inverse modeling.

In this work, a DNAPL infiltration and dissolution experiment conducted in a $21.5 \times 9 \times 8.5$ cm flowcell packed with 1 cm cubes of different sand types is simulated with a previously validated multiphase model [1, 2]. This benchmark is unique because it included a well-controlled DNAPL release of known volume and because it provided a rich, high resolution experimental dataset of MRI-derived tracer concentrations that can be used for permeability estimation, and a rich dataset of DNAPL saturations and dissolved concentrations obtained at regular intervals through the course of the DNAPL experiment.

We perform forward simulations of the DNAPL experiment using permeabilities obtained through a highly parameterized geostatistical inversion of the tracer test conducted in the flowcell [3, 4]. We examine the effect of the inversion results on the predictions of the multiphase model for DNAPL fate, specifically looking at the impact of the quantity and density of conditioning data for inversion of the tracer test. We perform the inversion using the entire, high resolution tracer test dataset and using subsets of this dataset, and then evaluate the impact of using the inverted permeabilities in DNAPL simulations. We also investigate whether small scale features of permeability that cannot be detected by inverse modeling have a big effect on the predicted DNAPL behavior. Based on these results, we discuss the necessity and scope of characterization efforts for modeling DNAPL source zones, and implications for optimizing data sampling design and source zone identification. Finally, we investigate which metrics (e.g. time to % mass depletion, mass flux, dissolved concentration etc.) can be expected to have less uncertainty, information that can be useful in setting remediation objectives for DNAPL source zones.

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Modeling Contaminant Plumes in Fractured Limestone in 3-D: Comparison of Modeling Approaches

Klaus Mosthaf, Annika S. Fjordbøge, Mette M. Broholm, Poul L. Bjerg and Philip J. Binning
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Key words: contaminant transport, fractures, limestone

Understanding the fate and transport of contaminant plumes from contaminated sites in limestone aquifers is important because they are a major drinking water resource. This is challenging because they are often heavily fractured and contain chert layers and nodules, resulting in a complex transport behavior. Several modeling approaches have been developed to describe contaminant transport in fractured media, such as discrete fracture, equivalent porous media, and dual continuum models. However, these modeling concepts are not well tested for contaminant plume migration in real limestone geologies. Our goal is to develop and evaluate approaches for modeling the transport of dissolved contaminant plumes in fractured limestone aquifers in 3D and to determine the required flow and transport parameters.

Several fracture flow and transport models of different complexity are available. These include the established approaches of the equivalent porous medium model, discrete fracture model and dual continuum model. In addition to these, we present a new nested modelling approach, where a discrete- fracture model is embedded in an equivalent porous medium model to reduce computational efforts while accounting for the interplay between fractures and matrix. We also test a new hybrid dual porosity – discrete fracture model that resolves major flow features as discrete fractures and describes smaller-scale fractures and fissures as a matrix with the dual porosity approach.

The models were compared for a contaminated site in Denmark, where a plume of dissolved PCE has migrated through a fractured limestone aquifer. Field data includes information on spill history, distribution of the contaminant (multilevel sampling), geology and hydrogeology. To describe the geology and fracture system, data from borehole logs, packer tests, optical televiewers and cores was combined with an analysis of local heterogeneities and data from analogue sites. A pump and tracer test with contaminant sampling was performed at the site to determine flow and transport parameters of the fractures and matrix and to quantify the contaminant distribution in the aquifer.

The models were evaluated by examining their ability to describe the collected field data. Model parameters were determined using the shuffled complex evolution algorithm to optimize model fit. Fitting diagnostics were examined to determine parameter identifiability and to evaluate the appropriate level of model complexity.

The comparison with data showed that the models have substantially different representations of the contaminant behavior, with different consequences for evaluation of contaminant risk and potential remediation strategies. On the plume scale, the equivalent porous medium model and the dual- porosity model can reproduce the main transport features. However, small scale fracture-matrix interaction, such as diffusion of contaminant into the matrix, cannot be represented with an equivalent- porous medium model and require a more complex model. The paper concludes with recommendations on how to identify a suitable modeling approach for simulation of contaminant plumes.
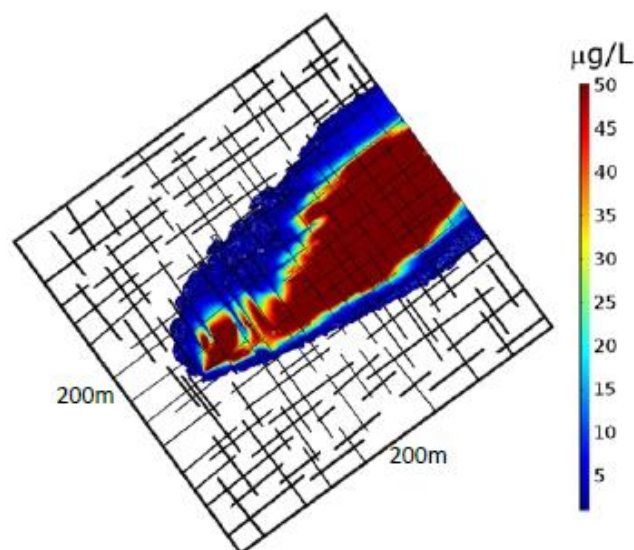

Figure 1: Dissolved PCE plume propagation in a fractured limestone using a 3D discrete-fracture model.

A Benchmark Laboratory Experiment for Saltwater Intrusion in Coastal Aquifers

Elena Crestani, Matteo Camporese, Paolo Salandin

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Key words: saltwater intrusion, laboratory experiment, benchmark

Introduction

Saline intrusion is a worldwide problem of increasing concern, due to overexploitation of coastal aquifers, rising sea levels, and climate changes. This issue can heavily affect the quality of both surface water and groundwater in coastal areas; therefore, many research projects and studies have been developed in recent years to identify possible countermeasures, mainly consisting of underground barriers.

Physical scale models are fundamental tools to study saltwater intrusion, as they can provide benchmarks for numerical model calibration and validation and allow the evaluation of efficient solutions to mitigate the salt wedge.

In this work, a benchmark laboratory experiment for the problem of saltwater intrusion in coastal aquifers is described, where the process is reproduced in a specifically designed sand-box, monitored by means of Electrical Resistivity Tomography (ERT), and numerically modeled.

Laboratory Experiment

A physical scale model has been built at the University of Padova to represent the terminal part of a coastal aquifer. The main purposes of the device are to study and describe the evolution of the salt wedge, the efficiency of underground barriers, and the minimum distance from the coast of a withdrawal that guarantees a continuous supply of freshwater. The model consists of a laboratory flume 500 cm long, 30 cm wide and 60 cm high, filled with a 48 cm-thick layer of glass beads, characterized by a d50 of 0.6 mm and a uniformity coefficient $d_{60}/d_{10} = 1.5$. The material is homogeneous, with porosity of about 0.37 and hydraulic conductivity of about 1.3×10^{-3} m/s. Upstream from the sand-box, a tank filled by freshwater provides the recharge to the aquifer. The downstream tank simulates the sea and red food dye is added to the saltwater to easily visualize the salt wedge. The volume of the downstream tank is about five times the upstream one, so that salt concentration variations (i.e., water density variations) due to the incoming freshwater flow are negligible. The water level in the two tanks is kept fixed during the tests ensuring a constant gradient and flow rate.

The saltwater wedge evolution is monitored during the experiments by means of photos collected with regular frequency and ERT. The experimental results are further validated with numerical simulations performed by the SUTRA model [1]. Figure 1 compares the photograph, electrical resistivity image, and numerical results referring to the same time, i.e., 20 h from the start of the experiment.
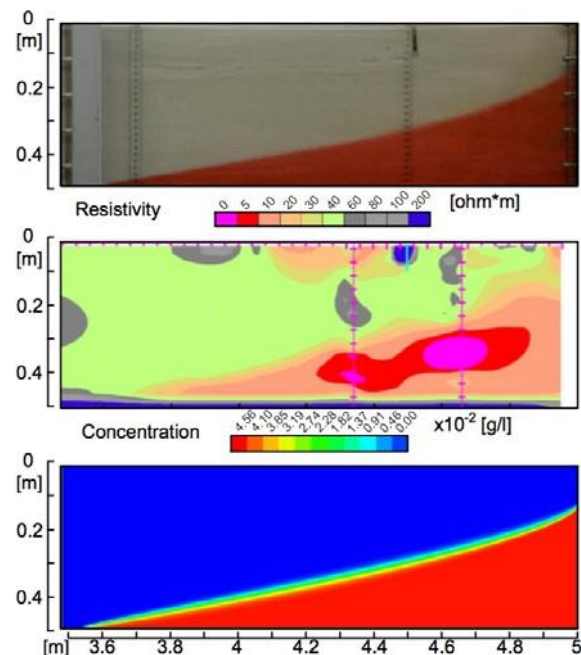

Figure 1: Saltwater wedge evolution at time 20 h: top) photograph, middle) electrical resistivity image and bottom) numerical model results.

Reference

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A Novel Optical Method for Quantifying Geological Properties of Oil Shale across Scales

Yashar Mehmani[1], Alan Burnham[1], Michael Vanden Berg[2], Francois Gelin[3], Hamdi Tchelepi[1]

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Key words: oil shale, kerogen, optics, spectroscopy, multiscale

This contribution introduces a simple approach for mapping the spatial distribution of kerogen content in oil shales, from scales of a few microns to hundreds of feet, using optical photographs. The method has been successfully and extensively validated for the immature oil shale deposits of the Green River Formation, in the United States. Implications for simulation and modeling studies of e.g. in-situ retort processes are substantial since most thermo- mechanical properties of oil shale formations are strong functions of kerogen content. Furthermore, the deterministic information obtained from this method can be cast into a statistical description that can be used in the lack of measurements. While our optical approach is not expected to easily extend to formations with high concentrations of "interfering minerals" such as clay and iron oxides, it introduces a new way for tackling multiscale characterization and modeling problems of source rock formations. A promising generalization of the method, based on near-infrared (NIR) spectroscopy, to problematic formations with interfering minerals is also discussed.
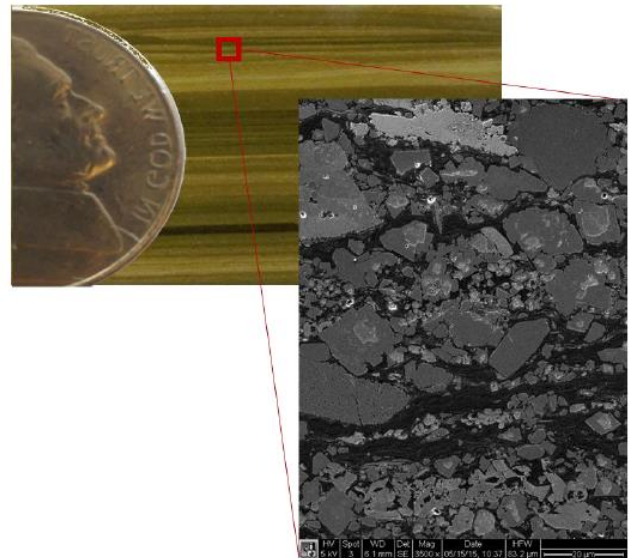

Figure 1: Depiction of a Green River oil shale sample (the nickel if for scale; ~2cm diameter), and a zoomed-in view of the microstructure shown by the SE-SEM image.

16-5: Advances in Experimental Techniques, Validation of Modelling Tools and Uncertainty in Predictions from Pore to Field Scale

Time: Friday, 24/Jun/2016: 2:30pm - 4:10pm – Location: MSB 3154

Wettability Control on Fluid-Fluid Displacements In Porous Media: Patterned Microfluidic Experiments And Dynamic Pore-Scale Model

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Multiple Scale Field Experiment to Determine Parameter Values for Modeling Water Transport in Unsaturated Soils

Annette Dathe[1], Matthew Petterson[2], Attila Nemes[1], Daniel Gimenez[2], Johannes Koestel[3], Mingming Qin[2], Helen K. French[4,1], Esther Bloem[1], Perrine M. Fernandez[4,1], Nicholas Jarvis[3]

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Immiscible Two-Phase Darcy Flow Model Accounting For Vanishing and Discontinuous Capillary Pressure: Application to The Flow in Fractured Porous Media

Kontantin Brenner[1,2], Mayya Groza[1,2], Roland Masson[1,2], Jeanne Pellerin[3]

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Simulating Infiltration of TCE and Water in Unsaturated, Discretely-Fractured, Porous Rock

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Wettability Control on Fluid-Fluid Displacements in Porous Media: Patterned Microfluidic Experiments and Dynamic Pore-Scale Model

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Key words: wettability, multiphase flow, microfluidics, pore-scale model

Abstract

Two-phase flow in porous media is important in many natural and industrial processes like geologic CO_2 sequestration, enhanced oil recovery, and water infiltration in soil. While it is well known that the wetting properties of porous media can vary drastically depending on the type of media and the pore fluids, the effect of wettability on fluid displacement continues to challenge our microscopic and macroscopic descriptions.

Here we conduct two-phase flow experiments via radial displacement of viscous silicone oil by water in planar microfluidic cells patterned with vertical posts. This model system approximates a porous medium by introducing microstructures, while allowing precise control over pore geometries and detailed visualization of the flow. In our system, the surface energy of the microfluidic cell can be tuned over a wide range of contact angles, allowing us to access different wettability conditions. In particular, we are able to achieve stable contact angles of $\theta = 150°$ (strong drainage), $\theta = 120°$ (weak drainage), $\theta = 90°$ (neutral), $\theta = 60°$ (weak imbibition), and $\theta = 7°$ (strong imbibition). In our experiments, we dye the injected water to characterize, via a calibration curve, the gap-averaged water saturation at high spatial and temporal resolution.

In drainage, we observe the classical capillary- number-dependent transition from capillary fingering to viscous fingering. In addition, the pore-scale displacement of the viscous silicone oil becomes incomplete as capillary number increases. In weak imbibition, we observe apparent stabilization of emerging flow instabilities, as a result of cooperative invasion at the pore scale. In strong imbibition, we find that the flow behavior is dominated by corner flow that connects the surface of neighboring posts via pendular rings. This process allows the injected water to propagate without filling the pore bodies.

Inspired by our experimental findings, we develop a pore-scale model for fluid-fluid displacement in porous media that captures the dynamic pressure redistribution and the wettability-controlled interface readjustments at the invasion front.
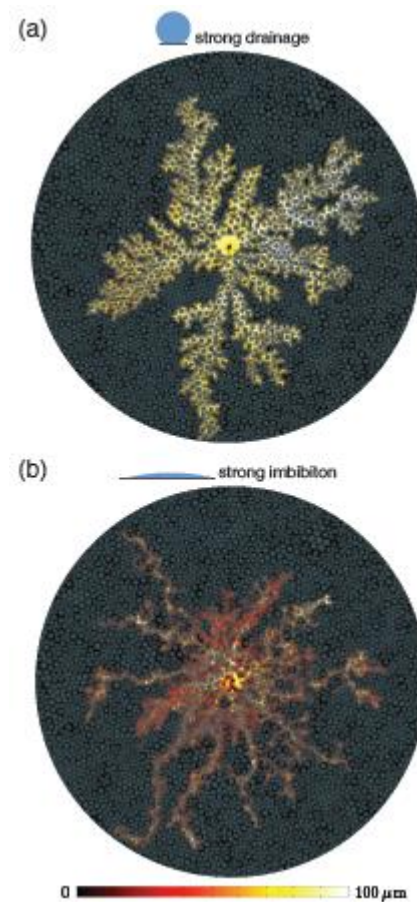
Figure 1: Experimental image of water displacing a viscous silicone oil in (a) strong drainage ($\theta = 120°$) and (b) strong imbibition ($\theta = 7°$) at Ca $= 3.69 \times 10^{-2}$. The colormap indicates the gap-averaged thickness of the invaded water.

Multiple Scale Field Experiment to Determine Parameter Values for Modeling Water Transport in Unsaturated Soils

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Key words: water transport, unsaturated porous media, parameter estimation

Introduction

Main challenges for modelling water transport in unsaturated soils are 1) the commonly used Richards equation is non-linear; 2) the conductivity term is a function of water content (or of the matrix potential); 3) a relation between soil water content and matrix potential has to be determined in order to solve the equation; and 4) processes like preferential water flow through macropores cannot be described with the simple Richards equation.

Saturated soil water conductivity Ksat can be measured in the field or in the laboratory. Soil-water retention can also be obtained experimentally or by applying pedo-transfer functions, which for example take grain size distribution and carbon content into account. Experimental measures of these properties are – strictly speaking – only true for the sample size they were derived from, while the underlying soil structure can vary considerable at different scales.

Experimental Setup

In the newly established SoilSpace project, we combine measurement tools from different disciplines in an attempt to quantify the heterogeneity of soil structure. A field experiment was set up on an agricultural field in southern Norway in a clayey soil (Stagnosol) with high macroporosity. The subsurface was initially investigated using electrical resistivity (ERT) on a 24 x 11 meter plot with 0.5 m spacing of the electrodes. Soil compaction caused by tire tracks was clearly visible from the ERT data and a 4.7 x 1 meter grid with 0.1 m electrode spacing containing this compaction and other features was chosen within the larger grid. Inside the smaller grid, a 2 x 1 x 0.8 meter (length x width x depth) intensively investigated soil volume (IISV) was instrumented with TDR (time domain reflectometry) probes and tensiometers to measure soil water content and hydraulic potential. After about two months, the probes were de-installed and more than 100 undisturbed soil samples were taken from different depths to determine Ksat and soil water retention, among other properties. From a chosen subset of these samples, we will directly quantify the spatial arrangement of soil pores using computer tomography (CT) scanning and image processing tools.
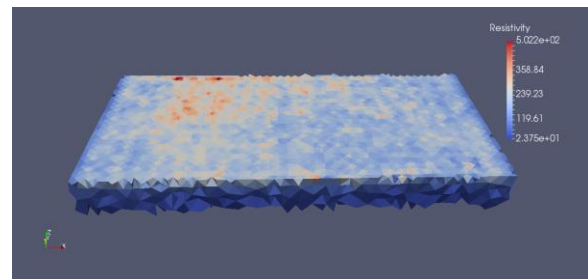

Figure 1: Resistivity values obtained for the large grid of 24 x 11 m. The small grid and the IISV are situated in the upper left third of the main area.

Outlook

This is ongoing work, and the results will guide in setting up a 3D model with distinguished volumes of changing soil water characteristics. We will compare the results obtained with different measurement tools and intend to develop methods for scaling up the information gained by CT to the IISV to the larger grid of 24 x 11 meter.

Immiscible Two-Phase Darcy Flow Model Accounting For Vanishing and Discontinuous Capillary Pressure: Application to the Flow in Fractured Porous Media

Konstantin Brenner[1,2], Mayya Groza[1,2], Roland Masson[1,2] and Jeanne Pellerin[3]

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Key words: Two-phase Darcy flow, vanishing capillary pressure, discontinuous capillary pressure, fractured porous media

In the framework of two-phase flows in fractured porous media, high contrasts of capillary pressures are expected at the interfaces between the matrix and the fractures. In addition the capillary pressure in the fracture network often can be neglected or assumed to be constant. The traditional approaches fail to cope with both of those difficulties. In particular the two-pressure formulation allows to deal with saturation jumps caused by the different entry pressures. In fact it can be used with general strictly monotone capillary curves, however it breaks down if the capillary pressure doesn't depend on saturation. On the other hand the pressure-saturation formulation is known to be more robust especially when dealing with vanishing capillary pressure. Unfortunately there is no way to extend it to the discontinuous capillary pressure case since the saturation jump is not in general a function of the saturations at both sides of the interface.

We propose an elegant mathematical formulation of two-phase flow in heterogeneous porous media, which bridges the gap between the two above mentioned approaches. It utilizes a single primary variable choice and doesn't relies on any variable switch or regularization techniques. This framework applies to general monotone capillary pressure curves and handles the saturation jumps at rock type interfaces (e.g. see Figure 1). It is also equivalent to phase-pressure or pressure saturation formulations as soon as one of those can be applied.

The new formulation is extended to the water gas two-phase flow in fractured porous media for which the fractures are modeled as interfaces of dimension one. The pressure is assumed to be continuous at the matrix-fracture interface corresponding to the case of conductive fracture network. The problem is discretized using an extension of the Vertex Approximate Gradient scheme to the case of hybrid dimensional Darcy flow models previously developed in [1]. Similarly to the two-pressure formulation, the new approach requires only two unknowns by degree of freedom. We illustrate it by several numerical experiments based on tight gas test case proposed in [2].
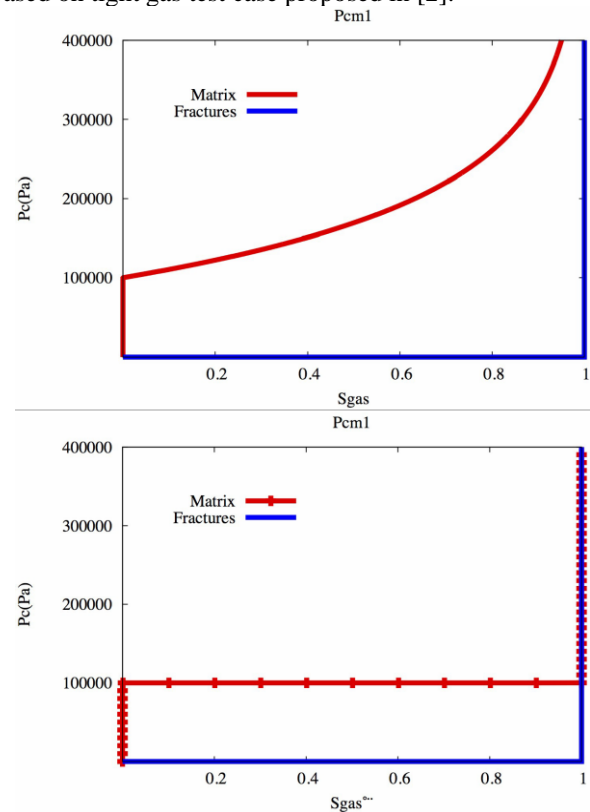

Figure 1: Possible form of capillary pressure curves in the matrix and the fracture network.

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Simulating Infiltration of TCE and Water in Unsaturated, Discretely-Fractured, Porous Rock

Kenneth M Walton[1], Andre JA Unger[2], Marios A Ioannidis[2], Beth L Parker[1]

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Key words: numerical model, multiphase flow, discrete fracture

Numerical simulation of flow of two or three mutually interactive phases is a standing challenge for model developers and practitioners. Applying such flow models in the context of fractured rock, an extreme case of heterogeneity, further increases the complexity of the problem. Depending on the rigour of the coupling of flow and transport equations and the geometric description of the domain, problems such as these quickly become intractable, or at best computationally burdensome.

In this presentation we introduce the Santa Susana Field Lab (SSFL) site, discuss key model parameters, and describe recent innovations in the discrete fracture-matrix numerical model CompFlow that permit us to examine such scenarios. Innovations include unstructured meshing techniques using node bisection local to fracture planes and asperity contact- bridged flow.

Conceptual Model

The SSFL is a former rocket engine research facility located on a topographic high near Los Angeles, California. It is underlain by fractured sandstone bedrock. Decades ago, TCE was released to the ground surface following engine tests. This is the real-world context for the following conceptual scenario: dense, non-aqueous phase liquid (DNAPL) contaminant migrates from the ground surface through the vadose zone and below the water table; a dissolved contaminant plume forms and is transported away from the source area. Relevant processes include three-phase flow, saturation dependent relative permeability and capillary pressure, equilibrium phase partitioning, and conservative tracer transport.

Numerical modeling focuses on the evolution of the architecture of the DNAPL source zone in the rock matrix and fracture network.

Numerical simulations

As a demonstration of the numerical model's capabilities, we present the results of several simulations (e.g. Figure 1). We discuss trade-offs in domain size and fracture network density. Smaller domains (~10 metres) permit three-phase simulations in 2D and 3D; larger domains (~100 metres) are possible in 3D with two phases and a more sparse fracture network.
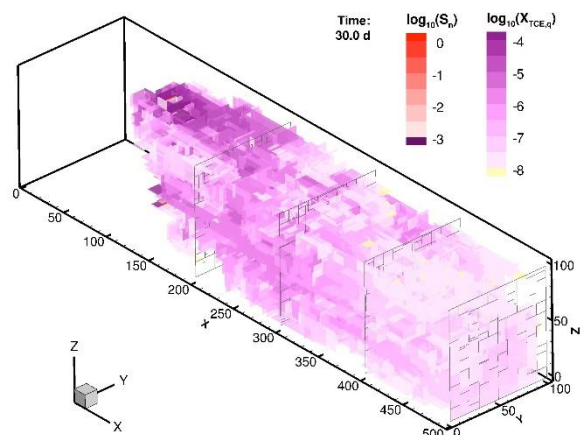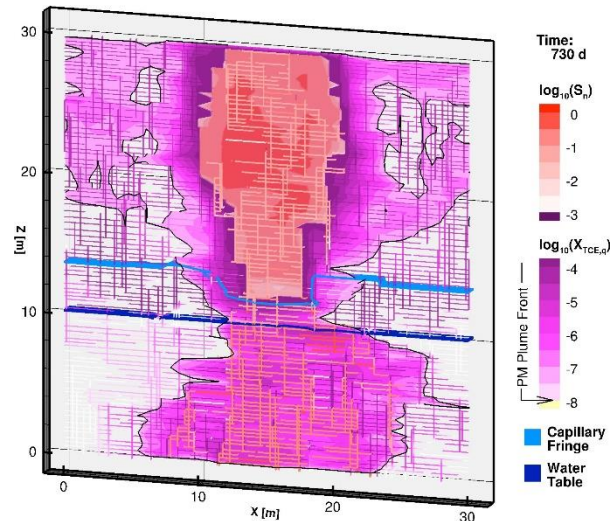

Figure 1: DNAPL saturation and dissolved mole fraction of TCE in discrete fractures and porous rock. Top: 30x30m 2D domain with 890 fractures. Bottom: 500x100x100m 3D domain with 2053 fractures.

