2010 InterPore Conference and Annual Meeting at Texas A&M University

Venue: *Rudder Tower, Room 601, Texas A&M University, College Station, TX*

Organizing Committee: *Yalchin Efendiev* (Texas A&M, co-chair*); Majid Hassanzadeh* (The Utrecht University); *Rainer Helmig* (University of Stuttgart); *Oleg Iliev* (Fraunhofer ITWM, Kaiserslautern); *Mary Wheeler* (UT Austin, co-chair)

Scientific Committee: *Todd Arbogast* (UT Austin); *Goodarz Ahmadi* (Clarkson University); *Lynn Bennethum* (University of Colorado, Denver); *Akhil Datta-Gupta* (Texas A&M University); *Louis Durlofsky* (Stanford University); *Rudolf Hilfer* (Stuttgart University, Germany); *Magne Espedal* (University of Bergen, Norway); *James Glimm* (SUNY Stony Brook); *Massoud Kaviany* (University of Michigan); *Seong Lee* (Chevron, San Ramon); *Knut-Andreas Lie* (SINTEF, Oslo, Norway); *Brent Lindquist* (SUNY Stony Brook); *Binayak Mohanty* (Texas A&M*); Laura Pyrak-Nolte* (Purdue); *Tinsley Oden* (UT Austin); *Dean Oliver* (U. of Tulsa); *Mattias Schmidt* (Procter & Gamble Service GmbH); *Kambiz Vafai* (University of California, Riverside); *Xiao-Hui Wu* (ExxonMobil, Houston); *Jay Walton* (Texas A&M); *Ivan Yotov* (U. of Pittsburgh); *Jinchao Xu* (Penn State)

Local Organizers: *Dylan Copeland, Kristy Delvo-Vela, Yalchin Efendiev, Carla Harris, Robyn Richards*

Supported by **IAMCS, ISC, Department of Mathematics, and College of Science**

Sunday, March 14, 2010

5:00 – 7:00pm -Registration at Hyatt Place Hotel

Monday, March 15, 2010

8:00-8:30am Opening Remarks and Registration

8:30-9:20am - Tom Russell (NSF, Arlington, USA) -- *Eulerian-Lagrangian methods for multiphase multicomponent transport*

9:20-9:45am - Paul-Eric Oeren (Numerical Rocks, Trondheim, Norway) -- *Computation of petrophysical and multiphase flow properties on rock microstructure images*

9:45-10:10am - Brent Lindquist (SUNY Stony Brook) -- *Up-Scaling Geochemical Reaction Rates*

10:10-10:40am - Break

10:40-11:05am – Laura Nolte (Purdue Univ.) -- *Films & Hysteresis in a Simple Channel*

11:05 –11:30am – Rudolf Hilfer (University of Stuttgart) -- *Percolation and hysteresis in immiscible displacement*

11:30-11:55am – Goodarz Ahmadi (Clarkson University) -- *Multiphase flows in porous and fractured media - applications to carbon dioxide sequestration*

Noon-1:30pm – Lunch

1:30-2:20pm – Kambiz Vafai (UC Riverside) -- *Porous Media Approach in Bioengineering Applications*

2:20-2:45pm – Louis Durlofsky (Stanford) -- *Generation of coarse-scale flow models for systems with complex subgrid interactions*

2:45-3:15pm - Break

3:15–3:40pm – Michael J. King (Texas A&M) -- *Comparison of Spatially Adaptive Upscaling Strategies for Tight Gas Reservoir Simulation*

3:40-4:05pm - Seong Lee (Chevron) -- *Developing Multiscale Finite Volume Algorithms for a "Next-Generation" Reservoir Simulator*

4:05-4:30pm - Ivan Yotov (Univ. of Pittsburgh) -- *Stochastic multiscale mortar mixed finite element methods for flow in random porous media*

4:30-4:55pm – Jinchao Xu (Penn State) -- *Efficient Iterative Solvers for Reservoir Simulations*

4:55-5:45pm - Business meeting

6:30-9pm - Conference Dinner (Interpore honorary award will be presented to Jacob Bear)

Tuesday, March 16, 2010

8:00-8:30am Opening Remarks and Registration

8:30-9:20am - J. Kuzan (ExxonMobil) -- *An Assortment Of Thoughts On Pores: Fractures, Scale-Up, and Wettability*

9:20-9:45am - Dani Or (ETH Zurich) -- *Inertial jumps, pressure bursts and acoustic emissions at displacement fluid fronts – pore scale dynamics affecting macroscopic properties*

9:45-10:10am – S. Majid Hassanizadeh (Utrecht) -- *There is no dynamic capillary pressure*

10:10-10:40am - Break

10:40-11:05am – Wolfram Ressel (University of Stuttgart) -- *Towards acoustical life cycle simulation of porous asphalt*

11:05 –11:30am – Rodrigo Rosati (Procter & Gamble) -- *Modeling and simulation across P&G porous media based products* (Thomas J. Lange and Rodrigo Rosati)

11:30-11:55am – Konrad Steiner (Fraunhofer-ITWM) -- Flow *problems in industrial porous media*

Noon-2:00pm – Lunch and **poster session**

2-2:25pm – Tom Hughes (UT Austin) -- *Mathematical Modeling of Coupled Drug and Drug-encapsulated Nanoparticle Transport in Patient-specific Coronary Artery Walls* (T. Hughes and Shaolie Hossain)

2:25-2:50pm - Rainer Helmig (University of Stuttgart) -- **Memorial Lecture dedicated to Magne Espedal --** *Corrected operator splitting combining streamline approach for porous media flow with gravity*

2:50-3:15pm - Lynn Bennethum (CU Denver) -- *Hybrid mixture theory for charged porous media with application to modeling a drug delivery system*

3:15-3:40pm – Eric Nauman (Purdue University) -- *A volume fraction-based mixture theory to predict capillary level transport of nanoparticles in tumors*

3:40-4:05pm - Break

4:05-4:30pm - Mansoor Haider (North Carolina State University) -- *Continuum mixture models of biomechanical cell-matrix interactions in articular cartilage*

4:30-4:55pm – Pawan S. Takhar (Texas Tech University) -- *Applications of hybrid mixture theory for studying transport mechanisms in food materials*

5:20-8:00pm - Poster session

Wednesday, March 17, 2010

8:00-8:30am Registration

8:30-8:55am - Mattias Schmidt (Procter & Gamble) -- *"Can I use (trust) the model?" – Some thoughts on modeling and simulation in an industrial application context*

8:55-9:20am – Randy Schunk (Sandia) -- *Partially saturated flows in poroelastic media: Theoretical approach and numerical challenges*

9:20-9:45am – David DiCarlo (UT Austin) -- *Modeling Saturation Overshoot at the Continuum and Pore-Scales*

9:45-10:10am – Matthew Balhoff (UT Austin) -- *Upscaling of macroscopic properties from the pore to continuum scale using mortars*

10:10-10:40am – Break

10:40-11:05am – Tim Wildey (UT Austin) -- *Multiscale Mortar Preconditioners for Flow in Porous Media*

11:05–11:30am – Felipe Pereira (Univ. of Wyoming) -- *A New Computational Strategy for the Approximation of Two-Phase Flows in Strongly Heterogeneous Poroelastic Media*

11:30-11:55am – Shuyu Sun (KAUST) -- *Numerical Simulation of Two-Phase Flow in Heterogeneous Porous Media*

Noon-1:30pm – Lunch

1:30-1:55pm – Masha Prodanovich (UT Austin) -- *Interfacial areas and triple contact lines at drainage and imbibition: theory, experiments and simulation*

1:55-2:20pm – Dan Marchesin (IMPA) -- *The injection problem for three-phase flow in porous media*

2:20-2:45pm- Gabriel Wittum (University of Frankfurt) -- *Simulation of density-driven flow in fractured porous media*

2:45-3:10pm – John Cushman (Purdue) -- *Stochastic processes run with nonlinear clocks as models for anomalous dispersion: complexity and ergodicity*

3:10-3:35pm - Guodong Jin (Baker Hughes Incorporated, Houston, TX) -- *Predicting Petrophysical Properties Of Downhole Earth Formation From Log-Derived Rock Models*

3:35pm – Closing Remarks

POSTER PRESENTATIONS:

- Flow simulation of fractured-vuggy media based on equivalent continuum model
  Li Yajun, Yao Jun, Huang Zhaoqin (China University of Petroleum)

- Discrete fracture-vug network model and its application to fractured vuggy porous media
  Huang Zhaoqin, Li Yajun, Yao Jun (China University of Petroleum)

- Physical controls of soil hydrauli parameter scaling at multiple scales
  Raghu Jana, Binayak Mohanty, Yalchin Efendiev (Texas A&M)

- Modeling biogeochemical processes in a comtaminated quifer-wetland system using ANN-HP1
  Bhanva Arora, Binayak Mohanty, Jennifer T. McGuire (Texas A&M)

- Using homogenization theory to calculate the effective diffusion tensor for human stratum corneum with corneocyte cells of tetrakaidekahedral geometry
  I. Muha, S. Stichel, A. Naegel, M. Heisig, Gabriel Wittum (University of Frankfurt)

- Multiscale simulations techniques for multi-phase flows using limited global information
  L. Jiang (U. of Minnesota), Y. Efendiev (Texas A&M University), I. Mishev (ExxonMobil)

- Some numerical results for modeling fractures as interfaces with nonconforming grids
  N. Frih, V. Martin, Jean E. Roberts, A. Saada (INRIA)

- Preferential flow paths in fractures
  Dustin Crandall (National Energy Technology Lab), M. Ferer (National Energy Technology Lab), Goodarz Ahamdi (Clarkson), D. Smith (National Energy Technology Lab)

- Damage modelling in non-isothermal unsaturated porous geomaterials
  C. Arson (Texas A&M)

- New methods for modeling productivuty index of the well for generalized Forchheimer flows in porous media
  L. Bloshanskaya, E. Aulisa, L. Hoang, A. Ibragimov (Texas Tech)

- *Modeling of effective parameters on permeability of porous media with application to fuel cell*
  A.M. Parvanian, M. Panjepour, Gh. Aryanpour (Isfahan University of Technology)

- Bayesian uncertainty quantification for flows in heterogeneous porous media using reversible jumo Markov chain Monte Carlo methods
  A. Mondal, Y. Efendiev, B. Mallick, A. Datta-Gupta (Texas A&M)

- Gas permeability measurement of very weakly permeabile porous media
  Y. Jannot (Nancy-Universite, CNRD) and Didier Lasseux (Lab. TREFLE)

