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Scaling up and modeling for transport and flow in porous media

Mise à l'échelle, homogénéisation & modélisation des écoulements de fluides en milieux poreux

DUBROVNIK, CROATIA
13-16 OCTOBER 2008

BOOK OF ABSTRACTS

Scaling Up and Modeling for Transport and Flow in Porous Media

Dubrovnik, Croatia, 13-16 October 2008

Book of abstracts

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Preface

Welcome to the International Conference on Scaling Up and Modeling for Transport and Flow in Porous Media, held at Dubrovnik, Croatia, 13–16 October 2008. This Conference was jointly organized by the Department of Mathematics of the University of Zagreb (Croatia), the Applied Mathematics Laboratory of the University of Pau & CNRS UMR 5142 (France), the Camille Jordan Institute of the University of Lyon & CNRS UMR 5208 (France), and the Groupement MoMaS/CNRS PACEN (France).

MoMaS is a French research program dedicated to mathematical modeling and numerical simulations related to underground nuclear waste storage. MoMaS has been launched in 2003 and is supported by several agencies and institutions, namely ANDRA, BRGM, CEA, EDF, IRSN and the PACEN program of CNRS. The main scientific activities of MoMaS (see http://www.gdrmomas.org for more insight) are grouped in a dozen of two years research projects that are reviewed on a yearly basis by a Scientific Committee. Current research projects focus on multiphase flows (hydrogen and water) in porous media, upscaling and homogenization, uncertainty quantification by stochastic and deterministic techniques and various numerical methods, including finite volumes, mixed finite elements, Discontinuous Galerkin, particle methods and domain decomposition. A benchmark on reactive transport has also been organized recently by MoMaS.

The aim of the conference was to bring together researchers, scientists, engineers, and students to exchange and share their experiences, new ideas, and research results about upscaling for modeling, analysis and simulation of flow and transport in porous media and application to problems including subsurface hydrology, petroleum exploration, contaminant remediation, carbon sequestration and nuclear waste storage.

The topics of the conference are: Flow and Transport in Heterogeneous Porous Media; Multiphase Flows; Multiscale Phenomena; Scaling and Heterogeneity; Scaling in porous media, in particular scaling of processes from the microscale to the mesoscale the use of coarse grid descriptions in modeling multiphase flow phenomena; Numerical Homogenization; Numerical simulation of multiphase flow in heterogeneous porous media; Mathematical modeling of multiphase flow in porous media.

This conference was attended by 75 participants from 15 different countries: Albania, Croatia, France, Germany, Israel, Italy, Morocco, The Netherlands, Norway, Russia, Slovakia, Tunisia, Ukraine, United Kingdom, and USA.

This conference is dedicated to our longtime friend and collaborator, Professor Alain Bourgeat, on the occasion of his 60th birthday. In particular, Alain Bourgeat supervised the MoMaS research program from its creation until 2006, and MoMaS owes him a lot. This conference contains 26 invited talks from the many collaborators and colleagues of him and 40 contributed talks. On the occasion of his 60th birthday, we wish Alain Bourgeat continuing creativity and a lot of great new ideas to further lead the way of mathematical and numerical modeling of flow and transport in porous media.

The conference could not have been held without the financial support of the organizing institutions and the following sponsors: Ambassade de France en Croatie; Institut Français du Pétrole (IFP); Institut de Radioprotection et de Sûreté Nucléaire (IRSN); Ministry

of Science, Education and Sport of Republic of Croatia; Total, Centre Scientifique et Technique Jean Feger and the Groupement MoMaS. We thank them for their financial support. The support of Institut National de Recherche en Informatique et en Automatique (INRIA), unité de recherche de Rocquencourt and Société de Mathématiques Appliquées et Industrielles is also greatly acknowledged.

We would like to thank Chantal Blanchard and Marie Laure Rius from CNRS & the University of Pau for their active role in the organization of the logistics of the conference. We also would like to thank Sandrine Craveiro from the University of Pau for the realization of the poster and the plaque of the conference.

Last, but not least, we want to acknowledge all participants for their contribution and efforts in making the conference an interesting, pleasant and successful event.

Wishing you a pleasant and fruitful meeting and hope you enjoy your stay in Dubrovnik.

Organizing committee:

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1. Grégoire Allaire, Ecole Polytechnique, France
2. Todd Arbogast, University of Texas at Austin, USA
3. Gilles Bernard-Michel, CEA, France
4. Jacques Blum, University of Nice, France
5. Guy Bouchitté, University of Toulon & Var, France
6. Guy Chavent, INRIA, France
7. Gregory A. Chechkin, Moscow Lomonosov State University, Russia & Narvik University, Norway
8. Jim Douglas, Purdue University, USA
9. Robert P. Gilbert, University of Delaware, USA
10. Jérôme Jaffré, INRIA, France
11. Peter Knabner, University Erlangen-Nuremberg, Germany
12. Roland Masson, IFP, France
13. Andro Mikelić, University of Lyon, France
14. François Murat, University Paris VI, France
15. Grigory Panasenko, University of Saint-Etienne, France
16. Mikhail Panfilov, LEMTA-ENSEM, France
17. Leonid Pankratov, FTINT, Ukraine
18. Andrey Piatnitski, Narvik University, Norway and Lebedev Physical Institute, Russia
19. Olivier Pironneau, University Paris VI, France
20. Michel Quintard, IMFT, France
21. Jean Roberts, INRIA, France
22. Thomas F. Russell, National Science Foundation, USA
23. Ralph E. Showalter, Oregon State University, USA
24. Peppino Terpolilli, Total, France

25. Damien Tromeur-Dervout, University of Lyon, France
26. Mary F. Wheeler, University of Texas at Austin, USA

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- Republic of Croatia: Ministry of Science, Education and Sport
- Société de Mathématiques Appliquées et Industrielles
- Total, Centre Scientifique et Technique

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Homogenization Approach to the Dispersion Theory for Reactive Transport Through Porous Media

Grégoire Allaire[1]

In this joint work with A. Mikelic and A. Piatnitski we consider the convection diffusion of a solute in a saturated flow through a porous medium. Taking into account the chemical reactions of the solute with the solid walls and for a regime of large Péclet and Damkohler numbers we obtain an homogenized model with an explicit effective drift and dispersion tensor.

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Aspects of Convergence for Mixed Multiscale Finite Elements and a New Approach for their Definition

Todd Arbogast[1], James M. Rath[2]

Key words: *multiscale finite elements, mixed methods, homogenization, heterogeneity, convergence*

AMS subject classifications: *65N15, 65N30, 76S05, 76M50, 76M10, 35B27*

Multiscale finite element numerical methods are used to solve flow problems when the permeability, i.e., coefficient in the elliptic operator, is heterogeneous. We show that a popular mixed multiscale finite element method fails to reproduce constant flow fields, and so fails to converge in any meaningful way. The problem arises when the permeability is an anisotropic tensor. This has implications for isotropic heterogeneous permeabilities, since the microstructure can lead to an anisotropic homogenized permeability. A new approach to multiscale finite elements is defined, and shown to produce a method that converges with respect to the microstructure.

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Transport of Radionuclides in a Synthetic Fractured Block. Comparisons between Different Approaches for the Numerical Simulations, Depending on the Degree of Connectivity of the Fractures

Gilles Bernard-Michel[1]

Modelling transport in fractured media is an important issue for the safety evaluation of a deep nuclear waste repository. The main challenge is to be able to derive a performance assessment model which is a simplified representation of the fractured media. This model has to be accurate enough to evaluate the retention properties of the studied block.

Our presentation is based on the following assumptions : at the block scale the fracture network can be simplied to a path of a few highly connected fractures ; for the lower scale (a few meters), the fractures may be strongly connected or on the contrary very isolated.

When the degree of connectivity is low enough, we illustrate that combined use of a Mixed Hybrid Finite Element method (for the transport modelisation in the fractures) and of Green functions (for the diffusion in the rock) will provide accurate simulations with acceptable computer costs [1]. On the other hand, when we are in the presence of a high connectivity network a the lower scale, homogeneization techniques [2] are more appropriate to represent the fractured media.

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Back to the Future: the Back and Forth Nudging Algorithm

Jacques Blum[1], Didier Auroux[2]

This paper deals with a new data assimilation algorithm, called Back and Forth Nudging (BFN), that consists in identifying the initial condition of a physical system from experimental data. The standard nudging technique consists in adding to the equations of the model a relaxation term that is supposed to force the observations to the model. The nudging method is a flexible assimilation technique, and computationally much more economical than variational data assimilation methods. First used in meteorology (Hoke and Anthes, 1976), the nudging method has been successfully introduced in oceanography in a quasi-geostrophic model (Verron and Holland, 1989). The nudging coefficients can be optimized by a variational method (Zou et al., 1992), where a parameter estimation approach is proposed to obtain optimal nudging coefficients, in the sense that the difference between the model solution and the observations is as small as possible. A drawback of this optimal nudging technique is that it requires the computation of the adjoint state of the model equations, which is not necessary in the standard nudging method.

The BFN algorithm, introduced in Auroux and Blum (2005), consists in repeatedly performing forward and backward integrations of the model with relaxation (or nudging) terms, using opposite signs in the direct and inverse integrations, so as to make the backward evolution numerically stable. The initial condition of this backward integration is the final state obtained by the standard nudging method. After integration of this backward equation, one obtains an estimate of the initial state of the system. We then repeat these forward and backward integrations (with the relaxation terms) until convergence of the algorithm. The BFN algorithm can be compared to the four-dimensional variational algorithm (4D-VAR, see e.g. Le Dimet and Talagrand, 1986), which also consists in a sequence of forward and backward integrations. In our algorithm it is useless to linearize the system, even for nonlinear problems, and the backward system is not the adjoint equation but the model equations, with an extra feedback term that stabilizes the numerical integration of this ill-posed backward problem.

This algorithm has first been tested on the standard Lorenz model with discrete observations (perfect or noisy) and compared with the variational assimilation method. The same type of study has then been performed on the viscous Burgers equation, comparing again with the variational method and focusing on the time evolution of the reconstruction error, i.e. the difference between the reference trajectory and the identified one over a time period composed of an assimilation period followed by a prediction period. The possible use of the BFN algorithm as an initialization for the variational method has also been investigated. Finally the algorithm has been tested on a layered quasi-geostrophic model and a shallow-water model, with sea-surface height observations. The behaviours of the two algorithms have been compared in the presence of perfect or noisy observations, and also for imperfect models (see Auroux-Blum, 2008). This has allowed us to reach a conclusion concerning the relative performances of the two algorithms. The BFN algorithm is hence very promising to obtain a correct initial state, with a smaller number of iterations than in a variational method and an easier implementation.

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About Existence for Optimal 1-Rectifiable Transports

Guy Bouchitté[1]

It is a work in collaboration with P. Seppecher and A. El Hajari (University of Toulon). Given two mass distributions μ_+, μ_- in $\mathbb{R}3$, we consider optimization problems of the kind

$$\inf \{\mathcal{F}(\lambda) \ : \ \mathrm{d}iv\, \lambda = \mu_+ - \mu_-\} \ ,$$

where the unknown λ is a vector measure (*transport* measure) and $\mathcal{F}$ is a cost functional.

In this talk we will focus on models where the admissible transports measures λ (those for which $\mathcal{F}(\lambda) < +\infty$) have to be concentrated on one-dimensional rectifiable subsets of $\mathbb{R}3$, that is of the form

$$\lambda \ = \ \theta(s)\, \tau_S\, \mathcal{H}1 \llcorner S \ ,$$

being $\theta(x) > 0$ a local flux intensity, τ_S an tangent vector and $\mathcal{H}1 \llcorner S$ the one -dimensional Hausdorff measure on S.