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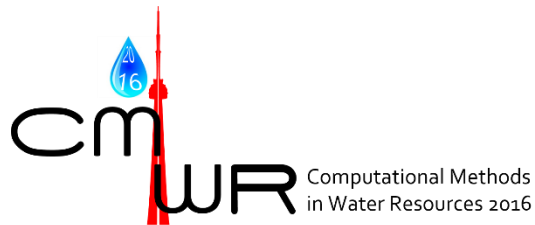
17-1: Data Assimilation in Water Resources Modelling

Time: Friday, 24/Jun/2016: 9:40am - 10:40am – Location: MSB 2170

Assimilation of Soil Moisture Data With The Integrated Terrestrial System Modeling Platform Terrsysmp at The Catchment Scale

Wolfgang Kurtz[1,2], **Mauro Sulis**[3], **Prabhakar Shrestha**[3], **Guowei He**[1,2], **Stefan Kollet**[1,2], **Harry Vereecken**[1,2], **Harrie-Jan Hendricks Franssen**[1,2]

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Assimilation of Soil Moisture Data with the Integrated Terrestrial System Modeling Platform Terrsysmp at the Catchment Scale

Wolfgang Kurtz[1,2], Mauro Sulis[3], Prabhakar Shrestha[3], Guowei He[1,2], Stefan Kollet[1,2], Harry Vereecken[1,2], Harrie-Jan Hendricks Franssen[1,2]

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Key words: Integrated modeling, Data assimilation, Soil moisture, Ensemble Kalman Filter, Uncertainty, High-performance computing

Abstract

Various studies have already shown that subsurface hydrology can have a profound influence on the estimation of land surface fluxes and the evolution of the atmospheric boundary layer [1, 2, 3]. Such dynamic feedbacks can be taken into account by the application of integrated terrestrial modeling platforms which combine different compartment models for the subsurface, the land surface and the atmosphere and therefore allow a better physical repressentation of processes across compartments. However, model predictions with such highly sophisticated models are generally prone to uncertainties regarding the model input variables, like subsurface parameters, meteorological input variables or vegetation parameters. In this respect, data assimilation techniques can help to better constrain the model predictions and parameters and the associated uncertainties by merging the uncertain model predictions with field observations of the modelled quantities. In this study, we perform data assimilation experiments with the integrated modeling platform TerrSysMP [2] consisting of individual component models for variably saturated subsurface flow (ParFlow), land surface processes (CLM3.5) and the atmosphere (COSMO). The component models are dynamically linked by the exchange of state variables and fluxes with the coupling software OASIS-MCT in a scale-consistent, modular manner. In a first step, we constructed a data assimilation framework for the land surface-subsurface part of TerrSysMP (CLM3.5 and ParFlow) by linking TerrSysMP with the PDAF (Parallel Data Assimilation Framework) software [4, 5]. The data assimilation framework uses a memory based communication between model and data assimilation routines and avoids frequent reinitializations of the model and is thus highly scalable and applicable to high-resolution hydrological models. The data assimilation system is also modular with respect to the model combination used in the forward simulations.

Data assimilation experiments are performed with a regional-scale hydrological model of the Rur catchment (TERENO/TR32-monitoring site, Germany). Soil moisture data from up to nine cosmiray stations are available for assimilation within this region. The effectiveness of the assimilation of these soil moisture observations is compared with respect to the chosen forward model (CLM versus CLM-ParFlow) in order to gain more insight into the role of the groundwater component on the assimilation results. Furthermore, the influence of subsurface parameterization on the assimilation results is investigated by using different subsurface parameter sets derived from soil maps of different data quality (regional versus local data sources). It could be shown that soil moisture characterization improved for both forward models but that the model dynamics are quite different. Differences in the initial subsurface parameterization were adapted by a joint update of model states and parameters.

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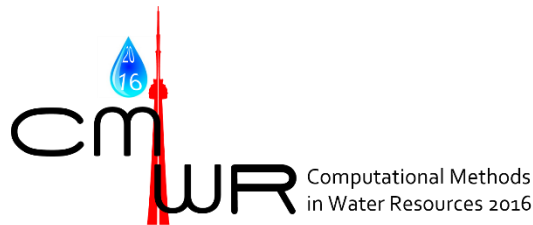
17-2: Data Assimilation in Water Resources Modelling

Time: Friday, 24/Jun/2016: 11:00am - 12:20pm – Location: MSB 2170

Land Subsidence Assimilation by a Generalized Polynomial Chaos Expansion-Based Ensemble Smoother

Claudia Zoccarato[1], Massimiliano Ferronato[1], Noemi Friedman[2], Pietro Teatini[1], Elmar Zander[2]

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Comparison of Eight Different Enkf Variants for Subsurface Data Assimilation: How to Achieve Sound Conclusions?

Johannes Keller[1], Harrie-Jan Hendricks-Franssen[1], Gabriele Marquardt[2]
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Recent Advances in Hydrologic Data Assimilation

Tara Razavi, Paulin Coulibaly

McMaster University, Canada; razaviz@mcmaster.ca

Multivariate Hydrological Data Assimilation on a Catchment Scale

Marc-Etienne Ridler[1], Henrik Madsen[1], Donghua Zhang[2], Karsten H. Jensen[2], Jens C Refsgaard[3]

[1]DHI, Denmark; [2]University of Copenhagen, Denmark; [3]Geological Survey of Denmark and Greenland, Denmark; mer@dhigroup.com

Land Subsidence Assimilation by a Generalized Polynomial Chaos Expansion-Based Ensemble Smoother

Claudia Zoccarato[1], Massimiliano Ferronato[1], Noemi Friedman[2], Pietro Teatini[1], Elmar Zander[2]

[1]University of Padova, Italy; [2]Technische Universität Braunschweig, Germany

Introduction

Numerical modeling of anthropogenic land subsidence due to the exploitation of subsurface resources is of major interest to avoid significant environmental impacts on the ground surface. The reliability of the predictions depends on the different sources of uncertainty introduced into the modeling procedure. In this study, the focus is on the reduction of the model parameter uncertainty via assimilation of land surface displacements. In particular, a test case application on a deep hydrocarbon reservoir is considered. The land settlements are predicted with the aid of a 3D Finite Element (FE) model [1] using a one-way coupled approach. The calibration focuses on the vertical uniaxial compressibility, c_M, which mostly controls the compaction of the rock formation caused by pressure depletion. Due to the geological compartmentalization of the reservoir into several blocks confined by sealing faults, cM is assumed to vary both with the vertical effective stress and within the horizontal plane [2].

gPCE-based Ensemble Smoother

The Ensemble Smoother (ES) as data assimilation technique can be easily implemented for parameter estimation problems. However, its convergence is guaranteed only with a large number of Monte Carlo simulations, which can be highly demanding from the computational viewpoint in large scale and complex systems. In this work, a meta-model is first built by using the generalized Polynomial Chaos Expansion (gPCE). Then, the ES is employed by sampling the ensemble members from the gPCE expansion. Because of the high computational cost of the forward model, the gPCE technique can be efficiently employed only with few random variables. Thus the discretization of the compressibility field is first achieved via the Karhunen-Loéve expansion (KLE). Figure 1 shows the first L=11 eigenfunctions from the KLE of the random field assuming a Matern function to describe the field covariance. The

proposed methodology is expected to reduce the overall computational cost of the original ES formulation and enhance the accuracy of the assimilation for parameter estimation. In fact, large ensembles can be sampled virtually at no additional cost, thus significantly reducing the associated errors [3].
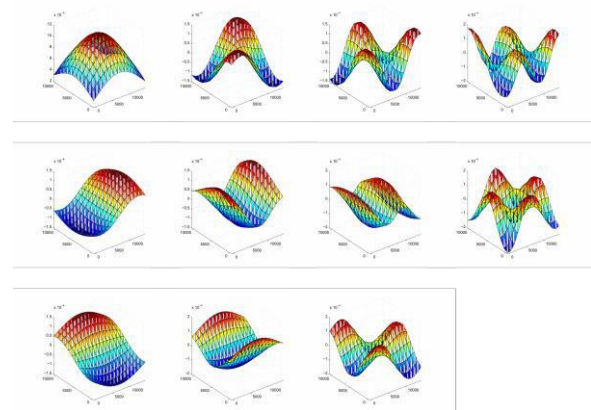

Figure 1: Eigenfunctions from the KLE expansion truncated at 11 terms.

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Comparison of Eight Different Enkf Variants for Subsurface Data Assimilation: How to Achieve Sound Conclusions?

Johannes Keller[1], Harrie-Jan Hendricks-Franssen[1], Gabriele Marquardt[2]

[1]Forschungszentrum Julich GmbH, Germany; [2]RWTH Aachen, Germany

Key words: data assimilation, EnKF, joint state-parameter estimation, comparison study

Introduction

Hydrological modelling involving the subsurface is affected by considerable uncertainty primarily related to large spatial variability of hydraulic conductivity and few measurement data. Sequential data assimilation offers an efficient methodology to estimate unknown subsurface parameters. However, it is also known that methods like the Ensemble Kalman Filter (EnKF) perform only optimal for Gaussian distributed states and parameters and extremely large ensemble sizes. Therefore, in the data assimilation literature different alternatives for the EnKF were formulated, like for example iterative filters. In the literature, many papers find that such alternative methods outperform the classical EnKF.

Study set-up

In this work we compared for a synthetic case eight different variants of EnKF: the classical approach, EnKF including dampening, EnKF including localization, the dual EnKF, the normal-score EnKF, an iterative approach, the Ensemble square root filter and finally a hybrid variant of classical EnKF and optimal interpolation. These variants should reduce problems with non-Gaussian distributions, non- linearity and small sample sizes. The synthetic case involved a groundwater flow and solute transport problem with the injection of a tracer.

The eight different methods were compared for six different ensemble sizes (50, 100, 250, 500, 1000 and 2000 ensemble members). In addition, each experiment was repeated 100 times, resulting in total in 4,800 data assimilation experiments.

Results and Conclusions

One main conclusion from the experiments is that the comparison of data assimilation methods on the basis of a single experiment, even if based on large ensemble sizes, is highly affected by sampling fluctuations. The study quantifies the risks that erroneously one method is considered to be better than another method.

This erroneous ranking of data assimilation methods is analyzed as function of the number of ensemble members in a study and as function of the number of synthetic studies.

Another main conclusion was that for larger ensemble sizes only few methods slightly outperform classical EnKF. For small ensemble sizes, classical EnKF is outperformed by most methods, and some methods show even a much better performance than classical EnKF.

Recent Advances in Hydrologic Data Assimilation

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Key words: Hydrologic Modeling, Data Assimilation

Data assimilation (DA), optimally merges information from model simulations and observations with appropriate uncertainty modeling. DA can account for various types of uncertainty involved in the prediction process including errors in model state variables and hydrometeorologic forcing data. Data assimilation techniques, assimilate the observations and remotely sensed retrievals of various quantities such as river flows, soil moisture, snow-covered area and snow water equivalent, surface water elevation, and land surface temperature to update hydrologic models state variables such as soil moisture content and routing storage as well as model parameters.

DA techniques can be broadly categorized into two major categories of sequential and variational approaches. Variational approach is a deterministic technique that minimizes the cost function of model performance to find the best model state estimates, while the sequential approach provide a stochastic forecast after updating the model states. Kalman and Particle filtering and their variations are among the sequential hydrologic DA techniques. Numerous research studies have proved the considerable potential of DA for improved hydrologic predictions in terms of both prediction accuracy and quantifying uncertainty.

In this study, we have reviewed the recent advances in hydrologic data assimilation with the focus on the recent studies in 2010-2015. In our review, the most common challenges in hydrologic data assimilation along with the proposed solutions are discussed. Among these challenges are the application of hydrologic DA in improved operational forecast systems, combining the strengths of DA and multi- model ensembles, the issue of time lag between the errors in model states and predicted discharge, DA application in improved flood forecasting with short lead times, and application of hydrological DA with distributed hydrological models.

Other challenges in an effective hydrologic data assimilation include the selection of techniques for quantifying model error, perturbations to model inputs and states, and quantifying observation errors. Among the discussed DA challenges, for example in a multi-model ensemble approach developing an effective strategy to optimally combine the individual models to achieve enhanced predictive skill and uncertainty estimation is one

major concern [1]. Potential solutions to the time-lag issue such as ensemble Kalman smoother (EnKS) [2,3] , variational DA techniques e.g. [5], recursive ensemble Kalman filter [4] have been proposed. A few generic tool boxes have been proposed to facilitate operational data assimilation such as the Data Assimilation Research Testbed (DART, http://www.image.ucar.edu/DAReS/DART/) and the Parallel DA Framework (PDAF, http://pdaf.awi.de/trac/wiki), and open source initiative for DA (OpenDA, www.openda.org/joomla/index.php) launched in 2010. OpenDA, an open interface standard which presents a set of tools to quickly implement data-assimilation and calibration for hydrological models, is specifically discussed.

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Multivariate Hydrological Data Assimilation on a Catchment Scale

Marc-Etienne Ridler[1], Henrik Madsen[1], Donghua Zhang[2], Karsten H. Jensen[2], Jens C Refsgaard[3]

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Key words: Data Assimilation, MIKE SHE, Hydrology

Introduction

Data assimilation in water resources modeling has shown great potential in improving forecasts. With the burgeoning of remotely sensed and in-situ data available, the challenge remains to assimilate several different variables in a hydrological system. These variables can represent different domains and measured in a range of temporal and spatial scales.

A flexible and powerful data assimilation system has been developed and allows users to optimally assimilate multiple variables using a number of filters.

Three hydrological variables are of particular interest on a catchment scale: 1) groundwater hydraulic head, 2) river discharge, and 3) soil moisture. Individually, their assimilation has been shown to significantly impact hydrological models. For the first time, using the state of the art data assimilation framework (see Figure), all three variables are simultaneously assimilated to holistically correct the entire system for improved model forecasts.

Methods

MIKE SHE is a fully distributed physically based hydrological model and is used to solve the major processes in the hydrological cycle including overland flow, unsaturated flow, groundwater flow, channel flow, and is coupled to the MIKE 11 river model.

The 1055 km2 Ahlergaarde catchment in Western Denmark, characterized by relatively low elevation gradients with predominantly sandy soils, is modeled in MIKE SHE and MIKE 11. In-situ measurements are used for assimilation and validation. Specifically, a network of 30 soil moisture sensors at depths 5, 25, and 50cm; hydraulic head measured at 10 locations, and 4 discharges along the river.

Results and Discussion

The assimilation of individual variables is shown to correct the model in the different hydrological domains. The gain from assimilating multiple variables simultaneously was found to depend on the correlation between variables and the frequency at which they are assimilated.

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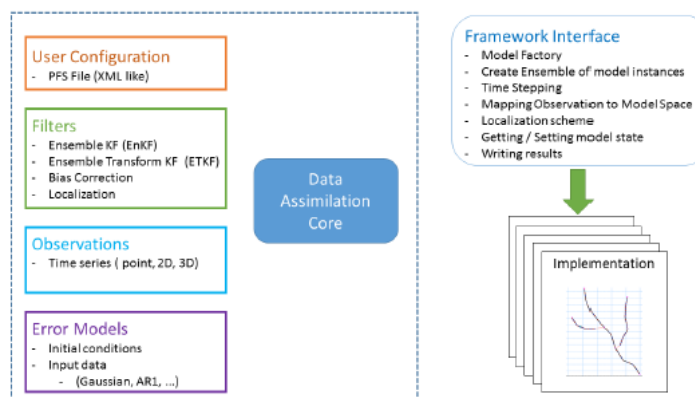
18-1: Multiscale Algorithms and Their Applications: From Upscaling to Scalable Solvers and Multiphysics Modelling

Time: Friday, 24/Jun/2016: 9:40am - 10:40am – Location: MSB 2172

A Multiscale Method for Heat Transport in Fractured Geothermal Reservoirs

Anna Nissen[1,2], Eirik Keilegavlen[1], Jan Martin Nordbotten[1,2], Tor Harald Sandve[3]
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Modelling CO_2-Storage in Fractured Porous Media: Early- and Late-Time Behaviour during Imbibition in Dual- Continua Representations

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Towards Extreme-Scale Applications with EXA-DUNE: Multiscale Methods and Uncertainty Quantification

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A Multiscale Method for Heat Transport in Fractured Geothermal Reservoirs

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Key words: geothermal reservoir, multiscale methods, fractured porous media, transport upscaling

Introduction

Numerical simulation of flow and transport in geothermal reservoirs can give valuable insight in order to improve and optimize geothermal energy extraction. Many geothermal reservoirs are characterized by fractures, where the large scale fractures tend to dictate the preferential flow paths. In order to accurately capture essential flow and transport characteristics it is therefore advantageous to explicitly represent fractures as lower dimensional objects in the computational grid. Compared to upscaled models, the explicit representation of fractures leads to a high number of degrees of freedom, calling for efficient numerical methods. Moreover, complex fracture geometries necessitate a great deal of flexibility in terms of grid generation and the design of numerical methods.

In this work we consider the discretization of advection-diffusion energy equations on unstructured grids with explicitly represented fractures. We seek to alleviate the computational burden by drawing upon ideas from computational multiscale methods and upscaling methods for fractured porous media.

Multiscale method

We develop a multiscale framework for the advection-diffusion transport equation, as an extension of the work presented in [1]. The coarse scale advection term is discretized using fine-scale velocities from the flow calculation (pressure equation), obtained either via a fine-scale simulation or a multiscale method. Motivated by [2], we allow for different coarse-scale grids in the flow and transport solve.

Our coarse-scale transport grids are inspired by the Multiple Interacting Continuum (MINC) Models [3], in that coarse cells are assembled based on the distance to the closest fracture. This type of coarse grid is typically strongly non-uniform and irregular, which makes the construction of basis functions a challenging task. We combine the MINC gridding model with an iterative framework for the construction of basis functions, where we have extended the method described in [4] to fractured systems. In this way the methodology is both theoretically justifiable (consistent) as well as applicable to complicated grid structures with explicitly represented fractures.

We verify our methodology by numerical examples, ranging from illustrative test cases to highly complex cases motivated by real geothermal fields. The examples show that the method accurately represents fine-scale details, and still has a computational cost comparable to that of upscaled methods.

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Modelling CO$_2$-Storage in Fractured Porous Media: Early- and Late-Time Behaviour during Imbibition in Dual-Continua Representations

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Fractured porous media are notoriously challenging to model but of significant importance for many subsurface applications, including geological CO$_2$-storage. In the common modelling approach a fractured geological formation is represented through distinct flow domains, the mobile fractures and the immobile matrix that provides additional storage for the fracture. The rate at which fluids exchange between the domains is represented by a transfer function. For imbibition during two-phase incompressible immiscible flow a simple first-order rate law can be formulated based on the saturation difference between the domains. While this is mathematically convenient it fails to capture the onset of imbibition at early times that is observed in simulations and experiments. Here we present an improved approach that captures the early time behaviour accurately by using semi-analytical self-similarity solutions for capillary driven flow. We also use this concept to predict the transitions from early to late-time-behaviour and construct a new hybrid transfer function. High resolution numerical simulations as well as experimental data are used to validate the results for different wetting and non-wetting phases viscosities and rock types that span a wide range of capillary diffusion coefficient for applications ranging from CO2 storage to oil recovery and beyond.

Towards Extreme-Scale Applications with EXA-DUNE:
Multiscale Methods and Uncertainty Quantification

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Key words: Multiscale, MsFem, DUNE, UQ, extreme-scale

In this contribution we are concerned with efficient numerical methods for uncertainty quantification (UQ) in the context of multiscale problems, in particular realted to single phase flow in heterogeneous porous media or the transport of pollutants in the groundwater. Typically, these models comprise physical properties that change rapidly and on a very small scale, as e.g. porosity, conductivity, or permeability of the medium. This results in rapidly varying and stochastic coefficient functions in the underlying partial differential equations. Hence, an efficient numerical treatment is still challenging and constitutes an active area of mathematical research. Such problems already lead to very large scale problems for single realizations and UQ involves solving a very large number of these realizations. Particular examples include ground water pollution risk analysis in the context of carbon dioxide sequestration or the evaluation of petroleum dig sites. In order to deal with these numerical and computational challenges we make use of efficient multiscale methods that are able to exploit a possible scale seperation inherent in a large class of such problems. Further- more, the Multi-Level Monte-Carlo Method (MLMC, [6]) is used, as it greatly improves algorithmic complexity over traditional UQ techniques.

We first introduce a mathematical abstraction for multiscale methods, following [5]. Based on this unified abstraction layer, we introduce a hybrid parallelization approach that reflects the different layers of multi- scale methods. We present our implementation based on the Distributed and Unified Numerics Environment DUNE [3] and the DUNE Generic Discretization Tool- box [2]. The presented approach and implementation results from the EXA-DUNE project [1] that is part of the DFG Priority Programme 1648 "Software for Exascale Computing". We combine shared- and distributed memory parallelization to achieve scalability and efficiency on current and future, potentially highly heterogenous, peta- and exa-scale computing clusters. We conclude our presentation with new scalability results for the Multiscale Finite Element [4] method and the integration of our implementation in MLMC.

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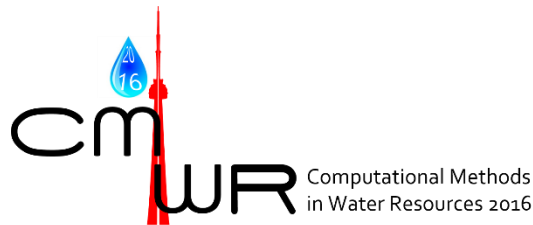
Computational Methods
in Water Resources 2016

18-2: Multiscale Algorithms and Their Applications: From Upscaling to Scalable Solvers and Multiphysics Modelling

Time: Friday, 24/Jun/2016: 11:00am - 12:20pm – Location: MSB 3153

F-AMS: A Flexible Multiscale Framework For Multiphase Flow Through Naturally Fractured Porous Media

Matei Tene[1], Mohammed Saad Al Kobaisi[2], Hadi Hajibeygi[1]
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Hybrid Mortar Domain Decomposition for Single-Phase Flow and Solute Transport

Yashar Mehmani[1], Matthew Balhoff[2]
[1]Stanford University, United States of America; [2]University of Texas at Austin, United States of America; yashar.mehmani@gmail.com

A Multiscale Method for Reservoir Geomechanics Simulation

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Multi-Resolution Discontinuous Galerkin Modelling Of Shallow Water Flow

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F-AMS: A Flexible Multiscale Framework for Multiphase Flow through Naturally Fractured Porous Media

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Key words: algebraic multiscale methods, multiphase flow, naturally fractured porous media, heterogeneous geological properties, scalable linear solvers.

Abstract

Mathematical formulations describing flow in porous media typically entail highly heterogeneous coefficients, changing over several orders of magnitude through the entirety of the domain. In addition, many of the target geological formations are fractured. Fractures are lower dimensional manifolds with properties that differ greatly from those of the surrounding porous rock. Therefore, given their significant role in establishing the patterns of the flow regime, accurate representation of fractures within flow and transport models is crucial for many geoscientific applications, including groundwater flow and geothermal energy exploitations [1]. Embedded Discrete Fracture Model (EDFM) [2] employs independent grids for matrix and fractures. This results in efficient computations, specially for complex fracture geometries, and cases with dynamic fracture creations (and closures) [6]. Even though small-scale fractures are homogenized within the matrix rock, the remaining explicit fractures (bigger than fine-scale grid resolution) along with heterogeneous matrix, for realistic cases, lead to linear systems which are beyond the scope of classical simulation methods. Multiscale finite element and volume (MSFE and MSFV, respectively) methods have been developed mainly for heterogeneous, but non-fractured, porous media [3, 4, 5]. In order to extend them to account for flow in heterogeneous fractured formations, here, F-AMS is introduced as a novel Algebraic Multiscale Solver [7]. It operates by defining coarse grids for both the porous matrix and the embedded discrete fractures. Then, by computing local basis functions, a general map between the fine- and coarse-scale systems, i.e. the prolongation operator, is obtained. These basis functions form a partition of unity and, in their present formulation, they allow for four degrees of fracture- matrix coupling: (1) Decoupled-AMS, in which the two media are completely decoupled, (2) Frac-AMS allows one-way coupling, where the fracture coarse solutions also affect the matrix fine-scale pressure, (3) Rock- AMS is the counterpart of Frac-AMS, where the matrix coarse solution is also employed to find the fracture fine-scale pressure, and (4) Coupled-AMS, in which matrix and fracture interpolators are fully coupled. If only one coarse degree of freedom (DOF) is considered for each fracture network, the Frac-AMS strategy becomes equivalent to the earlier method proposed by Hajibeygi et al. [6]. However, in order to maintain efficiency for general cases, the F-AMS framework permits full flexibility in terms of the definition of the fracture coarse grids and the level of matrix-fracture prolongation coupling. Moreover, by using the Finite Volume restriction operator after any iteration, a mass conservative velocity can be reconstructed and be used to solve the transport equations. Systematic numerical experiments for 3D heterogeneous fractured domains (from 10^5 to 10^7 grid cells, and fracture-matrix transmissibility contrasts of 10^1 to 10^8) are presented and discussed. In addition, the F-AMS is benchmarked agains SAMG [8], a commercial Algebraic Multigrid solver. These results illustrate that F-AMS is an efficient multiscale procedure for large-scale fractured reservoirs. It is important to note that for multiphase flow scenarios, only a few F-AMS iterations are sufficient to obtain good quality pressure solutions. These lead to the conclusion that F-AMS is an important multiscale development for the efficient simulation of flow in naturally fractured porous media.

