MODELING, ANALYSIS AND SIMULATION OF MULTISCALE NONLINEAR SYSTEMS

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PREFACE

This issue of the International Journal of Numerical Analysis & Modeling contains a selection of papers based on presentations at the Workshop *Modeling, Analysis and Simulation of Multiscale Nonlinear Systems*. It was held at Oregon State University, Corvallis, Oregon, June 25-29, 2007, in cooperation with Society of Industrial and Applied Mathematics (SIAM) Activity Group on Geosciences.

The Workshop. The participants were an interdisciplinary group of scientists working on various aspects of nonlinear coupled phenomena occuring at multiple spatial and temporal scales in natural and man-made environments. Their backgrounds ranged from internationally recognized senior researchers and mid-career scientists to recent Ph.D.'s and graduate students.

The focus of the workshop was on multiscale flow and transport processes and related multiscale phenomena in porous media. These topics were selectively augmented by presentations of atomistic to continuum modeling, continuum mechanics and materials sciences developments, problems from the biological sciences, and methods of numerical upscaling, stochastic modeling, and probability. In addition to the mathematical methods developed for and proven successful in these various areas, discussions of recent illuminating experiments were included. The objectives of the workshop were to highlight recent successes and methods and to identify and discuss outstanding problems of flow and transport in porous media and related multiscale or multiphysics issues from other disciplines. The Program included general overview talks on methods and applications as well as special topics. It is available at `http://www.math.oregonstate.edu/multiscale/workshop` together with many of the presentations.

The Workshop was sponsored by the United States Department of Energy Office of Science Multiscale Mathematics Initiative project 98089 "Modeling, Analysis and Simulation of Multiscale Preferential Flow" and by the National Science Foundation. It was organized by M. Peszyńska, R. Showalter, Anna Spagnuolo, Noel Walkington, and Son-Young Yi.

The Proceedings. All papers in this issue have been carefully refereed, and they represent the most recent progress in various directions. There follow brief descriptions of their contents.

A formulation for fully resolved simulation (FRS) of particle-turbulence interactions in two phase flows by S. Apte and N. Patankar describes the implementation of a refinement of the distributed Lagrange multiplier technique for the simulation of flows laden with rigid particles. Particle laden flows present many modeling and numerical challenges due to their multiple scale nature. It is difficult to develop rational macroscopic (mixture) models since the complex interactions between the particles and their boundary layers are poorly understood. It is hoped that numerical simulations that fully resolve the flow and particle motion will provide the insight to resolve this issue.

In *Multiscale feature detection in unsteady separated flows* by S. Apte, G. Chen, Z. Lin, D. Morse, S. Snider, J. Liburdy, and E. Zhang, the goal is to identify multiscale features in turbulent separated flows. Techniques based on vector and tensor fields are classified into global and local flow descriptors. The global descriptors are based on spatial integration of flow parameters and extract large-scale features. The local techniques are based on spatial derivatives of flow parameters and identify flow features on the scale of the flowfield grid size. These techniques are applied to two data sets, a velocity field obtained by experiment for flow over a thin airfoil, and velocity and pressure-gradient fields for flow over a square cylinder obtained from numerical simulation. In both cases, the flow separation generates large swirling flow patterns that are convected downstream as they change in size, shape and intensity.

The paper *Brownian Motion and Entropy Growth on irregular Surfaces* by C. Chevlier and F. Debbasch concerns mathematical models of physical processes that involve the diffusion of a density on a surface or, more generally, a manifold. For many applications, such as biological membranes, the surface is transported, so evolves with time. Here the authors investigate how irregularities or perturbations of the manifold, and it's metric tensor, affect the superimposed diffusion. Perturbation techniques are used to compare the evolution of a density on perturbations of a flat surface. It is shown that order $O(\epsilon)$ perturbations can lead to order $O(1)$ changes in the density. This transitioning of scales illustrates that evolution of the geometry must be carefully and accurately modeled.

