Mathematisches Forschungsinstitut Oberwolfach

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Reactive Flow and Transport Through Complex Systems

Organised by
Cornelius J. van Duijn (Eindhoven)
Andro Mikelić (Lyon)
Christoph Schwab (Zürich)

Oktober 30th – November 5th, 2005

Abstract. The meeting focused on mathematical aspects of reactive flow, diffusion and transport through complex systems. The research interest of the participants varied from physical modeling using PDEs, mathematical modeling using upscaling and homogenization, numerical analysis of PDEs describing reactive transport, PDEs from fluid mechanics, computational methods for random media and computational multiscale methods.

Mathematics Subject Classification (2000): 35B27, 80A32, 76V05, 35R60, 65C30, 65M60.

Introduction by the Organisers

The workshop *Reactive Flow and Transport Through Complex Systems*, organized by Cornelius J. van Duijn (Eindhoven), Andro Mikelić (Lyon) and Christoph Schwab (Zürich) was held October 30th–November 5th, 2005.

This meeting was attended by over 46 participants with broad geographic representation from all continents.

The theme of the conference,

modeling, analysis and numerical simulation of diffusion and transport processes in complex systems,

is a response to the need for more accurate, quantitative prediction in a growing number of scientific disciplines, particularly those related to biological applications. Here, simple mathematical models have been found, in particular due to the vastly increased available experimental data from these systems, to offer only inadequate and incomplete understanding of the observed phenomena.

This resulted in increased requirements for quantitative, verified predictions from sophisticated mathematical as well as computational models. The continuous development of complex mathematical and computational models and their

verification and validation against available experimental data is a continuous source of challenges for applied and computational mathematicians.

The complexity of the systems arises from several sources: highly irregular geometries of membranes and interfaces (as, e.g. in bone marrow, cell membranes, root systems of plants, membrane structures in human organs), physical or chemical properties of the systems (e.g., models for spread of pollution in underground medium which has uncertain material properties, where chemical reactions take place between constituents, and where strong transport effects on a macroscopic scale coexist with diffusion phenomena at the grain interfaces).

Quantitative mathematical and computational models of such phenomena are not only essential for a deeper understanding of these systems but, at least equally importantly, are a keystone in the development of new technologies which increasingly mimic and adapt biological phenomena for industrial purposes (e.g., root-reactor technology for the efficient production of organic compounds, bioinspired catalysts for waste processing, to name but a few).

Accordingly, the rather wide scope of the topic of the conference and the blend of researchers working in several areas of applied mathematics was a necessary condition to review modelling approaches across a number of application areas as well as across several mathematical disciplines.

Accordingly, during the meeting, talks were presented on homogenization, analysis and computation of multiscale problems, models of porous media, biological flow problems, to name but a few.

In addition to the regular presentations, there were three evening sessions organized "on the spot" based on the discussions which started in the first half of the meeting. These were in each case opened by a presentation from a person invited by the organizers, and were devoted to the topics:

(1) Mathematical Models in Biology – Results and challenges in the mathematical modelling of biological systems, (animated by W. Jäger, Uni and IWR Heidelberg),
(2) Density driven flows – analytical and computational results and challenges (animated by C. van Duijn, Einhoven and F. Otto, Bonn),
(3) Numerical Models of PDEs with stochastic coefficients (animated by H. Matthies, TU Braunschweig and by C. Schwab, ETH)

The presentations of the experts present at the meeting comprised, naturally, a much wider scope of topics:

- – Flow, transport and reactions in micro-reactors and micro-channels
- – Effective laws for processes on surfaces
- – Effective laws for transports and reactions in membranes
- – Polymer flow through porous media
- – Homogenization of processes in networks (neural networks, vessels .....)
- – Overall elastic properties of fiber structures and textiles
- – Flow through deformable structures with evolving process depending geometry
- – Growth of crystals, biological structures like dendrites or vessels.

- – Flow and transport in bifurcating vessels with rigid and flexible walls
- – Effects of walls
- – Wall laws and interface laws

These talks touched on advanced mathematical methods from dynamical systems, especially infinite dimensional ones arising with spatially heterogeneous problems (PDEs), asymptotic analysis, homogenization and averaging methods, numerical multiscale methods, methods from stochastic analysis and statistics.

Apart from advancing *disciplinary* mathematical methods in these areas, in the present meeting also qualitatively new mathematical developments emerged: for example, mathematical and computational modelling of PDEs with stochastic data which are spatially inhomogeneous and do *not* satisfy stationarity or ergodic hypotheses.

In processing experimental data (which becomes increasingly available at lower cost and, e.g. through modern scanning techniques, also at high volume and spatial and temporal resolution) new techniques of image and data processing have to be developed, and the mathematical models of complex systems have to allow for incorporation of statistical data extracted from these experiments.

This has repercussions for the mathematical research *and* implies that novel algorithms are needed to generate computational grids adapted to voxel data.

In the last five years mathematicians from analysis, stochastics and numerics started cooperation in this interdisciplinary field of research.

New journals specifically devoted to these issues such as the SIAM Journal of Multiscale Analysis and Simulation, have been successfully launched.

The previous meeting in Oberwolfach " Multiple Scale Systems - Modeling, Analysis and Numerics " from July 27 to August 2, 2003, gathered 42 scientists, among them approximately 15 junior scientists, from these areas.

Since multiscale tools are crucial in many of the above themes, in the previous meeting mainly diffusion problems were treated. Reactive flow and transport, which were central themes in the present meeting, emerged only recently as key issues.