- Coarse-scale models for high-contrast multiscale problems
  J. Galvis and Y. Efendiev (Texas A&M)

- A hybrid Ensemble Kalman Filter with coarse scale constraint for nonlinear dynamics
  S. Watanabe (Texas A&M), A. Datta-Gupta (Texas A&M), Y. Efendiev (Texas A&M), D. Devegowda (U. of Oklahoma)

- On Upscaling Flows in Highly Porous Media
  J. Willems (Texas A&M), O. Iliev (Kaiserslautern), R. Lazarov (Texas A&M)

- History matching in channel reservoirs using level set methods and Markov chain Monte Carlo
  X. Jiang, A. Mondal, A. Datta-Gupta, Y. Efendiev, B. Mallick (Texas A&M)

- A posteriori error estimates including algebraic error stopping criteria for iterative solvers
  P.Jiranek (Technical Univ. of Liberec), Z. Strakos (Academy of Sciences of the Czech Republic), M. Vohralik (Univ. of Paris 06)

- Analysis of the role of structural disorder on the inertial correction to Darcy's law
  Didier LASSEUX, Azita AHMADI and Ali Akbar ABBASIAN ARANI TREFLE - UMR CNRS 8508 - University of Bordeaux – Arts et Métiers ParisTech , Esplanade des Arts et Métiers, 3340, Talence Cedex France

Eulerian-Lagrangian methods for multiphase multicomponent transport (Thomas F. Russell, National Science Foundation)

Abstract: Transport in porous media is often advection-dominated. This leads to efforts to incorporate Lagrangian techniques into numerical schemes, in order to overcome CFL limitations, numerical dispersion, and non-physical oscillations. In multiphase transport, these efforts are made easier by working with an adjoint system, whose natural interpretation is in terms of mass movement rather than wave propagation. The talk will explain this in the context of Eulerian-Lagrangian methods for multiphase multicomponent transport and will outline some recent developments.

Computation of petrophysical and multiphase flow properties on rock microstructure images (Pål-Eric Øren, Numerical Rocks AS Trondheim, Norway)

Abstract: Due to great advancement in computer technology and software, the petroleum industry has made significant progress in describing detailed geological heterogeneities in hydrocarbon reservoirs and incorporating these in reservoir flow simulations. However, the description of the associated rock and fluid flow properties is not nearly as detailed. Measurements of flow properties are scarce and there is no easy way to account for spatial variations in these properties due to different pore structures and wettability trends. With recent advances in predictive pore-scale modeling and the power of today's high performance computers, rock and flow properties can now be derived directly through computations.

In the present work, we investigate the predictive capabilities of direct pore-scale simulations of material and transport related effective properties of sedimentary rocks. 3D rock microstructure images are obtained via X-ray microtomography and via thin section analysis combined with geological process based modeling of the rock forming processes. Petrophysical properties of the rock models, such as permeability, electrical resistivity, elastic properties, and NMR relaxation are computed and compared with experimental data. Multiphase flow properties such as capillary pressure and relative permeability are computed directly on the 3D images by two-phase Lattice Boltzmann simulations. The results are compared with measured data and with those obtained using network modeling techniques.

Our results demonstrate the potential and feasibility of combining rock microstructure images with numerical calculations to derive rock and flow properties for reservoir rocks and to augment the analysis and interpretation of experimentally derived data. This can lead to the development of type curves for properties and cross-property relations, which are more readily constructed numerically than by experimentation. This presents exciting possibilities of bridging the technology gap that exists today between detailed geological models and the lack thereof for the associated reservoir rock properties.

Up-Scaling Geochemical Reaction Rates (W. Brent Lindquist, Daesang Kim, and Catherine A. Peters, SUNY Stony Brook)

Abstract: Accurate modeling of reactive flow requires effective determination of reaction rates applicable for field scale models. We utilize network flow models in conjunction with X-ray computed tomography images to determine up-scaling from pore- to core-scales. In this talk we illustrate with dissolution and precipitation reactions that may accompany geological CO_2 sequestration in sandstone basins. Simulations of the injection of CO_2 saturated brine into the pore networks corresponding to three different sandstone samples were performed to study up-scaling of kaolinite and anorthite reaction rates. Computed tomography is used to capture both the sample pore network as well as map mineral distribution in the samples. True bulk reaction rates, as determined from the simulations, are compared with rates predicted by a volume-averaged-concentration method. For the anorthite reaction, which is effectively pH driven, the true bulk anorthite reaction rate is smaller than the volume averaged reaction rate by 25~40%. The kaolinite

reaction, which is effectively driven by the saturation state, is dominated by large spatial variation of values of this state value, particularly where precipitation occurs. In fact, the molecular-scale rate law in the precipitation regime for kaolinite is not well known experimentally. The three rate-law models investigated produce significantly different predictions for up-scaled reaction rates. Significantly, in all three cases, predicted volume-averaged reaction rates not only under-predict the magnitude of the bulk reaction rate, but the predicted bulk reaction type, dissolution vs. precipitation, is often opposite to that of the true up-scaled rate. Finally the observed up-scaled reaction rates show a flow-rate dependence that is not captured by molecular-scale reaction laws and must be quantified either by flow experiments or numerical simulation.

Films & Hysteresis in a Simple Channel (***Laura J. Pyrak-Nolte[1,2], Yihong Liu[1], David D. Nolte[1] and Nicholas J. Giordano[1])***

[1]Department of Physics, Purdue University, 525 Northwestern Avenue, West Lafayatte, IN 47907-2036
[2]Department of Earth and Atmospheric Sciences, Purdue University
Abstract: The hysteretic relationship between capillary pressure (P_c) on saturation (S) may suggest that additional state variables are needed to describe, fully, multiphase flow behavior in porous media. Studies in random micromodels have shown that the observed hysteresis is a projection of a higher-dimensional surface that depends on interfacial area per volume, A_V, as the additional state variable. However, these studies have not addressed the effect of films on the P_c-S-A_V relationship. Therefore, we report here the use of laser confocal microscopy to image the three-dimensional (3D) fluid distribution of two immiscible fluids in a simple wedge-shaped channel. We find that entrained films of wetting phase affect the P-S relationship during both drainage and imbibition and that these extensions of the fluid-fluid interface increase the interaction among the wetting, non-wetting, and solid phases.

Smooth-walled and rough-walled wedge-shaped channels were fabricated using two different approaches: 1) two-photon polymerization by femtosecond laser machining and 2) broadband photolithography. Both techniques use UV-sensitive photoresist (SU-8) to construct an all-SU-8 micromodel containing a wedge-shaped channel that is 100 μm wide at the outlet and 20 μm wide at the inlet with a constant depth of 40 μm. A Zeiss LSM 710 Confocal Microscope was used to image water (wetting phase) and air (non-wetting phase) distributions within the micromodels. By labeling the wetting phase with a fluorophore (Alex Fluor-488 water solution 1%w.t.), the water-air interfaces are clearly visible in the confocal microscopy images. The samples were initially saturated with water. A series of drainage and imbibition cycles were performed by incrementing or decrementing the air pressure. At each pressure, the system was allowed to reach mechanical equilibrium, and then a stack of scans in depth was collected to acquire the 3D fluid distribution for a given pressure. The confocal images were analyzed to extract the volume saturation of air and water, the curvature of the three-dimensional fluid-air interface, and the interfacial area per volume.

Hysteretic dependence of the capillary pressure (P_c) on the volume saturation (S_v) was observed even though the wedge-shaped channel has no complex geometry. The P_c – S_v hysteresis with and without films were compared. When films were present, higher capillary pressure was needed to drain the wetting phase. The film provided additional resistance during drainage and additional forces during imbibition.

Because S_v is proportional to the wetting phase volume variation, the energy DE cost to move the interface was calculated from the P_c – S_v graph between pressure steps, and the change in surface area DA between pressure steps was calculated from the saturation S_v. Linear relationships were found between DE and DA for drainage and imbibition. The slopes of the DE – DA lines with film are higher than those without film, suggesting that the system expends additional energy to move fluid-fluid interfaces when films are present.

Acknowledgments: This research is supported by the National Science Foundation (0509759-EAR and 0911284-EAR).

Percolation and hysteresis in immiscible displacement (Rudolf Hilfer, University of Stuttgart)

Abstract. The concepts of relative permeability and capillary pressure are crucial for the accepted traditional theory of two phase flow in porous media. Recently a theoretical approach was introduced that does not require these concepts as input [1][2][3]. Instead it was based on the concept of hydraulic percolation of fluid phases. The presentation will describe this novel approach. It allows to predict residual saturations and local spatiotemporal changes between imbibtion and drainage during two phase immiscible displacement [1][2][3][4][5].

References

[1] R. Hilfer. Capillary Pressure, Hysteresis and Residual Saturation in Porous Media,Physica A, vol. 359, pp. 119, 2006.
[2] R. Hilfer. Macroscopic Capillarity and Hysteresis for Flow in Porous Media, Physical Review E, vol. 73, pp. 016307, 2006.
[3] R. Hilfer. Macroscopic capillarity without a constitutive capillary pressure function, Physica A, vol. 371, pp. 209, 2006.
[4] R. Hilfer. Modeling and Simulation of Macrocapillarity, in: P. Garrido et al. (eds.) Modeling and Simulation of Materials vol. CP1091, pp. 141, American Institute of Physcis, New York, 2009.
[5] R. Hilfer and F. Doster. Percolation as a basic concept for macroscopic capillarity, Transport in Porous Media, in press, 2009.

Multiphase Flows in Porous and Fractured Media – Applications to Carbon Dioxide Sequestration (Goodarz Ahmadi, [1] Dustin Crandall,[2] and Duane Smith[2])

[1] Department of Mechanical and Aeronautical Engineering Clarkson University, Potsdam, NY 13699, USA
[2] National Energy Technology Laboratory, US Department of EnergyMorgantown, WV 26505, USA

Abstract. Recent experimental and computational modeling methods for studying multiphase flows in porous media and fractured rocks were reviewed. Connection with geological sequestration of carbon dioxide was discussed. The experimental setup of a laboratory-scale flow cell was described in details. It was shown that the gas-liquid flows generate fractal interfaces and the viscous and capillary fingering phenomena were discussed. Experimental data concerning the displacement of two immiscible fluids in the lattice-like flow cell were presented. The flow pattern and the residual saturation of the displaced fluid during the displacement were discussed. Numerical simulations results for the experimental flow cell were also presented.

