Project Title: Modeling, Analysis and Simulation of Multiscale Preferential Flow

PIs: Ralph Showalter, Malgorzata Peszyńska

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Oregon State University, Corvallis, OR 97331-4605

Award Number: DE-FG02-05ER25700

Organization and Support Activities

Personnel

- Ralph Showalter, Principal Investigator,
- Malgorzata Peszyńska, co-Principal Investigator,
- Son-Young Yi, Post-Doc supported 1/2 FTE September 2006 - June, 2009,
- Fernando Morales, Graduate Research Assistant,
- Ken Kennedy, Graduate Research Assistant,
- Viviane Klein, Graduate Research Assistant.

Additional undergraduate or short-term personnel: Kyle Augustson, Nicholas Stanford, John Osborne.

Equipment

Peszyńska used the project's funds as seed money for a project from OSU Research Equipment Reserve Fund which was funded. The project personnel thereby gained access to high performance computing nodes in a SWARM cluster in the OSU College of Engineering.

Workshop

The Workshop on "Modeling, Analysis and Simulation of Multiscale Nonlinear Systems" in cooperation with the SIAM Activity Group on Geosciences was held at Oregon State University, Corvallis, Oregon, June 25-29, 2007. The workshop brought together an interdisciplinary group of scientists working on various aspects of nonlinear coupled phenomena occuring at multiple spatial and temporal scales in natural and simulated environments. Additional funding for participants was obtained from a National Science Foundation grant.
See `http://www.math.oregonstate.edu/multiscale/workshop` for additional details.

Outreach & Education

The PIs maintained an interdisciplinary community weekly seminar on Applied Mathematics and Computation. See the http://www.math.oregonstate.edu/amc_seminar for past and current activities.

Research Visitors: Anna Spagnuola (October, 2006), Malte Peter (January 2007), Robert Lipton (February, 2007), Jim Douglas (May, 2007), Anna Trykozko (June-July 2007).

DOE Subsurface panel on coupled processes 9-12 January, 2007, Bethesda, MD (Peszynska as panelist).

Second AtC Coupling Methods Workshop 2-3 April, 2007, Austin, TX (Showalter as participant).

STOMP (Subsurface Transport over Multiple Phases simulator software at Pacific Northwest Laboratory, leaders: White, Oostrom) short course convened by Peszynska at Oregon State University, 24-25 May, 2009 (Peszynska, Showalter, Yi, Morales as participants).

DOE OSCAR-AMR Workshop, 22-24 May, 2007, Livermore, CA (Showalter as participant).

Northwest Consortium in Multiscale Mathematics Workshop on Multiscale Mathematics and Applications held three summer school workshops. The first was held in May 2006 in Tacoma, WA, drew more than 40 participants, and focused on critical issues forefront to multiscale modeling (Showalter, Peszynska, Morales as participants). The second workshop was held June 29-July 3, 2007 at Oregon State University in Corvallis, Oregon, and attracted 30 students from universities across the U.S. and instructors from over 15 universities and national laboratories (Peszynska, Showalter, Yi, Morales as participants).
See Computational Sciences & Mathematics Division Research Highlights.

The third DOE Summer School in Multiscale Mathematics and High Performance Computing *http://multiscale.emsl.pnl.gov/about.shtml* was held August 4-6, 2008 at Washington State University – Tri-Cities (Showalter, Peszynska, Morales, Klein as participants and the first two as speakers).

The PIs, postdoc, and students gave over 100 conference, and seminar presentations on the research that resulted from grants, including over 20 colloquia and plenary talks.

Research Agenda

1. Modeling of preferential transport from mesoscale to macroscale (Showalter, Peszynska and Yi)

This part of the project was motivated by experimental results of Zinn and Haggerty et al presented at the SIAM meeting in Portland, OR in July 2004. Their results showed that the double porosity models do not work well for *intermediate* regimes of flow and specifically for some ratios of preferential versus non-preferential flow (immobile zones) conductivities. The length scales used in the description of flow through natural porous media are the pore scale at which one recognizes the local pore geometry ($10^{-8} - 10^{-4}[m]$), the laboratory scale at which traditional models are used ($10^{-2} - 10^{1}[m]$), and the field scale which describes flow in a reservoir ($> 10^{2}[m]$).

Our goal here was to develop a better model which would be the basis for future unsaturated flow models. We used an approach different from the classical double porosity models in that instead of locally piecewise constant approximations to concentrations on the boundary of immobile zones we employed more precise piecewise linear approximations. As a result, the upscaled model contains both the usual terms appearing in the double porosity models and which are most significant for large contrasts of conductivities as well as additional terms which become more significant in other regimes of conductivity ratios. The resulting nonlocal advection-diffusion-dispersion models appear similar to nonlocal models of dispersion such as those considered by Cushman et al.