The meeting was, exactly because of its wide scope, successful particularly in cross fertilizing different areas of applied mathematics and also raised a huge number of questions and challenges to participants documenting that the applications of mathematics to biological, social and other "complex systems" which has been emerging in the past years, is in the process of gaining momentum and, more importantly, stimulates development of new techniques and approaches in applied and computational mathematics at an increasing rate.

List of all talks

- Monday, October 31, 2005:
  - 9h15–10h: Andrea BRAIDES: A Model for a Weak Membrane with Defects
  - 10h-10h45: Gregory A. CHECHKIN: Prandtl boundary layer equations in the presence of rough boundaries
  - 11h30–12h30: Eduard MARUŠIĆ-PALOKA: Rigorous Justification of Compressible Reynolds Equation for Gas Lubrication
  - 16h-16h45: Maria NEUSS-RADU : Homogenization of thin porous layers and applications to ion transport through channels of biological membranes
  - 16h45–17h30: Angela STEVENS: Propagation speed in inhomogeneous media
  - 17h45–18h30: Barbara NIETHAMMER: A statistical mechanics approach for effective theories of domain coarsening
- Tuesday, November 1, 2005
  - 9h00–9h45: Hermann G. MATTHIES: Computational Approaches for Stochastic Models in Flow Through Stochastic Porous Media
  - 9h45-10h30: Assyr ABDULLE: Fully Discrete Heterogeneous Multiscale Methods and Application to Transport Problems in Microarrays
  - 11h–11h45 Radu A. TODOR: Sparse Perturbation Algorithms for Elliptic Problems with Stochastic Data
  - 15h30–16h15: Guy BOUCHITTÉ: Some asymptotic problems on optimal transportation.
  - 16h15-17h: Michel LENZINGER: Viscous fluid flow in bifurcating channels and pipes
  - 17h15–18h René de BORST: Stability and Dispersion in Damaging Multiphase Media
- Wednesday, November 2, 2005
  - 9h00–9h45: Michel KERN: Reactive Flow and Transport Through Complex Systems
  - 9h45-10h30: Vincent GIOVANGIGLI: Gaseous flows with multicomponent transport and complex chemistry
  - 11h–11h45 Sorin I. POP: Dissolution and Precipitation in Porous Media
  - 11h45 – 12h30: Giovanna GUIDOBONI: Uniqueness of weak solutions for a fluid-structure interaction problem

- Thursday, November 3, 2005
  - 9h00–9h45: Björn ENQUIST: The Heterogeneous Multiscale Method for Flow in Complex Systems
  - 9h45-10h30: Peter KNABNER: Efficient Accurate Simulation of General Reaction Multispecies Transport Processes in Porous Media by Reduction and Selective Decoupling
  - 10h45–11h30 Raúl TEMPONE: Spectral Collocation for Partial Differential Equations with Random Coefficients
  - 11h30-12h15: Leonid BERLYAND: Two analytical models of random composites: polydispersity and correlations
  - 15h15–16h: Jérome JAFFRÉ: Riemann solvers for flows through rocks changing type
  - 16h00–16h45: Ben SCHWEIZER: Averaging of unsaturated flow in stochastic porous media
  - 16h45-17h30: Rudolf HILFER: Can homogenization solve the upscaling problem for 2 phase flow equations in porous media?
  - 17h45–18h30 Alain BOURGEAT: Some Problems in upscaling source terms in a waste disposal
- Friday, November 4, 2005:
  - 9h00–9h45: Jérome POUSIN : Order 2 in time schemes for discontinuous reactive terms operator splitting for reaction diffusion with a singular reaction term.
  - 9h45-10h30: Peter BASTIAN: ADG method for flow in complex domains
  - 10h45–11h30 Eric BONNETIER: Can one detect a misplaced inclusion in a periodic composite by boundary measurements ?

Reactive Flow and Transport Through Complex Systems

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Abstracts

Fully Discrete Heterogeneous Multiscale Methods and Application to Transport Problems in Microarrays

Assyr Abdulle

Physical systems encompassing a variety of strongly coupled scales pose major computational challenges in terms of analysis modeling and simulation. In this report we first discuss a multiscale modeling approach for the transport of particles such as DNA in heterogeneous devices (microarrays). The model involves a multiscale elliptic equation coupled with a multiscale advection-diffusion equation. We introduce a numerical method for the solution of the coupled system of equations. We first discuss a new multiscale finite element method for the solution of the elliptic problem. We then explain how it is possible to use an explicit stabilized method (ROCK) for the numerical solution of the stiff system of ordinary differential equations of large dimension, originating from the method of lines discretization of the advection-diffusion equation.

DNA separation in microarrays. We consider a (square) device with periodic asymmetric obstacles and model the transport of injected mixture with concentration $c(t,x)$ as an advection-diffusion equation given by

$$\frac{\partial c^\varepsilon}{\partial t} + \nabla \cdot (v^\varepsilon c^\varepsilon) = D\Delta c^\varepsilon, \tag{1}$$

where $v^\varepsilon = -\rho k^\varepsilon \nabla u^\varepsilon$ is the velocity field, u^ε is the electrical potential, k^ε is the electrical conductivity and ρ is the charge density of the electrical device. We assume for simplicity that ρ is constant and set it to one. The obstacles of the microdevice introduce a typical self-similar structure (which will also be called a "periodic cell"), and we denote by ε the length of these cells. The equation for the potential u^ε is given by

$$-\nabla \cdot (k^\varepsilon \nabla u^\varepsilon) = 0, \tag{2}$$

with Neumann boundary conditions at the corner of the device and Dirichlet conditions at the charged sites of the boundary. The homogenization problem corresponding to equations (1) and (2), where the heterogeneous fine scale structure is transferred into a homogeneous large scale model, shows that the heterogeneities of the device have no impact on the large scale drift [6]. Thus, the large scale drift does not depend on the diffusion constant or the molecular weight of the particles. The heterogeneous microarrays have an impact only on the large scale diffusion. This gives a quantitative explanation of the model proposed in [11],[12] and explain the experimental results of [10]. In [9] transport problems with compressible flows are studied and it is shown that for such flows, the large scale drift can depend on the small scale diffusion coefficient. In the sequel we explain how to solve numerically the coupled equations (1) and (2).