We present a method of existence which allows to extend the case

$$\mathcal{F}(\lambda) = \int_S \theta^\alpha \, d\mathcal{H}1 \quad \text{with} \quad 0 < \alpha < 1 \ ,$$

considered by many authors for modelling irrigation problems.

As a by-product we are able to consider well posed dynamic formulation of transport problems for countably many travellers taking into account the speed (with possibly positive parking cost) and the economy due to sharing the same convoy.

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Global Pressure Revisited: Three Phase Compressible Flows

Guy Chavent[1], Raphaël Di Chiara[2], Gerhard Schäfer[3]

Key words: *three-phase flow, global pressure, mathematical modeling*

The global pressure has been introduced in the seventies to simplify the mathematical formulation of three-phase flows [CJ]. Despite its recognized computational efficiency [ZE], it did not not gain a wide use, because of two hampering factors:

- it required the relative permeability and capillary pressure curves to satisfy a "total differential condition",

- the volume factors and viscosities where evaluated at the global pressure value, and not at the corresponding phase pressure, which could lead to unacceptable errors for large capillary pressures.

Recently, global pressure has received attention again for the simulation of unsaturated water flow, and we shall present some progress relative to the above difficulties.

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Homogenization of Random Multilevel Junctions

Gregory A. Chechkin[1], Tatiana P. Chechkina[2]

Key words: *Homogenization, partial differential equations, domain with random oscillating boundary*

AMS subject classifications: *35B27, 76M50, 35P05*

We consider the following homogenization problem:

$$\begin{array}{rcll} -\Delta_x\, u_\varepsilon &=& f, & \text{in} \quad D_\varepsilon; \\ \frac{\partial u_\varepsilon}{\partial \nu} + u_\varepsilon &=& p, & \text{on} \quad \Gamma_\varepsilon; \\ \frac{\partial u_\varepsilon}{\partial \nu} + \varepsilon\, u_\varepsilon &=& \varepsilon\, q, & \text{on} \quad \Upsilon_\varepsilon; \\ u_\varepsilon &=& 0, & \text{on} \quad \Gamma_1; \\ \frac{\partial u_\varepsilon}{\partial \nu} &=& 0, & \text{on} \quad \gamma_\varepsilon. \end{array} \tag{1}$$

Here the domain $D_\varepsilon \subset \mathbb{R}^3$ (see Figure 1) is the union of the fix domain $D_0 = \{x \in \mathbb{R}^3 : \widehat{x} = (x_1, x_2) \in Q,\ \ 0 < x_3 < \psi(\widehat{x})\}$, $Q = (0,a) \times (0,a)$, $\psi \in C^1(\overline{Q})$, $\min\limits_{\widehat{x}\in\overline{Q}} \psi(\widehat{x}) = \psi_0 > 0$, large number of thin cylinders $G_\varepsilon = \bigcup\limits_{i,j=0}^{N-1} \Big(\big\{ x :\ \big(\varepsilon^{-1}\, x_1 - i,\ \varepsilon^{-1}\, x_2 - j\big) \in B,\ \ x_3 \in (-l_2, 0] \big\} \Big)$, and the layer $\Pi_\varepsilon = \{x \in \mathbf{R}^3\ :\ \widehat{x} \in Q,\ \varepsilon g(\widehat{x}) F\left(\frac{\widehat{x}}{\varepsilon}, \omega\right) < x_3 \le 0\}$, where $g(\widehat{x})$ is a smooth nonnegative function with *supp* $g(\widehat{x}) \subset Q_0 \equiv \{x \in \mathbb{R}^3, (x_1, x_2) \in Q, x_3 = 0\}$, and $F(\widehat{\xi}, \omega)$ is a random statistically homogeneous ergodic nonpositive function with smooth realizations, ω is an element of a standard probability space $(\Omega, \mathcal{A}, \mu)$.

We assume that $B \subset \mathbb{R}^2$ is 1-periodic in $\widehat{\xi}$ translation of the fix smooth domain belonging to $[0,1] \times [0,1]$. We denote also $\Gamma_\varepsilon = \{x \in \Pi_\varepsilon\ :\ \widehat{x} \in Q,\ \varepsilon g(\widehat{x}) F\left(\frac{\widehat{x}}{\varepsilon}, \omega\right) = x_3\}$, Υ_ε is the union of lateral and lower surfaces of the cylinders, $\Gamma_1 = \{x :\ x_3 = \psi(\widehat{x}),\ \widehat{x} \in Q\}$, $\gamma_\varepsilon = \partial\Omega_\varepsilon \setminus \big(\Gamma_\varepsilon \cup \Upsilon_\varepsilon \cup \Gamma_1\big)$.

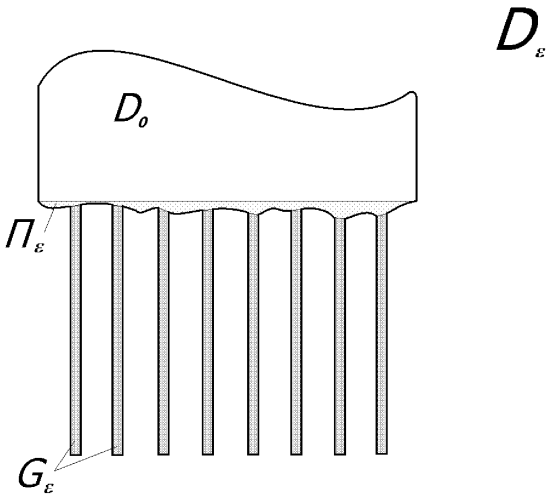

Figure 1: Random multilevel junction

Under the assumption that $f \in L_2(\Omega_0 \cup D_2)$, p, q are constants, we prove that the homogenized problem is

$$\begin{aligned}
-\Delta_x\, u_0^+ &= f \quad \text{in} \quad D_0 \\
u_0^+ = 0, \quad \text{on} \quad \Gamma_1, \qquad & \tfrac{\partial u_0^+}{\partial \nu} = 0, \quad \text{on} \quad \partial D_0 \setminus \big(\Gamma_1 \cup Q_0\big), \\
-\tfrac{\partial}{\partial x_3}\big(|B|\,\tfrac{\partial u_0^-}{\partial x_3}\big) + |\partial B| u_0^- &= |B|\, f + |\partial B| q \quad \text{in} \quad D_2, \\
u_0^+ &= u_0^- \quad \text{on} \quad Q_0, \\
|B|\tfrac{\partial u_0^-}{\partial x_3} - \tfrac{\partial u_0^+}{\partial x_3} + \Xi\, u_0^+ &= \Xi\, p \quad \text{on} \quad Q_0, \\
\tfrac{\partial u_0^-}{\partial x_3}(\widehat{x}, -l_2) &= 0, \quad \widehat{x} \in Q,
\end{aligned} \tag{2}$$

where $D_2 = Q \times (-l_2, 0)$, and Ξ is the mathematical expectation $\mathbb{E}\left(\sqrt{1 + \Big(g(\widehat{x})\, \nabla_\xi F(\widehat{\xi}, \omega)\Big)^2}\right)$.

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Several Operator Splitting Methods for Flows in Porous Media

Jim Douglas, Jr[1]

The lecture will give a survey of recent operator-splitting methods based on physics, rather than dimension, for multiphase and multicomponent flows in porous media. In particular, splittings based on separating transport from diffusion will be discussed. Significantly different approximation methods will be applied to transport and diffusion. The lecture will cover joint work with E. Abreu, F. Pereira, and F. Furtado.

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Homogenizing the Acoustic Properties of Cancellous Bone: The Non-Newtonian Fluid Case

Robert P. Gilbert[1], Alexander Panchenko[2], Ana Vasilic[3]

Key words: *porous media, acoustics, non-Newtonian fluids*

AMS subject classifications: *35A05, 76B40*

Osteoporosis can be characterized as a decrease in strength of the bone matrix. Various parameters, such as bone density, pore size, shear and bulk modulii, have a significant effect on bone rigidity. Ultrasound techniques have been used to characterize the elastic properties of bone for some time. However, there is still a need for a better mathematical background for understanding the use of ultrasound methodology.

We form a mathematical model describing the acoustic behaviour of cancellous bone. Bone is approximated by a porous material with periodic micro-structure. The solid part is represented by a visco-elastic porous matrix while the fluid (the blood-marrow mixture) inside the pores is assumed to be a non-Newtonian shear thinning fluid. Using the method of 2-scale convergence (and theory of monotone operators), we obtain the equations describing the effective properties of bone. The effective equations are written in terms of both the leading order term (depending on slow variable only) and the first order corrector term (depending on both slow and fast variables). The effective stress captures both visco-elastic and memory effects.

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Phase Exchange for Flow in Porous Media and Complementary Problems

Jérôme Jaffré

A benchmark from the GNR Momas (http://www.gdrmomas.org) considers the problem of modeling the migration of hydrogen produced by the corrosion of waste packets in a nuclear waste disposal. The problem is a liquid-gas system with water and hydrogen components, and phase exchange. We discuss physical formulations of the problem like Henry's law vs phase diagrams and, we formulate the problem as a system of nonlinear PDE's with complementary constraints. We show how to solve the problem and give some first numerical results.

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Large General Reactive Multicomponent Transport Processes in Porous Media: Modeling, Analysis and Efficient Simulation

Peter Knabner[1], Serge Kraeutle[1], Alexander Prechtel[1]

Key words: *flow and transport in porous media, reactive transport, Ljapunov method, complementarity system, reaction extents, Newton's method*

AMS subject classifications: *76S05, 35K55, 35K85, 35K57, 65M60, 65F30, 49M15*

Detailed modelling of reactive transport processes in the underground often requires the consideration of a wide range of reactive species. A prominent example is natural attenuation, that is the assessment and monitoring of microbially catalysed degradation processes of organic contaminants in the subsoil or aquifer. The reactions exhibit a wide range of reaction times, which advises to model those reactions being much faster than the time scale of the transport processes in a quasistationary manner, e.g. as (algebraicly described) equilibrium processes. Additionally not only mobile species (in solution) appear, but also immobile ones (attached to the porous skeleton). Reactions with minerals play a special role as their equilibrium desciption is rather a complementarity system than an algebraic equation with consequences for the kinetic description. In summary, the resulting system is not semilinear and parabolic, but rather quasilinear and couples partial differential equations (pde), ordinary differential equations, algebraic equations and complementarity conditions. For such a system without growth bounds in the nonlinearity no general existence theory is possible, but recent results indicate that for special structures of the nonlinearities resulting e.g. from the mass action law, a global existence theory is possible on the basis of a generalized Ljapunov approach. We will review the current state of the analysis. Concerning the numerical simulation of such systems, an often used approach is operator splitting, in which transport and reaction become (iteratively) decoupled. This procedure either introduces a further consistency error (in the non-interative version) which can only be controlled by the time stepping, or applies a fixed point type iteration of unclear convergence properties. We rather propose, after appropriate (mixed) finite element discretization, to deal with the full discrete nonlinear system (by a damped Newton's method). To make the problem still feasible we advise two means: The first is concerned with the continuous model and aims at a transformation of the dependent variables such that as many as possible are determined by decoupled linear pde's or by local algebraic relations, leading to a smaller coupled system. The problem lies here in the combined appearance of kinetics and equilibrium and mobile and immobile species. Alternatively to this exact a priori decoupling we use an a posteriori decoupling on the level of the linear system of equation in the Newton's method by ignoring weak couplings in the Jacobian matrix. The resulting benefit in the solution of the linear system should supersede a possible deterioration in the convergence of the iterative method, being now only an approximate Newtons's method. The approaches are all illustrated with realistic problems, including the MoMas benchmark.