Classical approaches to modeling of saturated preferential flow were achieved by extending the traditional models to field scale within the family of *two-scale* models including *double-porosity* models. The main premise in these is that flow is of traditional Darcy type in both the fast and slow flow regions, and that the regions are coupled by local equilibrium interface conditions. Such models were originally developed in the petroleum industry and were later applied in hydrology. Double-porosity models are only partly able to capture delay effects in response to dynamic transient inputs known as *tailing behavior*, i.e., some of the tailing behavior cannot be described by any of the existing models. Our recently developed non-local multiscale models perform remarkably well, and the corresponding numerical simulations yield the observed effects over a very wide range of conditions and parameter values. They perform as well as the classical models in the low-contrast range and as well as the two-scale models in the high-contrast range. Additionally, these new models are mass conserving, contain the effects of local advective transport, and they are the first to capture the break-through concentration profiles throughout the entire range of contrast. All of this is achieved over a wide range of mixing scales of the two regions, and it opens up a gallery of multiscale modeling issues for development. See [1, 2, 3] below plus manuscripts in preparation.

2. Modeling of fast flow in narrow fractures in porous media (Showalter and Morales)

A related objective was to model the *fast channel flow* through a system of fissures with substantially higher fluid velocities than the surrounding medium. Similar phenomena occur along the interface of a porous medium with a solid, since there the porosity increases substantially due to the lower efficiency of the arrangement of the porous matrix cells. The traditional filtration-flow models have been insufficient to represent this fast flow, and the construction of an appropriate fissure-flow model requires a substantial refinement to represent the additional scale separation. We obtained such a model for this fast channel flow through a very thin surface in the form of a Brinkman-type equation on this surface coupled to the Darcy flow through the surrounding porous medium. It was obtained as the asymptotic limit of a Stokes flow model in the fissures coupled to Darcy flow in the porous medium. This is the first justification of the Brinkman equation in such a situation, since it has been proven to arise only in situations where the porosity is too large to relate to a porous medium, i.e., it usually describes flow around a sparse array of obstacles. Here the lower dimension of the surface forces most of the fluid to flow near the porous medium, so it develops the required drag forces which account for the Darcy-like terms added to the Stokes system. Preliminary work involved the analysis of more traditional models in which the channel flow is modeled by a Darcy system with large permeability, as would occur in debris-filled fractures. See [4, 5, 6, 7] below.

3. Pseudo-parabolic Models of Dynamic Capillary Pressure (Showalter, Peszynska and Yi)

Recent experimental evidence on fast preferential flow indicates that the capillary pressure function is not uniquely determined when large flow rates are present. The OSU group investigated new models of *dynamic capillary pressure* since these perform better than the traditional equilibrium models, and they permit the extension to full two-phase flow models. Additionally we coupled the dynamic capillary pressure approach to the double porosity models to determine the regimes in which these effects are significant in preferential flow. Related work consisted of an analysis of the homogenization of pseudo-parabolic equations or systems that arise in these models. Such systems were known classically to behave in non-standard ways, and these were observed and clarified in this work.

The classical Richards equation for flow through a partially-saturated porous medium with porosity $\phi(x)$ and permeability $K(x)$ takes the form

$$\phi(x)\frac{\partial u(t,x)}{\partial t} + \nabla\cdot K(x)\frac{k_w(u(t,x))}{\mu_w}\nabla\left(P_c(u(t,x)) - \rho G D(x)\right) = 0,$$

where u denotes saturation, and gravitational effects depend on depth $D(x)$ and (constant) density ρ. Here $k_w(u)$, $P_c(u)$ denote relative permeability and capillary pressure relationships, respectively. This standard model follows from Darcy's law extended to multiphase flow and conservation of mass with the assumption that atmospheric pressure of air is constant.

The experimental determination of the pressure-saturation relationship $p = -P_c(u)$ is based on the assumption that this is an instantaneous process, although in reality it requires substantial time to approach an equilibrium before measurements can be taken. This led to the introduction of *dynamic capillary pressure* by Hassanizadeh and Gray in which $P_c(u)$ is replaced by $P_{c,dyn}(u) \equiv P_c(u) - \tau \frac{\partial u(t,x)}{\partial t}$ with $\tau > 0$. Similar dynamic models had been introduced earlier by Barenblatt, and a related model was derived by Bourgeat and Panfilov by homogenization from standard two-phase models with special interface conditions. The dynamic capillary pressure model of Hassanizadeh and Gray leads to the nonlinear pseudoparabolic equation

$$\phi(x)\frac{\partial u(t,x)}{\partial t} + \nabla \cdot K(x)\frac{k_w(u(t,x))}{\mu_w}\nabla\left(P_c(u(t,x)) - \rho G D(x)\right) \\ - \nabla \cdot K(x)\frac{k_w(u(t,x))}{\mu_w}\nabla \tau(x)\frac{\partial u(t,x)}{\partial t} = 0$$

When written in terms of pressure $u \mapsto -P_c(u)$ and linearized about a known solution u_0, with $\kappa(x) \equiv K(x)\frac{k_w(u_0)}{\mu_w}$, ϕ replaced by $\phi \frac{\partial u}{\partial p}|_{u_0}$ and τ by $\frac{\tau}{\phi}$, the equation takes the form

$$\phi(x)\frac{\partial u(t,x)}{\partial t} - \nabla \cdot \kappa(x)\nabla\big(u(t,x) + \tau(x)\phi(x)\frac{\partial u(t,x)}{\partial t}\big) = \nabla \cdot \kappa(x)\rho G D(x).$$

In this project, the analysis of the linear pseudo-parabolic equation was completely described and the formal asymptotic limits of homopgenization were obtained for the nonlinear model. Furthermore, numerical methods were studied together with convergence and extensions to heterogeneous porous media. See [8, 9] below.