Numerical simulation results and experimental data for single and multiphase flows through rock fractures were also presented. Fracture geometry studied was obtained from a series of CT scan of an actual rock fracture. Computational results showed that the major losses occur in the regions with smallest apertures. An empirical expression for the fracture friction factor was also described. Applications to CO_2 sequestration in underground brine fields depleted oil reservoir stimulation were discussed.

Keywords: Carbon dioxide sequestration, multiphase flows, flows in porous media, flows in fractured media, immiscible flows, computer model, reservoir engineering

Porous Media Approach in Bioengineering Applications (K. Vafai, UC Riverside)

Abstract. Flow, heat and mass transfer in biological tissues based on porous media modeling are synthesized in this talk. Pertinent models and six primary areas are presented in order to show how transport models in porous media advance the progress in biology. The main concepts presented in this talk are transport in porous media using mass diffusion, different convective flow models and selective convection. Energy transport in tissues is also presented. Progress in development of the bioheat equation (heat transfer equation in biological tissues) and evaluation of the applications associated with the bioheat equation are utilized in these areas. Prominent examples of diffusive applications and momentum transport

by convection in these works are mentioned. Porous media modeling in biological tissues is found to be quite an appropriate route for analyzing transport within biological tissues.

Generation of coarse-scale flow models for systems with complex subgrid interactions (Louis J. Durlofsky, Stanford)

Abstract. In computational upscaling, coarse-model parameters such as grid-block permeability are typically determined based on fine-scale computations over appropriately defined local regions of the model. In many cases, the coarse-scale properties can be computed directly from these local fine-scale simulations by relating the integrated flux to the imposed driving force. When multiple nonlinear effects are present or when the subgrid variation in state variables is large, however, the direct and accurate determination of coarse-scale parameters is difficult. Another complication that arises is the impact of the local boundary conditions on the coarse-scale properties.

In this talk, procedures for addressing these challenges are presented. Although the approaches are general, the target application here is the coarse-scale modeling of oil, gas and water production in reservoir simulation. We define appropriate near-well domains and then determine coarse-scale parameters by minimizing the discrepancy in flow quantities between fine and coarse solutions over these local regions. This minimization is achieved through the use of gradient-based optimization techniques, with gradients computed using an adjoint method. Boundary conditions for the local near-well computations are determined using a local-global procedure. Under this approach, the necessary boundary information is interpolated from (inexpensive) global coarse-scale solutions. The overall procedure is applied to simulate fluid production in 3D models involving heterogeneous near-well permeability descriptions and two and three-phase flow, including gas that is liberated from the oil phase during production. Simulation results demonstrate the consistent accuracy provided by this new upscaling procedure and its significant advantages relative to existing approaches.

Comparison of Spatially Adaptive Upscaling Strategies for Tight Gas Reservoir Simulation (Yijie Zhou and Michael J King, Department of Petroleum Engineering, Texas A&M University)

Abstract. Tight gas reservoirs provide an interesting and complex spatial pattern of partially or intermittently connected fluvial sand packages within a non-pay background. Detailed 3D geologic models of these reservoirs show that gas sands immediately adjacent to a producing well may not be effectively drained due to the lack of local connectivity. This is consistent with field performance data. In contrast, the coarser reservoir simulation models used for performance prediction have been forced to over-homogenize the reservoir description, leading to systematic errors in the estimates of gas recovered.

We report on our recent work in which we utilize a local connectivity analysis to design an effective reservoir simulation grid by grouping adjacent fine cells of the geologic model. This cell grouping operation is constrained to preserve the connectivity of both sands and barriers within the reservoir description. Different strategies are possible within these constraints. We report upon the relative success of several of them.

Developing Multiscale Finite Volume Algorithms for a "Next-Generation" Reservoir Simulator (by S. H. Lee, Chevron ETC, San Ramon)

Abstract: Recent advances in multiscale methods show great promise in efficiently simulating a high-resolution model for highly heterogeneous media. The current multiscale approach in reservoir simulation is designed to devise an efficient numerical algorithm in two scales. We first frame a fully implicit multiscale finite volume algorithm (MSFV) with prolongation and restriction operations of flow and transport equations. We then propose numerical, adaptive operators that will greatly improve numerical efficiency over the conventional finite difference reservoir simulation. We also discuss iterative methods that can improve the quality of the localization assumption in MSFV.

Stochastic multiscale mortar mixed finite element methods for flow in random porous media (Ivan Yotov, Department of Mathematics, University of Pittsburgh)

Abstract. We discuss a multiscale stochastic framework for uncertainty quantification of flow in porous media. The governing equations are based on Darcy's law with stochastic permeability represented with a Karhunen-Loeve (KL) expansion. We consider a domain decomposition formulation with different KL expansions in different subdomains. This approach allows to model efficiently heterogeneous media with different rock types. The approximation is based on multiscale mortar mixed finite elements in the spatial domain coupled with tensor product or sparse grid stochastic collocation. We precompute a multiscale basis, which involves solving subdomain problems for each realization of the local KL expansion. The basis is then used to solve the coarse scale mortar interface problem for each global KL realization. The resulting algorithm is orders of magnitude faster than a global stochastic collocation approach. Error analysis for the statistical moments of the pressure and the velocity is performed and numerically verified. The method is applied for simulations of single phase flow in highly heterogeneous porous media.

ABSTRACTS (Tuesday, March 16)

An Assortment of Thoughts on Pores: Fractures, Scale-up, and Wettability (John Kuzan, ExxonMobil)

Abstract. The presentation reviews the approach to life-cycle reservoir management and the areas in which approaches are highly numerical versus those that are more concept-based. Two examples of reservoir performance prediction application in the oil business are discussed in light of these different approaches. Pore-level features (fractures and wettability) are then examined in the same light, using scale-up approaches a macroscopic bridge between these two fine scale features.

Inertial jumps, pressure bursts and acoustic emissions at displacement fluid fronts – pore scale dynamics affecting macroscopic properties (Dani Or and Franziska Möbius, Soil and Terrestrial Environmental Physics (STEP), Department of Environmental Sciences, Swiss Federal Institute of Technology (ETH) Zurich, Switzerland)

Abstract. The macroscopically steady and regular motion of fluid displacement fronts through porous media often conceal considerable activity occurring at the pore scale involving rapid interfacial motions and pressure bursts at the front line. Experimental results using different fluids and flow rates supported by high speed imaging (1000 images/s) document local interfacial displacement velocities exceeding 1 m/s (Re>100). Characteristics of bursts resulting from rapid air-water interfacial reconfiguration through are quantified via their acoustic emissions (AE) and pressure measurements. The results challenge the pore scale basis for the laminar-viscous Darcy-Buckingham representation of unsaturated hydraulic conductivity for characterizing the transient displacement regimes of imbibitions and drainage fronts. Capillary processes associated with very short capillaries and pore throats are inherently different than those postulated for long capillaries under equilibrium and are in part responsible for the highly dynamic processes. The sensitivity of displacement front morphology to local force balance often expressed in terms of dimensionless Bo and Ca numbers is accentuated by inertial forces. We use Tallakstad et al. (2009, PRE) characteristic length to define the transition from highly transient regime at the front (in which continuum-based hydraulic functions and driving forces do not apply), to more stable interfacial configurations region where hydraulic properties regain their definition. The dynamic nature of displacement front passage leaves its mark in the resulting phase distribution and hydraulic properties and thus provides the physical basis for phenomena such as hysteresis and dynamic capillary pressure.

There is no dynamic capillary pressure (Majid Hassanizadeh, Utrecht University)

Abstract. Traditional equations of two-phase flow in porous media assume an algebraic relationship between the so-called "capillary pressure" and saturation. This algebraic relationship is consistent with an assumption of instantaneous equilibrium between fluids pressure difference and saturation. Commonly, this pressure difference is referred to as the "static capillary pressure." Both experimental and theoretical evidence points to a moregeneral dynamic relationship between pressures and saturation, with the traditional algebraic relationship being reached only at equilibrium. Under dynamic conditions, the difference in fluid pressures is commonly referred to as "dynamic capillary pressure." This terminology suggests that capillary pressure is not just a property of the fluids-solid system, but also depends on dynamics of the flow. In this presentation, we put forward the concept that the capillary pressure is an intrinsic property of the fluids-solid system, and is uniquely defined under dynamic as well as static conditions. Using data from pore-scale simulations and micromodel experiments, we show that macro-scale capillary pressure for a given set of fluids and solid, defined as the average of pore-scale capillary pressure, is uniquely related to saturation and specific interfacial area,. What IS different under static and dynamic conditions is the fluids pressure difference. Finally, the relationship between fluids pressure difference, capillary pressure, and time rate of saturation is investigated.

Towards acoustical life cycle simulation of porous asphalt* (*Wolfram Ressel, University of Stuttgart)

Abstract. The wearing course constitutes the top layer of asphalt pavements and is typically designed for a lifespan of about one decade. Wearing courses are usually made of densely graded, compact asphalt. Alternatively, porous asphalt can be used which is primarily designed with respect to a good noise reduction characteristic. Due to its hollow structure it is able to reduce the noise pressure level significantly. In addition, the hollow structure results in a good water drainage capacity. This implies that, together with water, road debris is infiltrated into the asphalt. If the debris accumulates on the bituminous surface of the pores the outstanding acoustical properties worsen and the acoustical life cycle of porous asphalt decreases notably in comparison to the structural life cycle.

The simulation of two phase flow including the deposition of particles on a pore scale helps to understand the emergent behavior on a laboratory scale. Further the relationship between slightly modifications of the pore geometry and the main acoustic parameters can be included. With this new numerical approach the simulation time for a life cycle of porous asphalt will be significantly reduced compared to laboratory experiments. Further the flexibility in testing modifications of existing asphalt types will be increased. The geometry is reconstructed from tomographical measurements in combination with three-dimensional image reconstruction techniques. It serves as input for pore scale simulation using the lattice Boltzmann method.

Modeling and simulation across P&G porous media based products (Thomas J. Lange (Modeling and Simulation, Corporate R&D, Procter&Gamble), Rodrigo Rosati (Core Technology, Baby Care, Procter&Gamble))

Abstract. Understanding and optimizing fluid flow and mechanical behavior for porous media is critical for developing superior consumer products, based on porous media, at Procter&Gamble, such as baby diapers, paper towels, wipes, feminine pads, packed bed filters for water, etc. This talk will provide first an overview of physics, modeling applications and challenges across a range of P&G products based on porous media. Then as a specific example the talk will provide an introduction into fluid flow in hygiene consumer products with the focus on baby diapers: in this case typical challenges are that the porous materials are soft and can deform due to wet collapse or external conditions, adjacent materials have a large contrast of key hydraulic parameters and they can be very thin such that the validity of the fluid flow

equations is questionable. In addition, swelling of materials such as super-absorbers leads to dimensional changes of the pore structure during the fluid transport: we will share how the flow and deformation processes in swelling porous media have been modeled and how a finite element solution strategy has developed and implemented in the FEFLOW commercial simulator. As well the talk will highlight some examples of thin layers in hygiene products and establish a number of challenges associated with them.