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Cell Centered Finite Volume Schemes for Multiphase Porous Media Flow Problems with Applications in the Oil Industry

Roland Masson[1], Léo Agelas[1], Daniele Di Pietro[1], Ivan Kapyrin[1]

Many applications in the oil industry require the efficient simulation of compositional multiphase Darcy flow. Cell centered finite volume schemes are often used for this purpose owing to their robustness, their low computational cost, and their ability to include complex physics. However, this requires a discretization of the diffusion operator which (i) shows good convergence, stability and complexity properties; (ii) can be used on general polygonal or polyhedral meshes; (iii) can handle heterogeneous and anisotropic diffusion tensors. In this talk we will first present the basic framework used in the oil industry for the finite volume discretization of multiphase Darcy flow compositional models. Then, we will focus on cell centered finite volume discretizations of diffusion fluxes on general meshes and for L^∞ diffusion tensors. Several approaches mainly using a discrete hybrid variational formulation framework will be discussed and assessed numerically.

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Analysis of Model Equations for Stress-Enhanced Diffusion in Coal Layers

Andro Mikelić[1]

Key words: *degenerate pseudoparabolic equation, entropy methods, stress enhanced diffusion*

AMS subject classifications: *35K70, 35K65, 76R50, 80A17*

This paper is motivated by the study of the sorption processes in the coal. They are modelled by a nonlinear degenerate pseudo-parabolic equation for stress enhanced diffusion of carbon dioxide in coal

$$\partial_t \phi = \partial_x \left\{ D(\phi)\, \partial_x \phi + \frac{D(\phi)\, \phi}{B} \partial_x \left(e^{-m\phi} \partial_t \phi \right) \right\},$$

where B, m are positive constants and the diffusion coefficient $D(\phi)$ has a small value when the CO_2 volume fraction ϕ is $0 \leq \phi < \phi_c$, representative of coal in the glass state and orders of magnitude higher value for $\phi > \phi_c$, when coal is in the rubber like state.

These type of equations arise in a number of cases when non-equilibrium thermodynamics or extended non-equilibrium thermodynamics is used to compute the flux.

For this equation existence of the travelling wave type solutions was extensively studied. Nevertheless, the existence seems to be known only for sufficiently short time. We use the corresponding entropy functional in order to get existence, for any time interval, of an appropriate weak solution with square integrable first derivatives and satisfying uniform L^∞-bounds. Due to the degeneracy, we obtain square integrability of the mixed second order derivative only in the region where the concentration ϕ is strictly positive. In obtaining the existence result it was crucial to have the regularized entropy as unknown for the approximate problem and not the original unknown (the concentration).

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Finite Elements Approximation of Second Order Linear Elliptic Equations in Divergence Form with Right-Hand Side in L^1

François Murat[1]

In this lecture I will report on joint work with J. Casado-Díaz, T. Chacón Rebollo, V. Girault and M. Gómez Marmol which was recently published in Numerische Mathematik, vol. 105, (2007), pp. 337-510. We consider, in dimension $d \geq 2$, the standard $P1$ finite elements approximation of the second order linear elliptic equation in divergence form with coefficients in $L^\infty(\Omega)$ which generalizes Laplace's equation. We assume that the family of triangulations is regular and that it satisfies an hypothesis close to the classical hypothesis which implies the discrete maximum principle. When the right-hand side belongs to $L^1(\Omega)$, we prove that the unique solution of the discrete problem converges in $W_0^{1,q}(\Omega)$ (for every q with $1 \leq q < \dfrac{d}{d-1}$) to the unique renormalized solution of the problem. We obtain a weaker result when the right-hand side is a bounded Radon measure. In the case where the dimension is $d = 2$ or $d = 3$ and where the coefficients are smooth, we give an error estimate in $W_0^{1,q}(\Omega)$ when the right-hand side belongs to $L^r(\Omega)$ for some $r > 1$.

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Asymptotic Partial Decomposition Strategy for Modelling of Flows in Thin Tube Structures

Grigory Panasenko[1]

The tube structures are the domains of a small measure which are connected finite unions of of thin cylinders (or rectangles in the 2D case). The small parameter here is the ratio of the diameter to the height of the cylinders. We consider the Stokes, the Navier-Stokes equations as well as the micropolar flows in such domains. The boundary conditions are either of the Dirichlet type (absolutely rigid walls) or the elasticity of the wall is taken into account (some examples of this kind of settings and its asymptotic analysis could be found in [1-7]). In the last case the rigidity of the wall is the second (great) parameter [8].

For these problems an asymptotic expansion of the solution is constructed. This asymptotic analysis is applied then for the implementation of the method of asymptotic partial decomposition of domain [1,3,9,10]. This method reduces the dimension to one in the main part of the tube structure, keeps the initial dimension in some small neighbourhoods of the ends of thin cylinders and prescribes the appropriate interface conditions between the reduced 1D parts of the cylinders and the 3D (or 2D) parts containing the junctions of the cylinders (rectangles) and their ends.

The main application of this analysis is the first step in the modelling of the blood circulation. Partially the results are obtained in collaboration with Ruxandra STAVRE (Institute STOILOW of Mathematics of Romanian Academy of Sciences), Delphine DUPUY (LaMUSE, Saint Etienne University) and Ivan SIRAKOV (PPF ALLIANA, Saint Etienne University) .

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Macro-kinetic model and oscillatory regimes of gas-liquid flow in porous media with boiling and bubble coalescence

Mikhail Panfilov[1], Irina Panfilova[2]

Key words: *Phase transition, two-phase flow, porous media, oscillations, dynamic theory, bifurcations*

A number of experimental data show that the flow of miscible gas-liquid systems in porous media is characterized by the appearance of stable high-amplitude and low-frequency oscillations. In the present paper we develop the theory of these processes which predicts and explains the oscillatory regimes as the result of the competition between several non equilibrium processes occurring on the pore-scale, as the evaporation, the coalescence of gas bubbles, the secondary liquid condensation and liquid/gas evacuation. The kinetic models of all the processes are developed and homogenized next over the ERV. The obtained

macro-kinetic model represents a generalization of the Volterra model which predicts the nonlinear oscillatory regimes and the bifurcation to other regimes. Some parameters describing the kinetics on the pore-scale are obtained by comparison the results of simulation with experimental data.

The model is used to simulate the natural depressurization of a heavy oil reservoir, and the gas flow with condensation in a gas-condensate reservoir.

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On the Homogenization of some Double Porosity Models with Periodic Thin Structures

Leonid Pankratov[1], Brahim Amaziane[2]

Key words: *Double porosity models, fractured media, thin fissures*

AMS subject classifications: *35B27,74Q15, 76M50, 76S05*

Models describing global behavior of incompressible flow in fractured media are discussed. A fractured medium is regarded as a porous medium consisting of two superimposed continua, a continuous fracture system and a discontinuous system of medium-sized matrix blocks. We derive global behavior of fractured media versus different parameters such as the fracture thickness, the size of blocks and the ratio of the block permeability and the permeability of fissures, and oscillating source terms. The homogenization results are obtained by mean of the convergence in domains of asymptotically degenerating measure.

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Homogenization of Spectral Problem for Elliptic Differential Operators with Sign-Changing Density

Andrey Piatnitski[1]

The talk will focus on homogenization of Dirichlet spectral problem in a bounded domain for divergence form elliptic operators with periodic rapidly oscillating coefficients in the case of sign-changing periodic density function. It will be shown that for any small enough value of the microstructure period the spectrum is discrete and consists of two sequences, one of them converges towards plus infinity, and another - towards minus infinity. Then we will discuss the asymptotic behaviour of spectrum as the microstructure period tends to zero. It turns out that this behaviour depends crucially on whether the average of the spectral density is positive, negative or equal to zero. We will construct the asymptotics of eigenpairs in all three cases.

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Pros and Cons of the Finite Element Methods for Option Pricing

Olivier Pironneau[1]

The finite element method is particularly well suited to the numeri- cal solution of the partial differential equation of finance for two reasons: mesh adaptivity and a posteriori error estimates; however it can be slow. The main applications of the method will be recalled here and these ad- vantages illustrated; a computation mixing Monte-Carlo and Partial Dif- ferential equation for a basket option will also be presented.

Ito Calculus applied to the Stochastic definition of option pricing models yields partial differential equations or integro-differential partial differen- tial equations for which three or four classes of numerical methods can be used. Finite Difference Methods are by far the simplest, except when mesh adap- tivity is required in which case it is rather difficult to control the numerical error. Finite Volume Methods are not really natural, except in the case of Asian options and so are the Spectral Methods because the volatilities are not constant in the interesting cases Finite Element Methods seem at first unnecessarily complex for finance where a large class of problems are one dimensional in space and yet rather easy to implement in practice as we shall see. The Finite Element Method has been invented for solid mechanic engi- neering around 1950; it is an extension of the theorem of virtual work. Its generalization to other problems has been done by applied mathemati- cians mostly through the concept of variational formulations and weak forms of the partial differential equations. Consequently it is indifferent to uniform or arbitrary mesh and since a posteriori error indicators are available it is possible to tune the mesh accordingly; this

property is very useful to compute accurately the exercise region of an American option or a multidimensional basket option. Large drift terms can be handled by the Galerkin-Characteristic method, a technicality which is not always known, but essential for Asian option. Finally the curse of dimension can be dealt with in a number of ways, from sparse grids to mixed Monte-Carlo/PDE methods.

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Upscaling dissolution mechanisms in porous media

Michel Quintard[1]

Dissolution mechanisms are found frequently in many porous media applications: geochemistry, karstification, environmental issues with, for instance, the dissolution of partially miscible pollutants, nuclear engineering (concrete walls dissolution by corium, ...), acid injection in reservoir engineering, aerospace industry, and many others. Different aspects are at the core of ongoing research, including chemistry modeling, numerical modeling. One aspect is paramount to the achievement of good models: the consideration of the many scales involved.

In this paper we will discuss several problems, with illustration taken from the above cited applications:

- the introduction of effective surfaces replacing the real, heterogeneous, rough surface. Effective surface properties are obtained through different techniques (volume averaging, domain decomposition), the impact of the interface recession on the effective properties is emphasized.
- non-equilibrium Darcy-scale models are discussed following results obtained from volume averaging, and comparison with available experimental data.
- the instability behavior of the resulting Darcy-scale model is discussed, many new aspects are emphasized, such as the impact of the porous domain extension.
- Subsequent up scaling may be needed to take into account large-scale effects (instabilities (wormholing), heterogeneity). Different models are proposed, depending on process parameters.

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Single-Phase Flow in Porous Media with Fractures: Modeling Fractures as Interfaces

Jean E. Roberts[1]

In this talk we are concerned with the numerical modeling of single-phase flow in porous media with fractures. In particular we are interested in domains having fractures of known form and location. Though larger than the fine fractures in regular systems of fractures which are usually taken into account using double porosity models, such fractures are still of width too small to be captured by a regular grid, and they require special treatment. Some models simply consider flow in a network of such fractures ignoring the interaction with the surrounding medium. However this is not an appropriate tactic for all applications and we consider here a model in which the fractures are treated as interfaces in a domain decomposition setting with nonstandard interface conditions. The issues of intersecting fractures, of non-matching grids and of nonlinear flow in the fractures will be discussed. Some numerical results will be shown.