Y. Epshteyn and B. Riviere in their paper *Convergence of high order methods for miscible displacement* consider a fully discrete discontinuous Galerkin FE discretization of a problem of miscible displacement in porous media. It includes several variants of formulation (NIPG, IIPG, SIPG) by varying a parameter in the formulation. The problem of miscible displacement is coupled, and solved for pressure and concentration, while velocity which provides the coupling depends on both pressure and concentrations. The resulting discrete nonlinear coupled system is shown to have a solution using a strategy similar to one in Ortner/Suli via a version of "second Schauder theorem".

In *Wavelets, a numerical tool for multiscale phenomena: from two dimensional turbulence to atmospheric data analysis*, P. Fischer and K. Tung illustrate how wavelet decompositions of multiscale data can provide insight into these interactions. This paper starts with a concise review of wavelet decompositions and then considers two case studies. The first study reveals the energy and entrophy cascades in two dimensional turbulent flow, and the second example illustrates a fundamental difference between atmospheric data from the stratosphere and troposphere.

The report *Physics of fluid spreading on rough surfaces* of M. Dragila and K. Hay presents results of a study of regimes of spreading of a viscous fluid on a rough surface, with applications to unsaturated flow in fractured rocks. A mathematical diffusion model is presented and matched with experimental results.

D. Kinderlehrer, K. Barmak, M. Emelianenko, D. Golovaty, and S. Ta'asan contributed *A new perspective on texture evolution.* Here the evolution of microstructure, specificially grain boundaries and interfaces, on the network level and the associated critical events are studied in a simplified system to determine the effect on texture. In order to gain insight into the influence of critical events on the coarsening dynamics, the evolution of stochastic characteristics of a one-dimensional system of grain boundaries moving under a gradient flow are studied as a prototype of interacting grain boundaries in a typical polycrystalline microstructure. Two kinetic models are proposed, solutions are computed and compared, and these differ in the choice of phase space, the type and number of variables that are used to describe an individual boundary.

S. Meier and M. Böhm presented *A Note on the Construction of Function Spaces for Distributed-Microstructure Models with Spatially Varying Cell Geometry.* They construct important Lebesgue and Sobolev spaces of functions that generalize a special case of the Bochner spaces. In addition, a special Lebesgue space of functions defined on the boundaries of a continuous distribution of domains is introduced. Existence, uniqueness, and upper and lower bounds for a distributed-microstructure model of reactive transport in a heterogeneous porous medium are proven.

The paper *Numerical Methods for Unsaturated Flow with Dynamic Capillary Pressure in Heterogeneous Porous Media* by M. Peszyńska and Son-Young Yi focuses on numerical modeling of unsaturated flow models that incorporate dynamic capillary pressure terms. These result in nonlinear degenerate pseudo-parabolic equations following either Richards' equation or the full two-phase flow model. Numerical difficulties associated with a cell-centered finite difference method and a locally conservative Eulerian- Lagrangian method based on finite differences are systematically studied, and convergence as well as extensions to heterogeneous porous media with different rock types are discussed.

M. Peter and R. Showalter discuss *Homogenization of secondary-flux models of partially fissured media.* Double-porosity models can account for direct cell-to-cell diffusion paths with the associated secondary-flux, and discrete versions were recently developed to describe flow and transport accurately over a wide range of scales. These discrete models are particularly effective in the presence of advection. In this report, the two-scale convergence of the discrete secondary-flux model to the corresponding continuous double-porosity secondary-flux model is described.

The paper *Downscaling: a complement to homogenization* by A. Trykozko, G. Brouwer, and W. Zijl presents an introduction to the *double constraint* (DC) method as well as some applications to downscaling of hydraulic conductivities. The DC method belongs to the class of direct inversion methods and aims to determine spatially distributed conductivities within a modeling domain from specified hydraulic potentials and flow rates at the same location on the domain's boundary. Flow fields based on the thus-obtained solution for the conductivity field do not only satisfy the continuity equation and Darcy's law, but also satisfy the two boundary conditions, both specified potential and specified flow rate. DC inversion is based on two runs with a standard groundwater flow model complemented with a simple back projection run. Implementation of the DC method's back projection module is relatively simple compared to the effort required to implement other direct inversion methods.

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