Fully discrete finite element heterogeneous multiscale methods. Applying a standard finite element method to the variational form of (2) requires usually

a meshsize $h < \varepsilon$ for convergence, i.e., to resolve the small scale of the problem. This lead to a complexity of $\mathcal{O}(\varepsilon^{-d})$, where d is the spatial dimension, which makes the direct numerical simulation impossible if ε is small. When the data of the problem are oscillatory with small period, classical two-scale approaches are well established, and the analytical treatment lead to homogenized equations. However, the fine scale behavior, i.e. the oscillations of the solution, are lost in the homogenization process. It can be recovered through the solution of additional "corrector" problems. But these corrector problems again exhibit rapidly oscillating coefficients so that their accurate numerical solution is as expensive as solving the original problem.

In the sequel, we present a new multiscale finite element method for the numerical computation of problems with multiple scales. Define a quasi-uniform macro triangulation $\mathcal{T}_H$ of the domain Ω, assumed to be a convex polygon. The finite element heterogeneous multiscale method (FE-HMM) is based on the following ideas [13],[3],[14],[4].

(1) Associated to the macro triangulation, we define a macro finite element space and a modified bilinear form with unknown input data.
(2) Within each macro triangle we define a sampling domain K_ε of length scale comparable to ε, a micro finite element space and a micro bilinear form based, upon the original multiscale tensor k^ε, which provides input data for the macro problem.

The FE-HMM gives a procedure to obtain an approximation u^H of the homogenized solution u^0, without computing explicitly the homogenized equations. By a post-processing calculation, it is possible to compute an approximation $u^{\varepsilon,h}$ of the fine scale solution u^ε of (2) at a much lower cost than solving the original fine scale problem. Indeed, we solve the fine scales only in sampling domains of size ε^d in the periodic case, within a macro mesh of Ω. Furthermore, the micro problems are independent and can be solved in parallel. In the non-periodic case, K_ε should be chosen as to sample enough information of the local variation of k^ε. Semi-discrete analysis of the method has been given in [3],[14]. In these works, the fine-scale problem involving the micro solver was assumed to be computed exactly. In [4], the first fully discrete analysis of the FE-HMM has been given. This analysis show that the macro and the micro meshes have to be refined *simultaneously*. This has been generalized for elasticity problems in [8].

Solving an advection diffusion problem with ROCK methods. Discretizing the advection-diffusion equation by the method of lines leads to a stiff system of ordinary differential equation of large dimension. Such ODEs, originating from the space discretization of (1) are called *stiff* in the literature [15]. It is also known that implicit solver have better stability properties, but at the expense of solving linear systems of large dimension if the spatial discretization mesh is small.

Chebyshev methods are a class of explicit one step methods with extended stability domains along the negative real axis. With such methods, large time steps can be used. This contrasts with the severe time step restriction given by the CFL condition for standard explicit methods.

Recently, a new strategy to construct higher order Chebyshev methods with "quasi" optimal stability polynomials has been proposed [1],[2]. These methods, called ROCK, together with the FE-HMM have been combined to solve transport problems described by equations (1) and (2) [5]. The numerical simulation of the DNA transport problem has been addressed in [7].

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Solving Partial Differential Equations in Complicated Domains

Peter Bastian

(joint work with Christian Engwer)

1. Introduction

Many practical applications require the solution of partial differential equations (PDEs) in complicated domains. We are especially interested in computing the flow around root networks of plants or in the pore space of porous media.

Classical numerical methods require a grid resolving the complicated geometry. Creating such grids is a highly involved process especially if coarse grids and high quality are required. Several methods have been developed that circumvent this problem. They are based on the use of a structured background mesh that encloses the domain. The Fictitious Domain method [GPP71] discretizes the PDE on the background mesh and adds the boundary conditions as additional constraints. This leads in general to a saddle point formulation that might be difficult to solve. The Composite Finite Element method [HS97] constructs piecewise linear basis functions on the fine background mesh and truncates them at the true boundary. Coarse grid basis functions for a geometric multigrid solver are constructed as combinations of fine grid basis functions. This method has been designed with emphasis on the fast solution of the arising linear system.

Our new method is based on the observation that in discontinuous Galerkin finite element methods the form of the element can be quite arbitrary. Thus the elements can be taken as the intersection of the structured background mesh with the complicated geometry. Assembling the stiffness matrix then requires integration over the interior and boundary of those non-standard elements. This is accomplished by constructing a local triangulation within each element. Note that the local triangulations of different elements are completely independent.

In the following sections we will describe the discontinuous Galerkin finite element method for an elliptic model problem, the construction of the local triangulation and give some numerical results.

2. Discontinuous Galerkin Scheme

Consider the following elliptic model problem in d space dimensions

$$\nabla \cdot j = f \quad \text{in } \Omega \subseteq \mathbb{R}^d \qquad j = -K\nabla p, \tag{1}$$

subject to boundary conditions

$$p = g \quad \text{on } \Gamma_D \subseteq \partial\Omega, \qquad j \cdot n = J \quad \text{on } \Gamma_N = \partial\Omega \setminus \Gamma_D. \tag{2}$$

We approximate the pressure p in the space of discontinuous finite element functions of order k

$$V_k = \{ v \in L_2(\Omega) \mid v|_E \in P_k, E \in \mathcal{T}(\Omega) \} \tag{3}$$

where $\mathcal{T}(\Omega) = \{E_1, \ldots, E_n\}$ is a partition of Ω into non-overlapping elements and P_k is the set of polynomials of at most degree k. By Γ_{int} we denote the set of interior faces of the elements with an arbitrarily chosen normal direction n and Γ_{ext} is the set of element faces intersecting with the domain boundary.