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Stochastic Modeling of Multiphase Transport in Subsurface Porous Media: Motivation and Some Formulations

Thomas F. Russell[1]

In practical simulation of multiphase subsurface transport, for example in aquifers or oil reservoirs, consideration of stochastic modeling is appropriate for two reasons. First, the formation and fluid properties are never precisely known, so that it is natural to allow for multiple realizations and to formulate results in probabilistic terms. Second, and more importantly for our purposes, small-scale heterogeneities and fluid phenomena can contribute significantly to large-scale behavior of the multiphase system, and computational limitations preclude the possibility of modeling these small-scale features directly in the large-scale system. When viewed through a coarser lens, the small-scale behavior can take on aspects of randomness, suggesting stochastic processes as worthwhile models for small-scale effects in large-scale systems. In particular, the physics of multiphase flow at material interfaces (capillary discontinuities) in porous media is not well understood, and a stochastic formulation that matches small-scale experimental observations could be beneficial in constructing efficient, accurate large-scale models. We will discuss some related background, concepts, and calculations that have been compared to experiments.

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Flow with Dynamic Capillary Pressure over Multiple Scales

Ralph Showalter[1], Malgorzata Peszyńska[2]

Key words: *Mathematical modeling, pseudoparabolic, homogenization, double-diffusion model, two scale convergence*

AMS subject classifications: *Primary 35B27, 76S05; Secondary 35K65, 35K90*

Recent models of partially saturated flow through porous media include dynamic effects in the capillary pressure curves. These lead to partial differential equations of pseudo-parabolic type with multiple nonlinearity and degeneracy. We describe properties and numerical computation of solutions of appropriate initial-boundary-value problems and the upscaling from various types of heterogeneous media.

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Some Flow Problems in Porous Media: an Industrial Point of View

Peppino Terpolilli[1]

The upstream oil industry finds and produces crude oil and natural gas. The upstream is sometimes known as the exploration and production sector. In this presentation we want to present two situations where the development of the oil industry projects leads to interesting applied mathematical problems. We are interested in techniques used by reservoir engineers to give prospective about the production of an oil field. Most of the time this is accomplished using tools which model the flow of fluids in porous rock and in the well. In recent years, many reservoirs with complicated physical and geological properties have been developed. Fundamental problems of enhancing oil and gas recovery from rocks have been intensively analysed.

In the first situation we will focus on uncertainty assessment and up scaling issues to devise more reliable forecasting figures; in the second one we shall see how to process new kind of data coming from new optical fibre sensor.

Uncertainty assessment is becoming a crucial step for the appraisal of a new field and/or for the decision of development. In the last decades we have witnessed a big change in the practise of reservoir engineering. Actually, a characteristic point for the applications of subterranean hydrodynamics is that the information concerning the underground is always rather poor and limited. It includes geophysical information coming from interpretation surveys, geological data from core analysis, logs along the wells, petrophysics measurements and well testing. When the wells are in production, we also collect the production history of the fields. However, even if the total amount of such information were available, which is by no means always the case, it is still insufficient to enable an unambiguous construction of an adequate reservoir model. Indeed, any model requires the interpolation over the whole field of the data measured in majority in the wells and the near vicinity. Under these circumstances, the basic goal of the reservoir engineer until recently was to establish qualitative features of the field under study, stable trends as well as certain quantitative predictions, stable with respect to the variation of the input data, poorly known. Nowadays the situation has drastically changed with the appearance of geostatistical tools enabling the construction of detailed geologic models constrained by the data at the wells. The level of details of these stochastic models must be consistent with the resolution of the data collected at the wells. Geostatistics offers efficient tools to interpolate between the wells but each such models is by no means the reality but a possibility, linked with the probabilistic framework inferred from the data. This very fact leads to the development of uncertainty assessment studies in the field of reservoir engineering trying to figure out the propagation of uncertainty from the data- like porosity and permeability fields- to the solutions like production rates and so on. Several methodologies are now available as alternatives to the direct ensemble averaging, hindered by the cost of a single run for a possible model. A prospective way is the solution by stochastic partial differential equations (SPDE) governing the different moments of quantity of interest. We also have at our disposal experimental design methodology, with which were already developed industrial tools in reservoir engineering. In this presentation we focus on upscaling theory which could be used to enable uncertainty assessment

The development of optical fiber sensor offer good promise for the monitoring of the deep offshore fields. We can now have at low cost permanent sensors along the well which provide continuous measurement of temperature. The challenge is then to interpret these measurements and extract useful information for the monitoring of the field. Here we are in a deterministic world where we need to make precise all the physic necessary to model the new measurements and then to design a mathematical representation suitable for a computer implementation. Actually we model the flows into the porous medium using Darcy law, including a tight energy balance equation coupled with a thermodynamic package which compute the properties of the fluid. There is also a coupling with the flow into the well where the sensors are located. We give an overview of the work done and some perspective on the inversion step when we try to extraxt information from the measurement.

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Meshfree Adaptative Aitken-Schwarz Domain Decomposition for Darcy flow

Damien Tromeur-Dervout[1]

Key words: *PDE of Elliptic Type, Schwarz Domain Decomposition, Aitken's acceleration of convergence, Parallel Computing, Darcy flow*

AMS subject classifications: *35J25, 65B99, 65N55, 65Y10.*

Schwarz DDM main drawback is its slow convergence especially for elliptic problem. The Aitken-Schwarz (AS) DDM, introduced by M. Garbey and D. T.-D. does not need an "optimal" choice for the artificial boundary condition but takes advantage of the pure linear convergence of the error at the artificial interfaces generated by the DDM of the Schwarz method when is applied to solve linear problems on regular meshes. The AS-DDM consists not to build directly an algebraical representation of the Dirichlet to Neumann mapping (DtN), but consists to build numerically the operator of error at the artificial interface (related to the DtN) which depends neither of the problem's right hand side nor of the Schwarz's iterate. One can apply the acceleration of the convergence of Aitken to obtain the discrete exact solution at the artificial interfaces. In this work we keep the two salient features of the AS which are: a basis, orthogonal with respect to an hermitian bilinear form, in order to represent the trace on the artificial interfaces of the solution of the Schwarz iteration , and a decrease of coefficients that represent this trace in this basis. This allows to build a P* matrix that approximates P with involving only some of the vector of the basis. Then, the values of these coefficients in the basis allow to provide an a posteriori tool to select in an adaptive way the modes that must be involve in the building of P*. We will show the last developments of the AS-DDM where the building of the matrix P* is no longer associated to the properties of the mesh. Some results on Darcy flow problems div(K grad H)=b where the permeability K follows a lognormal random distribution that leads to very high contrasted values and non separable operator, will be given. This part of the work is funded by the ANR CIS 2007 MICAS.

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Multiscale Discretizations for Flow, Transport and Mechanics in Porous Media

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Key words: *mixed finite element methods porous media*

A fundamental difficulty in understanding and predicting large-scale fluid movements in porous media is that these movements depend upon phenomena occurring on small scales in space and/or time. The differences in scale can be staggering. Aquifers and reservoirs extend for thousands of meters, while their transport properties can vary across centimeters, reflecting the depositional and diagenetic processes that formed the rocks. In turn, transport properties depend on the distribution, correlation and connectivity of micron sized geometric features such as pore throats, and on molecular chemical reactions. Seepage and even pumped velocities can be extremely small compared to the rates of phase changes and chemical reactions. The coupling of flow simulation with mechanical deformations is also important in addressing the response of reservoirs located in structurally weak geologic formations.

We will focus on the mortar mixed finite element method (MMFE) which was first introduced by Arbogast, Cowsar, Wheeler, and Yotov for single phase flow and later extended to multiphase flow by Lu, Pesyznska, Wheeler, and Yotov for multiphase flow. The MMFE method is quite general in that it allows for non-matching interfaces and the coupling of different physical processes in a single simulation. This is achieved by decomposing the physical domain into a series of subdomains (blocks) and using independently constructed numerical grids and possibly different discretization techniques in each block. Physically meaningful matching conditions are imposed on block interfaces in a numerically stable and accurate way using mortar finite element spaces. The mortar approach can be viewed as a subgrid or two scale approach. Moreover, the use of mortars allows one to couple MFE and discontinuous Galerkin approximations in adjacent subdomains. We will also discuss the use of mortars for poroelastic problems. In this presentation we will discuss theoretical a priori and a posteriori results and computational results will be presented.

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A Hybrid finite Scheme for a Diffusion Problem, Satisfying a Local Principle of Maximum

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Key words: *Single phase, hybrid finite volume and anisotropic*

Numerical modeling of two-phases flows in heterogeneous and anisotropic porous media is an important stake for petroleum engineering or for the storage of nuclear waste.

Numerous schemes have been developed especially for diffusion problems such as hybrid finite volume schemes. The originality of this scheme lies in the fact that we are able to use it with weak hypothesis on the mesh and that the unknowns are the values at the center of the control volumes and at some internal interfaces. However, it doesn't respect the local principle of maximum with strong heterogeneities. We need a scheme who satisfies it because the saturation remain between 0 and 1.

In this paper we focus on the single phase problem. We first present an hybrid finite volume scheme for heterogeneous and anisotropic diffusion problems on nonconforming meshes.
With the intention of satisfy the local principle of maximum, we have etablished a constraint thanks to Uzawa algorithm. The convergence properties of this scheme will be shown and finally an error estimator will be given for an isotropic case.

Finally, some numerical results will be presented for a single phase problem corresponding to a benchmark on discretization schemes for anisotropic diffusion problems on general grids (R.Herbin and F. Hubert,*"Benchmark on discretization schemes for anisotropic diffusion problems on general grids"*,2008).

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Small-Amplitude Homogenisation of Parabolic Problems

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Key words: *H-convergence, small-amplitude homogenisation, diffusion equation, H-measure*

AMS subject classifications: *35B27, 35K05, 35Sxx*

Abstract theory of non-periodic homogenisation for non-stationary diffusion equation is much less known than the corresponding theory for stationary diffusion.

However, the main results of G-convergence and H-convergence were already obtained by Sergio Spagnolo in the seventies, with some extensions by Vasilij V. Žikov and collaborators in the eighties, and Andrea Dell'Aglio and François Murat in the nineties.

We shall prove that the smoothness (with respect to a parameter) is preserved in the process of taking the H-limit, which is essential for our purposes.

The small-amplitude homogenisation consists in taking a sequence of coefficients which difference is proportional to a small parameter, and then computing the first correction in the limit. The explicit formula for the correction in the elliptic case can in general be obtained by using H-measures, a tool introduced arround 1990 by Luc Tartar and Patrick Gérard.

For parabolic problems, those classical H-measures are not well suited. Recently, the first author (jointly with Martin Lazar) introduced several parabolic variants, which allowed a number of applications to be extended from elliptic to parabolic equations. By using such a variant of H-measures we were able to write the explicit expression for the correction in the parabolic case.