Flow problems in industrial porous media (Dr. Konrad Steiner, Head of Department: Flow and Material Simulation, Fraunhofer Institut für Techno- und Wirtschaftsmathematik, Fraunhofer-Platz 1, 67663 Kaiserslautern, konrad.steiner@itwm.fraunhofer.de)

Abstract. The world is porous! Nearly all materials are porous -- at least on some fine scale. Typical examples are soils or body tissues, which all are multi-scale materials. Normally, one associates flows in porous media with geophysical applications like multiphase transport in petroleum engineering or nowadays with biological tissue engineering. Beside this, more and more industrial porous media used in process technology and material production need the assistance of modelling and simulation to design and optimize their performance. In addition to geophysical and biological application, in industrial porous media it is not only interesting to understand per se the porous media; moreover the manufacturing process and the functionality performance of the final product have to be simulated and optimized by varying the porous structure.

The talk will show applications and numerical methods to simulate and optimize industrial porous materials along their process chain, which include flow dominated multi-scale problems in porous materials. Examples will be the design of technical filter media and systems, the optimization of porous fabrics and felts for paper dewatering and manufacturing of fibrous or particle enforced hybrid materials. As well, the related manufacturing processes are often complex fluid dynamical problems like particle suspension flows with varying concentrations (fibre or particle injection moulding) or granular transport processes in the range from dilute particle flow up to compaction to packed grains.

Mathematical Modeling of Coupled Drug and Drug-encapsulated Nanoparticle Transport in Patient-specific Coronary Artery Walls (Tom Hughes, Shaolie Hossain, UT Austin)

Abstract. Heart attacks occur due to rapid progression of plaque buildup in the coronary arteries that supply blood to the heart muscles. The diseased arteries can be treated with drugs delivered locally to vulnerable plaques—ones that may rupture and release emboli, resulting in the formation of thrombus, or blood clot that can cause blockage of the arterial lumen. In designing these local drug delivery devices, important issues regarding drug distribution and targeting need to be addressed to ensure device design optimization as physiological forces can cause the local concentration to be very different from mean drug tissue concentration estimated from *in vitro* experiments and animal studies. Therefore, the main objective of this work was to develop a computational tool-set to support the design of a catheter-based local drug delivery system that uses nanoparticles as drug carriers by simulating drug transport and quantifying local drug distribution in coronary artery walls.

A three dimensional mathematical model of coupled transport of drug and drug-encapsulated nanoparticles was developed and solved numerically by applying finite element based isogeometric analysis that uses NURBS-based techniques to describe the artery wall geometry. To gain insight into the parametric sensitivity of drug distribution, a study of the effect of Damkohler number and Peclet number was carried out. The tool was then applied to a three-dimensional idealized multilayered model of the coronary artery wall to demonstrate the capabilities of the methodologies developed. Preliminary results indicated that use of realistic geometry is essential in creating physiological flow features and transport forces necessary for developing catheter-based drug delivery design procedures. Hence, simulations were run on a patient-specific coronary artery wall segment under normal and diseased conditions with a typical vulnerable plaque characterized by a lipid pool encased by a thin fibrous cap.

Results show that plaque and artery wall inhomogeneity modulate drug distribution. Furthermore, the lipid core recruits and retains hydrophobic drug from neighboring healthy branches of the coronary artery facilitated by the highly anisotropic diffusion, indicating that the nanoparticles that are off-target might still contribute significantly to the overall drug tissue concentration in the target region.

The computational tool-set developed was able to successfully capture trends observed in local drug delivery by incorporating a multitude of relevant physiological phenomena, and thus demonstrated its potential utility in optimizing drug design parameters including delivery location, nanoparticle surface properties and drug release.

Hybrid Mixture Theory for Charged Porous Media with Application to Modeling a Drug Delivery System ***(Lynn Schreyer-Bennethum and Keith Wojciechowski, Department of Mathematical and Statistical Sciences, University of Colorado Denver, Campus Box 170; 1250 14th St., Suite 600; P.O. Box 173364; Denver, CO 80217-3364 E-mail: Lynn.Bennethum@ucdenver.edu)***

Abstract. In this talk we will give an introduction to hybrid mixture theory (HMT) as a means for modeling charged swelling porous media. The assumptions and general procedure for arriving at governing equations and differences between some different mixture theoretical approaches will be discussed. We will discuss different interpretations for liquid pressure in a charged porous material. As an application we will consider swelling drug delivery polymers.

Swelling drug delivery polymers are a means of delivering drugs such as Aleve into our bodies in such a way that the drug is ideally released in a sustained and constant rate manner. The polymer itself is usually viscoelastic, e.g. hydroxypropyl methylcellulose (HPMC), and positively charged. The drug can be either attached to the solid phase or trapped in the pores so that as the polymer is exposed to a solvent (fluid), the polymer swells and the drug diffuses out. As the polymer swells it plasticizes – the polymer chains transition from the glassy to the rubbery state producing a front. We present some numerical results for the non-charged case.

A Volume Fraction-Based Mixture Theory to Predict Capillary Level Transport of Nanoparticles in Tumors ***(Mary M. Schuff, Jay P. Gore, and Eric A. Nauman, School of Mechanical Engineering, Purdue University, 585 Purdue Mall, West Lafayette, IN 47907. E-mail: enauman@purdue.edu)***

Abstract. Nanoparticle-based therapies have been proposed for improving tumor detection and treatment because a modification to their molecular structure provides control of their electromagnetic properties, surface chemistry, and binding affinity. In order to take advantage of these physico-chemical characteristics, the transport of the nanoparticles in the tumor and other tissues must be optimized. The limitations of existing transport models indicate the need for a comprehensive model that includes transport in the vessel lumen, the vessel wall, and the interstitial space and considers the effects of the solute concentration on fluid flow.

In this study, a volume fraction-based mixture theory was used to develop a general model to describe the transient distribution of fluid and multiple solutes at the microvascular level. The mixture theory formulation included a number of components not accounted for in the traditional transport equations. Mixture theory captured the dependence of the hydraulic permeability coefficient of the capillary wall on the concentration of solutes present as has been observed experimentally. The hydraulic conductivity of the tissue had a similar dependence on the solute concentration. The fluid flows across the capillary wall and in the interstitium were related to the solute concentration as well as the hydrostatic pressure. The mixture theory model allowed for the application of external body forces, uptake of solutes by cells, aggregation of the solutes, and solid tissue deformation. We will present the calibration and validation of the model as well as the effects of electromagnetic fields on the particle distribution.

Continuum Mixture Models of Biomechanical Cell-Matrix Interactions in Articular Cartilage ***(Mansoor A. Haider, Department of Mathematics, North Carolina State University, Box 8205, Raleigh, NC, 27695 E-mail: m_haider@ncsu.edu)***

Abstract. Articular cartilage is the load-bearing connective tissue lining the surfaces of diarthrodial joints such as the knee, shoulder and hip. Continuum mixture models of articular cartilage account for the biphasic (fluid-solid) or triphasic (fluid-solid-ion) composition of the tissue, and share common aspects with poroelastic mixture models. Articular cartilage is comprised of roughly 80% water (by volume), an extracellular matrix (ECM) with charged (proteoglycan) and uncharged (collagen) constituents, and a single population of specialized cells called chondrocytes. Since cartilage is avascular and aneural, these cells maintain the homeostatic balance between degradation and repair in the cartilage ECM, and are known to alter their metabolic activity in response to changes in their local environment. Chondrocyte shape varies with depth and individually (or in small groups) these cells are surrounded by a distinct, narrow tissue region, termed the pericellular matrix (PCM). Relative to the ECM, which is dominated by type-II collagen, the PCM contains mostly type-VI collagen as well as a higher concentration of negatively charged proteoglycans. Together, the chondrocyte and PCM have been termed a chondron. In the microscopic environment of cartilage, the PCM is hypothesized to have a dual role as both a protective layer and a mechanical transducer for the chondrocyte. In this context, mathematical models are used to determine tissue material properties from in vitro experiments performed on isolated tissue samples, as well as to simulate the biomechanical environment of individual chondrocytes within the cartilage ECM under a variety of loading conditions. This talk will focus on the development of continuum mixture models for the PCM in articular cartilage. A variety of analytical and computational approaches will be presented including the use of theoretical solutions, finite element methods, and boundary element methods integrated with optimization algorithms for inverse analysis of in vitro experimental data.

Applications of Hybrid Mixture Theory for Studying Transport Mechanisms in Food Materials ***(Pawan S. Takhar, Department of Animal and Food Sciences, International Center for Food Industry Excellence, Texas Tech University, Box 421141, Lubbock,TX, 79409. E-mail: pawan.takhar@ttu.edu)***

Abstract. During fluid transport processes such as drying, sorption and frying, physical and chemical changes take place in the biopolymers. A hybrid mixture theory based multiscale approach was developed that allows incorporating these changes into transport models. Two and three-scale transport and thermomechanical equations were developed and solved using the finite element method to predict moisture and stress profiles during continuous and intermittent moisture transport in foods.
The model validation was performed by making comparisons to experimental data. The solution of equations provided information on the role of glass transition on Fickian (or Darcian) and non-Fickian (or non-Darcian) modes of fluid transport, and stress development in foods. NMR imaging experiments were conducted to validate the model's prediction that fluid transport in foods is non-Darcian near glass transition. The experiments also showed that by carefully controlling the time-step in combination with high and low temperatures during intermittent drying, greater amount of moisture could be removed and more uniform moisture distribution could be obtained. This would allow saving energy consumption during drying and obtaining foods with fewer stress cracks.