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Hybrid Mortar Domain Decomposition for Single-Phase Flow and Solute Transport

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Key words: hybrid modeling, mortar domain decomposition, parallel computing

Flow and transport processes in the subsurface occur over a multitude of spatial scales, from a few microns to several kilometers. In modeling such processes, it is quite desirable if pore-scale details can be ignored and a macroscopic conservation equation can be written. Such an equation often describes spatial averages of the state variables (e.g. pressure/concentration) over a given support, often referred to as the representative elementary volume (REV). Geologic properties (e.g., permeability, dispersivity) appearing in these equations can be obtained, either numerically or experimentally, in a single step by solving a closure problem. While several applications do lend themselves to such a simplified descriptions, there are many that do not. These include scenarios involving wormholing in acidification, viscous fingering in miscible flooding, and reactive transport in CO_2 sequestration. The common characteristic of all these processes is that variances in the dependent state variables are too large to be averaged out to form a purely macroscopic equation. This scenario is often referred to one where scales are inseparable. From a modeling standpoint, this entails that pore-scale information cannot be transferred to the field scale in a single step anymore, and instead, a dynamic communication between the two is required.

The current contribution presents one such approach, among several others recently proposed in the literature, which establishes a communication between a pore-scale and a continuum-scale model. The approach is based on representing part of the computational domain directly with a pore-scale model, and coupling it to the surrounding continuum. The approach is useful when one has an a priori knowledge or estimate of where scales might become inseparable e.g., near wellbores. There are several benefits to our approach that result from its mortar domain decomposition based framework. These include generality in coupling various model types (e.g., Lattice Boltzmann, Finite-Element, Pore Network), with possibly different numerical schemes (e.g., explicit, implicit time marching), and effective parallel scalability for high performance computing.
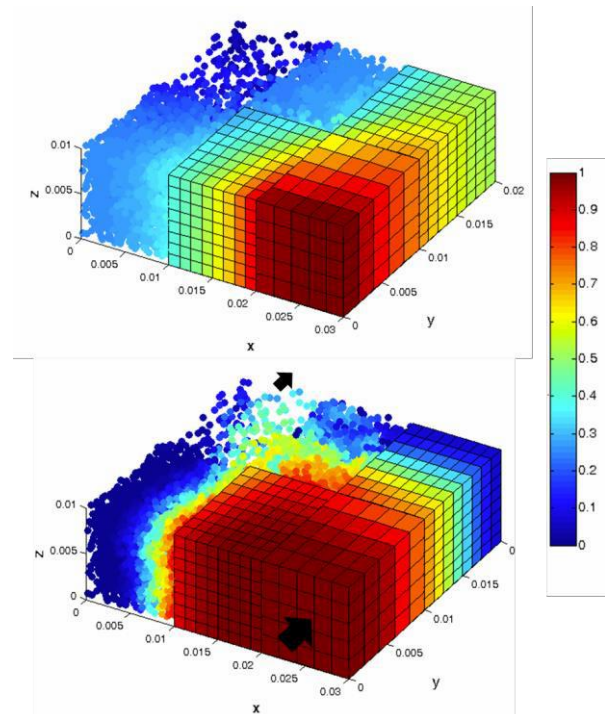

Figure 1: Normalized (by the inlet value) pressure (top) and concentration (bottom) fields of a hybrid domain consisting of coupled pore-scale and continuum subdomains.

A Multiscale Method for Reservoir Geomechanics Simulation

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Key words: multiscale methods, multiscale finite ele- ment method, reservoir geomechanics, preconditioning

Abstract

Geomechanical effects play a crucial role in many applications involving significant fluid withdrawal and injection in the subsurface—e.g. unconventional oil and gas reservoirs, hydraulic fracturing operations, geothermal systems, geologic carbon storage projects, and waste- water disposal sites—both from the effective design and environmental safety assessment perspective. The demand for accurate and efficient simulation of geomechanical effects is widely increasing in the geoscience community. For an applicable method, a number of factors are required to be accounted for at both the withdrawn/injected formation and the ground surface level, including [1]: (a) formation of earth fissures, (b) fault reactivation, (c) induced or triggered microseismic and seismic events, and (d) land surface stability (land subsidence/uplift). The mathematical formulation that describes deformation of a geological formation coupled with flow and transport entails heterogeneous coefficients with a wide range of length scales. Very high resolution, i.e. fine-scale, character- izations are essential for improving modeling predictions. Such detailed descriptions of hydro-mechanical properties impose severe computational challenges and motivate the development of multiscale solution strategies. Multiscale finite volume (MsFV) methods [2] have been developed and evolved during the past decade, as a conservative reform- ulation of its finite-element counterpart [3], to address this computational challenge for subsurface flow simulation purposes. Recent advancements of the method include iterative error reduction strategies within an algebraic framework, complex non-linear compressibility and compo- sitional fluid physics, adaptive flow-transport simulation strategies, flow and transport in fractured, and faulted media with complex wells. However, the focus of these work has been mainly on flow and transport, i.e. the mechanical deformation of the reservoir has been typically neglected.

The multiscale finite element (MsFEM) method has been applied to consolidation of heterogeneous porous media in [4]. Beyond the original idea of multiscale methods, namely providing approximate solutions at low computational cost, the multiscale basis functions allow also for the construction of coarse-scale solvers in the context of two-level domain decomposition preconditioners. Recent approaches to the elasticity equations combine a MsFEM method with additive Schwarz local solver [5].

The primary objective of the present work is to extend the algebraic multiscale solution framework presented in [6, 7] to the simulation of the mechanical response of heterogeneous geological porous media. Constructed on finite element fine-scale system, we show that the framework developed for flow through porous media can be quite naturally generalized to the geomechanical equili- brium problem. After imposing a coarse- scale grid, which is a non-overlapping decomposition of the domain, local basis functions are computed for the displacement vector. These basis functions form the restriction and prolongation operators used to obtain the coarse-scale system for the displacement. Then, a two- stage preconditioner, which combines the multiscale system with a local smoother, is derived for the iterative improvement of the multiscale solution. Numerical experiments, with synthetic and realistic parameters, are presented to illustrate the accuracy and robustness of the method with respect to distorted mesh, material anisotropy and boundary/loading conditions.

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Multi-Resolution Discontinuous Galerkin Modelling Of Shallow Water Flow

Georges Kesserwani[1], Daniel Caviedes-Voullième[1], Nils Gerhard[2], Siegfried Müller[2]

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Key words: Multiwavelets, Automated mesh adaptivity, Shallow water equations.

Introduction

Numerical modelling of the multiplicity of physical-length scales, which are involved in Shallow Water (SW) flows, has been a long-lasting challenge in computational hydraulics. The combination of Multi- Wavelets (MW) and the Runge-Kutta discontinuous Galerkin methods (RKDG) has resulted in a new philosophy (referred hereafter to MW-RKDG) to readily achieve multi-resolution modelling, which is driven by the local variability of the numerical solution. In an MW-RKDG numerical approach, spatial-resolution adaptivity is driven by one user- input parameter, the use of a very coarse baseline mesh is straightforward, data connectivity across various resolutions is rigorous, and quantitative control of the perturbation-error from the finest-uniform mesh (i.e. reference mesh) is feasible [1-3]. In light of the recent theoretical progress in MW- RKDG adaptive methods, this work aims to closely examine practical merits and potential implications of the MW-RKDG approach, i.e. in terms of how far it contributes to address the key challenge above. Two adaptive SW-MW-RKDG2 models are deployed for solving the shallow water equations with friction and topography source terms, and with presence of wetting and drying. The adaptive models are tailored and studied based on two reference RKDG2 schemes [4-6]. The SW-MW-RKDG2 models are exhaustively tested for several hydraulic benchmarks, and then assessed in replicating dam- break flow experiments. All adaptive simulations have been run for a baseline coarse mesh consisting of (only) 2 computational cells and allowing a maximum of 8 refinement levels (i.e. 512 cells for the reference scheme). The adaptive results have been analysed (qualitatively and quantitatively) comparing with analytical and experimental data, and with the outputs of the reference schemes (i.e. on several uniform meshes). When possible, further comparison with a third-order SW-MWRKDG model (SW- MWRKDG3) has been included. The performances of the SW-MW-RKDG2 models are analysed in detail considering subjects of: stability for SW modelling, adaptivity response to the features of the reference scheme, impact of accuracy-order increase on adaptive mesh predictability, choice for the sole parameter driving the MW adaptivity process, operational and runtime saving, and 2D extendibility.

Steady state results

Example of second and third-order adaptive SW- MW-RKDG simulations for the McDonald steady state (test No. 6). In Figure 1, the adaptive results (L8-A, P = 2 and L8-A P = 3) are compared with uniform mesh simulation (U46, P = 3), with the purpose to jointly illustrate the potential added value of MW-based modelling to h- & p-adaptivity.
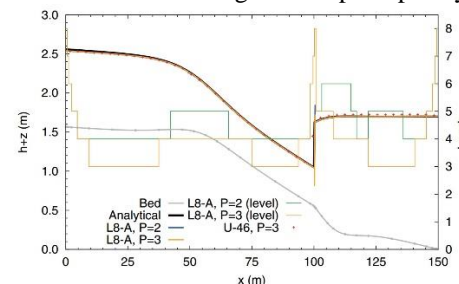

Figure 1: SW-MW-RKDG2 and SW-MW-RKDG3 (adaptive) steady state simulation.

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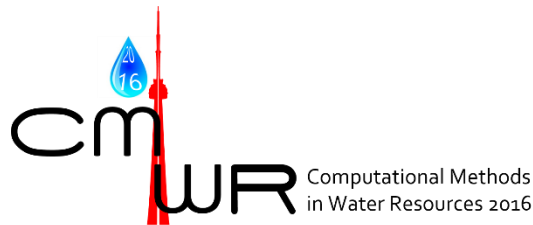
18-3: Multiscale Algorithms and Their Applications: From Upscaling to Scalable Solvers and Multiphysics Modelling

Time: Friday, 24/Jun/2016: 2:30pm - 4:10pm – Location: MSB 3153

Upscaling Reservoir Properties Using Single Well Tracer Tests

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Comparison of MINC Modelling Approaches for Two Phase Porous Media Flow

Alexandru Tatomir[1], Nicolas Schwenck[2], Bernd Flemisch[2], Holger Class[2], Rainer Helmig[2], Martin Sauter[1]
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Pore Network Extraction and Upscaling: a Big-Data Approach

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Crouzeix-Raviart MsFEM for Stokes-Oseen Problems in Heterogeneous Porous Media

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Upscaling Reservoir Properties Using Single Well Tracer Tests
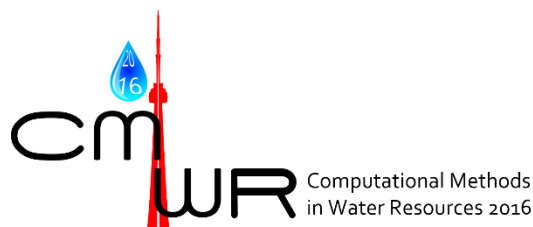
Mary Wheeler, Gurpreet Singh

The University of Texas at Austin, United States of America

Key words: Upscaling, SWTT, homogenization

Abstract

Accurate predictions of reservoir production and flooding scenarios for CO_2 sequestration, groundwater remediation and oil and gas production relies upon an accurate numerical reservoir simulation. This in turn depends upon the approach used to populate reservoir properties such as permeability, porosity, etc. at a spatial scale determined by numerical discretization. Well logs provide good estimates of near well bore reservoir property variation with depth. However, the spatial scales associated with these observed properties are quite small and therefore prohibitive to be used directly for numerical simulations. Upscaling provides a pragmatic solution by computing effective properties at the coarse spatial scale corresponding to the numerical discretization.

Another restriction of well logs is that the information extracted is valid for near well bore region. Single Well Tracer Test (SWTT) has been used extensively for evaluating the enhanced oil recovery (EOR) potential by determining the in situ fluids. A number of other works in literature utilize SWTT for estimating reservoir property heterogeneity. In this research, we use a two-scale homogenization approach to upscale the conservation equations associated with Single Well Tracer Test for estimating effective reservoir properties at the coarse scale. We first validate our upscaling approach by predicting the observed SWTT effluent concentration history with numerical simulations using effective reservoir properties. Secondly, we suggest coarse spatial scale for computations, which corroborate with SWTT effluent concentrations taking into account far from well bore reservoir properties.

Comparison of MINC Modelling Approaches for Two Phase Porous Media Flow

Alexandru Tatomir[1], Nicolas Schwenck[2], Bernd Flemisch[2], Holger Class[2], Rainer Helmig[2], Martin Sauter[1]

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[2]Institute for Modelling Hydraulic and Environmental Systems, University of Stuttgart, Germany

Keywords: MINC, upscaling, two-phase flow, fractured porous media, double porosity

Multiple interacting continua (MINC) model represents an extension of the classic double porosity model (Warren and Root, 1963) which accounts for the non-linear behaviour of the matrix-fracture interactions. The fully transient representation of inter-porosity two phase flow is relevant for a series of engineering applications e.g, oil-recovery, high-temperature geothermal reservoirs, unconventional shale gas exploitation, CO_2 storage in geological reservoirs, etc.

A two phase flow MINC simulator is implemented in the free-open source numerical toolbox DuMux (www.dumux.org). This study demonstrates the utility of the MINC model in a series of benchmark examples (e.g., idealized 1D reservoir, five-spot gas migration in a radial symmetric fractured reservoir, randomly generated fractured system). The transient behaviour of the matrix block is realized by considering in each fracture continuum-vertex an arbitrary number of one-dimensional control volumes. Different upscaling techniques for determination of the MINC nested volume element effective parameters are compared and discussed in terms of accuracy and computational efficiency. A discrete fracture model is used as reference solution.

Results show that the standard double porosity model with constant shape factors leads to large errors whereas, the MINC model coupled with multiple subregion upscaling technique maintains the accuracy and has speed-up factors up to two orders of magnitude. Increasing the number of sub-grids leads to an increase in accuracy, but also in computational time. The optimal number of element grids is determined according to each sub-gridding procedure.

Pore Network Extraction and Upscaling: a Big-Data Approach

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Key words: Network Extraction, Network Modeling, Graph Theory, HPC, Big-Data, 3D Visualization

Abstract

Pore networks provide practical descriptions for porous media to model multi-phase fluid flow by incorporating physically-based displacement mechanisms at the pore scale. To do so, generated networks should retain important features of the pore space topologies affecting fluid flow behavior. In this work, we are specifically interested in capturing pore level connectivity and concavity in a network of pore bodies connected by throats for larger scale sample sizes. We use direct pore-scale images of porous media as an input for the model presented in this work. Three-dimensional (3D) stacks of high-resolution images are obtained using computed X-ray micro-tomography for each rock sample. The network contains information about the location, size, shape, and connectivity for each pore and throat. 3D digitalization technologies have been rapidly developing, particularly over past 10 years. Consequently, data sets become larger in size and more complex because of the higher resolutions. Therefore, it is necessary to develop efficient algorithms to handle with such data.

We proposed a new algorithm to construct pore networks from a very large stack of images with realistic physical and flow properties. The advantages of our new algorithm over the published literature ([1], [2], [3]) are the utilization of: (1) a Big-Data approach to modernize the design of algorithms ([4], [5]); (2) HPC to optimize global and local processes; and (3) Computer Graphics to reconstruct and accurately analyze digital clustered objects. This would in turn enable us to simulate fluid flow on larger sample sizes without sacrificing on resolutions.

We assessed the quality of the extracted pore networks using both qualitative and quantitative means. A 3D computerized visualization is used to create an overlay of the extracted network on the original stack of 3D images. This allows us to perform a qualitative comparison. For the quantitative analysis, two- phase drainage and imbibition flow cycles were simulated and compared against their corresponding experimental measurements ([6], [7], [8]).

The computational efficiency of the newly proposed approach is demonstrated through several different studies in various rock samples.
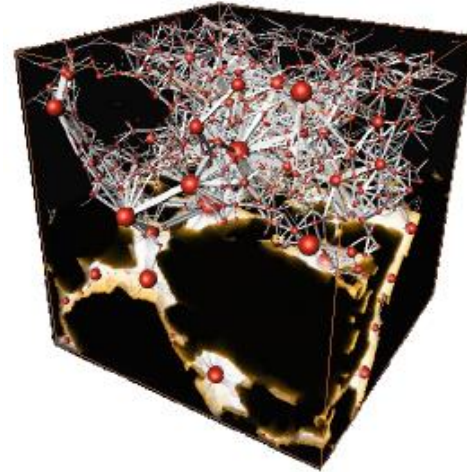
Figure 1: The 3D overlay of pore network representation on the segmented micro-CT image. At each pore body and throat, various properties such as volume, surface area, inscribed and effective radii, shape-factor, sphericity, aspect ratio, coordination number, and mineralogies are stored.

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Crouzeix-Raviart MsFEM for Stokes-Oseen Problems in Heterogeneous Porous Media

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Key words: Multiscale Finite Element Method (Ms-FEM), Crouzeix-Raviart Element, Oseen Equation, Heterogeneous Porous Media

Introduction

The Multiscale Finite Element Method (MsFEM) [1] is developed in the vein of Crouzeix-Raviart (C-R) element [2] for solving incompressible flows with linearized inertial term in heterogeneous porous media—where the geometries of the problems are complicated with aperiodic grain-pore interfaces. The weakly enforced continuity of C-R function space across element edges leads to a natural boundary condition for the multi- scale basis functions which relaxes the sensitivity of our method to complex patterns of pore structure; all without having to utilise any oversampling techniques. The application of penalization method [3] allows extensive use of simple Cartesian meshes.

Formulation of Problem

First, we introduce a grain-pore domain $\Omega \subset R^d$ within which a set B^ϵ of grains is included. The pore domain with voids left by the grains is denoted $\Omega^\epsilon = \Omega \setminus B^\epsilon$ illustrated in Fig. 1, where ε denotes the minimum width of grain. The Stokes-Oseen problem is to find $u : \Omega^\epsilon \to R$ which is the solution to

$$-v\Delta\vec{u} + \rho(\vec{\omega} \cdot \nabla\vec{u}) + \nabla p = \vec{f} \quad in \quad \Omega^\epsilon \ (1)$$
$$\nabla \cdot \vec{u} = 0 \quad in \quad \Omega^\epsilon$$

Where ν is dynamic viscosity, ρ is density of the fluid and $\vec{\omega}$ is known velocity field.

Construction of Crouzeix-Raviart Basis

First, we ntroduce a mesh T_H on Ω consisting of N_H polygons/polyhedrons of diameter at most H. Let $\mathcal{E}_H$ denote the set of all the edges/faces of T_H including those on the domain boundary $\partial\Omega$. The explicit construction of the C-R basis functions is as follows: for any $E \in \mathcal{E}_H$ we construct $\vec{\Phi}_{E,i} : \Omega \to R^d$ and the accompanying pressure $\pi_{E,i} : \Omega^E \to R$ such that $\vec{\Phi}_{E,i}$ and $\pi_{E,i}$ vanish outside the two triangles T1, T2 adjacent to E and they solve on each of this two triangles:
$$-v\Delta\vec{\Phi}_{E,i} + \rho(\vec{\omega}.\nabla\vec{\Phi}_{E,i}) +$$
$$\nabla\pi_{E,i} = 0, \quad on \ \Omega^\epsilon \cap T_k,$$
$$\nabla.\vec{\Phi}_{E,i} = const., \quad on \ \Omega^\epsilon \cap T_k$$

$$\vec{\Phi}_{E,i} = 0, \quad on \ B^\epsilon \cap T_k$$
$$\nabla\vec{\Phi}n_{E,i} - \pi_{E,i}n = const. on \ F \cap \Omega^\epsilon$$
$$\int_F \vec{\Phi}_{E,i} = \begin{cases} \vec{e}_i, & F = E \\ 0, & F \neq E \end{cases}, \forall F \in \varepsilon(T_k)$$
$$\int_{\Omega^\epsilon \cap T_k} \pi_{E,i} = 0. \quad (2)$$

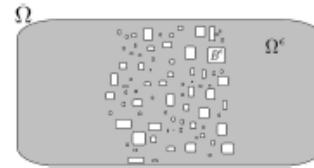Fig. 2 shows the numerical results of our method along with the comparison with a reference solution.

Figure 1: An illustration of the grain-pore domain Ω comprising the pore domain Ω^E with voids left by a set of grains B^E.
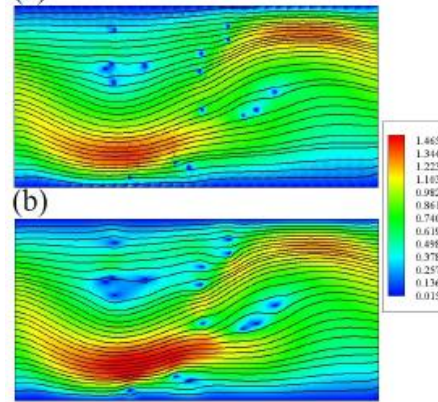

Figure 2: Inertial flows in rock pores. Velocity magnitude contours and streamlines are computed with CR-MsFEM on (a) 16×32 elements, and (b) the reference solution calculated on 1280×2560 elements. The speed-up in computational time is 4 orders of magnitude.

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19-1: Computational Developments in Modelling Climate Change and Water Resources

Time: Friday, 24/Jun/2016: 11:00am - 12:20pm – Location: MSB 2172

Seasonal Forecasting for Water Resource Management: Reservoir inflows and uncertainties

Michael B Butts[1], **Yuachao Xu**[1], **Henrik G Mueller**[1], **Roar A Jensen**[1], **Jacob K Larsen**[1], **Peter N Godiksen**[1], **Bertrand Richaud**[1], **Peter T Larsen**[2], **Miguel Ángel Corcuera Barrera**[3]

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The Impact of Changing Weather and Climate on Recharge and Groundwater

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Evaluating Reliability, Resiliency and Vulnerability of Water Resource System: A Bayesian Approach

Samiha Tahseen, Bryan W. Karney
University of Toronto, Canada; samiha.tahseen@mail.utoronto.ca

Seasonal Forecasting for Water Resource Management: Reservoir inflows and uncertainties

Michael B Butts[1], Yuachao Xu[1], Henrik G Mueller[1], Roar A Jensen[1], Jacob K Larsen[1], Peter N Godiksen[1], Bertrand Richaud[1], Peter T Larsen[2], Miguel Ángel Corcuera Barrera[3]

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Ke y words: climate variability, forecasting, climate adaptation, wat er resources management, reservoir operation

Introduction

Seasonal forecasting has the potential to impact decision making in many related sectors such as like water resources, energy, tourism, and agriculture, where outcomes are dependent on climate variability. Hydrological forecasting over a period of weeks to months can be particularly useful where future flows are strongly influenced by storages in the hydrological system. Typically, these would include reservoir operations for hydropower irrigation and water supply or accumulation of water as snow, ice or groundwater. Other applications include

- long-term contingency planning for floods and droughts
- water demands and allocation for irrigation or domestic/industrial water use
- energy production forecasting
- environmental monitoring
- climate adaptation

Despite its potential value both in terms of economics and for climate adaptation, seasonal forecast information is currently under exploited. This is being addressed in the European FP7 project EUPORIAS, (http://www.euporias .eu/, using the latest generation seasonal forecasts from climate models.

Case study

One of the important challenges is the need to quantify uncertainties and evaluate decisions against this uncertainty. In this paper we will examine the reliability and uncertainties related to seasonal hydrological forecasts for reservoir inflow and operations.

Many reservoirs must operate in order to fulfill a number of different requirements such as hydropower, water supply and flood protection that operate on different time scales . The Urumea catchment, located in the northern Spain is representative of many areas in southern Europe that are vulnerable to floods, droughts and water scarcity and where the rainfall distribution varies over a relatively small distance from the coast. On the Añarbe River, the Añarbe reservoir is operated by Aguas de Anarbe (AGASA). This reservoir is used for water supply to the city of San Sebas tian as well as hydropower, and the reservoir is operated to provide flood protection downstream and to maintain environmental flows within the Urumea River. The catchment rainfall exhibits a clear seasonal behavior and it is therefore of interest to inves tigate the accuracy and reliability of EUPORIAS seasonal predictions for inflows to the Añarbe reservoir.

A hydrological model for the rainfall-runoff processes in the Urumea catchment and the reservoir operation has been developed and successfully calibrated on historical data. Ensemble seasonal forecasts upstream of the reservoir have been developed using both historical streamflow measurements, (ESP-Q) and historical precipitation measurements (ESP-P).

Our initial comparisons with climate model forecasts highlight two important aspects of seasonal hydrological forecasts. Firstly, bias correction of the rainfall forecasts is essential. In this example, just using simple scaling provides a substantial improvement. Our initial results suggest that while the reliability of the rainfall forecasts may be low, the reservoir storage and operation strongly influence the hydrological response and therefore improve the reliability of the seasonal hydrological simulations.

The Impact of Changing Weather and Climate on Recharge and Groundwater

Jonathan F. Sykes, Stefano D. Normani, Mikko I. Jyrkama

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Key words: groundwater recharge, climate change, Toms River

Introduction

While the scale and long residence times of many groundwater systems provides a buffering function to short-term climatic variability, many groundwater systems are potentially vulnerable to the direct and indirect effects of climate change on recharge. Climate change affects surface water resources at the local scale directly through changes in the major long-term climate variables such as air temperature, precipitation, solar radiation, wind speed, relative humidity and the resulting evapotranspiration. Groundwater resources are affected by climate change through the direct interaction with surface water resources, and indirectly through the recharge process. Therefore, quantifying the impact of climate change on the quantity and quality of groundwater resources requires not only reliable forecasting of changes in the major climatic variables, but also accurate estimation of groundwater recharge and discharge. Estimating the renewable flux (i.e., sustainable limit) of the hydrologic system in both its present and projected future state is the prerequisite for groundwater management.