The finite element problem then reads: Find $p \in V_k$ such that

$$a(p, v) = l(v) \qquad \forall v \in V_k \tag{4}$$

where the bilinear form is given by

$$a(p,v) = \sum_{E\in\mathcal{T}(\Omega)} \int_E (K\nabla p)\cdot\nabla v \; dV + \sum_{\gamma_e\in\Gamma_{\mathrm{D}}} \int_{\gamma_e} (K\nabla v)\cdot n \; p - (K\nabla p)\cdot n \; v \; ds$$
$$+ \sum_{\gamma_{ef}\in\Gamma_{\mathrm{int}}} \int_{\gamma_{ef}} \langle (K\nabla v)\cdot n\rangle [p] - \langle (K\nabla p)\cdot n\rangle [v] \; ds$$

and the right hand side is the linear form

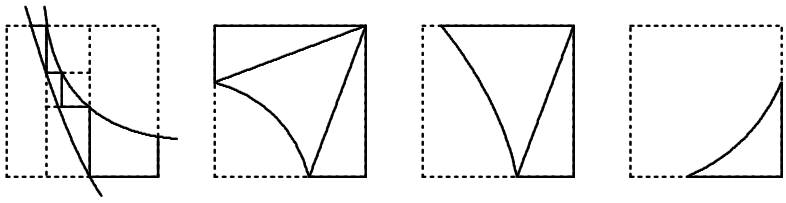
$$l(v) = \sum_{E\in\mathcal{T}(\Omega)} \int_E f \; v \; dV + \sum_{\gamma_e\in\Gamma_{\mathrm{N}}} \int_{\gamma_e} J \; v \; ds + \sum_{\gamma_e\in\Gamma_{\mathrm{D}}} \int_{\gamma_e} \epsilon\,(K\nabla v)\cdot n \; g \; ds.$$

Here $\langle\cdot\rangle$ denotes the average at the discontinuity and $[\cdot]$ denotes the jump at the discontinuity. This scheme has been introduced in [OBB98].

3. Local Triangulation Algorithm

The triangulation $\mathcal{T}(\Omega)$ used in the finite element algorithm is generated by intersecting a structured background mesh with the domain Ω as is indicated in the following figure:

The bilinear form and right hand side now require the computation of certain integrals over the interior and boundary of the non-standard elements. This is accomplished by constructing a triangulation of each element. This is illustrated in the following figure:

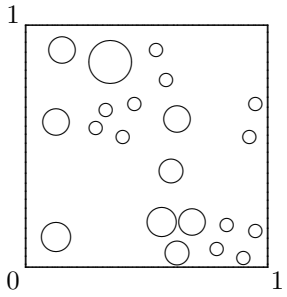


Since the we assume that the geometry of the non-standard element is not too complicated and the background mesh is structured we first do an adaptive bisection and then have a lookup table that generates triangulations for certain standard situations. Note that curved boundaries are approximated by using parametric elements of order 2. This can lead to non-standard elements having a cusp. It turns out that the approximation properties of the DG scheme are not harmed also for this case. A proof of this is not available yet. In [DFS03] a convergence proof

for DG is given for star-shaped elements. For further details of the triangulation algorithm we refer to [EB05].

4. Numerical Results

As an example we solve $-\Delta u = f$ in Ω with $u = g$ on $\partial\Omega$ where $\Omega \subset (0,1)^2$ is shown in the figure below. The functions f, g are chosen according to a prescribed solution $u \in C^\infty(\Omega)$. The algorithm has been realized within the software framework Dune [BDE+04]. The table below shows that experimental order of convergence is optimal when using polynomials of degree $k = 3$. Note that the error in the boundary approximation is not included.



Mesh	EOC L_2	EOC H^1
16×16	3.73	2.90
32×32	3.94	2.95
64×64	3.93	2.96
128×128	3.98	2.98

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Two analytical models of random composites: polydispersity and correlations

Leonid Berlyand

In this talk we discuss mathematical models of heterogeneous materials with random microstructure amenable to rigorous mathematical analysis when analytical solution in some form can be obtained.

We distinguish two classes of such models:

(A) simple (e.g., linear) PDE (constitutive law) with complex geometry (e.g. disordered arrays of densely packed particles of various sizes and shapes)

(B) complex (e.g. nonlinear) PDE or variational problem with simple geometry

We first present a problem from class (A) which models increase and decrease of the effective conductivity of two phase random composites due to polydispersity. Here we present a two–dimensional mathematical model of a composite material with conducting inclusions (fibers) randomly embedded in a matrix. Our main objective is to study how polydispersity (two different sizes of particles) affects the overall conductivity of the composite. If the conductivity of inclusions is higher than the conductivity of the matrix, then previous studies suggest an increase of the effective conductivity due to polydispersity. We prove that for high volume fraction when inclusions are not well–separated and percolation effects play a significant role, polydispersity may result in either an increase or decrease of the effective conductivity. This is a joint work with V. Mityushev [1].