Unsaturated transport equations were developed and utilized for studying oil uptake and moisture loss during frying of foods. Studying these transport mechanisms are needed to minimize oil uptake during frying for improving the health benefits of fried foods without compromising with taste, color and texture. Frying is an unsaturated porous media problem involving transport of water, oil and gas (vapors+air) in the food matrix over a hierarchy of spatial scales. Numerous novel equations such as generalized Darcy's law based fluid transport equations for various phases; near-equilibrium equation governing phase change from liquid water to vapor or *vice versa*; generalized stress-strain relations; swelling/shrinking behavior and generalized Laplace law of heat transfer were obtained. The equations were solved using the finite element method implemented in Comsol Multiphysics package to predict frying mechanisms in rice crackers. Rice crackers are obtained by performing high temperature frying (>200C) for a short time (~1 min). Reduction of fat uptake in foods such as rice crackers is a difficult task because they are thin and rigid initially and form a puffy and expanded structure in a few seconds. The model could predict the experimental moisture and oil content data with reasonable accuracy. The rate of moisture loss and oil uptake was found to be

directly related to the pressure development, evaporation rate and frying temperature. Simulations indicated that most physical processes during frying of rice crackers attain a steady state in the first 20 sec. After 20 sec, the vapor pressure inside crackers reduces to the atmospheric pressure, which leads to greater oil penetration afterwards. Thus, in the rice cracker industry, energy can be saved and oil uptake can be reduced by reducing the frying time from 60 sec to 20 sec.

ABSTRACTS (Wednesday, March 17)

"Can I use (trust) the model?" – Some thoughts on modeling and simulation in an industrial application context (Mattias Schmidt, Procter & Gamble)

Abstract. The adoption of modeling & simulation practices has proven critical to improve innovation productivity at P&G. As an example, understanding and optimizing fluid flow in absorbing porous media is critical for developing superior consumer hygiene products such as paper towels, wipes, feminine pads and baby diapers. Fluid flow models have proven very valuable for the development of Pampers based on multi-year investments in the fundamental understanding of transport mechanisms, numerical simulation tools, computation infrastructure and lab methods for both input data generation as well as validation of the models.

The complexity of the models requires strong cooperation of a wide range of specialists and practitioners across P&G and with key cooperation partners. In addition, the application to real-time business decision requires models to be trusted by the decision makers and simulation results available with fast feedback.

We present some experience and best practices for collaboration that have advanced both capability and capacity for the development and application of these models.

<u>About the author:</u>Dr. Mattias Schmidt is a Research Fellow and member of the Victor Mills Society. He joined P&G with a PhD in Physics from University of Leipzig and has worked in the area of fluid flow, absorbent core design and super-absorbent polymer development since 1991. He has and is contributing to drive adoption of modeling and simulation in R&D throughout P&G.

Partially Saturated Flows in Poroelastic Media: Theoretical Approach and Numerical Challenges (P.R. Schunk, Sandia)

Abstract. We present a general Darcy-equation formulation for flow in deforming porous media with several complicating features. Specifically, we derive governing equations (mass-balances) for liquid solvent, gas, and solid for imbibing/swelling media. Capillary pressure hysteresis, anisotropic microstructure, liquid-absorbing solid particles, and coupling with nonporous, continuous liquid/gas phase flow regions are several of the complicating features we discuss. The formulation has been implemented in a multiphysics finite element code. After introducing the relevant features of this code, we verify our formulation with several standard test problems reported in the literature. We then explore several complex applications, including forced flow with externally applied mechanical loads on a soft porous material and more natural flow from capillary-flow-induced deformation. We also demonstrate the capability on a coupled continuous fluid/porous media application of liquid-delivery to an imbibing porous medium. This presentation lays out successes and outstanding challenges of this development effort.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Modeling Saturation Overshoot at the Continuum and Pore-Scales (David DiCarlo, Bedhad Aminzadeh, Rony Wallach, UT Austin)

Abstract. For certain media, constant flux infiltrations produce nonmonotonic saturation profiles, which is also known as saturation overshoot. This overshoot is the cause of gravity driven preferential flow and cannot be described by traditional unsaturated continuum flow models (Richards Equation). In this talk, we describe how overshoot depends on the grain size and infiltrating fluid. We use these results to a) constrain the continuum extensions to the multi-phase flow equations, and b) show analytically how the overshoot can be calculated from pore scale physics.

Upscaling of Macroscopic Properties from the Pore to Continuum Scale using Mortars (Matthew T. Balhoff, UT Austin)

Abstract. Pore-scale network modeling has become an effective method for accurate prediction and upscaling of macroscopic properties (such as permeability, relative permeability, and capillary pressure) in porous media. In many cases these models compares favorably to experimental measurements. However, computational and imaging restrictions generally limit the network size to the order of 1.0 mm^3 (few thousand pores). For extremely heterogeneous media these models are not large enough to capture the petrophysical properties of the entire medium and inaccurate results can be obtained when upscaling to the continuum scale. Moreover, the boundary conditions imposed are artificial; a pressure gradient is imposed in one dimension so the influence of flow behavior in the surrounding media is not included.

In this work we upscale permeability for single-phase flow and generate for relative permeability and capillary pressure curves for heterogeneous media using pore-scale network models. A more efficient, novel domain decomposition method is used for upscaling the permeability of pore-scale models. The medium is decomposed into hundreds of smaller networks (sub-domains) and then coupled with the surrounding models to determine accurate boundary conditions. Finite element mortars are used as a mathematical tool to ensure interfacial pressures and fluxes are matched at the interfaces of the networks boundaries. The results compare favorably to the more computationally intensive (and impractical) approach of upscaling the media as a single model. Moreover, the results are much more accurate than traditional hierarchal upscaling methods. This upscaling technique has important implications for using pore-scale models directly in reservoir simulators in a multiscale setting.

Multiscale Mortar Preconditioners for Flow in Porous Media (Tim Wildey, UT Austin)

Abstract: The mortar mixed finite element method can be viewed as a multiscale method, with recent developments showing that the construction of a multiscale flux basis can greatly reduce the computational cost for the domain decomposition problem. Computing this multiscale basis can be expensive, but we show that the basis does not need to be recomputed for each time step if used as a preconditioner. This approach can also be extended to nonlinear interface problems and we provide numerical results illustrating the efficiency of this technique on fully implicit formulations for multiphase flow.

A New Computational Strategy for the Approximation of Two-Phase Flows in Strongly Heterogeneous Poroelastic Media (Felipe Pereira, Department of Mathematics and School of Energy Resources, University of Wyoming)

Abstract. We develop a new computational methodology for solving two-phase flows in highly heterogeneous porous media incorporating geomechanical coupling subject to uncertainty in the poromechanical parameters. Within the framework of a staggered-in-time coupling algorithm the numerical method proposed herein relies on a Petrov-Galerkin post-processing approach projected in the Raviart-Thomas space to compute the Darcy velocity of the mixture in conjunction with an operator splitting procedure for the computation of the porosity and a locally conservative finite volume TVD discretization of the nonlinear transport equation for the saturation. A notable feature of the numerical modeling proposed

herein is the local conservation property inherited by the discrete fluxes, which is crucial to capture correctly fingering patterns arising from heterogeneity and nonlinear coupling.

The water-flooding in a a poroelastic geological formation subject to an overburden load is simulated, subject to multiscale absolute permeability and Young modulus random fields. Statistical moments of the poromechanical unknowns are computed within the framework of a high resolution Monte Carlo algorithm. Numerical results illustrate the necessity of adopting locally conservative schemes in order to obtain reliable predictions of secondary recovery in heterogeneous deformable media.
This is joint work with Marcio Murad (Brazilian National Lab for Scientific Computing - LNCC) and Marcos Mendes (University of Wyoming).

Numerical Simulation of Two-Phase Flow in Heterogeneous Porous Media (Shuyu Sun, King Abdullah University of Science and Technology (KAUST) Thuwal 23955-6900, Kingdom of Saudi Arabia)

Abstract. Multiphase flow and transport in porous media have important applications in petroleum reservoir engineering and environmental science. Numerical modeling of subsurface multiphase flow is computationally challenging as it may involve multiple time and spatial scales, long simulation time periods, and many coupled nonlinear components. In particular, the advection-dominated saturation equation and the nonlinearity from the capillary pressure and relative permeability often result in sharp and moving saturation fronts. Accurate simulation of these phenomena not only requires local mass conservation to be retained in discretization, but it also demands steep gradients to be preserved with minimal oscillation and numerical diffusion. The heterogeneous permeability of the media often comes with spatially varied capillary pressure functions, both of which impose additional difficulties to numerical algorithms. To address these issues, we solve the saturation equation by discontinuous Galerkin (DG) method, a specialized finite element method that utilizes discontinuous spaces to approximate solutions. Among other advantages, DG possesses local mass conservation, small numerical diffusion, and little oscillation. The pressure equation is solved by a mixed finite element (MFE) scheme. In this talk, we will present the theory and numerical examples of a combined DG and MFE method for simulating two-phase flow in porous media, with emphasis on treating heterogeneous capillary pressure functions and resolving sharp moving saturation fronts.

Interfacial areas and triple contact lines at drainage and imbibition: theory, experiments and simulation (Maša Prodanović, Center for Petroleum and Geosystems Engineering, University of Texas at Austin, masha@ices.utexas.edu)

Abstract. Capillary pressure - saturation relationships are most commonly used to describe the pore scale fluid displacements in subsurface formations, yet they are not sufficient to describe the state of the system. Most of the work done during displacement is spent on creating interfacial areas. Thus the knowledge of areas is hypothesized to be the missing link that would explain e.g. hysteresis between drainage and imbibition curves (Gray & Hassanizadeh '93).

Numerical and imaged-based area computation provides an appealing alternative to experimental gas adsorption based methods because they provide information of a spatial nature in addition to sample-averaged properties. We compare interfacial areas, their contribution to capillary pressure (Gray & Hassanizadeh '93) as well as drainage efficiency (Morrow '70) computation based on a novel numerical method (level set progressive quasi-static algorithm) and experimental measurements (based on image analysis) directly in three different unconsolidated systems (two glass beads packs and a crushed volcanic tuff). Finally, we discuss the match with the aforementioned theory, computation and experimental findings in light of pore geometry differences (pore-throat sizes and aspect ratios, grain shapes).

We then present preliminary calculation of air-water-solid (AWS) contact line based on the aforementioned level set methodology. While AWS contact line length is not a sizeable contribution to capillary pressure, competing theories trying to explain colloid retention mechanism in soils currently discuss the contribution of straining at the AWS contact line. Our objective is to quantify the contribution of the AWS contact line to retention in simple geometries and granular materials and compare the computation to experimental observation.

Joint work with Dorthe Wildenschild (Oregon State University), Elena Rodriguez Pin, and Steven L. Bryant (University of Texas at Austin), Yan Jin (University of Delaware)

The injection problem for three-phase flow in porous media (Dan Marchesin, A. Azevedo, P. Castaneda, F. Furtado, A. deSouza, B. Plohr)

Abstract: If two fluids are available to displace oil from a virgin reservoir, what is the injection strategy that maximizes recovery? This question is considered here. Suppose that the densities of the oil in the reservoir and the two injected fluids are similar, so that gravity segregation can be neglected; and suppose that the injected fluids and the oil form three immiscible phases with no mass interchanges. What is the mixing proportion for injected fluid slugs that optimizes the oil recovery? We determine analytically the saturation profiles and recovery history for any proportion of continuously injected fluids, including the case for the optimal injection. The results are obtained for Corey-type quadratic permeabilities, but they are qualitatively the same for any convex permeability.