Temporal Change in Recharge

The impact on groundwater of a changing climate is investigated at the Reich Farm Superfund site in Toms River, New Jersey for the approximately 45 year period from October 1971 to April 2014. Temporally and spatially varying groundwater recharge to the phreatic aquifer is estimated using the hydrologic model HELP3. Data for the analysis includes the land- use/land-class (LULC), soil characteristics and daily meteorological records of precipitation, maximum daily temperature and minimum daily temperature. LULC distributions at three different times were used in the analysis. The aquifer response to recharge and municipal pumping at wells approximately 1.6 km south of the Reich Farm site was monitored using continuous loggers and manual measurements at observation wells. MODFLOW 2005 was used to model transient groundwater flow and verify the recharge estimates. Among other metrics that were investigated, the relationship between the temporal change in recharge and water table elevation can be illustrated in a plot of the cumulative monthly recharge minus the average recharge

for the period of analysis (Figure 1). Positive slopes in the upper plot indicate periods with recharge excess while negative slopes indicate periods of recharge deficit. For the Toms River site, from approximately 1996 to 1998, the recharge was generally above average resulting in the rise in the water table from 1996 to 1998. From 1998 to 2002, recharge tended to be less than average resulting in a decline of the water table to a low observed in 2002. A significant rise in the water table in 2010 can also be explained by recharge excess and recharge deficits. At the Toms River site, the high water table events occur on a cycle of approximately 12 years with peaks in 1974, 1985, 1998 and 2010.

A twelve month forward moving average of the monthly average recharge can also identify periods of recharge excess as compared to periods with a recharge deficit. The analysis indicates that the 12 month average recharge peaked in 1973, 1984, 1997, 2003 and 2009 with high water table levels occurring at some time in the year following these dates. The analysis of the Toms River data set supports the hypothesis that rather than single rainfall events, multi-year periods of either recharge excess or periods of recharge deficit are required to significantly perturb the water table elevation and define extreme recharge. This hypothesis is also supported by the fact that hurricanes Irene (August 2011) and Sandy (October 2012), that directly hit the Toms River area, had little to no impact on water table levels. The temporal patterns of recharge can be explained by the large scale patterns of change observed in the Atlantic Multi-decadal Oscillation (ocean temperature) and the North Atlantic Oscillation (air pressure). Correlations between the temporal recharge and the North Pacific Oscillation are also observed.
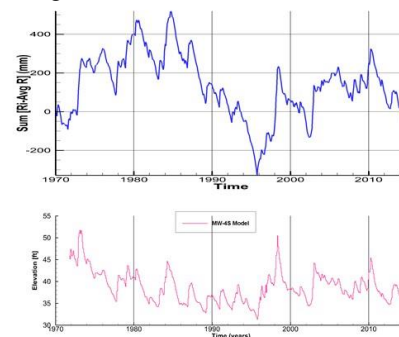

Figure 1: Cumulative recharge minus average recharge and simulated water levels at a monitoring well near Reich Farm.

Evaluating Reliability, Resiliency and Vulnerability of Water Resource System: A Bayesian Approach

Samiha Tahseen, Bryan W. Karney

University of Toronto, Canada

Key words: Climate change, Bayesian Network, the Great Lakes

Introduction

Considering that the world's water resources face increasing challenges within the context of a changing climate, there is a need to reassess the resulting impact on water usage, ecology, energy and environment. Understanding the possible impact is a key to develop appropriate management tools for mitigation. This study contributes to the existing knowledge base by quantifying several impacts in terms of probable system performance under future climate projections.

A warmer temperature and changing precipitation pattern across the Great Lakes watershed pose economic threats to numerous industries that rely on the lakes water supply. The direct economic impact of changing water level is estimated to be $9.61B and $18.82B over the period from the present through 2030 and 2050 respectively [1]. Lake Erie, being the shallowest with an average of depth of 19 m, makes it the most vulnerable to a changing climate. Identifying the resulting impacts (both favourable and adverse) is critical for the lake ecosystem as well as the tourism and hydroelectric resources downstream. The current study builds a Bayesian Network [2], specifically a probabilistic graphical model, using the historical climate and hydraulic data of the lower the Great Lakes. Historic climatic variables, such as temperature, precipitation, wind speed and direction, etc. and their corresponding hydrological data, such as water level, river flow, surface temperature, lake ice concentration etc. are extracted from resources such as Global Historical Climatology Network (GHCN), National Oceanic and Atmospheric Administration (NOAA), the Great Lakes Ice Atlas. The structural learning, i.e., conditional probability of different variables, is conducted employing EM learning algorithm with the imposed restrictions, such as requiring that hydrologic variables do not have causal effect on climate variables. Following these boundary conditions, the constructed Bayesian Network is presented as Figure 1. The developed model is used to define specific performance criteria, such as reliability, resilience and vulnerability, that capture the ability of the resource system to operate satisfactorily under wide range of possible conditions. The model output of system state can be partitioned into two set: S, the set of all satisfactory outputs, and F, the set of all unsatisfactory (failure) outputs. The reliability of a system can be described by the probability that a system belongs to S (satisfactory state). Resiliency describes how quickly the system is likely to recover from failure once a failure has occurred; this is estimated by inverse of expected value of the length of time a system's output remains unsatisfactory. Vulnerability refers to the likely magnitude of a failure, weighted by the likelihood of it occurring [3].

A Bayesian Network, which is a combination of a directed acyclic graph constructed with model variables and their conditional probabilities, provides a highly flexible modeling architecture. It allows incorporation of new variables, partially updating the model or made predictions with missing data, etc., which is highly conducive to the ongoing progress in climate change research and manifestations.
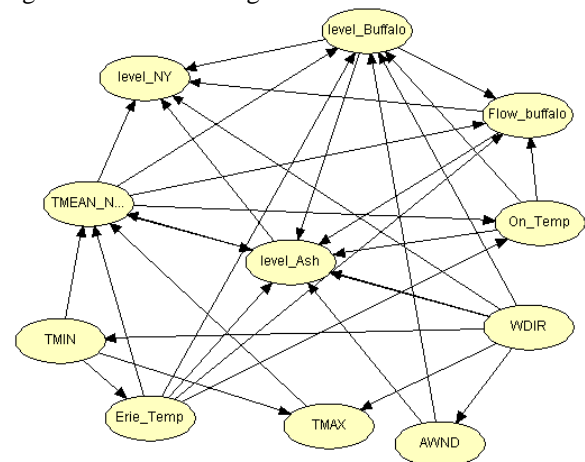

Figure 1: The Bayesian Network model

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19-2: Computational Developments in Modelling Climate Change and Water Resources

Time: Friday, 24/Jun/2016: 2:30pm - 4:10pm – Location: MSB 2172

Climate Change and the Niagara River: Is Lake Regulation Part of the Broader Solution?

Samiha Tahseen, Bryan W. Karney
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Simulation-Optimization of Multiple LIDs in an Urban Watershed

Kyle Eckart, Tirupati Bolisetti
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Climate Change and the Niagara River: Is Lake Regulation Part of the Broader Solution?

Samiha Tahseen, Bryan W. Karney

University of Toronto, Canada;

Key words: Climate change, the Great Lakes, HEC-ResSim

Introduction

Water resource management is a complex issue that requires comprehensive investigation involving social, economic, ecological, technical and policy dimensions. Considering that the world's water resources face increasing challenges, there is a need to assess the resulting impact on water usage, ecology, energy and environment.

Stretched at the border between Canada and the US, the Niagara River is currently operated for recreation, hydropower generation, and low flow augmentation. This study utilizes HEC-ResSim to simulate the existing power system at Niagara with an aim to assess generation under varying climate and operating conditions. The work of others on the Great Lakes basin found that the temperatures are likely to increase by 2-3°C by 2050 [1]. At the same time, precipitation is projected to increase by 9.5-25% [1][2]. The rising temperature has the potential to alter lake evaporation pattern which plays an important role in determining water availability. Historical data for the lakes in northwestern Ontario demonstrate that evaporation increases by an average of 35 mm/1°C increase in mean annual air temperature or 68 mm/1°C increase in mean summer air temperature [3][4]. Considering the same for southern Ontario, a 3°C temperature increase may lead to a 105 mm annual increase in lake evaporation. The study explores a wide variety of "what if" scenarios with increased evaporation ranging from 30-105 mm and a 20% increase in precipitation. The analysis is further extended to evaluate an ambitious lake regulation plan with storage infrastructure development. Figure 1 shows Lake Erie pool elevation under projected climate scenarios.
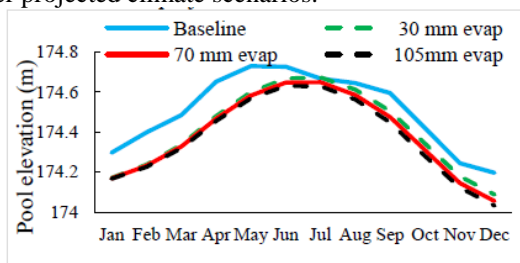

Figure 1: Lake Erie water level

The outcome suggests that though the change in pool elevation is quite subtle for summer and fall, low precipitation in combination with increased evaporation during winter and spring can lead to a drop in water level as high as 0.2 m. The changing climate apart from a sustained low water level, can reduce flow availability by 7-11% annually at the downstream hydropower stations. The novel lake regulation, which allows additional storage during the night and consequently releasing it during the peak demand hours, results in a 25-35% increased generation during peak hours (while decreasing during the rest of day) (Figure 2). When aggregated on a yearly basis, this can lead to a 360-470 GWh increase in power generation potential at Beck Complex.
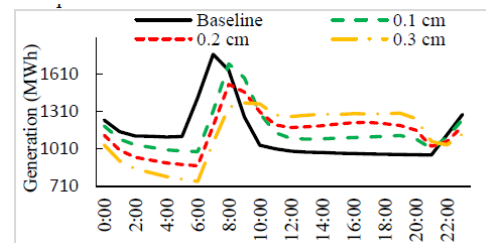

Figure 2: Generation with lake regulation

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Simulation-Optimization of Multiple LIDs in an Urban Watershed

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Key words: LIDs, SWMM, BorgMOEA, third keyword

Introduction

Urban stormwater management has become increasingly challenging due rapid urbanization, aging infrastructure, and budget shortages. These problems are compounded by climate change conditions and more stringent regulatory frameworks. Engineers have been focusing on alternate/innovative solutions such as Low Impact Development (LID). LIDs aim to replicate pre-development hydrological conditions and water balance. The addition of LID stormwater controls has a site specific, non-linear hydrological response on a watershed. Therefore, modeling is an important tool to understand the abilities of LIDs to affect the total runoff volume, peak flows, and pollutant loadings. It is also imperative to be able to predict the cost of implementing LID controls.

The objective of the present research is to investigate the response of the watershed to the implementation of multiple combinations of LID controls through a simulation-optimization modeling approach. The simulation-optimization model coupled Storm Water Management model (SWMM) with a genetic algorithm, Borg Multi-objective Evolutionary Algorithm (MOEA).

Methodology

The coupled model combines a next generation multiobjective optimization model, BorgMOEA [1] and the most extensively used stormwater management model, SWMM 5 [2]. A SWMM model was developed for study area watershed. The model was calibrated using local rainfall data and observed stormwater flows obtained via the flow monitoring of a stormsewer. The SWMM model simulated the hydrological response of the urban watershed to the LID combinations being tested by the optimization model. The optimization model evaluated 1000s of alternative combinations of LID controls before arriving at various optimal solutions that are non- dominated in the multiple objectives.

Study area The coupled model was tested in a 77 ha watershed located in the City of Windsor, Ontario, Canada. The study area is mostly residential and has portions of wooded areas. The developed areas have 49.5% impervious cover and utilizes curb and channel drainage. The predominant soils in this area are Brookston Clay and Brookston Clay Loam.

LID Controls

LID controls considered in the present study include rain barrels, bioretention cells, rain gardens, infiltration trenches and permeable pavements. The study considered three different levels of adoption (unrestricted, high and low levels) in order to understand the impact of the acceptance by stakeholders.

Conclusions

The present study demonstrated the power of a MOEA in evaluating solutions with different levels of acceptability in the presence of conflicting objectives.

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20-1: Advances in Computational Methods for Surface Hydrological Processes

Time: Thursday, 23/Jun/2016: 9:40am - 10:40am – Location: MSB 2170

Hydrologic Model Development Based on Diagnostic Data Analysis Utilized to Identify Flow Pathways

Mahyar Shafii, **Nandita Basu, James R. Craig, Philippe Van Cappellen** University of Waterloo, Canada; mshafiih@uwaterloo.ca

Parallel Multiresolution Techniques for the Simulation of Rain-Induced Floods on Large-Scale Terrain Data

Roland Wittmann, Hans-Joachim Bungartz
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Modeling Flood Hazard using a GPU-based 2D Hydraulic Model

Shuangcai Li
RMS, United States of America; lishuangcai@gmail.com

Adding Contaminant Transport Capabilities to a Modular Hydrological Modelling Framework

James R. Craig, **Mahyar Shafii, Nandita Basu**
University of Waterloo, Canada; jrcraig@uwaterloo.ca

Hydrologic Model Development Based on Diagnostic Data Analysis Utilized to Identify Flow Pathways

Mahyar Shafii[1], Nandita Basu[2], James R. Craig[2], Philippe Van Cappellen[1,3]

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Key words: hydrology, model identification, flow pathways, hydrological signatures

Introduction

It is often argued that advancing hydrologic science relies on new methods for analyzing hydrologic data and intelligent ways to comprehensively test hydrologic models. In order to trust that our models are adequately capturing the nonlinear dynamics of hydrological systems, we need data analysis tools which can ascertain the hydrological realism of a given model. Such tools enable the modeler to compare models against data more incisively. Recent work has shown that hydrological signatures (for example, flow duration curve) can be used successfully as a diagnostic tool in the model development process [e.g., 1]. While these signatures are effective in evaluating the consistency of model predictions, they rarely give the modeler an insight into the governing flow pathways in the system. In this study, we apply a conceptual model of the annual water yield that partitions the flow into different components (e.g., infiltration, baseflow, etc.), and subsequently, we quantify a number of signatures that are used to constrain the flow partitioning in a semi- distributed hydrologic model. The main objective of this research is to take steps towards getting the right answer for the right reasons [2], which eventually has implications in biogeochemical modelling that is dependent on proper characterization of the flow pathways. The proposed methodology is being used to model streamflow in multiple headwater subbasins in the Grand River Watershed in Southern Ontario. Preliminary results demonstrate the applicability and merits of the proposed approach to identify correct flow pathways simulated by hydrologic models.

Methods

Flow partitioning model: The water yield of a given watershed is a fundamental problem in hydrology. Partitioning of the water yield into different components, however, is even more important. Different conceptual models have been developed to use the hydrologic budget equation to filter precipitation into various components, e.g., wetting front, overland flow, etc. We use a conceptual model developed in [3] and recently employed by [4] in several catchments in the United States to get an insight into flow partitioning at the annual scale. This model has proven to be suitable under a wide range of climatic conditions. It relies on a two-stage filter to separate annual precipitation into surface runoff and infiltration (in the first stage) and then the infiltration into baseflow and vaporization (in the second stage).

Diagnostic approach: Based on the results of the aforementioned model, we quantify four signatures (and their corresponding acceptability limits) for surface runoff, infiltration, baseflow, and evaporation. These signatures are then utilized in the calibration of a semi-distributed model developed in a flexible hydrological modelling framework called RAVEN. Comparisons are conducted between the results of a typical model calibration and the flow pathway constrained, signature-based diagnostic approach. Note that this methodology can be used to assess flow partitioning in any conceptual hydrologic model.

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Parallel Multiresolution Techniques for the Simulation of Rain-Induced Floods on Large-Scale Terrain Data

Roland Wittmann, Hans-Joachim Bungartz

Technische Universität München, Germany

Key words: multiresolution analysis, local time- stepping, finite volume, vectorization

Abstract

Over the past decades, extreme weather events have increased in number and in power, causing widespread flooding and destruction. Through numerical simulation we have a tool to both predict and to study these events in order to find potential countermeasures to better protect civilians and their property. Different numerical approaches have been proposed in [1, 2, 3] to simulate these kind of scenarios. In this work, we use two open source finite-volume solvers for the shallow water equations to run our simulations: The first solver, Full Shallow Water equations for Over- land Flows (FullSWOF2D), was specifically designed for hydrodynamic purposes [4] but is not optimized in terms of vectorization or parallelization. The second solver, the SWE teaching code [8], was originally designed for the simulation of tsunami waves using vectorization and shared memory parallelization. As part of this work, we have added additional source terms to handle rain and friction as well as support for drying and wetting to this solver. In our recent work [7], we have shown that block-structured adaptive mesh refinement combined with local time stepping allows an efficient simulation of flood scenarios incorporating the FullSWOF2D solver. We extend this approach in three ways: First, we use multiresolution analysis techniques [9, 10] to determine significant details in our terrain dataset and to evaluate the smoothness of our numerical solution more effectively. Second, we use the concept of block fusion/splitting as presented in [6] to dynamically adjust the block size throughout the simulation to benefit from vectorization. Third, we use both shared and distributed memory parallelization techniques to handle the simulation of larger scenarios with higher accuracy. We demonstrate our approach on two digital elevation models: The first dataset is of a size of 16km by 9km and covers the mountain area of Mecca, Saudi Arabia of the 1960s, with a spatial resolution of about 1m. This dataset was digitally reconstructed from old maps as part of an ongoing effort to preserve the cultural heritage of Saudi Arabia [5]. The second dataset is of a size of 358km by 370km and covers the state Bavaria in Germany with a spatial resolution of about 25m. This dataset was provided by the Bay- erische Vermessungsverwaltung and by the European Environment Agency.

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Modeling Flood Hazard Using a GPU-based 2D Hydraulic Model

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Abstract:

Recent extreme floods (e.g. US Midwest flood 2008, US Northeast flood, 2010) have increased the concern of flood risk. Consequently, there are growing needs to adequately assess the flood risk. The objective of this study is to develop a numeric model to provide fast and reliable prediction of fluvial flood for the continent United States. In this paper a numerical model based on an upwind finite volume method is developed on Graphics Processor Units (GPUs) to solve shallow water equations. The HLLC approximate Riemann solver is adopted to calculate the flux because of its robustness, efficiency, and superior performance in handling discontinuities and wetting/drying processes. To preserve non-negative water depths and 'lake at rest' property (C-property), a robust positivity preserving method is used. Model efficiency and stability are treated using an explicit-implicit method for temporal discretization with operator splitting. The model is implemented on the Graphics Processor Units (GPUs) to achieve a significant faster speed compared to traditional CPUs. This model is used to generate the multiple return period flood maps for the continental United States. The performance of the model is demonstrated by comparing to the observation and published data

Introduction

The risk of flooding has evidently increased world- wide in the recent years [e.g., Milly et al., 2002; Brissette et al., 2003; Kundzewicz et al., 2005; Teng et al., 2006; Chang et al., 2009]. The increased number of extreme flood events caused significant loss of life and property damage, e.g., 2011 Mississippi River, 2011 Thailand floods, 2013 Colorado flood, and 2015 Texas floods. Hence the needs for insurers and reinsurers to understand and manage flood risk have been growing. Having recognized these needs, RMS has been developing models to quantify both inland and coastal flood risk globally. One important tool to assess the damage is the inundation model which is represented by 2D shallow water equation. However, fast and accurate modeling of inundation for inland floods remains a fundamental impediment, especially for large-scale probabilistic catastrophe models at high resolution. A novel numerical solution implemented on fast parallel computing architectures could be a solution.

With their specialized parallel processing architecture, Graphics Processing Units (GPUs) are well suited for this purpose. A GPU is a computer chip that performs fast mathematical calculations (specifically floating-point), primarily for the purpose of rendering images. In contrast to a CPU consisting of a few cores optimized for sequential serial processing, a GPU consists of thousands of smaller, more efficient cores designed for handling multiple tasks simultaneously. The resulting high performances have made GPUs popular chips for other resource-intensive tasks unrelated to graphics. Nowa- days, GPUs from NVIDIA are widely used with the CUDA, a C-based programming language for parallel execution on GPUs. The NVIDIA GPUs consists of a set of SIMD (single instruction multiple data) processors that execute blocks in parallel. Each block consists of a predefined number of threads. Threads in the same block can cooperate and share data using shared memory.

A novel GPU-based numerical solution of shallow water equations has been developed to simulate the hydrodynamics of both inland and coastal floods over complex natural domain topography across a wide range of spatial and temporal scales. This model is based on a first-order upwind finite volume method. The HLLC (Harten, Lax and van Leer) approximate Riemann solver [Toro, 1994] is adopted to calculate the flux because of its robustness, effi- ciency, and superior performance in handling discontinuities and wetting/drying processes. To preserve non-negative water depths and 'lake at rest' property (C-property), a robust positivity preserving method is used. A linear reconstruction and slope limiter are implemented, achieving second-order spatial accuracy. In order to increase the model efficiency and circumvent numerical instabilities caused by very small water depth especially near wet/dry boundaries, an explicit-implicit method is implemented for temporal discretization with operator splitting, i.e., a forward Euler for flux and bed slope and a backward Euler for friction slope. This model is used to generate the multiple return period flood maps for the continental United States. The performance of the model is demonstrated by comparing to the observation and published data.

Results

The 1959 Malpasset dam break in France is a bench mark test case to validate the shallow water flow models. The computation domain is discretized into 1148x612 cells at 15m resolution. To simulate the first 50 minutes after the

breach, the GPU-based model only used 6 seconds. Figure 1a shows the maximum flood depth and extent, which agrees well with the survey by police (the dark triangle in the figure). Figure 1b further shows the model compares well with the measured data of maximum water surface elevation at the gauges and the police survey locations.
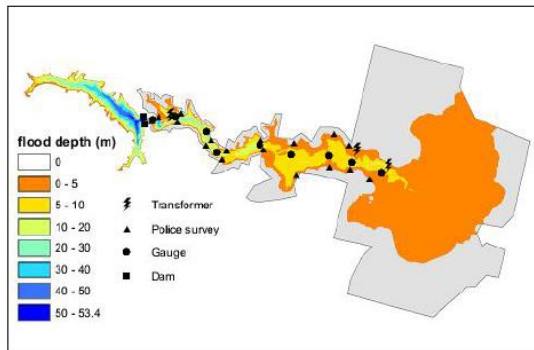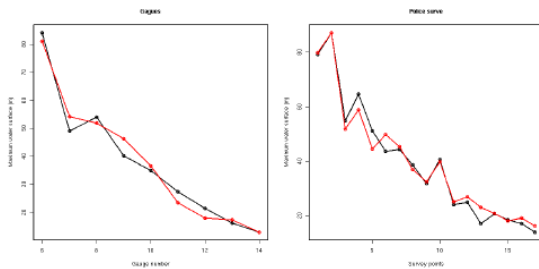

Figure 1a. Maximum flood depth and extent

Figure 1b. Maximum water surface elevation (black: observed; red: model)

By coupling with RMS rainfall-runoff and rout- ing models, the GPU-based model simulates the flood maps for multiple return periods among which there are 100-yr and 500-yr. Application of the GPU-based model on 2010 Tennessee shows the model compared well with the observations [Nash- ville.gov, 2010] (Figure 2). For a catchment with 1329x1053 cells at 30m resolution, the running time is around 2 minutes for the event. Furthermore, the simulated 100-yr flood maps are compared with the FEMA extent, BFE depth and USGS rating curve. An example is shown in Figure 3. The full paper will show the complete view of model performance and the flood risk for the continental United States.

Conclusions and Future Work

In short summary, comparing with the observations and the state-of-art models, the RMS GPU-based numerical model shows robust performance with significantly higher computational efficiency. Pow- ered by this GPU-based model and coupled compu- tations, an accurate and comprehensive view of the flood risk is presented for the continental United States.
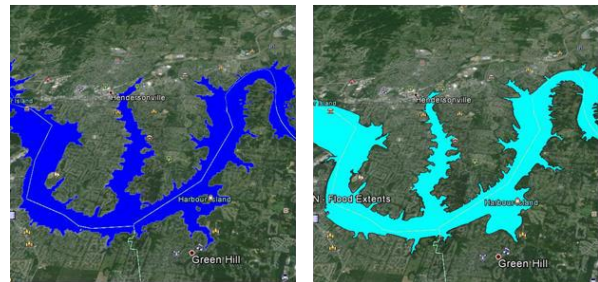

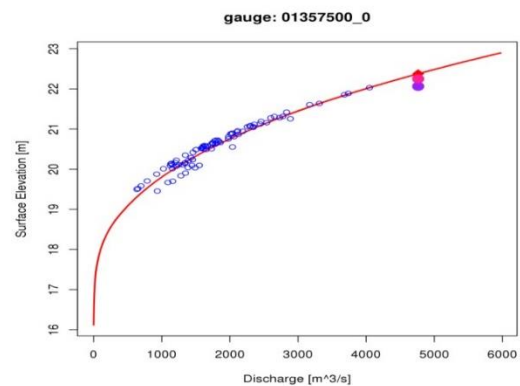*Figure 2.* 2010 Tennessee flooding (left: model; right: ob- served)

Figure 3. 100-yr water surface elevation (blue circle: observa- tion; red line: rating curve; purple dot: model; pink dot: BFE)

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Adding Contaminant Transport Capabilities to a Modular Hydrological Modelling Framework

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Key words: hydrological model; transport; compartment modelling

Introduction

The hydrological modelling framework Raven is a flexible modelling tool for semi-distributed simulation of watershed hydrology. Raven is unique in its adaptability – any modelling decision (e.g., discretization approach, algorithmic representation of physical processes, generation and interpolation of forcing functions, parameter generation, etc.) is userspecified and may be modified from the input files. This enables application to a variety of landscape types and scales, but also enables testing of model choices, hypothesis testing about model structure and function, and identification of the influence of model structural uncertainty upon model output.

The open-source object-oriented software code has recently been updated to additionally support the simulation of advective-dispersive-reactive transport of constituents with catchments and in the surface water network. Uniquely, the transport algorithm has been developed such that it works – without processspecific revision – with arbitrary configuration of modeled hydrologic processes. This means that new or revised algorithms for moving water (either hydrologic process or routing algorithms) may be added without modification of the transport code. This is only possible due to Raven's unique abstraction of hydrologic process and routing algorithms. The transport capabilities of Raven are here benchmarked and demonstrated for simulation of basins in British Columbia, Alberta, and Southern Ontario. Interesting applications include source identification of streamflow and nitrogen modeling in the Grand River, Ontario.