Next we present a model of a laminated random polycrystal with n grains. The orientation of each grain is given by an uncorrelated random sequence of the orientation angles θ_i, $i = 1, \cdots, n$. Under the imposed boundary conditions each grain undergoes a stress free transformation that depends on its orientation angle and result in transformation strains $\epsilon_i^T,\ i = 1, \cdot, n$. The sequence of random variables $\epsilon_i^T,\ i = 1, \cdot, n$ is obtain as the solution of a nonlinear optimization (variational) problem.

While the random variables θ_i, $i = 1, \cdots, n$ are uncorrelated, the random variables $\epsilon_i^T,\ i = 1, \cdot, n$ may or may not be correlated – this is the central issue of our analysis. We investigate this rise of correlations in three different scaling limits. Our proofs use the de Finetti's Theorem as well as the Riesz rearrangement inequality. This is a joint work with O. Bruno and A. Novikov [2].

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Asymptotics of the potential in a perturbed periodic composite medium containing misplaced inclusions

Eric Bonnetier
(joint work with Fehmi Ben Hassen)

We consider a conduction problem for a composite material made of identical inclusions of conductivity $0 < k < \infty, k \neq 1$, embedded in a matrix of conductivity 1. In a reference configuration, the medium lies in a smooth bounded domain $\Omega \subset \mathbf{R}^3$ and the distribution of the inclusions is perfectly periodic. If $Y = [0,1]^3$ and $D \subset Y$, the associated conductivity has the form $a_\varepsilon(x) = a(x/\varepsilon),\ x \in \Omega$, where a is the Y–periodic function equal to k in D and to 1 in $Y \setminus \overline{D}$.

Given Neumann boundary data $g \in L^2(\partial\Omega)$, such that $\int_{\partial\Omega} g = 0$, the potential u_ε solves

$$(1) \qquad \left\{ \begin{array}{lcll} \mathrm{div}(a_\varepsilon(x)\nabla u_\varepsilon) & = & 0 & \text{in } \Omega, \\ a_\varepsilon(x)\partial_n u_\varepsilon & = & g & \text{on } \partial\Omega \\ \int_{\partial\Omega} u_\varepsilon & = & 0. & \end{array} \right.$$

We compare this reference configuration to a medium where one of the inclusions has been misplaced: Instead of $\omega_{\varepsilon,1} = \varepsilon(p + D)$, the p–th inclusion occupies the set $\omega_{\varepsilon,2} = \varepsilon(p + \delta + D)$. We assume that $|\delta| = O(1)$, that the p–th inclusion is $O(1)$ away from the boundary $\partial\Omega$, and that, in its modified position, it does not intersect another inclusion. The conductivity of the perturbed configuration is denoted by $a_{\varepsilon,d}$ and we have

$$a_{\varepsilon,d}(y) \quad = \quad \left\{ \begin{array}{ll} a_\varepsilon(y) & \text{in } \Omega \setminus \omega_\varepsilon, \\ 1 & \text{in } \omega_{\varepsilon,1} \setminus \omega_{\varepsilon,2}, \\ k & \text{in } \omega_{\varepsilon,2}, \end{array} \right.$$

where $\omega_\varepsilon = \omega_{\varepsilon,1} \cup \omega_{\varepsilon,2}$. The corresponding potential, $u_{\varepsilon,d}$ solves (1), with coefficient $a_{\varepsilon,d}$ instead of a_ε.

We view the misplaced inclusion as a defect in the composite, compared to a perfectly periodic medium. We are interested in comparing the potentials $u_{\varepsilon,d}$ and u_ε, far from ω_ε, to study if one could detect such periodicity defect using boundary measurements. To this end, we give an asymptotic expansion for $u_{\varepsilon,d} - u_\varepsilon$, as $\varepsilon \to 0$. We present the result in the case of a single misplaced inclusion. However, our analysis extends to more general situations where the periodicity defects are localized and of size comparable to the period (for instance inclusions with conductivities different from k).

Let A^* denote the matrix of homogenized coefficients, defined by

$$A \quad = \quad \int_Y a(y)\,(I + \nabla\chi(y))\,dy,$$

in terms of the solutions $\chi \in (W^{1,2}_{\#}(Y))^3$ of the cell problems

$$\begin{cases} -\mathrm{div}(a(y)\nabla(\chi(y)+y)) = 0 \quad \text{in } \mathbf{R}^3 \\ \int_Y \chi(y)\, dy = 0. \end{cases}$$

Let u^* denote the solution to the homogenized equation

$$\begin{cases} \mathrm{div}(A^*\nabla u^*) &= 0 \quad \text{in } \Omega, \\ A^*\nabla u^* \cdot n &= g \quad \text{on } \partial\Omega \\ \int_{\partial\Omega} u^* &= 0, \end{cases}$$

and let G_ε (resp. G^*) be the Green's functions, vanishing on $\partial\Omega$, of the periodic (resp. homogenized) medium.

Theorem 1. *Assume that D has a smooth boundary ($C^{1+\alpha}$ for some $\alpha > 0$) and that ω_ε is centered at the origin. Then, for $|x| >> \varepsilon$, we have*

$$\begin{aligned} & u_{\varepsilon,d}(x) - u_\varepsilon(x) + \int_{\partial\Omega} \partial_n G_\varepsilon(x,y)\, (u_{\varepsilon,d}(y) - u_\varepsilon(y))\, d\sigma(y) \\ &= \varepsilon^3\, M : \nabla u^*(0) \otimes \nabla G^*(0,x) \;+\; o(\varepsilon^3). \end{aligned} \tag{2}$$