The optimal quantities are essentially determined by the viscosities of the three phases. The formulae are based on a recently-developed method-of-characteristics theory for immiscible three-phase flow. We present numerical simulations to illustrate this theory and the dependence of the saturation profiles and production histories on the injection proportion. We also show simulations that demonstrate how alternating injection of pure fluids in this proportion yields the same oil recovery.

Simulation of density-driven flow in fractured porous media (Alfio Grilloa, Dmitry Logashenkob, Sabine Stichela, Gabriel Wittum, University of Frankfurt)

Abstract. We consider a porous medium of hydrogeological interest consisting of a fluid-phase which filtrates the porous rocky matrix. The rocky matrix is assumed to be rigid and at rest, while the fluid-phase is a mixture comprising water and a dissolved contaminant. The latter undergoes both diffusion and transport. We assume that, in a region of observation, either a single fracture or a fracture network is present. We regard a given fracture as a porous medium on its own, which has physical properties different from those of the surrounding system. Within this setting, we aim to determine the evolution of the contaminant both in the fracture and in the surrounding medium under the following hypotheses: i) the thickness of the fracture is much smaller than the smallest characterstic length scale of the surrounding porous medium, and ii) the fracture and the embedding medium interact through ideal interfaces. We consider density-driven flow, and we approach the modelling of our problem by means of the averaging technique known as “averaging along the vertical”. The numerical simulations are performed by employing a finite volume procedure.

Stochastic Processes Run With Nonlinear Clocks as Models for Anomalous Dispersion: Complexity and Ergodicity (John H Cushman, Department of Earth and Atmospheric Sciences and Department of Mathematics, Purdue University)

Abstract. A diffusive process is said to be anomalous if in any given direction the average square of the separation a particle experiences from its origin grows nonlinearly with time. Any diffusive process is anomalous if viewed on a short enough time scale, but interestingly, many diffusive processes remain anomalous over longer times. We study several such processes here; diffusion in a laterally confined rare

gas nano-film, turbulent diffusion in the atmosphere and diffusion in three dimensional porous media. We illustrate how a novel processes, Brownian motion run with a nonlinear clock, statistically mimics trajectories generated via Newton's force law, turbulent diffusion and trajectories in 3-d porous media. Ergodicity and complexity are examined. The model is easily generalized to more complicated random processes and has application to anomalous problems in most fields. We also illustrate how Fractional Brownian motion run with a non-linear clock can generate anomalous diffusion with trajectories that have fractal dimension independent of the mean-square separation.

Predicting Petrophysical Properties Of Downhole Earth Formation From Log-Derived Rock Models (Guodong Jin, Chun Lan, Wei Shao, Margarete Kopal, and Songhua Chen, Baker Hughes)

Abstract. The successful modeling of physical processes at the pore-scale demands an accurate representation of the complex geometry of the pore space. Nowadays it is usually achieved either by working with actual core images (X-ray micro-CT images or thin sections data) or by creating numerical models. Extracting CT-images from core samples is necessary, but it is time-consuming, expensive, and not applicable to damaged core material or drill cuttings. On the other hand, the input data for reconstructing rock models are conventionally obtained from analysis of high resolution SEM images of thin sections. As an alternative, we introduce a new integrated micro-structural rock modeling approach from the first principles to reconstruct a representative rock model of an earth formation for each depth of interest. Downhole logging measurements and geological information provide directly or indirectly the necessary input data to the rock modeling process, such as porosity, grain mineralogy, cement/clay, grain size distribution. Examples are given in details to illustrate the approach and the facing challenging. Simulation results are compared with those derived from empirical relations, log measurements and experimental data.

POSTER ABSTRACTS.

Flow simulation of fractured-vuggy media based on equivalent continuum model (*Yajun Li and Jun Yao, China University of Petroleum)*

Abstract. Modeling and numerical simulation of fluid flow in fractured-vuggy media (FVM) is a challenging problem due to the multiscale and complexity of the FVM. An equivalent continuum approach is proposed for estimating the equivalent permeability tensors (EPTs) of fractured-vuggy-media blocks, and modeling fluid flow in the whole research region described by full tensorial permeabilities. First, a coupled Darcy-Stokes model is developed to estimate EPT of FVM which is the critical property for flow simulation. FVM is divided into porous flow regions and free flow regions (fractures, vugs) according to the structure of FVM and flow characteristic in different spheres at multiple scales, Darcy-Stokes equations with coupled boundary conditions is presented to describe fluid flow in FVM. Equivalent principle and theory is proposed for calculating the EPTs of FVM numerically. Then, the real FVM is replaced by continuous media characterized by EPTs calculated by the efficient procedure we presented. The methodology of simulating fluid flow in the new reseach region considering EPT of each grid block is proposed. We present some numerical examples to illustrate the theory, which proves that this methodology integrates the complexity of the flow calculation offered by continuum model with the realism of fracture and vug systems as captured by discreted model. This research provides theoretical bases to determine the parameters and the flow performance of FVM.

Discrete fracture-vug network model and its application to fractured vuggy porous media (*Zhaoqin Huang and Jun Yao, China University of Petroleum)*

Abstract. Modeling and numerical simulations of fractured vuggy porous media is a challenging problem due to the presence of cavities called macro vugs which are connected via discrete fractures networks. The main difficulty is the co-existence of porous and free-flow region in such media on macro scale. In this study, a novel conceptual discontinuum model i.e. discrete fracture-vug network (DFVN) model has been proposed to this problem.

In DFVN conceptual model, naturally fractured vuggy porous rock masses are considered as a composite porous material, consisting of (1) macro fractures system, (2) porous rock matrix system, and (3) macro vugs system. Macro fractures and vugs are embedded in porous rock, and the isolated vugs are connected via discrete fracture network. The flow in porous rock matrix and fractures follows Darcy's law, and the vugs system is free fluid region. The Beavers-Joseph-Saffman boundary condition is used on the interface between two regions.

Both 2D DFVN models with homogeneous isotropic rock matrix and heterogeneous anisotropic rock matrix are simulated and studied. The numerical results have shown that DFVN model provides a natural way of modeling realistic fluid flow in fractured vuggy porous media. And then a numerical procedure for the evaluation of equivalent permeability tensor for fractured vuggy porous media is presented. Based on two-scale homogenization theory, we obtained an equivalent macroscopic Darcy's law on coarse scale from fine-scale Discrete Fracture-Vug Network model. The method is verified through application to a periodic model problem and then is applied to the calculation of equivalent permeability tensor of porous media with complex fracture-vug networks. The applicability and validity of the method for these more general fractured vuggy systems are assessed through a simple test of the coarse-scale model.

Physical controls of soil hydraulic parameter scaling at multiple scales (*Raghu Jana, Binayak Mohanty, Yalchin Efendiev, Texas A&M University)*

Abstract. Understanding how soil hydraulic parameter values are affected at different scales by the spatial variability of influencing factors such as soil structure and texture, vegetation, and topography, as also the atmospheric forcings such as precipitation, is an inherent requirement of efficient scaling schemes. Inter-

connections often exist between information across scales. However, the mathematical and/or physical nature of these connections is generally unknown. In order to provide better input data to hydrological, ecological and meteorological models, it is very much essential to understand the physical processes underlying the spatial variations of these soil hydraulic properties. We present here a study where we investigated the influence of topographic variations on the effective, upscaled soil hydraulic parameters under different hill-slope configurations. A mathematical form to describe the effect of the physical controls at this scale is presented. The power averaging operator algorithm is adapted to aggregate fine scale soil hydraulic parameters to coarser resolutions. Soil moisture state and water flow scenarios are simulated using the HYDRUS-3D software for different numerically generated topographic configurations to test the equivalence of the upscaled soil hydraulic parameters. The algorithm produces reasonably good estimates of effective soil hydraulic parameters at coarse scales. Further, the theoretical basis is validated with data from the Little Washita watershed in Oklahoma, where it was found to perform reasonably well. The simulated soil moisture and hydraulic parameters are compared across scales, time, soil type distributions, vegetative covers, and with respect to topographic indices. Based only on the topography, the scaling algorithm was able to capture much of the variations in soil hydraulic parameters required to generate equivalent flows and soil moisture states in a coarsened domain. This approach takes a first step towards addressing the need to include physical controls into upscaling algorithms for soil hydraulic parameters when applied at large extents.

Modeling biogeochemical processes in a comtaminated quifer-wetland system using ANN-HP1 (*Bhanva Arora, Binayak Mohanty, Jennifer T. McGuire, Texas A&M University)*

Abstract. Fate and transport of contaminants in subsurface systems is controlled by various biogeochemical processes such as precipitation, sorption-desorption, ion-exchange, redox, etc. The interactions between biogeochemical processes becomes complex in the presence of contaminants. Thus variability in measured hydrological, geochemical and microbiological parameters corresponds to multiple processes simultaneously. The objective of this study is to evaluate interactions and develop quantitative relationships between hydrological (initial and boundary conditions, hydraulic conductivity ratio, and soil layering), geochemical (mineralogy, surface area, redox potential, and organic matter) and microbiological factors (MPN) that alter the biogeochemical processes at different microzones (hydrologic and structural interfaces) in the soil column. Experimental soil columns were designed with different levels of soil structural heterogeneity to better represent the contaminated aquifer-wetland system of the Norman Landfill research site. The Norman Landfill is a closed municipal facility with prevalent organic contamination. The sources of variation in the laboratory dataset were explored using multivariate statistics and dominant biogeochemical processes were obtained using principal component analysis (PCA). Furthermore, artificial neural networks (ANN) coupled with multicomponent variably-saturated flow and transport model HP1 was used to develop mathematical rules identifying different combinations of factors that trigger, sustain, accelerate/decelerate, or discontinue the biogeochemical processes. Preliminary results indicate: i) certain variables (anion, cation concentrations, etc.) do not follow normal or lognormal distributions throughout the column but within certain structural units of the column, ii) strong correlations exist between microbial presence and redox geochemistry (e.g. MPN with pH and S^{2-} concentrations), and iii) PCA suggests shifts in interacting variables (e.g. iron and sulfate reduced concentrations to multiple geochemical and flow parameters) as structural heterogeneity is increased.