P1: Poster Session 1

Time: Tuesday, 21/Jun/2016: 6:00pm 8:00pm – Location: MSB Stone Lobby

Flexible Simulation Framework to Couple Processes in Complex 3D Models for Subsurface Utilization Assessment

Thomas Kempka, Benjamin Nakaten, Marco De Lucia, Natalie Nakaten, Christopher Otto, Maik Pohl, Elena Tillner, Michael Kühn
GFZ German Research Centre for Geosciences, Fluid Systems Modelling, Germany

Impacts of Climate Change on Electric Power Systems

Dariush Fooladivanda, Joshua Taylor
University of Toronto, Canada

Performance Evaluation of a Conceptual and a Numerical Integrated SurfaceSubsurface Hydrologic Model: A Comparative Study

Mohammad Bizhanimanzar, Robert Leconte, Mathieu Nuth
Université de Sherbrooke, Canada

Numerical Modelling of the Transport of Corrosion Agents in a Geological Repository

Scott Briggs[1], Brent Sleep[2], Jennifer McKelvie[3], Magdalena Krol[1]
[1]York University, Canada; [2]University of Toronto, Canada; [3]Nuclear Waste Management Organization

Inverse Modeling of Saltwater Intrusion in Heterogeneous Coastal Aquifers

Amir Safi[1], Mutasem ElFadel[1], Joanna Doummar[2], Majdi Abou Najm[1], Ibrahim Alameddine[1]
[1]Department of Civil and Environmental Engineering, American University of Beirut; [2]Geology Department, American University of Beirut

A Hybrid and Parallelized Advection-Diffusion-Reaction Model for Biofilm Growth in Porous Media

Artin Laleian[1], Albert J. Valocchi[1], Charles J. Werth[2]
[1]University of Illinois, UrbanaChampaign, United States of America; [2]University of Texas, Austin

A Hydro-Geochemical Model for Variably Saturated Flow with Multicomponent Gas Diffusion: Application to Predict Pollutant Fate and Transport in Technosols

Hossein Davarzani, Samuel Coussy, Geoffrey Boissard, Philippe Blanc, Philippe Bataillard French geological survey (BRGM), France

Simulation of Carboxymethyl Cellulosemodified Nanoscale Zerovalent Iron (CMCNZVI) Transport in Porous Media under Different Scenarios; Effects of Heterogeneity, Attachment, and Aggregation

Salman Sabahi, Brent Sleep
University of Toronto, Canada

Parameter Estimation for Modelling Microbial Degradation of Propylene Glycol Following a Monod Kinetics

Annette Dathe[1], Perrine M. Fernandez[2,1], Lars Bakken[2], Esther Bloem[1], Helen K. French[2,1]
[1]Norwegian Institute of Bioeconomy Research (NIBIO), Norway; [2]Norwegian University of Life Sciences (NMBU), Norway

Multirate Iterative vs Explicit Coupling Schemes for Coupling Flow with Geomechanics in Fractured Reservoirs: Efficiency vs Accuracy

Tameem Almani[1], Kundan Kumar[2], Gurpreet Singh[1], Mary Wheeler[1]

[1]The University of Texas at Austin, United States of America; [2]Department of Mathematics, University of Bergen, Norway

Modelling Of Twophase Flow in Roughwalled Fracture Using Level Set Method

Yunfeng Dai, Zhifang Zhou

Hohai University, China, People's Republic of China

Modelling and Parametric Study of Kinetic Interface Sensitive Tracer Transport in Laboratory Column Experiments

Alexandru Tatomir[1], Friedrich Maier[1], Alexander Kissinger[2], Johannes Hommel[2], Rainer Helmig[2], Martin Sauter[1]

[1]University of Göttingen, Germany; [2]University of Stuttgart, Germany

Modeling of DensityDependent Flow based on the Thermodynamically Constrained Averaging Theory

Timothy Weigand[1], Pamela Schultz[1], Deena Giffen[2], Carl Kelley[2], Cass Miller[1]

[1]University of North Carolina at Chapel Hill, United States of America; [2]North Carolina State University, United States of America

Improved Flowbased Capture Zone Delineation Using Flowsource

Mashrur Anam Chowdhury

University of Waterloo, Canada

Impacts of Soil Heterogeneity on the Transverse Dispersion Related Isotope Fractionation

Bruce S. Xu, Brent E. Sleep, Barbara Sherwood Lollar

University of Toronto, Canada

Impact of the ViscousCapillary Force Balance on Flow in Layered Porous Media

Yacine Debbabi, Matthew Jackson, Gary Hampson, Peter Fitch, Pablo Salinas

Imperial College London, United Kingdom

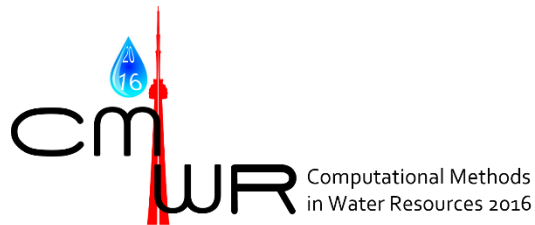## Impact of Fractures on Diffusion Dominated Reactive Transport: Application to Radioactive Waste Storage Studies

Benjamin Delfino[1], Jean Raynald de Dreuzy[2], Jocelyne Erhel[3], Benoit Cochepin[4], Yves Méheust[5]

[1]INRIA Rennes, France; [2]Géosciences Rennes; [3]Inria, Rennes; [4]ANDRA; [5]Géosciences Rennes;

Dfnworks: A HighPerformance Computing Suite for Subsurface Flow and Transport Modeling Using Discrete Fracture Network

Nataliia Makedonska[1], Satish Karra[1], Jeffrey D. Hyman[1], Hari S. Viswanathan[1], Carl W. Gable[1], Scott L. Painter[2]

[1]Los Alamos National Laboratory, United States of America; [2]Oak Ridge National Laboratory, United States of America;

Adaptive Higher Order Discontinuous Galerkin Methods for Strongly Heterogenous Twophase Flow in Porous Media

Birane Kane, Bernd Flemisch, Kunibert Siebert, Rainer Helmig
University of Stuttgart

Numerical Simulation of Turbulence and Air Entrainment in a Hydraulic Jump

S. Harada, S.S. Li
Concordia University, Canada

Formulation, Evaluation, and Validation of a Thermodynamically Contrained Averaging Theory Model for Two-Fluid-Phase Flow in Porous Media

Cass T Miller[1], James E McClure[2], Amanda L Dye[1], William G Gray[1]

[1]University of North Carolina, United States of America; [2]Virginia Tech, United States of America

Flow Regime Analysis for Geologic CO_2 Sequestration and Other Subsurface Fluid Injections

Bo Guo[1], Zhong Zheng[2], Karl Bandilla[1], Michael Celia[1], Howard Stone[2]

[1]Department of Civil and Environmental Engineering, Princeton University, United States of America; 2Department of Mechanical & Aerospace Engineering, Princeton University, United States of Ame

Flexible Simulation Framework to Couple Processes in Complex 3D models for Subsurface Utilization Assessment

Thomas Kempka, Benjamin Nakaten, Marco De Lucia, Natalie Nakaten, Christopher Otto, Maik Pohl, Elena Tillner, Michael Kühn

GFZ German Research Centre for Geosciences, Fluid Systems Modelling, Germany

Key words: multiphase fluid flow, geomechanics, geochemistry, heat transport, techno-economics, coupled simulation

Introduction

Utilization of the geological subsurface for production and storage of hydrocarbons, chemical energy and heat as well as for waste disposal requires the quantification and mitigation of environmental impacts as well as the improvement of georesources utilization in terms of efficiency and sustainability. The development of tools for coupled process simulations is essential to tackle these challenges, since reliable assessments are only feasible by integrative numerical computations. Coupled processes at reservoir to regional scale determine the behaviour of reservoirs, faults and caprocks, generally demanding for complex 3D geological models to be considered besides available monitoring and experimenting data in coupled numerical simulations.

Results and Conclusions

We have been developing a flexible numerical simulation framework that provides efficient workflows for integrating the required data and software packages to carry out coupled process simulations considering, e.g., multiphase fluid flow, geomechanics, geochemistry and heat transport (Figure 1). Simulation results are stored in structured data formats to allow for an integrated 3Dvisualization, result interpretation and data archiving. The main benefits in using the flexible simulation framework are the integration of data geological and grid data from any third party software package as well as data export to generic 3D visualization tools. Different spatial dimensions can be integrated, e.g., 0D batch with 3D simulations. User interaction is established via high-level programming languages. We present three case studies on the assessment of geological subsurface utilization based on different process coupling approaches and numerical simulations, i.e. hydrochemical [1] and hydromechanicalcouplings [2] as well as data integration with techno-economics [3].
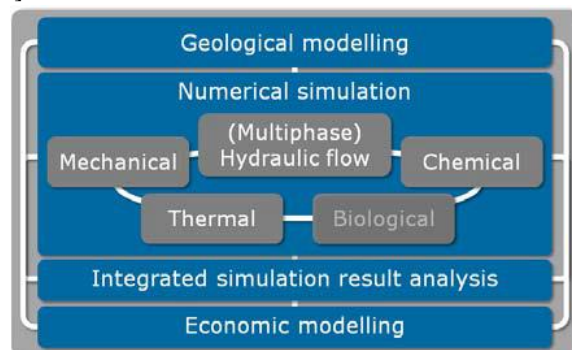

Figure 1: Flexible numerical simulation framework

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Impacts of Climate Change on Electric Power Systems

Dariush Fooladivanda, Joshua Taylor

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Key words: Climate change, water, energy

Introduction

Thermoelectric power plants are the major sources of power generation in several countries. The thermal energy conversion process used in these power plants is not highly efficient, and hence a large amount of the thermal input is converted into heat through the generation process. Dissipated heat will disrupt the operation of power plants. To improve the performance of power plants, several cooling systems, such as once- through and closed-loop systems, have been developed [1]. These cooling systems use large volumes of water for cooling, and reject waste heat either through air or though cooling water. Water use and waste heat at power plants have had several implications on climate and on ecological health of water resources worldwide [2].

Recently, several studies have been done on water use at power plants in the US based on field data [3]-[5]. In [1], Rutberg et al. propose a quantitative frame- work for evaluating the effects of changing technology on water use at power plants. The authors develop a system-level generic model of power plant water use with the objective of capturing the essential physics of the processes involved while minimizing computational complexity and number of input parameters. The model can be applied to fossil, nuclear, geothermal, and solar thermal plants, using either steam or combined cycles. The authors also present an application of the model to estimate water consumption at power plants. In [6], Lubega et al. use bond graphs to develop models that characterize the salient transmissions of matter and energy between the electricity, water, and wastewater systems. The proposed models enable engineers understand the coupling between a region's energy and municipal water consumption. Extensive work has been done on water-energy nexus, but none of them models the coupling between electricity generation and climate change constraints accurately.

Climate change has exposed the vulnerability of power utilities to low water availability and to high river temperatures for thermoelectric power plants. We focus on a large geographical area whose power system is controlled by an operator that relies on a set of thermal power plants to generate electricity. The thermo- electric power plants take their cooling water from a river shared by all the power plants, for cooling purposes. We study the multi-period optimal power flow problem in the presence of cooling water scarcity and climate change constraints. More precisely, we consider water constraints on the amount of water that can be consumed by the power plants, and heat constraints on the amount of waste heat that be transferred to the environment by the power plants. We then propose a general multi-period optimal power flow framework. The proposed problem is NP-hard even if we model the electric system using the linearized power flow model. We develop numerical techniques to compute sub-optimal solutions to the proposed problem, and to draw engineering insights. Finally, we show the impact of water availability, cooling water temperature, and heat constraints on electricity generation in a real-scenario.

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Performance Evaluation of a Conceptual and a Numerical Integrated Surface-Subsurface Hydrologic Model: A Comparative Study

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Key words: Integrated hydrologic models, MOBIDIC, MIKE-SHE

Over the past few decades substantial researches have been devoted to the development of numerically based coupled surface-subsurface hydrologic models. A recent intercomparison by Maxwell et al., [1] demonstrated the closer results between the models in infiltration excess (Horton) runoff generation mechanism than in saturation excess (Dunne) runoff generation or heterogeneous cases. In these models, the adapted form of Richard's equation (1D or 3D) is coupled to a variant of Saint-Venant surface flow equation (Kinematic wave or diffusion wave) and the resulted system of equations is solved using numerical methods. However, operational applicability of such models is made complicated due to intensive computational demand and data availability. In this study, the performance of a conceptual based integrated surface-subsurface model, namely, MOBIDIC [2], and a numerically based integrated hydrologic model , MIKE-SHE [3] in a virtual test cases i.e., a 3km×3.1km catchment were compared. The major difference between two models lies in representation of the unsaturated flow. While MIKE-SHE uses the one dimensional Richard's equation, MOBIDIC conceptualizes the unsaturated flow's process using two functionally different reservoirs (gravity and capillary) based on soil pore size. Using two synthetic hyetograph (a triangular rainfall with peak intensity of 1mm/min and base time of 60 minutes followed by 180 minutes of recession in Horton runoff generation case and a 1.5mm/min uniform rainfall for 240 minutes followed by 120 minutes of recession in Dunne runoff generation) on three different soil types i.e., loam, clay loam and sand, performance of two models in Horton and Dunne runoff generation mechanisms as well as dynamic of soil moisture and water table fluctuations are evaluated. The simulation results of the Horton runoff phase demonstrates larger volume of produced runoff in MOBIDIC due to simplifications in the infiltration mechanism.

However, in Dunne runoff generation phase both models produce the same outflow peak even though the soil layer becomes saturated earlier in MOBIDIC. It is concluded that improvements towards the infiltration mechanism and also extension of the conceptualized single layer dual reservoir unsaturated soil moisture approach to the multiple soil layers would reduce the discrepancies of the results between two models.

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Numerical Modelling of the Transport of Corrosion Agents in a Geological Repository

Scott Briggs[1], Brent Sleep[2], Jennifer McKelvie[3], Magdalena Krol[1]

[1]York University, Canada; [2]University of Toronto, Canada; [3]Nuclear Waste Management Organization

Abstract

Canada's Nuclear Waste Management Organization (NWMO) is designing an engineered barrier system (EBS) to contain and isolate used nuclear fuel from people and the environment. Due to the length of the EBS design life, computer models must be used to predict EBS evolution over thousands of years. In this study, the performance of the corrosion barrier, within the EBS, and its response to disturbances caused by the changing chemistry around and repository is considered. Modeling was undertaken to develop understanding of the fundamental evolution of the EBS by assessing the transport of corrosion agents such as sulphide.

Computer modeling permits accelerated evaluation of the performance of the EBS. This minimizes the need for expensive and difficult to implement long duration tests, while still identifying technology issues. The model in this study was developed using COMSOL Multiphysics, a finite element software package. The model is three dimensional and parametric (allowing for quick changes to the model geometry) and simulates the diffusive transport of sulphide within the NWMO EBS. The developed model simulates the entire NWMO placement room, as well as, a stand-alone used fuel container (UFC) and includes conservative assumptions such as a fully saturated system and constant concentration boundary conditions. For the Mark II UFC and Mark II placement room design, an optimal mesh size was chosen to maximise solution accuracy while still converging within a reasonable (hours) time scale.

Validation of the software package was conducted against analytical solutions of diffusion in 1D, 2D and for cylindrical and spherical shells in 3D. Mesh size and geometry are controlling factors that dictate the accuracy of the solution. Reducing mesh size increases solution accuracy at the expense of computational requirements. Mesh geometry also plays a role controlling the direction from which a solution converges, for example two geometries are investigated which over-predict and under-predict diffusion respectively. However, as these meshes are refined, they both converge to the same solution.

The model showed that with a constant concentration boundary conditions applied at the host rock and at the UFC surface, the sulphide flux driven through the EBS was the highest at the semi-spherical end caps. This demonstrates the importance of 3D modelling, highlighting the non-linear diffusion through semi- spherical surface

Inverse Modeling of Saltwater Intrusion in Heterogeneous Coastal Aquifers

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Key words: Saltwater intrusion, heterogeneity, Pilot points

Abstract

In this study, a 3D variable-density flow and solute transport model was used to assess the dynamics of saltwater intrusion under anthropogenic interventions and global climate change, and their synergistic impacts. The model was also used to examine the potential impacts of heterogeneity on the exacerbation of saltwater intrusion by linking the use of spatial distribution of salinity and inverse modeling based on an advanced pilot parameterization for characterizing spatial heterogeneity. The study area consists of a karstified limestone aquifer of Cretaceous age located along the Eastern Mediterranean (Beirut, Lebanon) and overlain by Upper Tertiary and Quaternary unconsolidated deposits. The choice of the proper pilot points distribution to be adopted depended on the least difference between simulated results and observed head and salinity data. Since the number of pilot points is much larger than the number of head observations, a decomposition technique was used to define a small number of model parameters referred to as super parameters to be estimated using available head observations to reduce the number of model runs. However as the concurrently use of both pilot points and the decomposition technique may cause structural noise that leads to bias estimation of super parameters, Tikhonov regularization was included in the model parameterization to safeguard the model against such numerical instability. Prior to the transient calibration, a steady-state calibration for historical water levels was relied upon to reduce potential numerical instabilities associated with inadequate initializing base parameters in the transient calibration.

The transient calibration results suggested a high degree of heterogeneity in the middle parts of the aquifer and along western coastlines with specification of a high hydraulic conductivity and low storativity in fault networks. Figure 1 presents a water velocity contour map to understand the dominant mechanism of intrusion and the role of heterogeneity in forming and controlling intrusion over time.
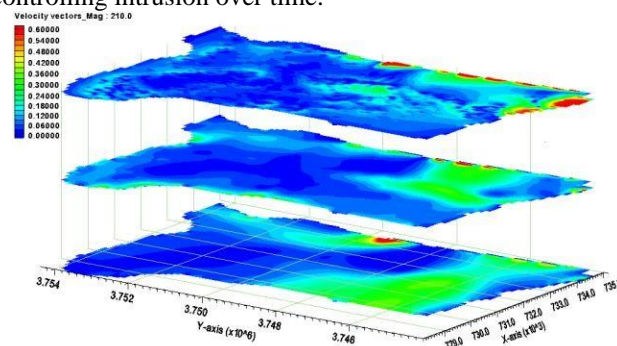

Figure 1: Water velocity contour map

While the lateral encroachment of salinity is of most concern due to high horizontal hydraulic conductivity in the wave direction, the final outcome of the model supports a potential for upward leakage of salinity due to potential fast flow pathways in fractured networks that tend to exacerbate the vertical movement of salinity within the macropores of the soil matrix across the middle parts of the domain as well as the northwestern coastline (Figure 2).
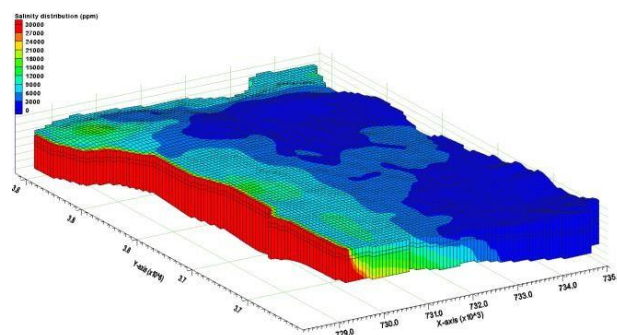

Figure 2: Salinity distribution (TDS concentration) in the pilot aquifer

This stresses that while anthropogenic activities, particularly groundwater abstraction, plays a major role in encroachment of salinity, a high degree of heterogeneity also exhibited a significant impact on the exacerbation of this intrusion.

A hybrid and Parallelized Advection-Diffusion-Reaction Model for Biofilm Growth in Porous Media

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Key words: hybrid, mortar, biofilm

Pore structure is uniquely altered by the presence of biofilm, thereby affecting solute transport within the porous medium. While pore-scale models capture these important dynamics, they are computationally expensive, making them infeasible for large domains, or when details of the pore geometry are unknown. The complex nonlinear feedbacks among transport, reaction, and biofilm growth lead to changes in porosity and permeability that cannot be captured by fully continuum models. In some applications, such as modeling groundwater contaminant plumes, hybrid models, which couple pore-scale and continuum-scale models, may effectively reduce computational expense while preserving accuracy. Because most reaction occurs along the plume fringe, or mixing zone, this region is resolved at the pore-scale with a fine grid. Away from the mixing zone, a continuum approximation using a coarser grid is sufficient and less computationally intensive. We present a hybrid and parallelized two-dimensional model for biofilm growth consisting of connected pore-scale and continuum-scale subdomains, which extends prior work [1] to include liquid advection.

Because the time scale of biofilm growth is much slower than those for flow and transport, the latter processes can be modeled as steady state. New steady state flow and concentration fields are computed following significant biofilm growth that alters the permeability. In the pore-scale subdomain, the velocity field is determined with a parallelized lattice Boltzmann method, the solute concentration field is determined with a finite volume method utilizing a parallel direct solver, microbial solute utilization is nonlinear and given by dual Monod kinetics, and biofilm spreading is determined by a cellular automaton method [2]. In the continuum-scale subdomains, the velocity field and solute concentration field are determined by finite volume methods solving upscaled governing equations. A mortar space method [3] is employed on boundaries between pore- and continuum-scale subdomains to ensure continuity of fluid and solute mass. We find the hybrid model has a significantly reduced CPU run time relative to a complete pore-scale model, while producing a consistent result in terms of biofilm growth and distribution.

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A Hydro-Geochemical Model for Variably Saturated Flow with Multicomponent Gas Diffusion: Application to Predict Pollutant Fate And Transport in Technosols

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Key words: hydro-geochemical modeling, Technosol, pollutants

Introduction

The prediction of the long term trace element transport in Technosols, defined as soils containing at least 20 % of human-made materials within the 100 cm upper soil horizon, would be a way to anticipate land management. These soils, usually abandoned for decades, contain pollutants resulting from industrial processes. The main objective of this study is to develop a model to predict the hydro-geochemical and mechanical evolutions in Technosols. In this study, the model developments have been made in order to consider the multi-component soil gas phase diffusion whereas the original COMSOL- Phreeqc coupling model [1] does not take it into account. Therefore, the coupling model is able to (i) take into account soil hydro-geochemical heterogeneity (such as permeability and porosity contrasts), (ii) manage multi-component gas diffusion, consumption and generation in unsaturated soil and (iii) take climatic variations, such as rain infiltration, into consideration.

Model concept and validation

The COMSOL® and IPhreeqc procedures alternate for the calculation of liquid water flow, gas and solute transport and reactions using a non-iterative sequential split-operator approach. Data from the output of one procedure is passed back to the Matlab® workspace and reformatted for the following procedure. The gas phase mole numbers and volume are updated using IPhreeqc's method GAS_PHASE_MODIFY. As for flow and transport calculations, a function is used to create valid initial conditions for gas transport calculations in COMSOL. The coupling developed model has been validated using CrunchFlow [2] in a 1-D and fixed soil water saturation case.

Model application and results

The coupling model was applied on a case study consisting in a Technosol developed on dredged sediments. The mineralogical compositions of two samples, from fractured oxidation crust and soil block center, were characterized by X-Ray Diffraction spectroscopy. The mineralogical assemblage of the block center sample is used as the composition of the initial sediment deposited 30 years ago. The model axisymmetric geometry consists of a heterogeneous soil profile with a fracture region (about 0.5 m large, 1 m depth). The atmospheric oxygen and carbon dioxide diffuse permanently into the soil and fracture over the time at their respective diffusion coefficients. The modeling results over 30 years have shown that the Technosol weathering leads to dissolution of galena with consumption of the soil oxygen, as well as precipitation of lead carbonates and formation of ferrihydrite. These mineralogical transformations take place more in poorly saturated zones in the profile such as cracks and soil surface. An example of the results is shown in Figure 1 for gaseous oxygen diffusion into the soil and related kinetic of galena dissolution after 30 years. The model can capture well the soil evolution trend at least for about 30 years.
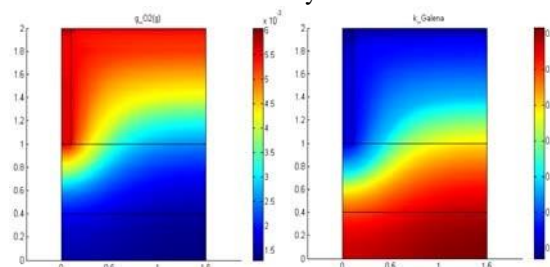

Figure 1: Oxygen concentration in soil air (mol/L) and galena concentration (mol/kgw) after 30 years.

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Computational Methods
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Simulation of Carboxymethyl Cellulosemodified Nano-Scale Zero Valent Iron (CMCNZVI) Transport in Porous Media under Different Scenarios; Effects of Heterogeneity, Attachment, and Aggregation

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Key words: CMC-NZVI transport, aggregation, attachment, heterogeneity

Different parameters and mechanisms influence carboxymethyl cellulose-modified nano-scale zero-valent iron (CMC-NZVI) transport in the subsurface. In this study the effect of particle-collector attachment, particle-particle attachment, and physical heterogeneity of porous media were considered. To calculate particle-particle attachment, an empirical correlation was used to modify the rate of aggregation of nanoparticles. In addition, the effect of aggregation on the attachment of nanoparticles to collectors was evaluated over the time and space domain. Meanwhile, the effect of change in hydraulic conductivity of porous media was taken into account. The change in hydraulic conductivity influences attachment patterns and CMC-NZVI transport.