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Homogenizations of Integro-Differential Equations with Lévy Operators

Mariko Arisawa[1]

Key words: *Homogenization, Non local problem, Integro-differential equation, Levy operator, Viscosity solutions, Ergodic problem*

AMS subject classifications: *35B27 35B37 37A30*

Some homogenizations results of the integro-differential equations with the Levy operator are studied. The following is a simple example of the periodic homogenization of the pure jump process (without diffusion):

$$u_\epsilon - c(\frac{x}{\epsilon}) \int_{z\in\mathbf{R^N}} [u_\epsilon(x+z) - u_\epsilon(x) - \mathbf{1}_{|z|\leq 1}\langle \nabla u_\epsilon(x), z\rangle] q(z)dz - g(\frac{x}{\epsilon}) = 0 \quad x \in \Omega,$$

$$u_\epsilon(x) = \phi(x) \quad x \in \Omega^c,$$

where $\Omega \subset \mathbf{R^N}$ an open bounded domain, the Levy measure $q(z)dz$ satisfies

$$q(z) = \frac{1}{|z|^{N+\alpha}} \quad z \in \mathbf{R^N}, \quad \alpha \in (0,2) \quad \text{a constant},$$

$$c(x) \quad \text{is periodic in} \quad \mathbf{T^N}, \quad 0 < \exists c_0 < c(x),$$

$g(\cdot)$ is a Lipschitz continuous periodic function in $\mathbf{T^N}$, and ϕ is a continuous function defined in Ω^c. We are interested in two problems; (I): the existence of the unique limit: $\lim_{\varepsilon\to 0} u_\varepsilon(x) = \exists^! \overline{u}(x) \quad x \in \Omega$, (II) the effective nonlocal equation which characterizes $\overline{u}(x)$:

$$\overline{u} + \overline{I}(x, \nabla\overline{u}, \nabla^2\overline{u}, I[\overline{u}](x)) = 0 \quad x \in \Omega,$$

where $\overline{I}$ represents the effective nonlocal integro-differential operator.
To solve the above problems rigorously, we use first the formal asymptotic expansion method, and then a probabilistic method, which is connected to the ergodicity of the jump process. More general results than the above example will be presented, too. The purpose of this work is to show a enoughly general connection between the homogenization problem and the ergodic property of the system which exists in the multi-scale model.

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A Two-Level Enriched Finite Element Method for the Darcy Equation

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Key words: *Darcy equation, enriched finite element method, local mass conservation*

In this work we present an enriched Petrov-Galerkin finite element method to solve the Darcy equation in mixed form. Our starting point is the lowest order unstable $\mathbb{P}_1 \times \mathbb{P}_0$ finite element space. To recover stability we enrich this finite element space as follows: first, the trial finite element space, is enriched with functions belonging to an apriori unknown space, while the test function space is enriched with bubble-like functions, in such a way that we allow static condensation. This process is applied in order to give a precise characterization of the enrichment function as being the solution of local Darcy problems including the residual of the strong equation, and this characterization is included in the method leading to a stabilized-alike method. The enrichment strategy suggests a way of recovering the local mass conservation feature, which is a feature not shared by existing jump-based formulations. Finally, since the local problems may not be solved analytically, we present a tow-level strategy to implement the method showing that the basis functions may be computed using a cheap and accurate method. The final method is analyzed and several numerical results are presented to validate the method and confirm the theoretical results.

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Refinement Indicators for Adaptive Parametrization: Theory and Applications

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Key words: *refinement indicators, adaptive parameterization*

AMS subject classifications: *65N21*

We model our inverse problem of transmissity estimation as a minimization problem of an objective function defined as a least-squares misfit between measurements of piezometric heads and the corresponding quantities computed with chosen transmissivity T.
One of the difficulties in solving this problem is that, because of the high cost of experimental measurements, the data is usually insufficient to estimate the value of the hydraulic transmissivity in each cell of the computational grid. Therefore we have to find a parameterization of the transmissivity which reduces the number of unknowns. The idea of reducing the number of unknowns is in accord with the physical reality of the problem. Indeed, hydrogeological parameteters are space dependent functions defined by the particularities of the geological zone. These particularilities are usually the same for quite large zones. Our idea for solving this parametrization problem is to proceed in a progressive way. The parametrization is refined using refinement and coarsening indicators which give us information about the effect on the objective function of adding or removing some degrees of freedom. These indicators give us the information "where should we refine".

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Formulation of the Problem of Upscaling of Solute Transport in Highly Heterogeneous Formations

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Key words: *Flow and Transport in Heterogeneous Porous Media*

Solute transport in heterogeneous porous formations is generally solved by the following steps: the random permeability structure is characterized statistically; the flow problem is solved at the fine scale (numerical elements are much smaller than heterogeneity scale); transport of a solute plume is solved by using the resolved flow field and assumed additional physical processes (sorption, decay) for given initial and boundary conditions.

In the past (Dagan, 1994, Rubin et al, 1999), upscaling was investigated for weakly heterogeneous formations, by using a first-order approximation in the logconductivity variance to solve the flow and transport problems in both fine scale and upscaled domains. The basic Lagrangian approach was to compensate for the reduction of macrodispersion caused by the increase of the size of the initial solute parcels in the upscaled domain by the addition of a diffusion component. The adopted necessary conditions were that for mean uniform flow the centroid and the second spatial moment of a large, ergodic, plume should be the same for the fine scale and upscaled solutions. If the plume is Gaussian this is also a sufficient condition for the same configuration.

In the last few years we have studied solute transport in highly heterogeneous formations, characterized by logconductivity variances much larger than unity (e.g. Jankovic et al, 2003). For a structural model of blocks of different conductivities distributed lognormally, we have been able to derive by accurate numerical simulations and semi-analytical approximations the mass arrival distribution, i.e. pdf of solute particles travel times, at downstream control planes. Under same assumptions of mean uniform flow and large, ergodic, initial plumes, the fine scale solution was shown to be skewed, displaying a long tail for large travel times. This tail was associated with large residence times in blocks of low conductivity.

We propose to discuss the formulation of the upscaling requirements under these circumstances by using the same blocks model, whose size is increased. The salient question is if it is possible to recover the main features of the fine scale mass arrival distribution by the addition of a diffusion component to the molecular one in order to compensate for the loss of information caused by upscaling.

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Modeling of Thermal Dispersion in Heated Pipes

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Key words: *porous media, turbulence, thermal dispersion, macroscopic model*

AMS subject classifications: *76S05*

This work deals with heat transfer and dispersion for laminar and turbulent flows in heat exchangers and nuclear reactors. The geometrical complexity of such systems does not allow to calculate the details of the velocity and temperature profiles in each subchannel. However, the primary interest for industrial purposes is not the microscopic details of the flow, but rather description on a large scale of mean flow quantities and heat transfer. Such a macroscopic description may be obtained applying Whitaker up-scaling method (Whitaker, 1999) to derive closure problems for channels. The so-called double average procedure (Pedras *et al.*, IJHMT, 2001 and Pinson *et al.*, 2006) has been used and balance equations for mean flow variables have been derived within laminar and turbulent regimes. The heat flux at the solid surfaces is considered as a boundary condition for the fluid energy balance. This up-scaling procedure results in additional contributions, amongst wich dispersion predominates. Thermal dispersion might be seen as the sum of a first contribution, hereafter denoted "passive", due to velocity heterogeneities, and a second one, called "active", due to wall heat transfer. Fine scale simulations have shown that both passive and active dispersion achieve asymptotic behaviours for highly turbulent flows.

The aim of the present work is now to propose practical models for both passive and active thermal dispersion in ducts that account for the three regimes : laminar, transitional and turbulent. Embedded in hydrocode, they are validated against fine scale simulations. Our results confirm the importance of thermal dispersion for heated flows in ducts.

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An Unfitted Discontinuous Galerkin Finite Element Method for Numerical Upscaling in Porous Media

Christian Engwer[1]

Key words: *Discontinuous Galerkin, Finite Elements, Hydrology, Numerical Homogenization, C++, Flows in porous media*

AMS subject classifications: *65N30, 74Q99, 86-08, 86A05, 68N99, 76S05, 76B99*

Groundwater processes are generic multi scale processes. This implies that the understanding of the pore scale is necessary to describe the system as whole.

Numerical simulations of fluid flow and transport in porous media at the continuum scale require the knowledge of effective parameters. Hydraulic parameters (e.g. capillary pressure/saturation curve, relative permeability function) for the macroscopic models are often hard to measure.

Nowadays detailed measurements of the pore scale structure are possible. As the governing equations on the micro-scale are well known, macroscopic parameters can be obtained directly from the pore scale geometry by numerical upscaling.

Handling the pore scale in a numerical simulation is not easy. On the pore scale the solid phase forms a complex shaped geometry. Within pore scale simulations a good approximation of the geometrical shape of the is crucial to obtain reliable numerical results, at the same time the interest lies only in a solution on a coarser scale, which would allow a smaller number of unknowns.

A new discretization scheme for solving PDEs in complex domains, e.g. on the pore scale, was developed. It combines the idea of Unfitted Finite Elements with a Discontinuous Galerkin (DG) Finite Elements discretization. The degrees of freedom are determined by the structured grid, while the fine structures of the domains shape are preserved by limiting the support of the shape functions to the intersection of the structured grid cells and the domain. This method allows the minimal number of unknowns to be independent of the

shape of the domain, even if their size is significantly bigger than that of the structures in the shape of the domain.

In this paper the method is applied to numerical upscaling in porous media. For verification the method is used to estimate effective permeability for a given domain with known properties.

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A Numerical Method for an Underground Waste Repository Problem with Non Standard Interface Condition

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Key words: *Beltrami-Laplace Operator, mixed finite elements, a priori error estimate, a posteriori estimator.*

The mathematical model describing the leaking of an underground waste repository include several different geometric scales: from the meter in the detail of a waste container to several kilometers for the length of the global repository and several hundred meters for the repository height. Due to this high contrast in the caracteristic lengths, direct numerical simulations for performance assesment using such a local and detailed model is not realistic. To overcome this numerical difficulties, numerous authors have proposed to use homogenization theory to derive from this detailed model a global one where detailed geometry is no more considered . By this way, they obtain three limit problems depending the convection behaviour. One of these limit problems, presents a coupling between a partial differential equation living in the whole domain and a partial differential equation living in an hyperplan separating the whole domain in two parts. We propose, in this work, to give a numerical method to solve such a problem. Using a Mixed hybrid finite element method in the whole demain and a classical finite element method in the hyperplan and decoupling the two problem by a domain decomposition method, we obain an accurate and efficient method. We present mathematical analysis of a such method and numerical example showing its efficience.

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Comparison of Theory and Experiment for Solute Transport in Bimodal Heterogeneous Porous Medium

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Key words: *Mass transfer, upscaling, volume averaging, mobile-immobile, solute transport*

AMS subject classifications: *76S05, 76R05, 76M50*

In this work we compare the two-region mass transfer theory obtained within the framework of the method of volume averaging with experimental results from literature of solute transport in two dimensional bimodal porous media. We find that the constant mass transfer coefficient predicted by the steady-state closure to the theory, when used with the macroscale transport equation, provides a reasonable prediction of the observed breakthrough curve. However, for highly heterogeneous media, the use of a constant mass transfer coefficient does not allow a good representation of the tailing that is observed in the data. Indeed, the steady solution to the closure problem can be represented in terms of the eigenvalue expansion of a Green's function that leads to the effective mass transfer coefficient being defined in terms of the harmonic average of the eigenvalues of such expansion. To further investigate the influence of using a single, constant value for the mass transfer coefficient, we examine the solution to the mass transfer problem in terms of a mixed model, where the eigenvalues of one region (the inclusions) are kept, while the second region (the matrix) is treated as a homogenized material. The results from this comparison indicate that the mass transfer coefficient predicted via volume averaging using a quasi-steady closure could potentially be improved upon by development of new methods that retain more of the eigenvalues of the system. At last, the case of weakly heterogeneous media is also studied, especially for short-pulse injections, and the influence of the injection duration on tailing is discussed.

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Two-Phase Flow Numerical Modelling: Application to a Geological Nuclear Waste Disposal

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Key words: *two-phase flow, finite element, finite volume, nuclear waste disposal*

In the context of nuclear waste underground disposal, numerical modeling of gas-liquid two-phase flow is required. Those kind of problem involves several numerical difficulties : a very high level of heterogeneity due to the numerous materials, anisotropy, strong non linearities, coming out and vanishing of each phase etc. Beside, an accurate description of gas and liquid diffusion and transport is needed. For all this points, different numerical schemes are under consideration : finite element or finite volume, choice of the unknown,etc.