Using homogenization theory to calculate the effective diffusion tensor for human stratum corneum with corneocyte cells of tetrakaidekahedral geometry (*I. Muha, S. Stichel, A. Naegel, M. Heisig, Gabriel Wittum. University of Frankfurt)*

Abstract. The stratum corneum (SC), the outermost layer of the skin, is a biphasic membrane typically about 10-20 _m thick. It consists of attened and keratinized corneocyte cells embedded in the intercellular lipid matrix. Because of the different properties of these phases, they build a repellent layer and therefore the stratum corneum provides the main part of the barrier function of the skin against impacts from outside.

In [1] differences between several two- and three-dimensional models were evaluated. The study proved that the shape of the cells has an important impact on the permeability of the membrane. In three dimensions it has been found that the cells in the stratum corneum can be described by tetrakaidekahedra [2, 3]. This cell type has an almost optimal surface-to-volume ratio and provides a barrier, in which a minimal amount of mass is used very effectively. The shape has been confirmed by newer microscopic investigations [4]. Due to the complexity of the geometry and the difference in length scales involved in its microstructure, solving the equation directly on the detailed microstructure involves high computational costs. In [5] a macroscopic effective diffusion tensor was derived for brick-and-mortar structures using the method of asymptotic expansion [6]. It remained an open question whether the mathematical tools from homogenization theory can be applied to tetrakaidekahedral geometry. In this work the same technique is transferred to membranes with base cells of tetrakaidekahedral shape. We show (i) how the method of asymptotic expansion can be used to homogenize membranes consisting of tetrakaidekahedra. Furthermore, numerical results confirm that (ii) the effective diffusion tensor is of diagonal shape, and (iii) the transversal and lateral diffusivity can be described uniformly with different coefficients. We also report the necessary coefficients for many different cases. For example, we analyze the impact of different geometric parameters (e.g., edge length and overlap). Additionally, the effect of swelling corneocytes is examined. The application of homogenization theory significantly reduces the computational cost of modeling transdermal diffusion through SC, because there is no need to solve the model equations in a three-dimensional highly heterogeneous complex microstructure. This technique can, e.g., be used to study the influence of lateral diffusion in diffusion-cell experiments with finite dosages.

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Mixed MsFEMs for flows in heterogeneous porous media ***(L. Jiang (U. of Minnesota), Y. Efendiev (Texas A&M University), I. Mishev (ExxonMobil))***

Abstract. The use of limited global information in multiscale simulations is needed when there is no scale separation. The global fields typically contain small scale (local or global) information required for achieving a convergence with respect to the coarse mesh size.
In this poster, we demonstrate how the use of limited global information can efficiently improve the simulations that are performed on a coarse grid. We present mixed MsFEM using multiple limited global information. The simulations both on structured and unstructured coarse grids are performed and the accuracy of the methods is investigated. We also show how one can reduce the computation of global fields by performing partial upscaling and the applications of mixed MsFEM to stochastic flows.

Some numerical results for modeling fractures as interfaces with nonconforming grids (N. Frih, V. Martin, Jean E. Roberts, A. Saada, INRIA-Rocquencourt)

Abstract. In an earlier work we presented some theoretical results including convergence estimates for a numerical model for incompressible, single phase flow in a porous medium containing fractures. In the

model the fractures were modeled as interfaces and the grids were non matching. In this poster we present numerical studies to confirm our theoretical results. We present convergence curves for several variations of the model and compare the results.

Preferential flow paths in fractures ***(Dustin Crandall (National Energy Technology Lab), M. Ferer (National Energy Technology Lab), Goodarz Ahamdi (Clarkson), D. Smith (National Energy Technology Lab))***

Abstract. Preferential flow paths in a discrete fracture have been observed with simulations and experiments. By slowly injecting air into an initially water-saturated fracture micromodel a distinct flow path of low resistance along the fracture length was observed. The aperture distribution of the fracture, obtained from CT-scans of a fracture in Berea sandstone, conform to a log-normal distribution. Three-dimensional, finite volume, multi-phase flow simulations were performed within the same fracture geometry and largely agreed with the experimentally observed results, but were computationally expensive. The fracture geometry was ported to a pore-throat model by correlating the spatial aperture distribution to the throat radii in the computational domain. This pore-throat/fracture model has been shown to capture the same preferential flow paths observed in the experiments and the finite-volume simulations, but at a fraction of the computational expenditure. Furthermore, modified Invasion Percolation with trapping (IPwt) models showed even better agreement with the experiments at a much smaller fraction of the computational expenditure. This agreement of the IPwt simulations suggests that the flow is dominated by capillary forces.

Damage modelling in non-isothermal unsaturated porous geomaterials (*C. Arson, Texas A&M University)*

Abstract. The aim of this work is to study damage in non-isothermal unsaturated porous geomaterials. A Continuum Damage Mechanics model has been developed to account for cracking effects in non-isothermal, unsaturated porous media [2, 3]. Contrary to the huge majority of existing damage frames proposed for unsaturated materials [1], the proposed model is formulated in independent stress state variables (net stress, suction and thermal stress). The damage variable is a second-order tensor. The behavior laws stem from the combination of phenomenological and micromechanical principles. Helmholtz free energy is written as the sum of damaged elastic energies and residual-strain-potentials. The concept of effective stress, frequently used in Continuum Damaged Mechanics, is extended to the three stress state variables. The damaged rigidities are computed by application of the Principle of Equivalent Elastic Energy. The non-elastic strain components depend on the increment of damage, which is determined by an associative flow rule. Fracturing is also modelled in the transfer equations. The Representative Elementary Volume is assumed to be damaged by a micro-crack network, among which liquid water and vapour flows are homogenized. A damaged intrinsic conductivity, which plays the role of an internal length parameter, is introduced. The influence of damage on air and heat flows is taken into account by means of porosity, which is also involved in the transfer model in the intact state. The damage model has been implemented in Theta-Stock Finite Element software [4]. Basic mechanical tests have been simulated. The numerical results are in conformity with the reference data. Full-scale models of mine galleries and nuclear waste repositories have been designed. These engineering problems involve thermo-hydro-mechanical couplings and multi-phase flows. First, the resolution algorithm has been validated in the elastic domain, by comparing the results to the predictions of reference elastic models. Secondly, thermal damage trends have been studied for various types of repositories. The physical trends meet the theoretical predictions. After some further developments, the program is expected to become a useful engineering tool, dedicated to underground storage design.

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New methods for modeling productivuty index of the well for generalized Forchheimer flows in porous media (*E. Aulisa, L. Bloshanskaya*, L. Hoang, A. Ibragimov)*

Abstract. Motivated by the reservoir engineering concept of the well Productivity Index (PI) we analyze a time dependent functional for general non-linear Forchheimer equation. We are proposing an analytical tool for accurate evaluation of the PI for non-linear flows for slightly compressible fluid in an arbitral reservoir well system. Two types of boundary conditions are considered, given well-bore pressure and given total flux. We study, both theoretically and numerically, the effect of the non-linear nature of the flow filtration on the value of the diffusive capacity and estimate the deviation between PI for linear and non-linear case. Exact formula for skin factor in radial cases have been derived depending on the order of polynomial in g-Forchheimer equation and geometrical parameters. Next, following work of Peaceman for linear case we numerically observe that the well-block pressure for linear and non-linear case is essentially equal to the actual owing pressure at a radius proportional to the well-block size. Developed framework was applied to accurately reconstruct the owing pressure, and to evaluate the productivity index of the well by solving an auxiliary problem with reduced degrees of freedom. It was numerically proved that well-block radius is essentially the same for the polynomials of all degrees, and is determined only by grid geometry.

Modeling of effective parameters on permeability of porous media with application to fuel cell *(*A.M. Parvanian, M. Panjepour, Gh. Aryanpour (Isfahan University of Technology))

Abstract. Different components of proton exchange membrane fuel cells can benefit from porous media special characteristics; such as lightness, remarkable area to volume ratio, mechanical strength, etc. Various important factors specially permeability can control and optimize the properties of porous materials. The aim of this investigation is modeling of effective parameters on permeability such as pore size, pores per inch (PPI), connectivity and thickness. The Monte Carlo is used to geometry generation of porous layer and then fluid flow through it has been modeled using Lattice Boltzmann Method. The results could be used for designing of porous layers applicable in PEMFC.

Bayesian uncertainty quantification for flows in heterogeneous porous media using reversible jumo Markov chain Monte Carlo methods *(A. Mondal, Y. Efendiev, B. Mallick, A. Datta-Gupta (Texas A&M University))*

Abstract. In this paper, we study the uncertainty quantification in inverse problems for flows in heterogeneous porous media. The channelized structure of the permeability field is modeled by interfaces separating a high and low permeable region. Within each channel, the permeability is assumed to have a log-normal distribution. Uncertainty quantification in history matching is carried out hierarchically by constructing geologic facies boundaries as well as permeability fields within each facies using dynamic data such as production data. Karhunen-Loeve expansion is to reduce the dimension of the parameters for the correlated permeability field. The level-set approach is used to perturb the facies boundaries. Reversible jump Markov chain Monte Carlo (MCMC) algorithms is used to sample from the posterior distribution of the channelized permeability field condition on the water-cut data. The use of reversible jump MCMC allows us to vary the dimension of the parameter space in each iteration which is used effciently to move the points on the facies boundaries. The search with Metropolis-Hastings algorithm results in very low acceptance rate, and consequently, the computations are CPU demanding. To speed-up the computations, we use a two-stage reversible jump MCMC that utilizes upscaled models to screen the proposals. In our numerical results, we assume that the channels intersect the wells and the intersection locations are known. Our results show that the proposed algorithms are capable of capturing the channel boundaries and describe the permeability variations within the channels using dynamic production history at the wells.