The matrix M in (2) is a polarization tensor, that accounts at first order for the presence of a defect: for $1 \le i,j \le 3$,

$$M_{ij} \;=\; \int_{\partial\tilde{\omega}} (\frac{a^-}{a_d^-} - 1)(y_i + \chi^i(y)) \left(a^+(y) \frac{\partial \varphi_j^+}{\partial \nu_y} + a^-(y) \left(\nu_j + \frac{\partial \chi^j(y)}{\partial \nu_y} \right) \right) d\sigma_y,$$

where $a_d(y) = a_{\varepsilon,d}(\varepsilon y)$, and where the auxiliary functions φ_j are defined by

$$\begin{cases} \mathrm{div}(a_d(y)\nabla(\varphi_j(y) + y_j + \chi_j(y))) &= 0 \quad \text{in } \mathbf{R}^3, \\ \lim_{|y|\to\infty} \varphi_j(y) &= 0. \end{cases}$$

The expansion (2) has the same structure as that derived in [5] where perturbations of the potential are caused by small inclusions in a smooth background reference medium (see also [1] and the references therein). In our case, it is the Green's function of the homogenized medium that appears on the right–hand side, its singularity signaling the presence of a periodicity defect. This may prove interesting for detection purposes, using a MUSIC type algorithm, as in the case of a reference medium with constant coefficients [4].

The proof of (2) relies on pointwise estimates on the periodic potential and on its gradient, which are independent of ε [3]. The proof uses the '3 steps compactness method' of M. Avellaneda and Fang Hua Lin, who gave such estimates for elliptic operators with smooth coefficients [2]. The smoothness assumption can be loosened, as shown by L. Nirenberg and YanYan Li [6], using the fact that, in a composite medium made with $C^{1+\alpha}$ inclusions, the gradient of the potential is bounded, independently of the distance between the inclusions. These results may be adapted to obtain the following pointwise estimates on the Green's functions

Theorem 2. *Let $\omega \subset\subset \Omega \subset \mathbf{R}^3$ and $0 < r < diam(\omega)/4$. There is a positive constant C, independent of ε, such that, for all $B(y,r) \subset \omega$,*

$$\begin{aligned} \|G_\varepsilon(.,y) - G^*(.,y)\|_{L^\infty(\omega \setminus B(y,r))} &\leq C\varepsilon^{1/4}, \\ \|\nabla_x G_\varepsilon(.,y) - (I + \nabla\chi(./\varepsilon))\nabla_x G^*(.,y)\|_{L^\infty(\omega \setminus B(y,r))} &\leq C\varepsilon^{1/4}. \end{aligned}$$

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Some problems in scaling up the source terms in an underground waste repository model

Alain Bourgeat

(joint work with Eduard Marušić-Paloka, Olivier Gipouloux)

Introduction

We are interested in $\rho(x,t)$the evolution in time of the density of some quantity, such as heat or chemical concentration, which is transported by diffusion and convection from a "sources site" made of a large number of similar "local sources". This type of modeling could, for instance, describe contaminants transport and migration in aquifers from a long-lived nuclear waste underground repository.

General Equations. The process is described by a diffusion convection type equation:

$$R\omega\frac{\partial\rho}{\partial t} - \nabla\cdot(\mathbf{A}\nabla\rho) + (\mathbf{V}\cdot\nabla)\rho + \lambda R\omega\rho = 0 \tag{1}$$

- R the latency retardation factor,
- ω the porosity,
- $\mathbf{v}$ the Darcy's velocity
- $\lambda = \frac{\log 2}{T}$; T the element radioactivity half life time.

There are at least three levels where there is a need for scaling up the above model , from a detailed description to a global model: - from **Waste Packages** to a **Storage Unit** model (see [1],[2]) - from **Storage Units** to a **Zone** model (see [3]) - from **similar Zones** to a **Repository Site** global model.

From the Storage Units to a Zone Global Model

The technique and the results herein after (see [1],[2])would be the same for the scaling up from "Similar Zones" to a " Repository Site model" .

The Equations. For seek of simplicity, we will assume $R = 1$.

$$\omega^\varepsilon \frac{\partial \varphi_\varepsilon}{\partial t} - \operatorname{div}(\mathbf{A}^\varepsilon \nabla \varphi_\varepsilon) + (\mathbf{v}^\varepsilon \cdot \nabla)\varphi_\varepsilon + \lambda \omega^\varepsilon \varphi_\varepsilon = 0 \quad \text{in } \Omega_\varepsilon^T \tag{2}$$

$$\varphi_\varepsilon(0,x) = \varphi_0(x) \quad x \in \Omega_\varepsilon \tag{3}$$

$$\mathbf{n} \cdot \sigma = \mathbf{n} \cdot (\mathbf{A}^\varepsilon \nabla \varphi_\varepsilon - \mathbf{v}^\varepsilon \varphi_\varepsilon) = \Phi(t) \quad \text{on } \Gamma_\varepsilon^T \tag{4}$$

$$\varphi_\varepsilon = 0 \quad \text{on } S_1, \tag{5}$$

$$\mathbf{n} \cdot (\mathbf{A}^\varepsilon \nabla \varphi_\varepsilon - \mathbf{v}^\varepsilon \varphi_\varepsilon) = 0 \quad \text{on } S_2\ ; \tag{6}$$

with

$$\mathbf{A}^\varepsilon(x_2) = \mathbf{A}(\frac{x_2}{\varepsilon});\ \mathbf{v}^\varepsilon(x,t) = \mathbf{v}(x, \frac{x_2}{\varepsilon}, t);\ \omega^\varepsilon(x_2) = \omega(x_2/\varepsilon). \tag{7}$$