In this paper, we propose a numerical treatment of a classical problem of near-field modelling of a disposal cell for intermediate-level long-lived waste (exercise Couplex Gaz proposed by Andra). For this problem, we will use and compare two different schemes. The first we use is a classical finite element model. The second one is a "hybrid finite volume" scheme, first developed by Eymard et al. The idea of this scheme is to find approximation of the solution by setting up a system of discrete equations for values in the centers of control volumes and on the interfaces. Flux is approximated by a function of this values. This scheme has been developed to be adapted to anisotropic operator and non conforming mesh. We will present and detail the results we obtain. A comparison between physical results and performances (CPU times, number of degrees of freedom etc.) will be shown .

At least, we will present a three-dimensional application made with a finite element model : modelling of a fraction of the disposal area for high-level long-lived vitrified waste.

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Numerical Method for Elliptic Multiscale Problems

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Key words: *multiscale problem, heterogeneous coefficients*

A large class of multiscale problems are described by partial differential equations with highly oscillatory coefficients. Such coefficients represent the properties of a composite material or the heterogeneity of the medium in the computation of flow in porous media problem. The computation of an accurate discrete solution of such problems requires a very fine discretisation associated with a fine grid. For such a fine resolution, the storage and computation costs are very high. ¿From an engineer's perspective, we are interested in the average behaviour of the elliptic heterogeneous operator on a coarse scale taking into account the small scale features without fully resolving them. We intend to provide a smoother elliptic operator that behaves like the original operator on a coarse mesh. As a model problem, let us consider the elliptic boundary value problem on Ω, a bounded Lipschitz domain in $\mathbb{R}^d$,

$$\begin{cases} Lu = f\ , & \text{in } \Omega, \\ u = 0\ , & \text{on } \partial\Omega, \end{cases} \qquad \text{where} \qquad L = -\sum_{i,j=1}^{d} \frac{\partial}{\partial_j} \alpha_{ij} \frac{\partial}{\partial_i},$$

with the right-hand side f in $L^2(\Omega)$. The coefficients may be non smooth, e.g., $\alpha_{ij} \in L^\infty(\Omega)$ is an oscillatory or jumping coefficient. The eigenvalues of $\alpha(x) = (\alpha_{ij})_{i,j=1,\dots,d}$ have to be bounded, but there is no requirement on smoothness or periodicity of the coefficients. Here, we restrict ourselves to the one-dimensional case. In order to construct our operator, we consider the prolongation and restriction operators issued from the multi-grid method framework, and combine them with L. In the case of periodic coefficient α, we recover the operator provided by homogenisation theory. Numerical results for different types of coefficient α (periodic or not) demonstrate the choice of the operator we built.

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Particle Simulation of Unsaturated Flows

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Key words: *Particle method, Richards equation, biphasic, unsaturated porous media*

AMS subject classifications: *76S05, 65M99*

Richards equation describes the flow of water in a porous media paritially filled with gas. assuming that the gas pressure is equal to the atmospheric pressure and the fluid is incompressible. This equation is highly non linear because of the dependency of permeability and capillarity pressure on the moisture content. Beside this, a lot of practical interest simulations have two additional difficulties : the computational domain is unbounded and the water concentration presents abrupt fronts moving throughout this domain.

Because of all these characteristics, any numerical simulation is still a very challenging task and requires the use of specific techniques. The last two characteristics suggest that particles methods should be of some interest because of their ability to transport discontinuities and to naturally resolve external boundary conditions. However, the strong non-linearity constitutes a difficult obstacle for such simulation and only one partial attempt has been made yet by Rossi[1]

We present a complete solution of the problem based on the two usual alternative : Particle Strength Exchange and Dispersion Velocity . Because of the form of Richards equation, it was found that the last one is more affected by strong discontinuities than the PSE method which was not the case for a standard convection-diffusion problem[2]. However, the dispersion veocity method presents a definitive advantage in the representation of unbounded flows. Other type of boundary conditions like prescribed fluxes modelisation has been addressed as well and wil be discussed to some extent.

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On Numerical Upscaling for Stokes and Stokes-Brinkman Flows

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Numerical upscaling for Stokes and Stokes-Brinkman problems is considered. The particular motivation comes from simulating fluid filtration in connection with the automotive industry, however, the algorithms presented here are not limited to this application. Laminar incompressible flow through a filter element is considered. Stokes-Brinkman system is used to describe it. Stokes system describes the slow flow in the pure fluid region, while Brinkman system (sometimes considered as Stokes-type perturbation of Darcy equation) governs the flow through the porous filter media. The geometries of the filter media and of the housing of the filter element may be very complicated. The algorithm presented here relies on the numerical upscaling approach. A coarse and a fine grid is considered, with the fine grid being unaffordable on the existing computers, but resolving the geometry reasonably well. Each coarse grid cell is the union of fine grid cells. Only those coarse grid blocks are selected which contain unresolved geometry details, e.g. the coarse blocks containing a mixture of fluid, solid, and porous media on the fine grid. For each such blocks, an auxiliary cell problem is solved and a coarse grid permeability is calculated. In the homogenization theory, at least two different formulations of the boundary conditions for the cell problems are known when Stokes equations are upscaled: these are periodic boundary conditions and constant velocity boundary conditions. We study these two cases numerically, along with a formulation coming from the engineering literature. Results from numerical simulations are presented and discussed.

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Discontinuous Galerkin and Nonconforming in Time Optimized Schwarz Waveform Relaxation for Coupling Heterogeneous Problems

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Key words: *Discontinuous Galerkin in time, non conforming space-time grids, Optimized Schwarz Waveform Relaxation, time windows, heterogeneous problems*

In the context of long time computations in highly discontinuous media such as far field simulations of underground nuclear waste disposal it is of importance to split the computation into subproblems for which robust and fast solvers can be used. Optimized Schwarz waveform relaxation algorithms have been described for linear convection-diffusion-reaction problems in [1], and provide an efficient approach even with rotating velocity fields [3]. These algorithms have two strong points: first, they are global in time and thus allow non conforming space-time discretization in different subdomains, and second, few iterations are needed to compute an accurate solution, due to optimized transmission conditions. It has been proposed in [2] to use a discontinuous Galerkin method in time as a subdomain solver.

We present here the 2D analysis of the method. The time interval is split into time windows, and in each time window, a few iterations of an OSWR algorithm are computed, using second order optimized transmission conditions. The subdomain solver is the discontinuous Galerkin method in time, and classical finite elements in space. Coupling between subdomains is done by a simple and optimal projection algorithm without any additional grid. We present numerical results in two dimensions to illustrate the performances of the method.

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A New Formulation of Immiscible Compressible Two-Phase Flow in Porous Media Via the Concept of Global Pressure

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Key words: *Two-phase flow, Compressible, Immiscible, Water-Gas, Global pressure, Nuclear waste*

The understanding and prediction of fluid flow and transport processes through heterogeneous porous media is of great importance in various areas of research and industry. Petroleum engineers need to model multiphase and multicomponent flow for production of hydrocarbons from petroleum reservoirs. Hydrologists and soil scientists are concerned with underground water flow in connection with applications to civil and agricultural engineering, and, of course, the design and evaluation of remediation technologies in water quality control rely on the properties of underground fluid flow. More recently, modeling flow and transport of contaminant received an increasing attention in connection with disposal of radioactive waste and sequestration of CO_2.

Historically, there have been two main approaches to modeling multiphase flow in porous media. The first is based on individual balance equations for each of the fluids, while the second involves manipulation and combination of those balance equations into modified forms, with concomitant introduction of ancillary functions that we will refer to as the fractional flow or global pressure–saturation formulation. The notion of global pressure was first introduced by [3],[2] and was then revisited by other authors, see for instance [4]. It has been since used in a wide range of engineering specialities related to numerical simulation in hydrology and petroleum reservoir engineering, see for instance [5] and references therein. It has been proven that this fractional flow approach is far more efficient than the original two-pressure approach from the computational point of view [5].

Numerical methods are very sensitive to the choice of form of the governing equation. In the light of the new and continuing developments in numerical methods for the solution of the multiphase flow equations, it is worthwhile revisiting the question of the form of the governing equations and exploring the implications of this equation form for a numerical method based on it.

In this talk, we will present a new formulation [1] to describe immiscible compressible two-phase flow in porous media. The main feature of this formulation is the introduction of a global pressure. The resulting equations are written in a fractional flow formulation and lead to a coupled system which consists of a nonlinear parabolic (the global pressure equation) and a nonlinear diffusion-convection one (the saturation equation) which can be efficiently solved numerically.

Finally, we will present some numerical results to illustrate the performance of the new formulation for water-gas flow in the context of nuclear waste underground disposal.

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What Feeds Oscillations in the Schrödinger Type Equations?

Martin Lazar[1]

H-measures, as originally introduced by Luc Tartar and Patrick Gérard, are well adapted to hyperbolic problems. In a recent study we gave an attempt to apply the H-measure theory to parabolic equations. In order to accomplish this task, we proposed a new variant of H-measures, called the parabolic H-measure, which is better suited to such kind of problems.

The goal is to identify the microlocal energy, expressed by the parabolic H-measure, via oscillations in initial data and source terms. For the heat equation this can be achieved

by means of the localisation property for the new variant. In fact, due to the hypoelliptic character of the equation, the microlocal energy contained in the initial data dies out.

However, for the Schrödinger equation this is not the case. Similarly to the treatment of hyperbolic equations, the propagation property has to be developed. The preliminary results tell us that the microlocal energy is generated by the initial data, rather than by the source term function, as opposed to the situation involving the heat equation.

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Modeling and Numerical Approximation of Multi-Component Anisothermal Flows in Porous Media

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Key words: *Petroleum reservoir, multi-phase anisothermal flow, complex thermodynamics, finite volumes.*

AMS subject classifications: *65M60, 76T30, 80A20.*

With the increase of subsea wellheads and highly deviated wells, production log are less easy to be performed. Thus, new technologies such as permanent gauges and optical fiber sensors are emerging to help engineers monitor reservoirs. It is now critical to develop software allowing an interpretation of the temperature data for triphasic flows.

Here, we present a new model for determining the temperature of flows in porous media. We are interested in the thermal simulation of a multi-component, multi-phase (oil, gas and water) flow in petroleum reservoirs, with no mass transfer between water and hydrocarbon phases.

For this purpose, we have extended an existing isothermal simulator (GPRS : General Purpose Reservoir Simulator) by adding an energy equation and the corresponding thermodynamics. The governing equations are the mass conservation law for each hydrocarbon component coupled with extended Darcy's law for each phase, to which we add an exhaustive energy balance that takes into account viscous dissipation effects. The phase behavior is represented by an equation of state and by phase equilibrium relations. All the thermodynamic coefficients for the hydrocarbon phases are computed from the Peng-Robinson equation, whereas a different equation is used for the water phase.

The problem is time-discretized by means of Euler's implicit scheme and finite volumes are employed for the space approximation. The nonlinear system thus obtained is solved at each time step by Newton-Raphson's method. Numerical examples, including real test-cases and comparisons with the isothermal GPRS code, will be presented.