Gas permeability measurement of very weakly permeabile porous media (*Y. Jannot (Nancy-Universite, CNRD) and Didier Lasseux (Lab. TREFLE)*)

Abstract. Precise measurement of gas permeability of weakly permeable porous media (smaller than 1 □D) is a tricky task. In this range of permeability, very significant Klinkenberg effects are expected and must be accounted for in the physical model for gas flow as well as in the design of the experiments and procedures. For such porous media, stationary methods are inadequate mainly due to the fact that the experiments require the measurement of extremely small flow rates for which conventional flowmeters are inappropriate requiring the use of sophisticated devices. In addition, it is necessary to correctly estimate the time required to reach stationary flow in order to perform the experiment under steady conditions and interpret the results with the corresponding model. However, more precise estimates than the rough dependence of this characteristic time on the square of the sample length and on the inverse of the intrinsic permeability still leaves much to be desired. Unsteady methods are much more rapid and allow to circumvent these difficulties. They are based on the interpretation of the time evolution of the pressure decay of a gas pulse initially confined in a reservoir connected to the inlet of the sample. For these methods, the unsteady pressure signal must be interpreted with a fully non-stationary model for which no analytical solutions are available unless excessive simplifying assumptions are made. Consequently, the inversion requires a numerical procedure that can be cumbersome.
In this work a quasi-steady method is presented that takes some advantages of both steady and unsteady techniques. It is based on an unsteady method but makes use of conditions such that quasi-steady flow can be reached after a transient period. The characteristic time of this transient period is determined precisely. Under these conditions, an analytical solution to the governing equations is found allowing a simple interpretation of the experiment and a determination of the permeability. The precise measurement of the gas flow rate is performed indirectly avoiding the use of a flowmeter. The method is illustrated on two different materials. The first one is a 3mm thick sheet of glass/epoxy composite material. The apparent permeability on this sample was determined at an average pressure ≈ 4.5 bars and was found to be ~1.3 nD. The second material is a tropical wood (Bubinga) that is more permeable. Measurements were performed on a 25mm thick sample on which intrinsic permeability and Klinkenberg coefficient were determined to be ~10 □D and ~5 bars respectively.

Coarse-scale models for high-contrast multiscale problems *(J. Galvis and Y. Efendiev, Texas A&M University)*

Abstract. This poster discusses special coarse spaces for multiscale finite element and domain decomposition methods. These spaces allow a coarse-scale representation of the solution of multiscale flow problem. The focus will be on problems that have high variations in the media properties. It is known that the number of iterations in domain decomposition and many iterative methods is adversely affected by the contrast in the media properties. One way to decrease the number of iterations is to choose coarse spaces appropriately. In the proposed methods, the coarse spaces are constructed based on a local eigenvalue problem. We show that if domain decomposition methods use these coarse spaces then the condition number of preconditioned system is independent of the contrast in media properties. The coarse space can have large dimension. We discuss dimension reduction for the proposed coarse spaces and hierarchical computations of multiscale basis functions. The latter results to domain decomposition preconditioners that have the condition number which is independent of contrast. We will discuss the accuracy of coarse-scale solutions using these proposed coarse spaces.

A hybrid Ensemble Kalman Filter with coarse scale constraint for nonlinear dynamics *(S. Watanabe (Texas A&M), A. Datta-Gupta (Texas A&M), Y. Efendiev (Texas A&M), D. Devegowda (U. of Oklahoma))*

Abstract. The recent interest in Ensemble Kalman Filters (EnKF) in the Petroleum Industry is driven to a large extent by the need for continuous reservoir model updating and uncertainty assessments based on dynamic data. The EnKF approach relies on sample-based statistics derived from an ensemble of reservoir model realizations. Sampling error in these statistics, particularly with the use of modest ensemble sizes, can severely degrade EnKF performance leading to parameter overshoots and filter divergence. However,

for computational efficiency, the ensemble size needs to be kept small resulting in spurious sample correlations and loss of geologic realism during model updating. Moreover, facies-based non-Gaussian geologic models and the non-linearity of multiphase flow problems pose significant additional challenges for the EnKF. The EnKF updates are designed to be optimal only for Gaussian priors and linear model dynamics. For multiphase history matching, the posterior distribution will be non-Gaussian and the ensemble mean is not a good representation of the central tendency. As a result the EnKF can result in a poor match to the data or unrealistic model updates.

The hybrid multiscale EnKF proposed here provides an improved approach to operational data assimilation problems and tends to overcome many of the limitations associated with the classical EnKF implementation. Our approach combines non-linear inversion with the EnKF to account for the inherent non-linearities of multiphase inverse problems. Specifically, we update the ensemble mean in a conventional EnKF through a non-linear inversion at selected time intervals and replace the ensemble mean with the 'posterior mode' from the inversion. This explicitly recognizes the fact that for non-Gaussian distributions, the posterior mode is a better representation of the central tendency compared to the ensemble mean. Furthermore, the inversion results are imposed on the individual ensemble members via a coarse-scale constraint using a sequential second stage updating in the conventional EnKF and a flow-based upscaling. Our approach ensures that the ensemble members in the conventional EnKF will follow the trajectory of the non-linear inversion within a specified degree of tolerance. This not only allows us to account for non-linearities in the model updates but also prevents filter divergence arising from the use of limited ensemble size. We first illustrate the advantage of the hybrid approach using a synthetic example and present a detailed validation of our results. Next, the approach is applied to a west Texas carbonate reservoir to demonstrate its power and utility for practical field problems.

On Upscaling Flows in Highly Porous Media (J. Willems (Texas A&M), O. Iliev (Kaiserslautern), R. Lazarov (Texas A&M))

Abstract. Brinkman's equations modeling fluid flow in highly porous media are considered. They are discretized using a generalization of the DGFEM for Stokes equations by Wang and Ye. For computing the solution to the arising linear system of equations an iterative two-scale finite element method is presented. The method uses the concept of subgrid approximation developed by Arbogast for Darcy's equations. To reduce boundary layers and to ensure convergence to the global fine solution the method is put in the framework of alternating Schwarz iterations.

History Matching Channel Reservoirs using Level Set Methods and Markov Chain Monte Carlo (X. Jiang, A. Mondal, A. Datta-Gupta, Y. Efendiev, B. Mallick, Texas A&M University)

Abstract. We present a method for history matching and uncertainty quantification for channelized reservoir models using Level Set Method and Markov Chain Monte Carlo. Our objective is to efficiently sample realizations of the channelized permeability fields conditioned to the production data and facies observation at the wells. Traditional history matching algorithms typically smear the channel boundaries and also fail to converge if the initial model is far from the solution.

In our approach, the channel field boundary is first described by level set function (signed distance function) using the reinitialization equation. By solving the level set equation (motion in the normal direction), we are able to move the channel boundary and evolve the channelized reservoir. The Gaussian random field is used as velocity field in level set equation and Markov Chain Monte Carlo is used to perturb the velocity field to generate new channel reservoir model. One advantage of this approach is that it is easy to condition the channel model to the facies observations at well locations by conditioning the Gaussian random field to zero at wells. To speed up the computation and improve the acceptance rate of the MCMC algorithm, we employ two-stage methods where coarse-scale simulations are used to screen out the undesired proposals.

We demonstrate the effectiveness of the level set MCMC algorithm using both 2D and 3D examples involving waterflood history matching. In the 2-D example, the channel boundary is represented by the level set equation. We assume that the facies observation at well locations are known. This 2-D example shows that the proposed algorithm can determine the large-scale features of the reference channelized permeability field based on the production data and facies observation. In the 3-D example, the result shows that level set MCMC algorithm can successfully match the data and identify the orientation of the channels in the reference model. The MCMC algorithms naturally provide multiple realizations of the permeability field conditioned to well and production data and thus, allow for uncertainty quantification in the forecasting.

A posteriori error estimates including algebraic error stopping criteria for iterative solvers
(P.Jiranek, Technical Univ. of Liberec, Z. Strakos, Academy of Sciences of the Czech Republic,
M. Vohralik, Univ. of Paris 06)

Abstract. For the finite volume discretization of a second-order elliptic model problem, we derive a posteriori error estimates which take into account an inexact solution of the associated linear algebraic system. We show that the algebraic error can be bounded by constructing an equilibrated Raviart–Thomas–Nedelec discrete vector field whose divergence is given by a proper weighting of the residual vector. Next, claiming that the discretization error and the algebraic one should be in balance, we construct stopping criteria for iterative algebraic solvers. An attention is paid, in particular, to the conjugate gradient method which minimizes the energy norm of the algebraic error. Using this convenient balance, we also prove the efficiency of our a posteriori estimates, i.e., we show that they also represent a lower bound, up to a generic constant, for the overall energy error. A local version of this result is also stated. This makes our approach suitable for adaptive mesh refinement which also takes into account the algebraic error. Numerical experiments illustrate the proposed estimates and construction of efficient stopping criteria for algebraic iterative solvers.

Analysis of the role of structural disorder on the inertial correction to
Darcy's law (**Didier LASSEUX, Azita AHMADI and Ali Akbar ABBASIAN ARANI**
TREFLE - UMR CNRS 8508 - University of Bordeaux - Arts et Métiers ParisTech , Esplanade des Arts et Métiers, 3340, Talence Cedex France)

Abstract: This work focuses on the stationary one-phase Newtonian flow in a class of homogeneous porous media at large enough flow rates leading to a non-linear relationship between the filtration velocity and the pressure gradient. A numerical analysis of the non linear -inertial- correction to Darcy's law is carried out for model periodic structures made of arrays of square-section cylinders. The global aim is to determine and analyze the effective properties appearing in the macroscopic model resulting from the volume averaging of the mass and momentum (Navier-Stokes) equations at the pore scale

$$\langle \mathbf{v}_\beta \rangle + \mathbf{F} \cdot \langle \mathbf{v}_\beta \rangle = -\frac{\mathbf{K}}{\mu_\beta} \cdot \left(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right)$$

The effective permeability tensor, **K**, and the inertial tensor, **F,** are obtained by solving the microscopic flow and also the closure problems resulting from upscaling. From extensive analysis, general features of the tensor **F** and normalized correction f_c for ordered structures (regular array of cylinders) have been studied (Interpore Conf. 2009). It was shown, in particular, that the quadratic correction, classically referred to as the “Forchheimer correction”, is an approximation which does not hold at all for certain particular orientations of the pressure gradient for this type of regular structures. The aim of the present work is to investigate the robustness of the quadratic “Forchheimer correction” when disorder in introduced in the medium. The correction to Darcy’s law is studied for weakly and strongly disordered media for a given porosity with a pressure gradient aligned with the principal axes of the structure. Weak structural disorder is obtained as a result of random placement of identical square-section cylinders in a periodic unit cell, while strong disorder corresponds to both random placement and random size of the

cylinders. The correction obtained for 10 to 20 realizations is studied for each case as a function of the Reynolds number.

It is shown that for disordered structures, the linear velocity -dependence of the correction, f_c is a robust approximation in a very large interval of Reynolds numbers, featuring a quadratic Forchheimer correction to the filtration velocity in the strong inertia regime. Moreover, the crossover Reynolds number, corresponding to the transition from the weak inertia cubic regime to the strong inertia quadratic regime, as well as the magnitude of the correction in the weak inertia regime stay small in comparison to an ordered structure. This explains the fact that this regime is generally overlooked during experiments on naturally disordered porous media.

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