Parameter Estimation for Modelling Microbial Degradation of Propylene Glycol Following a Monod Kinetics

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Key words: parameter estimation, microbial degradation, Monod kinetics

Aim of the presented study is to model aerobic degradation of propylene glycol (PG), which is used in large amounts at airports during winter conditions to keep the runways and aircrafts ice-free. PG is relatively easily biodegradable in the subsurface but the oxygen demand is high. Microbial degradation of the substrate (PG and decayed biomass) was modeled following a Monod kinetics using the FME (Flexible Modelling Environment) package of R (Project for Statistical Computing). The model was calibrated against continuous measurements of O_2 depletion and CO_2 production obtained from an incubation experiment performed in the laboratory. Initial concentrations of O_2, CO_2 and PG are known and microbial yield and stoichiometric constants can be calculated from the measurements. Parameter values for the initial microbial population size, maximum microbial growth rate, the half saturation constant, and microbial degradation and respiration rates were estimated using the FME package. The model accounts for carbon from the substrate incorporated into the biomass. The long- term goal of implementing microbial degradation of a contaminant into a soil water and solute transport model is still a challenge because of the often ambiguous parameter space.
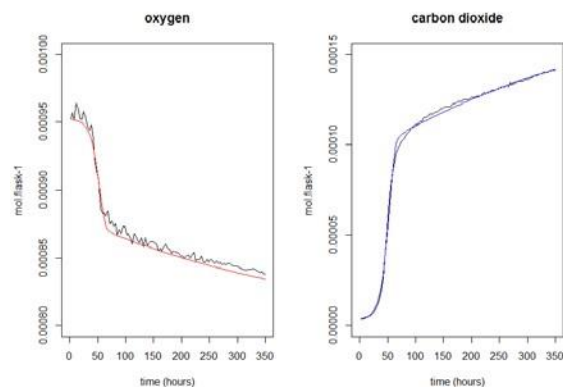

Figure 1: measured (black line) and modelled (red and blue lines) oxygen and carbon dioxide masses for one flask incubated with propylene glycol.

Multirate Iterative vs Explicit Coupling Schemes for Coupling Flow with Geomechanics in Fractured Reservoirs: Efficiency vs Accuracy

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Key words: Poroelasticity, Fractures, Iterative and explicit coupling, Multirate schemes, Efficiency, Accuracy

Introduction

Coupling of geomechanics and flow in fractured poroelastic media has several applications including hydrocarbon production, subsidence events, ground water remediation, enhanced geothermal systems, solid waste disposal, and hydraulic fracturing [2]. In addition, accurate computations for both flow and deformations are required for uncertainty quantification incorporating the geomechanical parameters. The geomechanical effects, as a result of the influence of deformations in the porous media driven by the changes in pore pressure, can be very important especially in the case of stress-sensitive and fractured reservoirs. The fact that fractures present in porous media can severely influence flow profiles and subsequently mechanical deformations motivates the development of efficient and convergent coupling schemes for coupling flow with geomechanics in fractured reservoirs.

Multirate Iterative vs Explicit Coupling

In this work, we compare the efficiency and accuracy of two major coupling approaches: iterative versus explicit coupling schemes. For both schemes, we consider multirate coupling, the one in which the flow takes several finer time steps within one coarser mechanics time step. Multirate schemes better exploit the different time scales of mechanics and flow by taking advantage of the fact that the mechanics problem can cope with a much coarser time step compared to the flow problem. For poro-elastic media, this introduces two different time scale levels, whereas in fractured poro-elastic media, three nested time-scale levels are introduced, as the fracture problem yet necessitates a much finer time step compared to the time step used for the flow in the matrix.

Model Equations

In this work, we assume a quasi-static Biot model in which fractures are treated as possibly non-planar interfaces. In particular, fractures are modeled explicitly as a lower dimensional geometric object, and the flow inside a fracture is described by a lubrication type of equation, coupled to the quasi-static Biot's equation in the reservoir matrix through a leakage term. Hence, the introduced multirate iterative coupling scheme is an adaptation of the classical fixed- stress split algorithm, due to the presence of fractures [1].

Theoretical & Numerical Results

For multirate iterative coupling schemes, inspired by the previous work of Mikelic and Wheeler [3], and the work of Girault, et al [1], we show that the multirate iterative coupling scheme is a Banach fixed point contraction. For multirate explicit coupling schemes, we consider stability rather than convergence, and show that under mild assumptions on the initial data, the corresponding explicit coupling scheme is theoretically stable. Numerically, we observe that multirate explicit coupling schemes reduce CPU time efficiency, with acceptable level of accuracy compared to their counterpart iterative coupling schemes. However, the accuracy and time savings of explicit coupling schemes over iterative coupling schemes are problem dependent.

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Modelling of Two-Phase Flow in Rough-Walled Fracture using Level Set Method

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Key words: Two-phase, Level Set Method (LSM), Fracture, Contact Angle, Continuum Model

Abstract

To describe the flow characteristic of rough-walled fracture level displacement of immiscible fluid accurately, an incompressible two-phase flow model with interfacial tension and nonzero contact angle is built in Comsol. The moving interface of the oil and water is tracked by using the Level Set Method (LSM). The wettability of the rough wall is illustrated by defining the contact angle and the slip length. The curve of capillary pressure-water saturation is created by using different invasion oil pressure during a sudden drainage. The simulation results using the LSM are compared with those results using the continuum model.

Modelling and Parametric Study of Kinetic Interface Sensitive Tracer Transport in Laboratory Column Experiments

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Keywords: Fluid-fluid interfacial area, KIS tracers, model validation, CCS, geological storage of CO_2
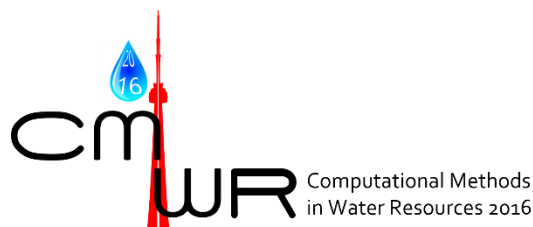
Abstract

Kinetic interface sensitive (KIS) tracers have the potential to describe the evolution of fluid-fluid interfaces advancing in two phase porous media systems. Intended to offer answers about the CO_2 plume movement and the efficiency of trapping in geological carbon storage reservoirs, KIS tracers are first tested in controlled laboratory conditions.

The aim of this study is to validate the newly developed numerical model with laboratory column experiments using an analog CO_2 – brine system with n-octane – water as working fluids. An initial model described in Tatomir et al. (2015) is extended from a two phase four component (2p4c) to a two phase five component (2p5c) model to account for mass depletion of the ester (KIS) component. The KIS tracer is dissolved in n-octane, which is injected as the nonwetting phase. Subsequently, the KIS tracer follows a hydrolysis reaction over the n- octane – water interface resulting in an alcohol and an acid which are both water soluble. The n-octane – water interfacial area is described with constitutive-relationships derived from the Brooks- Corey model and applying pore scale, or pore network models (Joekar-Niasar et al., 2008).

The KIS model is implemented into the DuMux (www.dumux.org) numerical framework using the box scheme for spatial discretization and the implicit Euler scheme for the time discretization.

Furthermore, we investigate the behavior of the KIS tracer in the column experiment with regard to different injection rates. Through parametric studies, the 2p5c KIS numerical model is validated with the experimental results. This result indicates that the model can successfully be used for further experiments and can be extended to real reservoir conditions with supercritical CO_2 – brine systems.

Modeling of Density Dependent Flow based on the Thermodynamically Constrained Averaging Theory

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The thermodynamically constrained averaging theory (TCAT) has been used to formulate general classes of porous medium models, including new models for density- dependent flow. The TCAT approach provides advantages that include a firm connection between the microscale, or pore scale, and the macroscale; a thermodynamically consistent basis; explicit inclusion of factors such as a diffusion that arises from gradients associated with pressure and activity and the ability to describe both high and low concentration displacement. The TCAT model is presented and closure relations for the TCAT model are postulated and a parameter estimation is performed on a subset of the experimental data. Due to the sharpness of the fronts, an adaptive moving mesh technique was used to ensure grid independent solutions within the run time constraints. The optimized parameters are then used for forward simulations and compared to the set of experimental data not used for the parameter estimation.

Improved Flow-Based Capture Zone Delineation Using Flowsource

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Key words: capture-zone delineation, directed acyclic graphs, transient, steady-state

Abstract

FlowSource is a capture zone delineation tool that uses directed acyclic graphs to represent groundwater flow path information. This enables it to volumetrically quantify where well water is coming from without the use of particle tracking or advective transport simulation. Thus, while most conventional capture zone delineation methods, which rely upon particle tracking, can provide information about which points within an aquifer are hydraulically connected to a well, FlowSource can provide explicit information about the degree of that connection.

However, an important limitation of FlowSource is that it implicitly assumes fully mixed cells, which can lead to numerical dispersion issues [1]. To address this limitation, a novel method was developed to track the distribution of groundwater flow within a threedimensional rectilinear cell by recreating the streamtube geometry within the cell (Figure 1 illustrates the streamtube geometry recreation for flow field with four inflows and two outflows). For any given set of flows at the cell faces, the volumetric flow from each inflow face to each outflow face is analytically evaluated using an extension of the equations from Pollock's semi-analytical particle tracking method [2].

This study demonstrates the use of FlowSource with our amendments in (1) delineating steady state flowbased capture zones of point abstractions and surface water bodies and, (2) capturing the impacts of transient conditions (i.e., changing recharge, changing water levels in the stream) on these capture zones.
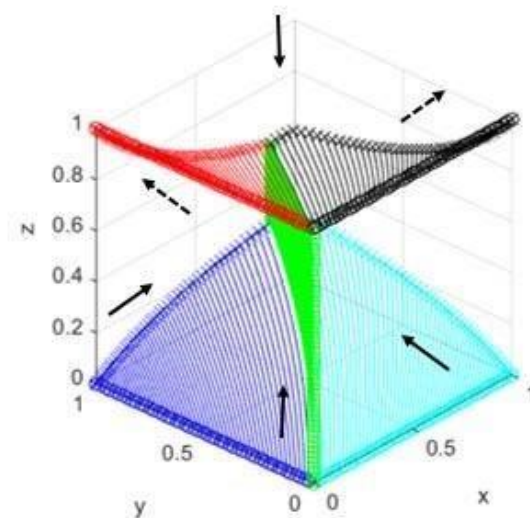

Figure 1: Streamtube geometry reconstruction of a flow field with four inflows and two outflows. Inflows shown with solid black arrows and outflows shown with dashed black arrows

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Impacts of Soil Heterogeneity on the Transverse Dispersion Related Isotope Fractionation

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Key words: stable isotope fractionation, dispersion, heterogeneity

Introduction

Use of compound specific isotope analysis for assessment of intrinsic biodegradation is now an accepted practice. Typically, in the use of isotopic signatures to assess biodegradation it is assumed that biodegradation is the only process causing significant isotopic fractionation. The impact of diffusion on isotopic fractionation due to differences in molecular weights of isotopologues has been demonstrated for systems that are diffusion dominated. However, processes such as mechanical dispersion may mask the detectable effects of molecular diffusion on isotopic fractionation. In considering transverse dispersion, transverse dispersivities may be small and may also be compound specific [1] due to the effect of molecular diffusion on transverse mixing. If transverse dispersion coefficients (D_T) are compound specific, this may accentuate isotopic effects at the local scale. In this study, the effects of transverse dispersion related isotope fractionation (TDRIF) are evaluated at the field scale using upscaling with compound specific D_T values.

Modeling Approach

The numerical model MT3DMS is coupled with fundamental isotope equations, including compound specific transverse vertical dispersion [1] to simulate transport of benzene isotopologues in heterogeneous porous media. The impacts on TDRIF at the field scale of standard deviation in log normally distributed soil permeability ($\sigma log_{10}k$) and of correlation length are investigated through flux-related upscaling [2].

Results and Conclusions

Typical simulation results for two realizations of simulated spatial development of $\delta^{13}C$ of benzene for 300 days conservative transport are illustrated in Figure 1 for different levels of heterogeneity. A range of values of $\sigma log10k$ from 0.3 to 1.0 were investigated for correlation length values varying by a factor of two. The upscaling results show that increasing heterogeneity results in

reduced TDRIF. For $\sigma log10k$ of 0.3 with compound specific D_T, TDRIF may be detectable on the lateral plume boundaries with high resolution discrete sampling strategies. At a $\sigma log10k$ level of 1.0, TDRIF is not detectable even on the lateral plume boundaries using a metric of ± 2 ‰ for detectable isotope effects. There was not a significant effect of correlation length on TDRIF over the range of correlation lengths investigated.
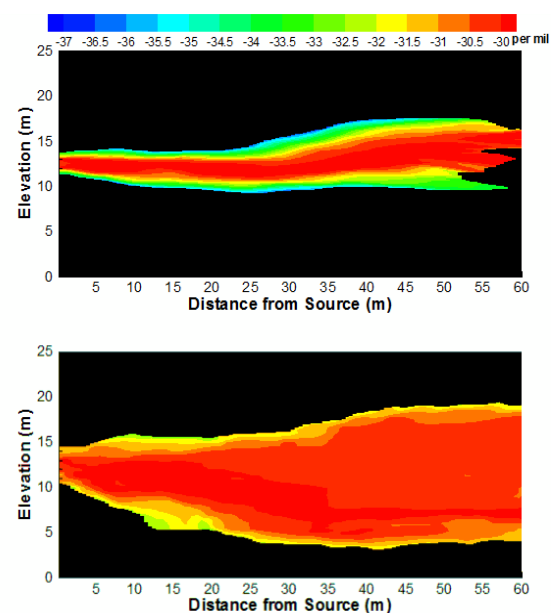

Figure 1: $\delta^{13}C$ of benzene after 300 days conservative transport in 2-D heterogeneous simulation domains. Source $\delta^{13}C$ = -30‰. Top figure: $\sigma log10k$ = 0.3, Bottom figure: $\sigma log_{10}k$ = 1.0.

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Impact of the Viscous Capillary Force Balance on Flow in Layered Porous Media

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Key words: Layered porous media, Dimensionless numbers, Crossflow, Capillary trapping

Motivation

Geological heterogeneity occurs over a broad range of length scales, from the pore- to the reservoir-scale, and exerts a first-order influence on multiphase flow relevant to geological carbon storage and hydrocarbon recovery. Most studies that investigate the interaction of multiphase flow and geological heterogeneity focus on a particular reservoir, outcrop or heterogeneity type, using a particular suite of fluid and rock properties and a particular flow scenario. It is usually not possible to extrapolate the results of such studies to new or alternative cases; moreover, they fail to provide simple criteria that can be used to rapidly assess the impact of heterogeneity on flow prior to the development of detailed models.

An alternative view is that geological heterogeneities can be captured by a number of key dimensionless geometries observed in numerous depositional environments and over a broad range of length scales. Likewise, flow through a particular type of heterogeneity geometry can be captured by a small set of dimensionless numbers. We investigate here whether the interaction between flow and geological heterogeneity can be captured by a small set of dimensionless heterogeneity models and dimensionless numbers. The aim is not to predict exactly the behaviour of a given system; rather, it is to (i) predict how the system will change as parameters are varied, and (ii) provide a framework to understand the behaviour of complex systems.

Focus of this work

Here we focus on the impact of viscous and capillary forces on flow parallel and perpendicular to continuous layers of contrasting material properties. Such layers are a ubiquitous geological heterogeneity observed at many length scales, including lamination (millimetre-thick layers), bedding (centimetre- to metre-thick layers) and laterally extensive genetic stratigraphic units that may correspond to flow zones in groundwater aquifers.

We define a set of dimensionless numbers, some of which are common to flow both parallel and perpendicular to layering, such as the longitudinal permeability ratio σx and the ratio R_s of the storage capacities (moveable pore volumes, MPV) in each layer, and some of which are specific to a given flow direction, such as the dimensionless capillary to viscous ratios N_{cv} defined differently for layer parallel and layer-perpendicular flow, and the effective aspect ratio R_L that quantifies crossflow for layer-parallel flow. We examine how variations in the dimensionless numbers affect the trapping efficiency, defined as the fraction of the MPV occupied by the injected phase after 1 MPV injected. The results are directly applicable to geological carbon storage.

Results

We find that the flow behaviour – expressed here in terms of the trapping efficiency – is clearly controlled by the dimensionless numbers. For example, when flow is perpendicular to layering, we show that heterogeneity only influences flow when capillary forces are significant ($N_{cv} > 0$). As N_{cv} is increased, a larger fraction of the non-wetting phase is trapped if the layers have contrasting capillary pressure curves 1. When flow is parallel to layering, both viscous and capillary forces are important. Viscous forces cause the ratio of the fluxes along each layer to be equal to the permeability ratio σx and, in the viscous limit ($N_{vc} = 0$), heterogeneity reduces storage efficiency if $\sigma x \neq R_s$ 2. As capillary forces become more significant (N_{cv} increases) and if crossflow between layers can occur ($R_L > 0$), the storage efficiency also increases in response to capillary crossflow and reaches a maximum at a given N_{cv}. At lower N_{cv}, capillary crossflow is reduced and the injected phase preferentially moves through the high permeability layers, yielding reduced storage efficiency. At higher N_{cv}, the benefit of crossflow is outweighed by along layer diffusion of the injected phase, yielding reduced storage efficiency 3.

Application of the results

The results allow for a rapid assessment of potential flow

regimes and of their consequences in terms of storage efficiency. The results can additionally be used to assist the scaling of laboratory core-flooding experiments.
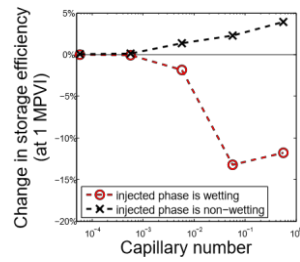

Figure 1: Change in storage efficiency (relative to efficiency obtained without heterogeneity) for flow across an alternation of identical layers vs. the capillary number.

Impact of Fractures on Diffusion Dominated Reactive Transport: Application to Radioactive Waste Storage Studies

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Key words: Fractured network, Porous media, Reactive transport, Radioactive waste storage

Abstract

Even in small numbers, fractures must be carefully considered for the geological disposal of radioactive wastes. They critically enhance diffusivity, speed up solute transport, extend mixing fronts and, in turn, modify the physicochemical conditions of reactivity around possible storage sites. Fractures occur at several places in the cement surrounding the containers and in the Excavation Damaged Zones (EDZ) of the galleries. They even occur in clays such as the French Callovo-Oxfordian formation mostly because of the desaturation conditions induced in the operational time of the galleries. Numerous studies addressing various applications (e.g. radioactive waste storage, CO_2 sequestration, geothermal storage, hydrothermal alteration) have shown that fractures cannot be simply integrated within an equivalent porous medium through a simple enhancement of its petro-physical properties (porosity and permeability). Fractures cannot either be accurately identified so that fully deterministic modeling approaches are precluded. We propose a combined numerical and experimental approach to determine the influence on reactivity of typical fracture patterns classically found in radioactive waste applications. We investigate the possibility of applying simplified modeling frameworks on the basis of some key properties:

(i) transport is mostly diffusive and much faster in the fractures than in the porous matrix [1],

(ii) reactions occur predominantly in the matrix because of the large surface to volume ratio favorable to dissolution/precipitation processes,

(iii) the reactivity within the surrounding matrix isat equilibrium, or equivalently much faster than the diffusive transport. Reactivity is assumed transport- limited rather than rate-limited.

Based on the separation of the fracture and matrix domains, we develop a reactive transport model with diffusion conditions differing between the fracture and in the matrix, appropriate flow-rock interactions at equilibrium in the matrix and fracture-matrix exchange conditions at their interface. Using preferentially existing software, we propose simulation methods that comply with much faster diffusion in the fracture than in the matrix, and validate them against elementary fracture structures and a simplified reactivity. We intend to use the developed methods on different fracture structures to simulate reactivity over long periods of time. We determine the possible relevance of the most classical simplified frameworks for fracture matrix including:

(i) fully homogenized models with porosity, permeability and surface adapted to volume ratio to recover localization effects,

(ii) models with isolated fractures within ''infinite matrix" assuming implicitly the localization of reactivity in the immediate vicinity of the fracture [2],

(iii) double porosity models characterized by single or multiple exchange coefficients [3].

Following the outcome of the numerical simulations, we will investigate experimentally the most critical limitation of reactivity. It might a priori be the fracture to matrix exchange law especially if the fracture is desaturated and the matrix saturated. Within the radioactive waste framework, we aim at including fractures in the safety assessment workflow. We intend to determine to which extent fractures facilitate the access to reactive surfaces, the increase in bulk reactivity, the corrosion potential and the perturbation of the chemical conditions. We frame as much as possible the reference simulations in realistic physical and chemical conditions including the main operational phases of the radioactive waste repository. Results will be reported as comprehensive evolution scenarios.

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dfnWorks: A HighPerformance Computing Suite for Subsurface Flow and Transport Modeling Using Discrete Fracture Network

Nataliia Makedonska[1], Satish Karra[1], Jeffrey D. Hyman[1], Hari S. Viswanathan[1], Carl W. Gable[1], Scott L. Painter[2]

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Key words: Discrete Fracture Network, Subsurface Flow and Transport, Unconventional hydrocarbon extraction

Flow and solute transport modeling using discrete fracture network (DFN) is an important approach for understanding the subsurface flow and transport in impermeable rock, where fractures provide dominant flow and transport pathways. It is challenging to obtain accurate transport results in three-dimensional DFNs because of the high computational burden and difficulty in constructing a high-quality unstructured computational mesh on simulated fractures. A recently developed computational suite, dfnWorks [1], generates discrete fracture networks of planar polygons; constructs a high quality conforming Delaunay triangulation of the intersecting fractures in DFNs; assigns fracture properties, such as aperture and permeability, using geostatistics; sets boundary and initial conditions; solves pressure and flow in single or multi-phase fluids using the parallel finite volume approach, PFLOTRAN [2], which is locally mass conserving and thus eliminates mass balance problems during solving for transport; simulates particle transport using Lagrangian particle tracking approach. dfnWorks enables accurate flow and particle tracking modeling on kilometer-scale DFNs with tens of thousands of fractures and millions of computational cells.

dfnWorks toolkit has been successfully applied for studying contaminant transport in nuclear waste repository [3], CO2 sequestration and extraction of unconventional hydrocarbons [4]. In this talk, the details of dfnWorks along with its application to hydrocarbon extraction from unconventional oil & gas, will be discussed. Numerical experiments on a realistic fractured shale system (Figure 1) are presented to identify how in-fracture heterogeneity of aperture and transmissivity affect the production curves. The contributions of main gas transport mechanisms, such as advection, desorption, and matrix diffusion to the production curve shape will be discussed.
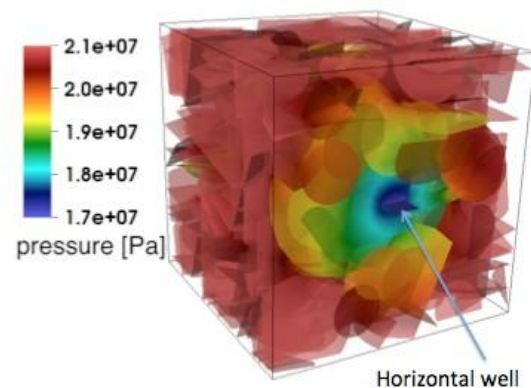

Figure 1: Discrete fracture network generated based on fracture statistics from a naturally fractured shale site. Horizontal well is located in the center of the simulation domain. Color represents obtained pressure solution.

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Adaptive Higher Order Discontinuous Galerkin Methods for Strongly Heterogenous Twophase Flow in Porous Media

Bernd Flemisch, Rainer Helmig, Birane Kane, Kunibert G. Siebert, University of Stuttgart

Key words: Discontinuous Galerkin, higher order discretization, h-adaptivity, porous medium, two-phase flow

Introduction

Simulation of multiphase flows arising in environmental problems such as infiltration and remediation requires careful numerical treatment due to the strong heterogeneity of the underlying porous medium. The spatial discretization requires locally conservative methods in order to be able to follow small concentrations [1]. Discontinuous Galerkin (DG), Finite Volume and Mixed Finite Element, are examples of discretization methods which achieve local conservation at the element level [2]. DG methods are based on weak formulations with finite dimensional piecewise polynomial solution space and test function space. The main difference to classical Finite Element methods is that the finite element function space corresponding to DG methods consists of piecewise polynomials which are allowed to be discontinuous across element interfaces. Numerical fluxes and penalty terms are added in order to enforce weakly the continuity of the solution and the boundary conditions. DG methods present attractive features such as an inherent local and global conservation, a high-order accuracy, a high parallel efficiency and a geometric flexibility (unstructured meshes and non-conforming grids) allowing an easier local h-p adaptivity. Furthermore, the ability of DG methods to treat rough coefficients problems and capture discontinuities in solutions allowed the DG methods to be a suitable candidate for the discretization of PDE's arising in Environmental Engineering.

Approach and Application

We implement and evaluate numerically interior penalty DG methods for 2d and 3d incompressible, immiscible, two-phase flow. We consider a strongly heterogeneous porous medium and discontinuous capillary pressure functions. We write the system in terms of a phase-pressure/phase-saturation formulation. A backward Euler scheme in time is combined with various interior penalty DG discretizations in space such as the Symmetric Interior Penalty Galerkin (SIPG), the Nonsymmetric Interior Penalty Galerkin (NIPG) and the Incomplete Interior Penalty Galerkin (IIPG) [3]. This implicit space

time discretization leads to a fully coupled nonlinear system requiring to build a Jacobian matrix at each time step for the Newton-Raphson method. We include in our implementation local mesh adaptivity on non-conforming grids. To our knowledge, this is the first time the concept of local h-adaptivity is incorporated in the study of a 3d two- phase flow with strong heterogeneity, discontinuous capillary functions and gravity effects. We also use higher order polynomial degree up to piecewise cubics.
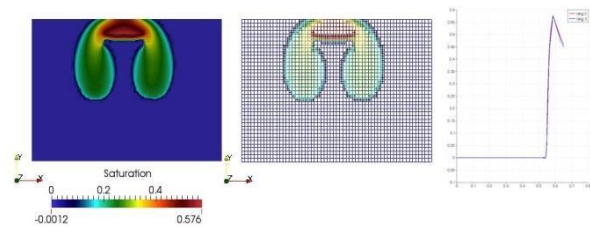

Figure 1: 2d-Problem, saturation distribution after 4000 s of injection with 0.075 kg/s of DNAPL in a depht of 0.65 m. Domain permeability 6e-11 m2. Lens permeability 7e13 m2. Polynomial order p = {2,3}.
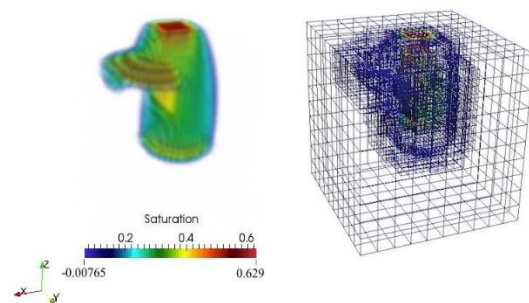

Figure 2: 3d-Problem, saturation distribution after 5000 s of injection with 0.25 kg/s of DNAPL in a depth of 1m. Domain permeability 6e-11 m^2. Lenses permeabilities 7.15e-13 m2, 7.15e-14 m^2.