A priori Energy estimates and Homogenized equation.
The following a priori estimates:

$$\varphi_\varepsilon \rightharpoonup \varphi \qquad \text{weak* in} \quad L^\infty(0,T;L^2(\Omega)) \tag{8}$$

$$\nabla \varphi_\varepsilon \rightharpoonup \nabla \varphi \qquad \text{weakly in} \quad L^2(0,T;L^{\beta*}(\Omega)) \tag{9}$$

with

$$\varphi \in L^2(0,T;H^1(\Omega))\ L^\infty(0,T;\ L^2(\Omega)), \text{ and } \beta* = \frac{2\beta}{3\beta - 2}.$$

And φ is then the solution of:

$$\omega^2 \frac{\partial \varphi}{\partial t} - \operatorname{div}(\mathbf{A}^2 \nabla \varphi) + (\mathbf{v}^2 \cdot \nabla)\varphi + \lambda \omega^2 \varphi = 0 \text{ in } \tilde{\Omega}^T \tag{10}$$

$$\varphi(x,0) = \varphi_0(x) \quad x \in \tilde{\Omega} = \Omega \backslash \Sigma \tag{11}$$

$$\varphi = 0 \quad \text{on } S_1 \tag{12}$$

$$\mathbf{n} \cdot (\mathbf{A}^2 \nabla \varphi - \mathbf{v}^2 \varphi) = 0 \quad \text{on } S_2 \tag{13}$$

$$[\varphi] = 0 \ , \quad \left[\mathbf{e}_2 \cdot (\mathbf{A}^2 \nabla \varphi - \mathbf{v}^2 \varphi)\right] = -|\tilde{M}|\Phi \text{ on } \Sigma\ , \tag{14}$$

where $[\cdot]$ denotes the jump over Σ, and $|\widetilde{M}|$ stands for the limit of a storage unit area; (M_ε) *area* $= |\widetilde{M}| + O(\varepsilon^{\beta-1})$

Remark 1. *We do not need exact periodicity in space, of the units; the same proof holds whenever each unit is randomly placed in a mesh of an $\varepsilon-$ net. The units do not even need to have the same shape as long as their thickness is small enough ($\ll \varepsilon$).*

The above result may be extended to a general case where the flux Φ depends also on the space $\Phi(x,t)$ and the units have different shapes $M_\varepsilon(x)$; then the right hand side of (14) would have to be replaced by $\lim_{\varepsilon\to 0}|M_\varepsilon(x)|\Phi(x',t)$.

Asymptotic expansion and Matching for the Short time.
We define first the Matched Expansion:

$$F_\varepsilon = \begin{cases} \varphi_\varepsilon^0 \qquad \text{in } \Omega\backslash\overline{G_\varepsilon}\ ; (\text{ Outer Expansion}) \\ \varphi_\varepsilon^0 + \varepsilon\left(\chi_\varepsilon^k(\frac{x}{\varepsilon})\frac{\partial\varphi_\varepsilon^0}{\partial x_k} + w_\varepsilon(\frac{x}{\varepsilon})\Phi - \varphi_\varepsilon^0\rho_\varepsilon^k(\frac{x}{\varepsilon})v_k^1\right) \quad \text{in } G_\varepsilon\ ; \end{cases} \tag{15}$$

where G_ε is the Inner Layer and the functions χ_ε^k, ρ_ε^k and w_ε are 1-periodic solutions of three auxiliary stationary diffusion type problems posed in an infinite strip.

Theorem 1. *For any $0<\tau<1$ there exists a constant $C_\tau>0$ non dependant on ε, such that*

$$|\varphi_\varepsilon - F_\varepsilon|_{L^2(0,T;H^1(B_\varepsilon))} \le C_\tau\,\varepsilon^\tau\ , \tag{16}$$

where $B_\varepsilon = \Omega\backslash\partial G_\varepsilon$.
The same estimate holds in $L^\infty(0,T;L^2(\Omega_\varepsilon))$ norm.

Remark 2. *The expansion (15) clearly points out two important terms: the zero order term φ_ε^0 and the first order term $\varepsilon\, w_\varepsilon(\frac{x}{\varepsilon})\Phi$.*
On one hand the diffusion in the low permeable layer around the units is small and on the other hand the leaking is intensive during a short time; then during this short time, the first order term $\varepsilon\, w_\varepsilon(\frac{x}{\varepsilon})\Phi$ will dominate in φ_ε; and after this short time the diffusion will become dominant, i.e. φ_ε^0 will become the most important term in the expansion.

From Waste Packages to a Storage Unit Global Model, with a possibly damaged zone

We are now seeking a mathematical model describing the global behavior of one **Storage Unit**(see [3]); assuming it is made of a high number of Waste Packages (or containers sets), lying on a hypersurface Σ and linked by parallel backfilled drifts ; all the parallel drifts being connected at the top to a main gallery, also backfilled. (see [3])
All the repository is embedded in a low permeability layer, called host layer . As in the previous section, for simplicity, we assume the convection field (Hydrology regime) is given.
Denoting ε the ratio between the width of a unit and the distance between two drifts; then in the renormalized model there are three scales: $O(1)$ for a disposal unit scale, $O(\varepsilon)$ for both the scale of a containers row and the drifts period, and $O(\varepsilon^\gamma)$,γ close to three, for the Waste Packages diameter.