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A Conservative Galerkin Characteristics Method for Contaminant Transport Problems in Porous Media

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Key words: *nonlinear diffusion, convection-adsorption, method of characteristics*

AMS subject classifications: *65M25, 35K57*

We continue investigate a numerical approximation based on the modified method of characteristics with adjusted advection combined with the relaxation scheme for solving a transport of contaminant :

$$\partial_t(\theta c + \rho s) + \operatorname{div}(qc - D\nabla c) = 0, \quad \rho \partial_s \partial t = kf(c,s) = k(\psi(c) - s) \tag{3}$$

Here c and s are the dissolved concentration and the adsorbed concentration, where $\rho > 0$ is the bulk-density, ψ is the sorption isotherm of porous media with porosity θ. Modified method of characteristics with adjusting advection MMOCAA is already proposed by [1] to conserve the mass globally. The implicit adjusting of the advection is studied in [2,3,4] for nonlinear degenerate parabolic problems (single porosity) combined with a relaxation scheme (W. Jäger, J. Kačur 1993 and J. Kačur, Mahmood 2003). In this work, we study the convergence of approximation scheme in addition the error estimate of the numerical solution. In the numerical experiment we have shown the rate of convergence besides to the numerical experiments for contaminant transport with different sorption isotherms.

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A Posteriori Estimators for a Model for Flow in a Porous Medium with Fractures

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Key words: *fracture model, a posteriori error estimate, mixed finite element method*

AMS subject classifications: *65N15, 65N30, 65N50*

We establish residual a posteriori error estimates for lowest-order Raviart-Thomas mixed finite element discretizations of a model for the flow of a single phase fluid in a porous medium with fractures. The model considered here is a model in which the fractures are identified with interfaces between subdomains (cf V. Martin, J. Jaffre, J. Roberts, SIAM J. Sci. comput., 2005). Interactions between the fractures and the surrounding porous medium are taken into account by imposing nonlocal transmission conditions at the fracture interfaces. We consider here a convex domain Ω in $\mathbb{R}^n$, $n = 2$ or 3, and we suppose that a fracture $\bar{\Omega}_f$ separate Ω into two connected subdomains $\Omega \backslash \bar{\Omega}_f = \Omega_1 \cup \Omega_2$, $\Omega_1 \cap \Omega_2 = \emptyset$. We suppose that the fracture can be identified to a hyperplane γ.

Global upper bounds and local lower bounds for the approximation error in the naturel norms are derived. We present an adaptive method and some numerical tests.

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Numerical Modelling of Porous-Fluid Flows Using the Penalisation Method

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Key words: *Penalisation method ; Porous-fluid interface*

AMS subject classifications: *65Z05, 76D05, 76D17, 76D55*

The aim of this work is to build an efficient model to compute the flow both in fluid and porous media. In the literature several approaches are proposed to study this problem. If the goal is to solve the fluid flow with a porous interface, one can avoid to solve the porous flow imposing correct porous-fluid boundary conditions [2]. This approach is widely used to study turbulent flows over permeable walls for instance. However some authors think that it is necessary to compute the flow in both regions to have a good representation of the porous flow [4]. Then a coupling between Stokes or Navier-Stokes equations and Darcy equations is required with a right treatment of the interface. In our opinion, it is easier to solve this problem by a unique model, namely Brinkman-Navier-Stokes equations or the penalisation method. This consist in adding a term U/K into the Navier-Stokes equations where K is a non dimensional permeability coefficient representing the medium. This method can be seen as a fictitious domain method which is very easy to implement, robust and efficient. It does need neither to have a mesh fitting the porous region nor to impose a boundary condition at the interface between the porous and the fluid media [1].

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A Fast-Reaction Slow Diffusion Limit for Propagating Redox Fronts in Mineral Rocks

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Key words: *Fast reaction – slow diffusion limit, moving-reaction fronts, free-boundary problem*

AMS subject classifications: *35 R 35, 35 K 65*

We consider a fast reaction-slow transport problem modeling the flow and molecular diffusion of an aqueous oxidant that reacts with a mobile reductant to produce mineral deposits. We investigate the fast reaction slow-diffusion limit and indicate that if ϵ goes to zero, then the limit problem becomes a hyperbolic Stefan-like problem wich allows for the presence of concentration jumps at the moving interface where the reaction is localized. We report on preliminary results obtained together with Sébastien Martin (Orsay, Université Paris 11, France).

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Time-Fractional Fick's Law for Dispersion with Memory Effects in Porous Media

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Key words: *diffusion equations, fractional calculus, stable probability distributions, random walks*

AMS subject classifications: *26A33, 45K05, 60E07, 60J60, 60J75, 35Qxx*

Many dispersion data in porous columns do not obey Fick's law. With certain tracers in some media, breakthrough curves increase very rapidly, and show a sharp pike, followed by heavy tailed trailing edge not compatible with Fick's law. The fractional Mobile/ Immobile Medium model

$$\partial_t C + \lambda \partial_t^\gamma C = K\Delta C - v \cdot \nabla C, \tag{4}$$

captures heavy-tailed trailing edges, and rules the density of a Brownian Motion with advection (at speed v), modified by inserting sticking times distributed according to a γ-stable random variable. The fractional Caputo derivative $\partial_t^\gamma C$ of the order of γ (between

0 and 1), is $I^{1-\gamma}\partial_t C$, where $I^{1-\gamma}$ represents the fractional integral of the order of $1-\gamma$, which is convolution by $t^{-\gamma}/\Gamma(1-\gamma)$, computed over $[0,t]$. And K is the diffusivity. The flux of tracer, compatible with (1) is

$$F(x,t) = (Id + \lambda I^{1-\gamma})^{-1}(-K\nabla C + vC). \tag{5}$$

Discretizing (1) yields the tracer concentration in a column, and also the flux. Issues are compared against Monte Carlo simulation of Brownian Motion with sticking, thus illustrating the fact that in a Brownian motion subordinate to a class of strictly increasing Lévy processes, modified by suitable shift, the density of walkers satisfies (1).

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Crystal Dissolution and Precipitation in Porous Media: Formal Homogenization and Numerical Experiments

Tycho van Noorden[1]

Key words: *homogenization, free boundary problem, porous media flow*

AMS subject classifications: *35B27, 35R35, 76S05*

We investigate a two-dimensional micro-scale model for crystal dissolution and precipitation in a porous medium. The model contains a free boundary and allows for changes in the pore volume. Using a level-set formulation of the free boundary, we apply a formal homogenization procedure to obtain upscaled equations. For general micro-scale geometries, the homogenized model that we obtain falls in the class of distributed microstructure models. For circular initial inclusions the distributed microstructure model reduces to system of partial differential equations coupled with an ordinary differential equation. In order to investigate how well the upscaled equations describe the behavior of the micro-scale model, we perform numerical computations for a test problem.

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Upscaling of Transport Processes in Porous Media with Biofilms in Equilibrium and Non-Equilibrium Conditions

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Key words: *biofilm, porous media, reactive transport, volume averaging*

AMS subject classifications: *74Q15, 76S05, 92C45*

Modeling transport in porous media of organic chemical species in presence of a bacterial population growing in the form of biofilms is an important area of research for environmental applications, including groundwater remediation. Biofilms, which are composed of bacteria and extracellular organic substances, grow on the grains of a porous medium. Bacterial metabolism converts the organic solute into biomass and thus may contribute to pollutant degradation. Bio-reactive transport of an organic solute is a complex process involving a wide variety of scales (from the bacteria scale to the aquifer heterogeneity scale) and processes (hydrodynamic, physicochemical and biochemical). The goal of this work is to develop macroscopic models of bio-reactive transport at the Darcy-scale from the method of volume averaging. In the general case, the macroscopic system obtained by averaging pore-scale equations is composed of two coupled equations (one equation by phase). However, under certain assumptions, such a complex formulation may be simplified and leads to the development of a one-equation model. Three distinct approaches can be considered: a local mass equilibrium model and two non-equilibrium models, if the biodegradation rate is limited whether by external mass transfer or by the kinetics of bacterial metabolism. The use of such upscaled models implies the numerical solving of closure problems or micro-scale problems, in order to assess the values of the effective coefficients (macroscopic dispersion tensor, macroscopic reaction rate). Computations of these effective coefficients have been performed in different situations of mass transport in porous medium, and a sensitivity study of these macroscopic parameters to microscopic features has been led. The validity domain of each model has also been identified in terms of hydrodynamic and physicochemical parameters of transport, i.e., the Péclet number and the Damkohler number.

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Stochastic Finite Elements in a Complex System: Non Stationary Fluid Flow, Mass Transport, Heat Conduction, Vibrating

Skender Osmani[1], Margarita Qirko[1]

The paper presents a view on applications of stochastic finite elements (S.F.E.) $\mathbb{R}^3$ in one complex system, considering a differential equation with random parameters,

$$\frac{\partial}{\partial x}\left(k_x\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_z\frac{\partial\phi}{\partial z}\right)-\frac{\partial}{\partial x}(V_x\phi)-\frac{\partial}{\partial y}(V_y\phi)-\frac{\partial}{\partial z}(V_z\phi)-d\frac{\partial\phi}{\partial t}-g\frac{\partial^2\phi}{\partial t^2}=Q$$

where, x, y, z are the 3D spatial coordinates, t- the processes time $\phi = \phi(x, y, z, t)$ is a process function (temperature, pressure etc)

Kij- the conductivity tensor. In general case it is:

$$(K) = \begin{pmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{pmatrix},$$

d- capacity coefficient (function), g- mass coefficient (function), Q- density of the volume flux, V - velocity vector. This equation in specific conditions goes to:

- non stationary fluid flow in porous medium (or/and) ,
- mass transport (or/and)
- heat transfer (or/and)
- vibrating system etc.

The paper contains:

1. An approach of the mean value estimation of the parameter distributions, using S.F.E.. The next is defined as a block v_i, with the random function $Z(x)$, where $x \in v_i$ is a random variable i.e. the value at point x determines the respective probability distribution $p(x)$. After the estimation of the mean value over the domain v_i, is calculated by

$$Z_{v_i} = \frac{1}{v_i}\int_{v_i} Z(x)dx$$

2. Development of the numerical model using S.F.E . applying a mixed algorithm at the , i.e. it is applied. The Galerkin approach not "as a whole" as it is often happened in the literature [3][15], but partly, combining it with other numerical procedure as Runge-Kutta of the fourth order etc. In this treatment, the initial and boundary conditions have been supposed to be treated specifically according by the given problem.

3. Several simple examples as particular case of the mentioned equation.

4. Conclusions, the good things of the S.F.E in stationary flow, mass transport, heat transfer, vibrating , subsidence, waving, deformations, consolidations, earthquakes and other phenomenon's.

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Adaptation of a Mortar Method to Model Flow in Large-Scale Fractured Media

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Key words: *Mixed Hybrid Finite Element Method, Mortar method, Fractured media*

AMS subject classifications: *65N30, 65N55, 65N22*

We simulate flow in fractured media with an impervious rock matrix. Flow is generally observed to be highly channelled and cannot be a priori homogenized as fractures occur on a very broad range of scales extending typically from the meter to the kilometer. We model flow by Poiseuille law within the fractures. Because of the large fractures number and configurations, classical mesh generation and management can be very insufficient. We propose to use non matching grids at the intersections of fractures with continuity of fluxes and heads enforced by a Mortar method. Globally, flow is solved with a Mixed Hybrid Finite Element Method. The challenge comes from the numerous intersections ($\approx 10^3$). The benefits will first be independant mesh generation within the fractures and secondly, the ability of easily refining or coarsening the mesh.