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Numerical Simulation of Turbulence and Air Entrainment in a Hydraulic Jump

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Key words: hydraulic jump, air entrainment, volume of fluid

Introduction

Hydraulic jump is a process through which supercritical flow transitions to subcritical flow. Its primary application is in energy dissipators downstream of hydraulic structures such as dams and weirs. Extensive effort has been made in experimental and analytical studies of hydraulic jumps in the past. Hydraulic jump is inherently turbulent, characterized by complex flow structures and significant air entrainment. As a result, geometrically similar models suffer from scale issues due to the difficulty in simultaneously achieving Froude number and Weber number similitude. The ability to simulate hydraulic jumps numerically, therefore, holds great potential.

Recent efforts, though limited in number, have been made to model hydraulic jump as a multiphase flow to account for the process of air entrainment. Nonetheless, previous studies do not include the open-channel aspect of the hydraulic jump. This study reports a numerical simulation of bubbly flow and internal flow structures of hydraulic jump.

Numerical Model

The numerical model is 2-D, unsteady, and multiphasic. Standard k-e model is adopted to close the set of RANS equations. The transient interfacial behavior is captured by explicit volume of fluid (VOF) method and piecewise-linear interface calculation scheme (PLIC). Solution methods are 2nd order accurate in space (momentum, turbulent kinetic energy, rate of dissipation) with 1E-5 convergence residual criterion.

Results

The simulation identified three distinct flow regions: the jet region, the turbulent shear layer and the recirculation region. Time-averaged air volume fraction field indicated increasing shear layer thickness along the streamwise direction. Turbulent kinetic energy was predicted, in descending order, at the toe of the jump, the turbulent shear layer and the recirculation region. Instantaneous air volume fraction contours captured the initial entrainment at the toe, advective transport of bubbles through the turbulent shear layer, bubble coalescence, and degassing of the resulting buoyancy-driven bubble packets (Fig. 1).
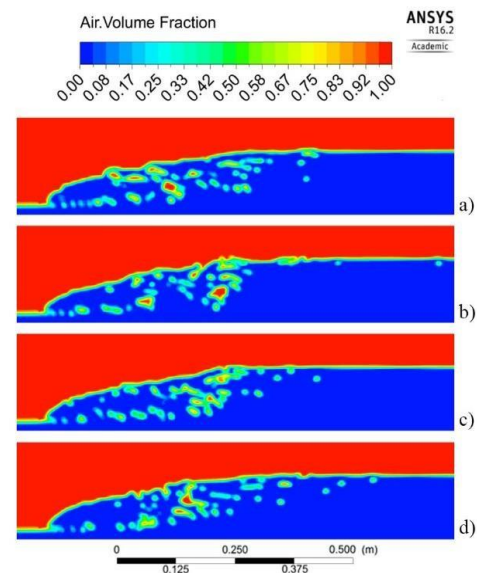

Figure1: Instantaneous air volume fraction contour at t=36s (a), 37s (b), 38s (c), and 40s (d)

To evaluate the capability of the model, simulation predictions were validated against experimental results in the literature [1]. The comparison showed fair agreement with time-averaged velocity profile and air volume fraction in the free shear layer.

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Formulation, Evaluation, and Validation of a Thermodynamically Contrained Averaging Theory Model for Two-Fluid-Phase Flow in Porous Media

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Key words: TCAT, lattice Boltzmann modeling, microfluidics

In response to the deficiencies in the traditional model for two-fluid-phase flow in porous media, a thermodynamically constrained averaging theory (TCAT) model has been derived [1]. While this model resolves many of the deficiencies associated with the traditional model, it requires non-standard closure relations and evaluation and validation of the formulated mechanisms included in the model.

We summarize the TCAT model formulation, and we evaluate and validate critical aspects of this model. Specifically, a specific TCAT model is extracted from a hierarchy of models of varying sophistication and formulated. The challenges to closure and application are highlighted. A two-fluid-phase lattice Boltzmann model (LBM) is formulated in three-dimensions based upon a 19-state lattice structure and a color scheme with a multiple-relaxation-time collision operator [2]. The LBM simulator is implemented to compute macroscale quantities of interest from the microscale state, matching macroscale variable definitions supported by the TCAT formulation. The LBM is used to evolve macroscale quantities by taking advantage of a firm connection to the microscale quantities obtained from simulation. Microfluidic experiments for two-fluid-phase flow are also used to examine the microscale details of displacement processes, which are compared to LBM simulations and used to evaluate and validate TCAT closure relations.

The results of this work show three important advancements. First, both experimental results and LBM simulations show that thermodynamic equilibrium in two-fluid-phase flow requires on the order of 3–4 hours to be achieved in a 500-micron domain, which suggests that a substantial fraction of extant capillary pressure saturation data is likely to be a representation of a dynamic state and not a true equilibrium state [3]. Second, a kinematic evolution equation formulated in the TCAT model is compared to the experimental data and LBM simulations showing that the posited TCAT form provides an improved description of the dynamics of changes in fluid pressures, capillary pressure, interfacial area, and fluid saturations compared to alternative formulations [4]. Third, the parameterization of capillary pressure, which is needed in the TCAT model and has been of significant interest in the community over the last two decades, is examined in unprecedented detail. A dense set of LBM simulations show that the average capillary pressure can be described accurately using the wetting phase saturation and the fluid-fluid interfacial area. The capillary pressure can be described even more accurately using the wetting phase saturation, the fluid-fluid interfacial area, and the Euler characteristic for the non-wetting phase. The results shown in Fig. 1 demonstrate that hysteresis can be essentially removed from the description of capillary pressure with parameterizations of the sort investigated in this work.
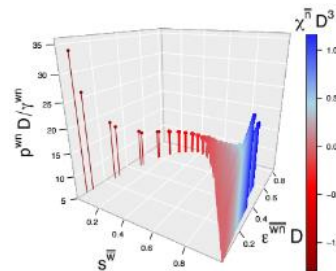

Figure 1: Capillary pressure as a function of fluid saturation, interfacial area, and Euler characteristic.

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Computational Methods
in Water Resources 2016

Flow Regime Analysis for Geologic CO_2 Sequestration and other Subsurface Fluid Injections

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Abstract

Carbon dioxide (CO_2) injection into a confined saline aquifer may be modeled as an axisymmetric two-phase flow problem. Assuming the CO_2 and brine segregate quickly in the vertical direction due to strong buoyancy, and neglecting capillary pressure and miscibility, the lubrication approximation leads to a one-dimensional nonlinear advection-diffusion equation that describes the evolution of the sharp CO_2-brine interface. The interface evolution is driven by two forces: the force from fluid injection, and buoyancy. Analytical solutions can be derived when one of the two forces is dominant. Those solutions depend on the viscosity ratio (M) between the displaced and injected fluids, and a buoyancy parameter that measures the relative importance of buoyancy and the driving force from injection. Different combinations of these two parameters give different forms of the solutions. But for all the solutions, the radius of the lateral spreading of the injected fluid follows $r \propto t^{1/2}$, with the proportionality coefficient differing for the different solutions. In this paper, we identify the kinds of solutions appropriate for practical CO_2 injection projects as well as other subsurface fluid injection applications. We use data from eight CO_2 injection projects, 24 acid gas injection projects, two liquid waste disposal projects, and one CO_2-WAG enhanced oil recovery project. The solutions provide a simple guidance tool for expected behavior of the different injection operations while providing general insights into overall fluid behavior.

P-2: Poster Session 2

Time: Wednesday, 22/Jun/2016: 6:00pm - 8:00pm – Location: MSB Stone Lobby

Optimal Estimation and scheduling in Large Scale Aquifer Management

Hojat Ghorbanidehno, Amalia Kokkinaki, Eric Darve, Peter Kitanidis
Stanford University, United States of America

Calibrating a Hydrologic Forecasting Model for the Madawaska River Basin

Hongli Liu, Bryan Tolson
University of Waterloo, Canada

Study on Stratified Reservoir of Dams Using Numeric Modeling

Redvan Ghasemlounia, M.Sedat Kabdasli
Istanbul Technical University, Turkey

Comparing a Ranking and Penalty Approach for Water Allocation Modelling

Bertrand Richaud, Roar Jensen, Eduardo Munoz, Michael Butts
DHI, Denmark

GPU-based Modeling of Tsunami Propagation and Inundation

Shuangcai Li
RMS, United States of America

Virtual Reality Catchment Simulations for Verifying Data Assimilation Methods

Bernd Schalge[1], Jehan Rihani[1], Gabriele Baroni[2], Barbara Haese[7], Daniel Erdal[3], Harrie-Jan Hendricks-Franssen[5], Insa Neuweiler[4], Gernot Geppert[6], Felix Ament[6], Stefan Kollet[1,5], Olaf Cirpka[3], Pablo Saveedra[1], Xujun Han[5], Sabine Attinger[2], Harald Kunstmann[7,8], Harry Vereecken[5], Clemens Simmer[1]

[1]University of Bonn; [2]Hemlholtz Institute for Environmental Research; [3]University of Tübingen; [4]University of Hannover; [5]Forschungszentrum Jülich; [6]University of Hamburg; [7]University of Augsburg; [8]Karlsruhe Institute of Technology; Germany

Toward a Joint Assimilation of SMOS Brightness Temperature and GRACE Terrestrial Water Storage Observations for Improved Soil Moisture Estimation

Manuela Girotto, Gabrielle De Lannoy, Rolf Reichle, Matthew Rodell
NASA/USRA, United States of America

To Study the Effects of the Maximum Scour Depth and Sediment Transport of the Dajia River, Taiwan

Dong-Sin Shih, Yuan-Ya Liao, Hui-Cheng Chang
National Chung Hsing University, Taiwan, Republic of China

Optimization of Bioenergy Crop Selection and Placement Based on a Stream Health Indicator Using an Evolutionary Algorithm

A. Pouyan Nejadhashemi[1], Matthew Herman[1], Fariborz Daneshvar[1], Mohammad Abouali[1], Dennis Ross[1], Sean Woznicki[1], Zhen Zhang[2]
[1]Michigan State University; [2]University of Chicago; United States of America

Numerical Investigations of Sulfur Water Formation Mechanisms in Sedimentary Basins

Mingliang Xie[1], Danyang Su[1], K. Ulrich Mayer[1], Kerry T.B. MacQuarrie[2]

[1]University of British Columbia; [2]University of New Brunswick, Canada

Non-Hydrostatic Pressure Shallow Flows: GPU Implementation in 2D-Domains Using Finite-Volume and Finite- Difference Scheme

Cipriano Escalante Sánchez[1], Tomás Morales[2], Manuel J. Castro[1]

[1]UMA; [2]UCO, Spain

A Nonlinear Second Order in Space Correction Preserving Maximum Principle for Diffusion Operators

Christophe Le Potier

CEA, France

The Integrated Hydrologic Model Intercomparison Project, IH-MIP2: A Second Set of Benchmark Results to Diagnose Integrated Hydrology and Feedbacks

Stefan Kollet[1,2], Mauro Sulis[3], Reed Maxwell[4], Claudio Paniconi[5], Mauro Putti[6], Giacomo Bertoldi[7], Ethan T. Coon[8], Emanuele Cordano[7,9], Evgeny Kikinzon[8], Emmanuel Mouche[10], Claude Mügler[10], Young-Jin Park[11], Simon Stisen[12], Edward Sudicky[13]

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Inter-Particle Effects on the Pore Clogging with Fine Particles

Shinichiro Hirabayashi, Toru Sato

University of Tokyo, Japan

Comparison of Chemical Exposure in Soil and Groundwater Using a Physics-Based Numerical Model

Soonyoung Yu[1], Sang-Il Hwang[2], Seong-Taek Yun[1], Gitak Chae[3]

[1]Korea University; [2]Korea Environment Institute; [3]Korean Institute of Geoscience and Mineral Resources, South Korea

Seasonal Forecasting of Reservoir Inflows: Case Study Applications of a Decision Support Tool

Michael B Butts, Basel Draw, Bibhab Mani Panthi, Roar A Jensen, Jacob K Larsen

DHI, Denmark

A Joint Geophysical and Flow Inversion Framework to Characterize and Constrain Subsurface Fracture Networks

Maruti Mudunuru, Satish Karra, Nataliia Makedonska, Ting Chen

Los Alamos National Laboratory, United States of America

Optimal Estimation and scheduling in Large Scale Aquifer Management

Hojat Ghorbanidehno, Amalia Kokkinaki, Eric Darve, Peter Kitanidis

Stanford University, United States of America

Key words: Optimal control, aquifer management, big data

Water resources systems, and especially groundwater reservoirs, are a valuable resource that is being endangered in many places around the world by contamination and overexploitation, threatening a vulnerable supply and its long-term sustainability. Optimal control techniques have been widely applied to groundwater management applications since the early days of dynamic programming. One such popular algorithm for aquifer management problems is the Linear Quadratic Gaussian Control (LQGC) method [2]. The objective of such methods is to quantify the controls (e.g. pumping schedule) such that a cost function is maximized while satisfying one or more constraints. However, LQGC is limited by its high computational cost for systems with a large number of states and a large number of controls as the computational cost increases quadratically with the latter.

This work presents a new method for optimal control in the linear Gaussian case with a linear cost that is applicable for large scale problems where limited information about the state of the system is available. The new algorithm reduces both the computational and storage cost by harnessing the structure of the large weighting and covariance matrices involved in the computations by using efficient low rank approximation methods. Embedded in the control algorithm is the Spectral Kalman Filter [1], a fast kalman filtering method that allows the assimilation of available data in order to improve the estimate of the state in the face of uncertainties related to unknown parameters and boundary conditions. The integration of filtering in the optimal control algorithm also allows the estimation of critical parameters such as aquifer properties in real time. Our joint control-estimation algorithm also provides real time estimates of uncertainty. The cost of the method increases linearly with the number of states and the number of controls, a significant improvement compared to the textbook version for KF and LQGC methods.

Our algorithm provides a practical approach for combined uncertainty quantification and optimal control for linear and weakly non-linear systems. We present a validation case for pumping schedule management in a small homogeneous aquifer, as well as a larger scale case with heterogeneities in aquifer properties and boundary conditions. We show an evaluation of our method in terms of accuracy and computational cost, and investigate the impact of the structure of the weighting matrix on the results. Extensions of the method to non-linear problems are discussed.

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Calibrating a Hydrologic Forecasting Model for the Madawaska River Basin

Hongli Liu, Bryan Tolson

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Key words: hydrologic forecasting, automatic calibration, uncertainty estimation, streamflow, water level.

Introduction

The heart of any hydrological forecasting system is a hydrological model (Serban and Askew, 1991). In order to make predictions resemble observations, a robust model calibration has to be implemented prior to the chosen hydrological model applied for practical use. Traditional calibration process usually adjusts model parameters by conducting a manual or automatic calibration experiment. Ontario Power Generation (OPG) requires a hydrologic forecasting system for the numerous hydropower generation locations in the Madawaska River Basin of Ontario, Canada.

Objectives & Methodology

The primary goals of this study are to calibrate a candidate hydrologic model of the Madawaska built in the RAVEN hydrologic modelling framework (Craig and Snowdon, 2015). A key challenge in this study includes making use of imperfect flow and water level data across the system. Many of the historical flow and water level measurements were measured once a day without the corresponding measurement time being recorded. Two calibration formulations will be posed and optimized. A baseline calibration formulation assumes the water level and flow data represent daily average data. The revised calibration explicitly acknowledges the instantaneous and unknown timing of each flow and water level sample. The RAVEN-based hydrologic model will be calibrated with the dynamically dimensioned search (DDS) algorithm (Tolson and Shoemaker, 2007).

The DDS- Approximation of Uncertainty approach (Tolson and Shoemaker, 2008) will also be utilized to evaluate how the model prediction uncertainty changes between the two calibration formulations.

The Madawaska River is a subwatershed of the Ottawa River, with length of 230 km and drainage area of 8505 km^2. Streamflow data from ten flow gauges managed by Environment Canada are available while once daily reservoir water level data/outflows are available from seventeen water level gauges managed by Environment Canada and Ontario Power Generation. The period for which most of the data is commonly available is 1996-2014.

Current Progress

A RAVEN-based model has been built and initially calibrated for a subwatershed of the Madawaska River.

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Study on Stratified Reservoir of Dams Using Numeric Modeling

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Abstract

Water is the most basic requirement of human, which covers 70.8 percent of surface of the world, approximately. From this amount of water on the earth, only fresh water is usable for human. Thus, it is important to save the water resources. In this way, numeric modeling has the basic role in the management and saving of water resources. But it is very difficult to modeling the real flows, which are be in the nature. The complexity of real fluid flow makes it impossible to solve the governing equations without making some form of simplifying approximation, even with the use of complex models and fast computers. In this study, changes in stratified reservoirs of dams, and also lakes, are studied for different inflow and reserved water conditions using FLOW-3D.Finally, results are shown and compared with each other with figures and tables.

Comparing a Ranking and Penalty Approach for Water Allocation Modelling

Bertrand Richaud[1], Roar Jensen[2], Eduardo Munoz[2], Michael Butts[1]

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Key words: water allocation, optimisation, global ranking, linear programming, penalty approach

Introduction

Water allocation problems, where supply has to match the demand in place and time, can be solved in different manners. This poster compares two methods for water allocation model on a case study in Sri Lanka. The first approach described in this paper, called Global ranking, is best on the sorting of all users in the basin in order of importance. At the same time, storages in reservoirs are also being assigned ranks, and the model will find the nearest storage able to supply users. The second method being compared is using penalties instead of ranks and is solved with a linear programming solver. Penalties are assigned to units of water user and hydropower deficit as well as reservoir storage depletion.

Methodology and Case study

Global ranking The global ranking algorithm is based on the assumption that water user demands irrespective of their location in the river basin can be assigned priority and water should be distributed according to this priority [1]. In some countries this is a common water allocation paradigm, based on the date they were given certain water right (first in time first to serve) also called "riparian rights". This algorithm is opposed to the simple model which solves the water allocation problem from upstream to downstream (first in line – first to serve). This means that if a high priority user is located downstream of a low priority user, the latter may take the water as it passes the node and leave no water to the high priority users.

Penalty concept Penalties are assigned to units of water user and hydropower deficit as well as reservoir storage depletion. The aim of water allocation optimisation model is to minimize the total penalties in the entire system at each time step. The problem is formulated as a linear problem where objective functions are solved under given constraints. The objective function are minimised by optimising a set of decisions variables [2].

Case study The case study is a part of the Mahaweli basin in Sri Lanka. A part of this basin has been selected as pilot model for the purpose of comparing different water allocation methods.

Both methods appear to be efficient in solving water allocation problems. However, the global ranking approach can be applied in a straightforward manner once the priorities between users have identified. The penalty approach requires calibration of the penalties, which may influence the overall results, and can be a tedious task for practitioners. Therefore the ranking approach appears to be a more efficient method for an initial screening of the water allocation, and could be refined by applying an optimisation method, such the linear approach.
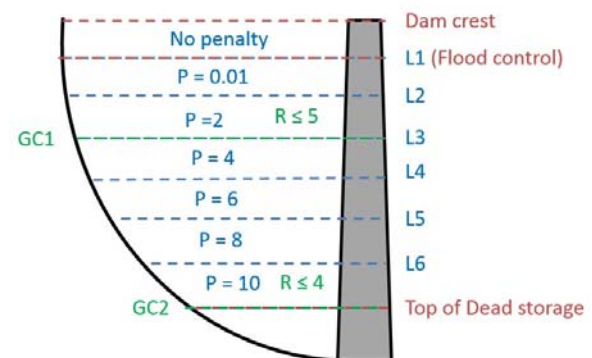

Figure 1: Comparison of guide curves (GC) for global ranking approach with penalty level (P) for Penalty approach in the Maduru Oya Reservoir.

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GPU-based Modeling of Tsunami Propagation and Inundation

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Abstract

Recent destructive tsunami (e.g., Sumatra 2004, Japan 2011) caused significant loss of life and property damage. The objective of this study is to develop a numeric model to provide fast and reliable estimate of the land inundation of a tsunami. In this paper a numerical model based on an upwind finite volume method is developed on Graphics Processor Unit (GPU) to solve shallow water equations. HLLC approximate Riemann solver is adopted to calculate the flux because of its robustness, efficiency, and superior performance in handling discontinuities and wetting/drying processes. To preserve non-negative water depths and 'lake at rest' property (C-property), a robust positivity preserving method is used. Model efficiency and stability are treated using an explicit-
.

implicit method for temporal discretization with operator splitting. The model is implemented on the Graphics Processor Unit (GPU) to achieve a significant faster speed compared to traditional CPU. The slip distribution and seismic moment of the earthquake driven tsunami events are introduced to the model as the initial condition including coastal uplift and subsidence. Its superior performance is demonstrated by applying the model to simulate 2011 Japan Tohoku Tsunami, Chile Maule tsunami (2010), and Indian Ocean tsunami (2004). Both near-field and far-field regions affected by the tsunami waves are numerically studied and the resulting run-up and tsunami inundations are compared with the recorded observation data including coastal tide gauges and eyewitness observation data

Virtual Reality Catchment Simulations for Verifying Data Assimilation Methods

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Key words: virtual catchment, coupled models, data assimilation

Abstract

The advantage of integrated terrestrial system models which encompass the subsurface, land surface and atmosphere (SLAS) is the physically consistent representation of states and exchange fluxes between compartments. However, these models need a large number of input parameters and are affected by large uncertainties. Data assimilation for such integrated models offers the possibility to narrow down uncertainties on model predictions and model parameters. No data assimilation system for integrated subsurface-land surface- atmosphere models has been developed yet. In order to develop and evaluate such data assimilation algorithms we generated a virtual (VR) catchment, including the subsurface, land surface and atmosphere.

Using a VR as a virtual truth allows us to evaluate data assimilation algorithms for SLAS models while mitigating the data scarcity issue. Virtual measurements at different spatial and temporal scales are extracted via forward operators of states and fluxes.

In this contribution, we describe the development of a high resolution VR catchment, which is based on the Neckar catchment in Germany, using the Terrestrial System Modeling Platform (TerrSysMP)[1].

We present a fully coupled TerrSysMP which includes the interactions of subsurface (Parflow), land surface (CLM) and atmosphere (COSMO), and allows for example the evaluation of the impact of soil moisture, which can influence near-surface temperatures, atmospheric boundary layer heights or the Bowen ratio. By considering cross-compartmental dynamics the physical consistency of the VR is enhanced which creates the best possible testbed for data assimilation. In addition to the fully coupled VR we consider also simulations without ParFlow, only including COSMO and CLM.

The model states simulated by the fully coupled system and the model which includes only the atmospheric and land surface component were compared. It was found that variables like land surface temperature or soil moisture can vary substantially between the two models, related to the improved representation of the hydrology in the fully coupled model.

We illustrate how the true state (the VR state) is reconstructed by extracting virtual observations at various temporal and spatial scales. In particular, we show how well the precipitation field can be estimated by using random samples of virtual station measurements like rain gauges and virtual radar observations.

For the fully coupled system we show how assimilating soil moisture changes state variables in the subsurface, land-surface and atmosphere component models.

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Toward a Joint Assimilation of SMOS Brightness Temperature and GRACE Terrestrial Water Storage Observations for Improved Soil Moisture Estimation

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Key words: GRACE, SMOS, data assimialtion, soil moisture

Abstract

Soil water profile is a key variable for understanding and predicting hydrological, weather, and biogeochemical Earth dynamics. Observations from recent soil moisture missions (e.g. SMOS and SMAP) have been used in innovative data assimilation studies to provide global high spatial (i.e. 40 km) and temporal resolution (i.e. 3-days) soil moisture profile estimates from microwave brightness temperature observations [1]. In contrast with microwave-based satellite missions that are only sensitive to near-surface soil moisture (0-5 cm), the Gravity Recovery and Climate Experiment (GRACE) mission provides accurate measurements of the entire vertically integrated terrestrial water storage column but, it is characterized by low spatial (i.e. 150,000 km2) and temporal (i.e. monthly) resolutions. Data assimilation studies have shown that GRACETWS primarily affects (in absolute terms) deeper moisture storages (i.e., groundwater) [2]. An example of the improvements brought by GRACE to the surface, rootzone, and groundwater components of the soil moisture profile is shown in Figure 1. Here, it is hypothesized that unprecedented soil water profile accuracy can be obtained through the joint assimilation of GRACE terrestrial water storage and SMOS brightness temperature observations. A particular challenge of the joint assimilation is the use of the two different types of measurements that are relevant for hydrologic processes representing different temporal and spatial scales. The performance of the joint assimilation strongly depends on the chosen assimilation methods, measurement and model error spatial structures. The optimization of the assimilation technique constitutes a fundamental step toward a multi-variate multi-resolution integrative assimilation system aiming to improve our understanding of the global terrestrial water cycle.