4. Adaptive computational upscaling of flow with inertia from porescale to mesoscale (Peszynska, Augustson, Garibotti, Kennedy, and external collaborator Anna Trykozko from University of Warsaw)

Since in preferential groundwater flow after rapid rain or flood events the flow rarely obeys models based on Darcy's law (or Richards' equation in the unsaturated case), it is hypothesised that an alternative model such as Forcheimer's or Forchheimer-Brinkman's would be appropriate when Reynolds number for the flow exceeds 1 or in large porosity regions. Specifically, the Darcy's law for momentum has the form $\mathbf{u} = -\mathbf{K}\nabla \mathbf{p}$ while Forchheimer's equation is $\beta\|\mathbf{u}\|\mathbf{u} + \mathbf{u} = -\mathbf{K}\nabla p$ and Brinkman's-Forchheimer $\beta\|\mathbf{u}\|\mathbf{u} + \mathbf{u} - \gamma\Delta u = -\mathbf{K}\nabla p$. (Note that coefficients of density and viscosity were supressed for simplicity). These models are essentially upscaled equations of Navier-Stokes at pore-scale.

However, measurements of the flow properties expressed by coefficients β, γ are rarely experimentally available. Therefore in this step we undertook a computational experiment in which β is derived from computational simulations of Navier-Stokes equations at pore-scale. Elements of the project included i) understanding of how to average the velocities and pressures, ii) sensitivity to mesh size and understanding of finding the coarsest grid possible for Navier-Stokes simulations at which β can be calculated along with the error bounds available. Additionally, iii) we used a very simple computational algortithm for Navier-Stokes solver (node-centered finite differences for vorticity-stream function formulation with higher order boundary conditions and relaxation of iterative solver). This is a simple and inexpensive computational algorithm which provides an attractive alternative to commercial CFD codes. We validated its results with results from Ansys Fluent and assesed accuracy of β. Recent highlights (Peszynska and Trykozko) include computations with real porescale geometries and coupled transport as well as an anisotropic model of inertia at corescale. See [10-14] below plus manuscripts in preparation.

4. Adaptive modeling of nonlinear coupled systems (Peszynska, and Klein, with collaborators Torres, Trehu)

Methane hydrates are an ice-like compound abundant in subsea sediments and unstable in standard conditions. They are simultaneously an environmental hazard and an energy source. A computational model for the evolution of methane hydrates in the seabed was developed and studied. The multiphysics model included multiphase multicomponent mass conservation equations and several variants of energy balance equation both with and without latent heat. Model adaptivity was used to assess and control the two sources of computational error, that is, the discretization error and the modeling error. For related models of methane evolution with kinetic exchange terms and kinetic phase transitions, error estimates for a corresponding system of degenerate reaction-diffusion equations were developed by adaptive multi-level finite elements modelling. See [16, 17, 20] below.

5. Adaptive modeling and a-posteriori estimators for coupled systems with heterogeneous data (Peszynska with Klein and Kennedy)

Consider the model problem, a system parametrized by $P = \{\lambda_1, \lambda_2, a, b, c\}$ (non-negative coefficients)

$$\lambda_1 u_t - \nabla \cdot (a \nabla u) + c(u - v) = f, \tag{0.1}$$
$$\lambda_2 v_t - \nabla \cdot (b \nabla v) - c(u - v) = g, \tag{0.2}$$

which appears in several applications in porous media and, in particular, in double–diffusion model, and pseudo-parabolic problems with $P = \{0, 1, a, 0, c\}$, and kinetic models of diffusion-adsorption with linear isotherms, when $P = \{1, 1, a, 0, c\}$. For this system and its stationary version, we developed robust a-posteriori residual-based estimators, and proved reliability and efficiency bounds [15,18]. The estimator is robust in the sense that it does not blow up when the coefficients change even by orders of magnitude, and works well for discontinuous coefficients. The highlight of this work is that it guides the use of multilevel grids, i.e., different grids for each component of the system; the use of such grids decreases the number of degress of freedom. Applications to MH and ECBM and examples were presented in [17, 19, 20].

We also investigated analytical and computational issues for Forchheimer's model (see (Section 3)). In particular, we addressed upscaling of the model [10], and computed sensitivity of the solutions, also of a coupled transport model [14]. While sensitivity to a few individual parameters can be assessed with forward sensitivity analyses, it is difficult, in general, to assess the impact of model truncation/modification on the accuracy of simulations. We have ongoing work with Kennedy on coupled flow and transport, and with Klein on systems of elliptic and parabolic equations relevant to coalbed methane recovery and methane hydrates. In the former case, we use sensitivity analysis, and in the latter, a-posteriori error analysis. Both projects are also reaching out to stochastic simulations.

Publications

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