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Fluid/Solid Coupled Convection/Diffusion in Unidirectional Flows

Charles Pierre[1], Franck Plouraboué[2]

Key words: *Convection-diffusion, variational formulation, Hilbert space, mixed formulation*

The general topic of this work is the mathematical and numerical analysis of stationary heat or mass transfer process by coupled convection diffusion between a solid and a fluid phase in a general *tube like* configuration: the fluid motion is unidirectional, thus taking place in a translationaly invariant domain of arbitrary cross section. Such heat or mass problems involving diffusion coupled with unidirectional convection is present in many types of equipments such as heat pipes, heat exchangers (shell, tube or plate), chromatographs and reactors and mass exchangers in micro-channel articial devices, and occurs in real biological tissues. This framework covers both parallel or counter flow configurations.

A common strategy in such a framework is based on a *separate variable solution* approach, separating the transverse and longitudinal directions. Although classical that procedure leads to theoretical and numerical difficulties, even in very simple geometrical configurations, such as a fluid flowing in a circular duct with longitudinal diffusion or with a solid wall, respectively known as the *extended* or *conjugated Graetz* problems.

We propose here a new mixed formulation of the problem in order to overcome these difficulties. In the one hand that formulation provides a theoretical framework for the definition of the separate variable solutions through a self-adjoint eigenvalue problem, whose properties are rigorously established. On the other hand it offers numerical tools in terms of mixed finite element for the computation of the solution.

One proposes to present both these theoretical results implications and the attached numerical simulations.

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Convergence of Generalized Volume Averaging Method on a Convection-Diffusion Problem

Franck Plouraboué[1], Charles Pierre[2]

Key words: *Convection-diffusion, volume averaging, spectral convergence*

This work presents a thorough investigation of the convergence of the volume averaging method as applied to convection-diffusion problems inside a cylinder. From considering generalyzed "closure relations" we introduce the property of λ-analyticity of the stationnary solutions of convection-diffusion axi-symetrical problems.

This property offers a general representation of solutions associated with any boundary conditions. It also permits to contruct an approximated spectral representation of the volume average description of the solution.

This spectral point of view is complementary with the Liapounov-Schmidt reduction technique and provides a precise framework for investigating convergence. It is shown for convection-diffusion inside a cylinder that the spectral convergence of the volume averaged description depends on the chosen averaging operator, as well as on the boundary conditions. A remarkable result states that only part of the eigenmodes among the infinite discrete spectrum of the full solution can be captured by averaging methods.

This leads to a general convergence theorem (which was already examined with the use of the centre manifold theorem and investigated with Liapounov-Schmidt reduction techniques in similar contexts).

Moreover, a necessary and sufficient condition for an eigenvalue to be captured is given. We then investigate specific averaging operators, the convergence of which is found to be exponential.

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Mathematical and Numerical Analysis of Reactive Porous Media Flows

Iuliu Sorin Pop[1]

Key words: *Reactive flow, porous medium*

AMS subject classifications: *65M12, 65M15, 65M60, 35K65, 35K55, 76S05*

In this presentation we focus on reactive porous media flow models. Such processes are typically modeled as coupled systems of nonlinear evolution equations, which are possibly degenerate. We emphasize here on dissolution and precipitation processes, involving a multi-valued dissolution rate.

After addressing some modeling details, we present results concerning the existence and uniqueness of a weak solution. Furthermore we consider a convergent numerical scheme for approximating the numerical solution.

This talk is based on the work done jointly with Florin Radu (Jena), C.J. van Duijn and Tycho van Noorden (both in Eindhoven).

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A Level Set Method for Non-Zero Contact Angle Drainage and Imbibition in Realistic Porous Media

Maša Prodanović[1], Steven L. Bryant[2]

Key words: *fluid displacement, porous media, level set method, contact angle*

AMS subject classifications: *76S05, 76Txx, 76M20, 65C20*

Slow displacement of immiscible fluids in a porous medium can be modeled as a quasi-static, capillarity-controlled process. At constant pressure and interfacial tension, pore scale fluid-fluid interfaces are modeled as constant mean curvature surfaces. Such surfaces are not guaranteed to exist at a location nor easy to calculate. Further, tracking the topological changes of the interface, such as splitting or merging, is nontrivial. The irregular pore spaces in natural porous media admit a multiplicity of such changes.

Assuming quasi-static displacement, we developed a simple but robust model based on the level set method for determining fluid interface position during both drainage (displacement of the wetting fluid by non-wetting) and imbibition (displacement of non-wetting fluid by wetting). The method arrives at geometrically correct interfaces, handles any wettability situation (contact angle between the fluid-fluid anf fluid-solid interface) and agrees with available theories and experiments. The level set based description allows for robust handling of topology changes and independence from the pore space complexity. Our simulations establish the exact position and shape of the interface in porous geometries, from which fluid volumes, contact areas and interface curvatures can be readily obtained.

We show 2D and 3D simulations in both simulated and imaged porous samples of real rocks. Finally, we explore application of the above method to flow in the fracture and through the adjoining rock pore space (that typically happens on two different length scales). These simulations can provide valuable insight in modeling transfer functions

in dual porosity continuum models and in identifying appropriate relative permeability models for fractures.

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Upscaling of the Reaction-Advection-Diffusion Equation in Porous Media with Monod-Like Kinetics

Falk Hesse[1], Florin A. Radu[1,2], Sabine Attinger[1], Martin Thullner[1]

Key words: *Upscalling, advection-diffusion-reaction equation, Monod kinetics, porous media*

AMS subject classifications: *65M60, 35K57, 35K55*

The contamination of groundwater is a severe problem in many industrial and developing countries as it imposes a severe threat to water resources. Therefore the biodegradation of these groundwater contaminants has been extensively investigated. The extrapolation of laboratory results on microbial degradation processes to in situ biodegradation processes in the field is challenged by finding an adequate description of the bioavailabilty of chemical species.

By explicitly resolving pore geometries, advective-diffusive transport and microbial degradation are simulated by making use of the software toolbox UG allowing for a quantitative analysis of bioavailabilty limitations on microbial contaminant degradation. These numerical simulation results are accompanied by analytical upscaling leading to the formulation of effective equations with effective degradation and effective dispersion coefficients for biodegradation processes at the pore scale. We will demonstrate that, in addition to the classical result of a reaction-and a diffusion-limited regime in case of first order degradation processes, a new transition regime appears for Monod kinetics. The new regime indicates a concentration limitation (this phenomenon is known from lab experiments). The three regimes and their implications for practical applications are discussed.

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Joint Structural and Petrophysical History Matching of Stochastic Reservoir Models

Thomas Schaaf[1], Bertrand Coureaud[1]

History matching is an integral part of reservoir production forecasting and uncertainties quantification workflows. One has to cope with the non-uniqueness issue as history matching is an ill-posed inverse problem, due to a lack in constraints and data. History matched solutions are obtained by minimizing an objective function that describes discrepancy between measured and simulated production data. Dealing with several history matched models is therefore critical and assisted history matching tools are of great interest to speed up the history matching process and thus to get multiple history matched models in the same timeframe. In practise, structural (e.g. faults location, horizon depths) as well as petrophysical, PVT, SCAL, etc. data are uncertain and the history matching process rarely tackles all these parameters in a single step. Classically, some of these parameters are considered as known while others are updated. This constitutes the 'by default' approach as all these parameters are interdependent and it may lead to sub-optimal history matched models. This manuscript presents an original history matching workflow that picks uncertain structural and petrophysical parameters anywhere in the "geomodeling to simulation" workflow, using a popular geomodeling software. Using efficient parameterization techniques of the geological model, both geological and simulation models are updated at the same time, preserving the consistency between each other. The assisted history matching software used in this work is versatile. An external software, such as a geomodeler, may be automatically launched in batch mode throughout the constructed workflow. Background scripts control each building step of the geological and simulation models, possibly capitalizing on an existing geomodel. This joint structural and petrophysical history matching leads to a more robust integrated geological stochastic reservoir model, as all uncertainties are simultaneously tackled and reduced. The results obtained on a 3D synthetic waterflooding scenario demonstrate that this history matching approach is very efficient since the throw and transmissivity of one fault as well as facies distribution, petrophysical and SCAL properties are updated to explain the production history. It makes this approach attractive both to update simultaneously various data types and reduce the bias in history matching process.

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Domain Decomposition for Multiscale Elliptic PDEs

Ivan Graham[1], Robert Scheichl[1], Jan Van lent[1]

More powerful (parallel) computers and better imaging and tomography tools have made it possible in recent years to carry out detailed simulations of biological, physical and engineering processes in complex geometries with highly varying heterogeneous material parameters. Consequently, the development of efficient and robust parallel solvers for such problems is of paramount importance. Here we are concerned with the convergence of two-level domain decomposition preconditioners in the context of multiscale heterogeneous second-order elliptic problems, in both the deterministic and (Monte-Carlo simulated) stochastic cases. In contrast to standard analyses, we do not assume that the coefficients can be resolved by the subdomain partition or the coarse mesh. We perform a new analysis of the preconditioned matrix, which shows rather explicitly, how its condition number depends on the variable coefficient in the PDE, as well as on the coarse grid/overlap size. The classical estimates guarantee good conditioning only when the coefficients vary mildly inside the subdomains. By contrast, our new results show that, with some modifications, domain decomposition preconditioners can still be robust even for large coefficient variation inside subdomains, where the classical methods fail to be robust. In particular our estimates prove very precisely the previously made empirical observation in the AMG literature that the use of energy minimising coarse spaces can lead to robust preconditioners. Numerical experiments on a variety of two-scale model problems confirm our theoretical results. The performance of the new preconditioners is greatly improved over standard preconditioners in the random coefficient cases. The proposed/investigated coarsening strategies (especially the explicit energy minimising coarse spaces) are also interesting in their own right, as numerical homogenisation or upscaling techniques.

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Two Phase Partially Miscible Flow and Transport Modeling in Porous Media; Application to Gas Migration in a Nuclear Waste Repository

Farid Smaï[1]

Key words: *Two-phase flow ; porous medium ; modeling ; underground nuclear waste management*

AMS subject classifications: *76S05 ; 76T10 ; 35K55*

The simultaneous flow of immiscible fluids in porous media occurs in a wide variety of applications. The most concentrated research in the field of multiphase flows over the past four decades has focused on unsaturated groundwater flows, and flows in underground petroleum reservoirs. Most recently, multiphase flows have generated serious interest among engineers concerned with deep geological repository for radioactive waste. There is growing awareness that the effect of hydrogen gas generation, due to anaerobic corrosion of the steel engineered barriers of radioactive waste packages, can affect all the functions allocated to the canisters, waste forms, buffers, backfill, host rock.

In this situation, the migration of gas through the near field environment and the host rock, involves two components, water and pure hydrogen ; and two phases "liquid" and "gas". An outstanding physical and mathematical problem in simulation of such multiphase flow is the appearance disappearance of one of the phases, leading to the degeneracy of the equations satisfied by the saturation. In order to overcome this difficulty, we discuss a formulation based on new variables (total hydrogen mass density and liquid pressure) which doesn't degenerate. We give an existence result for this formulation and we present some numerical simulations.

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Machine Learning in Reservoir Production Simulation and Forecast

Serge A. Terekhov[1]

Upscaling of numerical simulations of petroleum reservoirs is important problem not only from point of view of computer resources, but also due to natural limitations of knowledge about precise structure of porous fields. Both geometry and rock properties are not surely

known, so the model complexity should be consistent with available amount of experimental information.

This report is devoted to coarse level limit of upscaled simulations. Namely, it considers the resolution at the scale of producer and injector wells treated as the point super-elements. Simulation field is modelled via network of interconnected cross-talking wells.

Fluid consumption and production time series are represented by interlinked trained neural networks. Computations carried out for surrogate numerically simulated fields display promising results for two practical tasks: estimation of mutual wells influence, and the prediction of future production under some given injection rates. Second problem is important for optimal production control applications.

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