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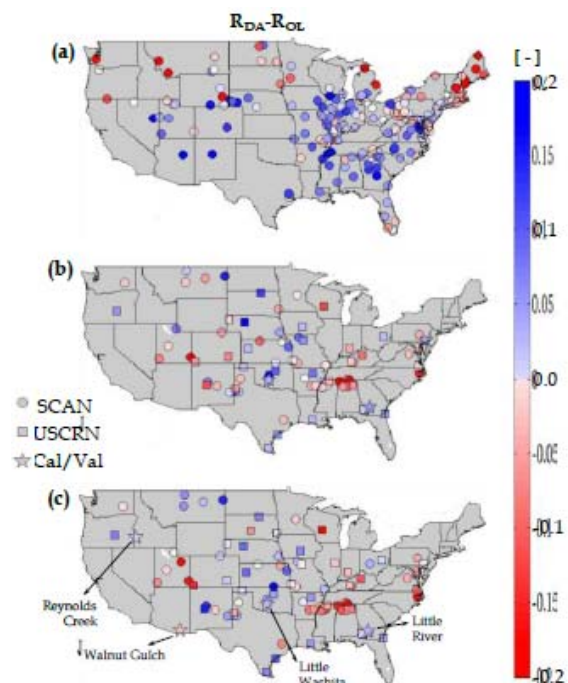

Figure 1: Differences in (a) groundwater, (b) root-zone soil moisture, and (c) surface soil moisture correlation coefficient (R) using the uni-variate GRACE TWS assimilation system relative to OL results. Positive differences (i.e. blue markers) indicate the locations where DA skill is improved over the OL experiment when assimilation was not used.

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To Study the Effects of the Maximum Scour Depth and Sediment Transport of the Dajia River, Taiwan

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Key words: river scouring, sediment transport, Dajia River

Abstract

This research used modeling approach to study the wave propagation of flow discharges, velocity distributions, maximum riverbed scouring, and sedimentation transports along the Dajia river of Taiwan. After Chichi earthquake occurred in 1999, some frequent flash floods have attacked central Taiwan, resulting in severe riverbed scoring and bring huge sedimentations into this river. Some dams spanned cross the river will easily block huge sedimentations in channels. Among these rivers, Dajia river can be labeled one of most important river in central Taiwan. In order to better understand the mechanism of sediment transport and riverbed scouring, form Maan dam to the estuary of Dajia river is examined to study. The WASH123D hydraulic model with combined modified empirical formula of Su&Lu (2013) and Blench (1969) are integrated to this simulation to further calculate maximum scoring depth along the river. Physiographic Soil Erosion- Deposition model (PSED) is applied to generate lateral sedimentations of Dajia river of our modeling system. The fragile geology with resulting in collapsed soils from hillside along channels is incorporated to this modeling. Simulation results from other well develop two-dimensional sedimentation models, SRH-2D and ARMB2D, are examined to compare with our results. And the effects of maximum scour depth and sediment transport of the Dajia River are discussed in this research.

Optimization of Bioenergy Crop Selection and Placement Based on a Stream Health Indicator Using an Evolutionary Algorithm

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Abstract

The emission of greenhouse gases continues to amplify the impacts of global climate change. This has led to the increased focus on using renewable energy sources, such as biofuels, due to their lower impact on the environment. However, the production of biofuels can still have negative impacts on water resources. This study introduces a new strategy to optimize bioenergy landscapes while improving stream health for the region. To accomplish this, several hydrological models including the Soil and Water Assessment Tool, Hydrologic Integrity Tool, and Adaptive Neruro Fuzzy Inference System, were linked to develop stream health predictor models. These models are capable of estimating stream health scores based on the Index of Biological Integrity. The coupling of the aforementioned models was used to guide a genetic algorithm to design watershed-scale bioenergy landscapes. Thirteen bioenergy managements were considered based on the high probability of adaptation by farmers in the study area. Results from two thousand runs identified an optimum bioenergy crops placement that maximized the stream health for the Flint River Watershed in Michigan. The final overall stream health score was 50.93, which was improved from the current stream health score of 48.19. This was shown to be a significant improvement at the 1% significant level. For this final bioenergy landscape the most often used management was miscanthus (27.07%), followed by corn-soybean-rye (19.00%), corn stover-soybean (18.09%), and corn-soybean (16.43%). The technique introduced in this study can be successfully modified for use in different regions and can be used by stakeholders and decision makers to develop bioenergy landscapes that maximize stream health in the area of interest.

Numerical Investigations of Sulfur Water Formation Mechanisms in Sedimentary Basins

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Key words: Sulfur water, reactive transport, hypersaline, sulfate reduction bacteria, salinity

Sulfur water is widely found in groundwater at intermediate depths of sedimentary basins, including regions of the Michigan basin in southeastern Ontario [1]. However, the mechanisms responsible for the occurrence of these brackish sulfur waters are not fully understood. Anaerobic microbial sulfate reduction is a common process resulting in the formation of sulfur water and has been intensively investigated in various fields of environmental engineering [2], and by the oil and gas industry [3]. Sulfate reduction rates depend on many factors including the concentrations of sulfate, the abundance of organic substances, redox conditions, temperature, salinity and the type of sulfate reducing bacteria (SRB) [4]. It is well known that the efficiency of sulfate reduction decreases with increasing salinity. This paper investigates the process of sulfur water formation in sedimentary basins using the reactive transport simulator MIN3P_THCm [5].

The reaction of sulfate reduction by SRB can be generally described by the following reaction [6]:

$$CH_2O + 0.5\ SO_4^{2-} \rightarrow CO_3^{2-} + 0.5H_2S + H^+$$
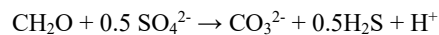
This reaction can be treated in the same way as mineral dissolution and precipitation reactions, and is best modeled as a kinetically controlled irreversible reaction. Sulfate reduction is here simulated using a simplified Monod-type rate expression of the form:

$$R = -K_{sal}K_{sulf}\left[\frac{[SO_4]}{K_s + [SO_4]}\right]$$

in which R is the rate of sulfate reduction, K_s is the half-saturation constant, and $[SO_4]$ is the total sulfate concentration. k_{sulf} is the rate constant at a reference salinity and k_{sal} is the salinity inhibition factor. Additional geochemical reactions that are considered include calcite dissolution, accounting for pH- buffering, as well as siderite, gypsum, and sulfide mineral precipitation, providing important controls on the solubility of Fe(II), SO_4 and H_2S.

The numerical simulations are undertaken for a simplified 2D model based on hydrogeological parameters typical for sedimentary basins. The kinetic reaction parameters for the sulfate reduction reaction are based on experiments in saline sediments in the Great Salt Lake (Utah, USA) [4]. Simulation results indicate that fresh/low salinity water penetrates to intermediate depth as a result of episodic recharge events beneath temperate ice-sheets, in the process mixing with more saline porewater, while the hypersaline pore water in the deep subsurface is high in density and remains unchanged. The groundwater at intermediate depth provides favorable conditions for sulfur water formation, i.e. rich in organic matter and sulfate, moderately saline and relatively warm.

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Non-Hydrostatic Pressure Shallow Flows: GPU Implementation in 2D-Domains Using Finite-Volume and Finite- Difference Scheme

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[1]Universidad de Malaga, [2]Universidad de Cordoba, Spain

Key words: Dispersive, Shallow-Water, FiniteDifference, Finite-Volume, GPU, Path Conservative, Solitary Waves, Tsunami Simulation, NonHydrostatic, Wave Breaking

Introduction

Shallow water equations are not appropriate for deep or moderate waters simulations where frequency dispersion effects may become more important that nonlinearity.

In this framework, Boussinesq type models are commonly used, and in recent years, non-hydrostatic pressure models have shown to be able to describe weakly dispersive waves as well as Boussinesq type models.

Jacques Sainte-Marie [2] and Yamazaki [6] described two non-hydrostatic pressure systems, when the vertical velocity component is included in the integrated motion equations.

These models, which are suitable for intermediate water, can be extended to cover the dynamics of the surf zone, by considering some mechanisms of wave breaking. A breaking mechanism similar to [4] is adopted, based in an eddy viscosity approach.

Numerical Scheme

Both non-hydrostatic models could be split into two parts: one corresponding to the non-linear shallow water system in conservative form and the other corresponding to the non- hydrostatic terms. An efficient second-order well-balanced numerical method, which combines finite-volume and finite-difference schemes is developed.

The hyperbolic part of the system is discretized using a PVM path-conservative finite-volume method [1, 3], and the non-hydrostatic terms with compact finite differences.

Finally, the resulting ODE system in time is discretized using a TVD Runge-Kutta method [5].

Implementation and Numerical Results

In order to optimize the performance, models have been implemented using CUDA, taking advantage of parallelization that provide graphics cards. Also, some numerical tests including comparisons with 1D and 2D laboratory data such as Figure 1 and Figure 2.

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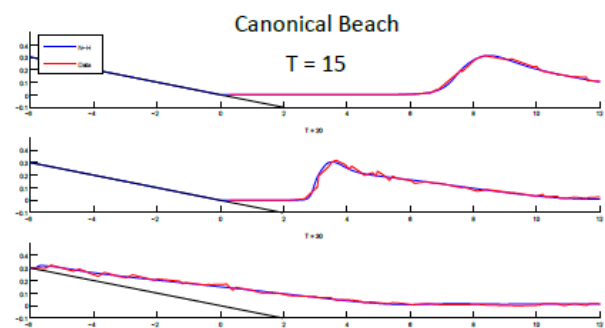

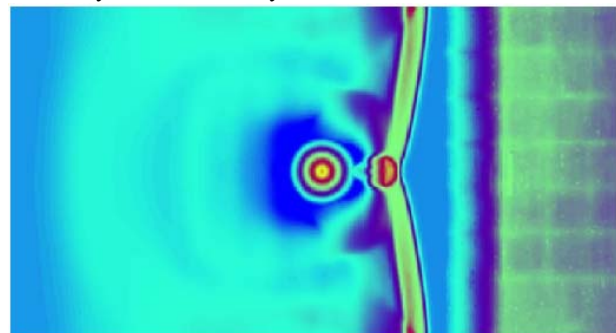*Figure 1:* 1D Canonical Beach. Comparison with laboratory data and Non-hydrostatic model.

Figure 2: 2D Conical Island. Comparison with laboratory data and Non-hydrostatic model.

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A Nonlinear Second Order in Space Correction Preserving Maximum Principle for Diffusion Operators

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Key words: Maximum principle, Diffusion Operators, Nonlinear schemes

Abstract

It is well known that classical linear methods discretizing diffusion operators do not always satisfy maximum principle for distorted meshes or high anisotropy ratio. A few years ago, a nonlinear finite volume scheme was proposed to discretize the diffusion operators [2, 4, 8]. For that scheme, we obtained discrete maximum principle for distorted meshes or highly anisotropic diffusion tensors. In the present work, we propose a nonlinear correction which gives nonoscillating solutions and which is in practice second order in space.

The scheme consists in mixing the two methods developed in [5] and [7]. We show that the new scheme is coercive. We explain why there exists at least one solution. We also show that the new scheme satisfies the LMP structure (definition 1.3 in [2]).

We also explain in the one-dimensional case, with a traditional discretization of the diffusion operator why the nonlinear correction is second order in space with regular functions.

Finally, numerical results are presented considering an analytical problem and using the finite volume scheme described in [8]. We first show the L2 error with respect to the analytical solution, the order in space, the minimum values and the percentage of negative values as a function of the discretization step h (Scheme 1). Then, we present the results obtained with the modified scheme (Scheme 2 and Scheme 3). Finally, we compare with the nonlinear correction developed in [7] (Scheme 4). We observe that scheme 2 and scheme 3 are second order in space and are even more accurate than the original scheme. We check there are non oscillating. On these numerical tests, scheme 4 remains first order in space and non oscillating. Note that it is easy to generalize this new correction to hybrid schemes [3] in the spirit of [6] or to DDFV schemes [1].

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The Integrated Hydrologic Model Intercomparison Project, IH-MIP2: A Second Set of Benchmark Results to Diagnose Integrated Hydrology and Feedbacks

Stefan Kollet[1,2], Mauro Sulis[3], Reed Maxwell[4], Claudio Paniconi[5], Mauro Putti[6], Giacomo Bertoldi[7], Ethan T. Coon[8], Emanuele Cordano[7,9], Evgeny Kikinzon[8], Emmanuel Mouche[10], Claude Mügler[10], Young-Jin Park[11], Simon Stisen[12], Edward Sudicky[13]

[1]Agrosphere Institute, Forschungszentrum Jülich GmbH, Germany. [2]Centre for High-Performance Scientific Computing in Terrestrial Systems, HPSC TerrSys, Geoverbund ABC/J. [3]Meteorological Institute, Bonn University, Germany. [4]Department of Geology and Geological Engineering, Colorado School of Mines, USA.[5]Institut National de la Recherche Scientifique, Centre Eau Terre Environnement, Université du Québec, Canada.[6]Department of Mathematics, University of Padova, Italy. [7]Institute for Alpine Environment, EURAC, European Academy Bolzano, Italy. [8]Computational Earth Science, Los Alamos National Laboratory, USA. [9]Rendena100, Engineering and Consultancy sole proprietorship, Tione di Trento, Italy.[10]Laboratoire des Sciences du Climat et de l'Environnement, CEA-CNRS-UVSQ, France. [11]Aquanty, Inc., Waterloo, Canada.[12]Department of Hydrology, Geological Survey of Denmark and Greenland, Copenhagen, Denmark. [13]Department of Earth and Environment, University of Waterloo,

Key words: Integrated Hydrologic Models, Models Inter- comparison, Variably saturated groundwater-surface water systems

Introduction

Emphasizing the physical intricacies of integrated hydrology and feedbacks in simulating connected variably saturated groundwater-surface water systems, the Integrated Hydrologic Model Intercomparison Project initiated a second phase (IH- MIP2) increasing the complexity of the benchmarks of the first phase [1].

Method

IH-MIP2 benchmarks included the tilted v-catchment with 3D subsurface; a superslab case expanding the slab case of the first phase with an additional horizontal subsurface heterogeneity; and the Borden field rainfall-runoff experiment. The analyses encompassed time series of saturated, unsaturated, and ponded storages, as well as discharge. Vertical cross sections and profiles were also inspected in case of the superslab and Borden benchmark.

Seven model codes took part in IH-MIP2: ATS [2], Cast3M, CATHY, GEOtop, HydroGeoSphere (HGS), MIKE-SHE, and ParFlow (PF).

Results

Results show generally good agreement between the different models, which lends confidence in the fundamental physical and numerical implementation of the governing equations in the different models. Differences can be attributed to the varying level of detail in the representation or parameterization of physical processes, in particular with regard to ponded storage and friction slope in the calculation of surface water flow (Figure 1). While these differences are quite subtle, they may become important for specific applications such as detailed inundation modeling or when strong inhomogeneities are present in the simulation domain.
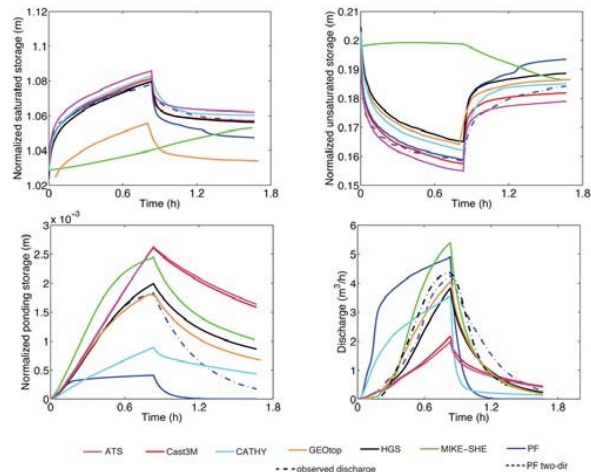

Figure 1: Storage and discharge time series of the Borden benchmark: a) unsaturated storage, b) saturated storage, c) ponded storage, and d) discharge. Note that storage values are normalized by the catchment area, which differs between the models because of different discretization schemes.

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Inter-Particle Effects on the Pore Clogging with Fine Particles

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Key words: porous media, clogging, electrostatic force, lattice Boltzmann method

Introduction

Methane hydrate is known to be one of the potential and promising energy resources, which is abundantly distributed in the environmental conditions of high pressure and low temperature. In Japan, methane hydrate reservoir was found in the sand sediment beneath the seafloor, and its development is expected. In the development of the methane hydrate, it is anticipated that the migrating fine particles, which are accompanied with produced gas and water, may clog the pore of sand sediments and consequently reduces the permeability near the production well. Although this phenomenon is well known and a lot of experimental approaches have been addressed (e.g. Wyss et al.), its microscopic mechanism is still unknown. Microscopic numerical simulation is useful to understand the behavior of fine particles. However, the inter-particles effects have not been well considered in the literature.

In this study, we take the inter-particles forces such as Van der Waals force and electrostatic force into account for the coupled analysis of fluid and particles in porous media and found their effects on the pore clogging event.

Methodology and Results

Numerical methods The lattice Boltzmann method was used for fluid analysis and the Discrete Eelement Method (DEM) was used to analyze particle dynamics. Both analysis of fluid and particles are coupled through the velocity boundary condition and the hydrodynamic force.

Inter-particle force The van der Waals force and the electrostatic force are considered as well as direct contact force of particles. The relationship between electrostatic force and salinity are modeled by using the experimental data in the literature.

Results Table 1 shows an example of calculation conditions with different salinity. An instantaneous snapshot is shown in Figure 1 for each cases and it is seen that more particles are concentrated on local pores in Case 2. Figure 2 shows time history of flow velocity and it is found that the clogging of local pores bring about the reduction of total flow velocity.

Table 1: Example of calculation conditions.

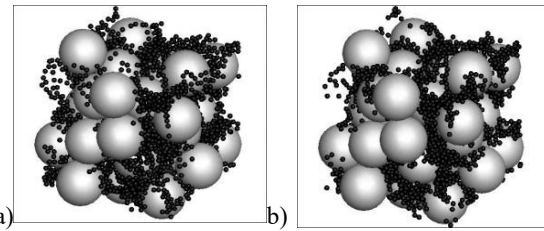|	Salinity (mol/L)	Surface potential (mV)
Case 1	0.001	220
Case 2	0.5	65

a)   b)

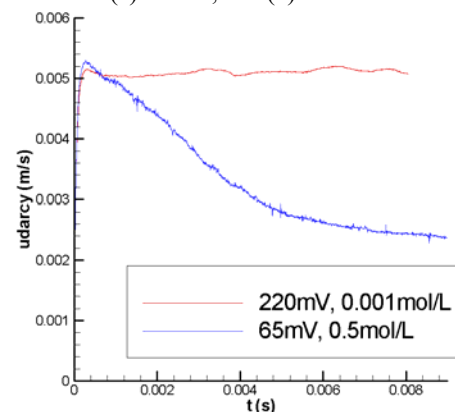*Figure 1:* Instantaneous snapshots of particle distribution in (a) Case 1, and (b) Case 2.

Figure 2: Time history of flow velocity.

Acknowledgements

References

[1] H.M. Wyss, D.L. Blair, J.F. Morris, H.A. Stone and D.A. Weitz. Mechanism for clogging of microchannels, Physical Review E, 74 061402 (2006).

Comparison of Chemical Exposure in Soil and Groundwater Using a Physics-Based Numerical Model

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Key words: chemical accident, exposure, subsurface pollutant loading, soil, groundwater

Abstract

Fate and transport of ten chemicals were assessed by using a multiphase compositional model. 1 ton of a chemical was assumed to leak 3.5m below ground surface. Simulation results showed that ethylbenzene and m-xylene were persistent until 100,000 days.

Then exposure to soil and groundwater contaminants were quantified above and below the water table, respectively using the numerical results. Exposure was assessed by multiplying concentration, impact area and duration, with assuming that a large impact area causes a high chance of intake. The concentration, impact area and duration address the intensity of contamination, mobility and persistency in an assessment of pollutant loading [1], respectively. Thus the multiplication can be used as point-source pollutant loading in tank leakage and accidental spillage in industry [1], and the pollutant loading can be combined with the aquifer vulnerability to assess the pollution potential.

Exposure assessment results showed that the exposure rank differed in soil and groundwater (Table 1). Dichloromethane caused the highest exposure score in both soil and groundwater because of the longest duration in soil and the widest impact area in groundwater. In groundwater, phenol and MTBE also had the high exposure scores because of the high concentration and the long duration.

Linear regression analysis showed that both duration and exposure had a significant correlation with vapor pressure in soil and water solubility in groundwater. Decay parameters were significantly correlated with the duration and exposure in both soil and groundwater. In contrast, soil partitioning coefficient was not a controlling factor for the duration and exposure. Multiple regression analysis using the dominant factors provided a tool to assess the pollutant loading (exposure) of a new chemical without site investigation in a chemical accident.

The work is distinct in that a physics-based numerical model was used to quantitatively assess the subsurface pollutant loading in chemical accidents, which can scientifically defend a simpler and more qualitative assessment of pollutant loading. Besides this study assessed exposure to chemicals in soil and groundwater together and discussed their interaction.

Chemical	Soil		Groundwater	
	Score	Rank	Score	Rank
TCE	4.5E+08	6	4.3E+08	5
PCE	8.5E+08	3	1.5E+08	7
Benzene	2.7E+08	7	2.2E+08	6
Toluene	2.5E+08	8	1.2E+07	8
Ethylbenzene	>6.5E+09	-	> 4.5E+10	-
m-Xylene	>6.0E+09	-	>2.7E+10	-
MTBE	6.3E+08	5	1.4E+11	3
Dichloromethane	1.1E+10	1	9.5E+12	1
Phenol	8.7E+08	2	5.6E+12	2
Tetrachloromethane	6.7E+08	4	2.3E+10	4

Table 1: Exposure based on the average concentration over the duration in case of a 1-ton leak 3.5m below ground surface.

References

[1] J. Chilton, O. Schmoll and S. Appleyard. Assessment of groundwater pollution potential. In: O, Schmoll, G., Howard, J. Chilton, I. Chorus (eds), *Protecting Groundwater for Health: Managing the Quality of Drinking-water Sources*. World Health Organization and IWA Publishing, London, UK, 375-409, (2006).

Seasonal Forecasting of Reservoir Inflows: Case Study Applications of a Decision Support Tool

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Key words: seasonal forecasting, decision support tools, climate model-based forecasting, reservoir management

Introduction

Within the EU FP7 project EUPORIAS) DHI is developing a prototype decision support system for water resources management that exploits the latest generation of climate model-based seasonal forecasts, http://www.euporias.eu/. Seasonal forecasts for water supply, hydropower production, irrigation, water quality management, habitat protection and navigation are particularly useful for water resources management where future flows depend on storages such as snow accumulation or man-made reservoirs. The accuracy and reliability of climate model-based seasonal forecasts depends both on our knowledge of the initial conditions in the reservoir or catchment and the accuracy of the long-term forecasts of temperature and precipitation. It is necessary to quantify the uncertainty if the forecasts are be used as the basis for operating reservoirs. Therefore, robust and reliable operation requires decision support tools including both short-term forecasting for flood management, seasonal forecasting for long-term operation and planning as well as the quantification of the uncertainty and reliability of these forecasts. In this poster, we present the key requirements for such a prototype decision support system and its application to forecasting reservoir inflow for two case studies.

Case studies

Upper Maule, Chile: The Colbún hydropower plant in the Maule Basin in the central Chile is one of the country's larger hydropower schemes generating 474 MW and making an important contribution to the interconnected electricity network of Chile (SIC). The optimisation of the water resources in this basin directly impacts the cost of electricity in the network as a whole. The reservoir relies on snowmelt from October to March to generate power. Therefore snow water availability forecasts are extremely important. In addition, heavy rainfall and melting snow from the Andes Mountains generate floods in the upstream basin and high inflows into the reservoir. So the challenges are; the difficulty of planning power production, and the safe and economical operation of the reservoir during flood events and the provision of water for irrigation.

Urumea catchment: The Urumea catchment, located in the northern Spain is vulnerable to floods, droughts and water scarcity. The rainfall distribution show a strong seasonal pattern but the amounts vary significantly from year to year. On the Añarbe River, in this catchment the Añarbe reservoir is operated by Aguas de Anarbe (AGASA). The challenges are that the reservoir is used for water supply to the city of San Sebastian as well as hydropower, and the reservoir is operated to provide flood protection downstream and to maintain environmental flows within the Urumea River.
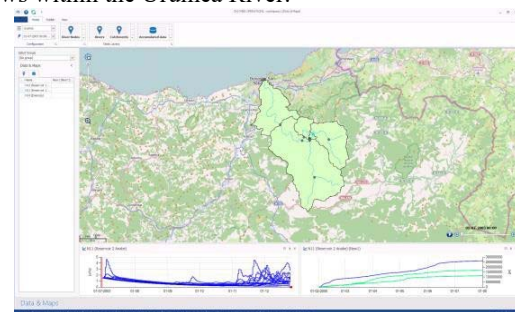

Figure 1: Prototype decision support system for seasonal forecasting in water resources management

Acknowledgements:

A Joint Geophysical and Flow Inversion Framework to Characterize and Constrain Subsurface Fracture Networks

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Subsurface applications including geothermal, geological carbon sequestration, oil and gas, etc., typically involve maximizing the extraction of energy or maximizing the storage of fluids. Characterizing the subsurface is extremely complex due to heterogeneity, and anisotropy. There are uncertainties in the geological, geomechanical, geochemical, thermal, hydraulic parameters, which need to be estimated from multiple diverse as well as fragmented data streams. State-of-art inversion approaches do not consider multiple data sets as well as confidence in experimental/field-scale measurements and models used. Joint inversion methods attempt to overcome these limitations by combining different sources of information and inverting multiple types of data residuals simultaneously. We present a coupled multi-physics framework, for integrating data from geophysical and flow sources, and constraining fractured subsurface system characteristics such as permeability. The subsurface system is modeled as a Discrete Fracture Network (DFN) where fractures are assumed to be two dimensional planes in three-dimensional space. Using a two-step joint inversion approach, we then evaluate and constrain the stochastics of the DFN based on microseismic and flow datasets. In this approach, we first estimate bounds on the statistics for the DFN fracture orientations and fracture sizes, using microseismic data.

These bounds are estimated either through a focal mechanism (physics-based approach) or through clustering algorithms (statistical approach). Then, using a Monte Carlo sampling based on these estimated fracture statistics, multiple realizations of DFNs are generated. On these realizations, we perform flow calculations, and compare with measured flow datasets, to obtain optimal probability distribution of the DFNs. The obtained DFNs can then be used to evaluate subsurface parameters of interest such as permeability and porosity, which can be eventually used for predictive modeling of state of- stress due to anthropogenic activities, for instance. The efficacy of this multi-physics based joint inversion is demonstrated with representative synthetic examp