The Model and Equations. The Darcy's velocity is:

$$\mathbf{v}^\varepsilon(x) = \begin{cases} \mathbf{v}^h(x) \text{ in the host rock } \Omega_\varepsilon \setminus S_\varepsilon \\ \varepsilon^{-\beta}\, \mathbf{v}^d(x', x_2/\varepsilon; x_3/\varepsilon) \text{ in the drifts } S_\varepsilon \end{cases} ;$$

the Diffusion/Dispersion is:

$$\mathbf{A}^\varepsilon(x) = \begin{cases} \mathbf{A}^h(x) \text{ in the host rock } \Omega_\varepsilon \setminus S_\varepsilon \\ d(x)\, \mathbf{I} + \varepsilon^{-\beta}\, \mathbf{A}^d(x_2, x_2/\varepsilon, x_3/\varepsilon) \text{ in the drifts } S_\varepsilon \end{cases} .$$

And, because the convection in a storage unit goes mainly in the direction of the drifts, we assume

$$\mathbf{A}^d(x_2, y_2, y_3) = a(x_2, y_2, y_3) \ (\mathbf{e}_1 \otimes \mathbf{e}_1 .)$$

With the above assumptions the "Microscopic" model of a Storage Unit is:

$$\omega^\varepsilon \frac{\partial \varphi_\varepsilon}{\partial t} - \operatorname{div}(\mathbf{A}^\varepsilon \nabla \varphi_\varepsilon) + (\mathbf{v}^\varepsilon \cdot \nabla)\varphi_\varepsilon + \lambda\, \omega^\varepsilon\, \varphi_\varepsilon = 0 \quad \text{in } \Omega_\varepsilon^T \tag{17}$$

$$\varphi_\varepsilon(0, x) = \varphi_0(x) \quad x \in \Omega_\varepsilon \tag{18}$$

$$\mathbf{n} \cdot (\mathbf{A}^\varepsilon \nabla \varphi_\varepsilon - \mathbf{v}^\varepsilon\, \varphi_\varepsilon) = \Phi_\varepsilon(t) \text{ on } \Gamma_\varepsilon^T \tag{19}$$

$$\mathbf{n} \cdot (\mathbf{A}^\varepsilon \nabla \varphi_\varepsilon - \mathbf{v}^\varepsilon\, \varphi_\varepsilon) = \kappa\ (\varphi_\varepsilon - g_\varepsilon) \quad \text{on } K_\varepsilon^T \cup H_\varepsilon^T \tag{20}$$

$$\varphi_\varepsilon = 0 \quad \text{on } Z_\varepsilon^T \ . \tag{21}$$

with H_ε^T the drifts Tops surface, Z_ε^T the drifts (sealed) Bottoms , K_ε^T the rest of the exterior boundary of Ω, and Γ_ε^T the Waste Packages boundary $\times(0, T)$.

Remark 3. *In the above model, g_ε will measure the concentration entering at the drifts tops; and $\varepsilon^{-\beta}$ the Darcy's velocity range inside the drifts.*

Results. Depending on β (the Darcy's velocity range), with a proper rescaling of the source flux and of the concentration on the shafts tops, we have three different global behavior :

- With $0 \leq \beta < 1$,

The shafts do not make any contribution, the repository behaves as if they were not there. Mainly $\varphi_\varepsilon \to \varphi$ the unique solution of a problem, similar to the Homogenized equation obtained in the previous section 10- 14, i.e. of same type as the microscopic problem.

- With $\beta = 1$

and a source term, $\lim_{\varepsilon \to 0} \Phi_\varepsilon(t) = \Phi(t)$ uniformly in t , and some concentration, $g_\varepsilon = \varepsilon^{-1}\, g^d$, entering the shafts tops H_ε.
This model could be seen as representing connected shafts, galleries and drifts with damaged sealings. The transport processes, inside and outside the "damaged" shafts are comparable and there is a strong interaction between them. The solution of the Microscopic model $\varphi_\varepsilon \to \varphi$ weakly in $L^2(0, T; W^{1,\gamma^*}(\Omega))$ and $\varphi_\varepsilon \longrightarrow \varphi^0 =$

$\varphi(x_1, x_2, 0)$, $d\mu^\varepsilon(x)2 - scale$, [4], where φ is the unique solution of a coupled problem:

$$\omega^h \frac{\partial \varphi}{\partial t} - \operatorname{div}(\mathbf{A}^h \nabla\varphi) + (\mathbf{v}^h \cdot \nabla)\varphi + \lambda\omega^h \varphi = 0 \text{ in } \tilde{\Omega}^T; \tag{22}$$

$$\varphi(0, x) = \varphi_0(x) \text{in } \tilde{\Omega}; \tag{23}$$

$$\mathbf{n} \cdot (\mathbf{A}^h \nabla\varphi - \mathbf{v}^h \varphi) = \kappa(\varphi - g^h) \text{ on } S^T \tag{24}$$

$$[\mathbf{e}_3 \cdot (\mathbf{A}^h \nabla\varphi - \mathbf{v}^h \varphi)] = -M\Phi - \frac{\partial}{\partial x_1}(\langle a\rangle \frac{\partial \varphi^0}{\partial x_1}) + \langle v_1^d\rangle \frac{\partial \varphi^0}{\partial x_1} \text{ on } \Sigma^T \tag{25}$$

$$\langle a\rangle \frac{\partial \varphi^0}{\partial x_1}(t, L, x_2, 0) + \langle v_1^d\rangle \varphi^0(t, L, x_2, 0) = \kappa g^d. \tag{26}$$

- With $2 > \beta > 1$

and a sufficiently strong source and some concentration entering the drifts tops $g_\varepsilon = \varepsilon^{-\frac{\beta+1}{2}} g^d$ on H_ε; then the transport process in the drifts is dominant and we do not see anything else in the corresponding global model . We have then: $\varepsilon^{(1-\beta)/2} \varphi_\varepsilon \longrightarrow \phi$, $d\mu^\varepsilon(x)2 - scale$,[4], to the global concentration φ^0, the unique solution of a 1-dimensional problem for any $x \in]0, L[$:

$$-\frac{\partial}{\partial x_1}\left(\mathbf{A}_{11}^d \frac{\partial \varphi^0}{\partial x_1}\right) + \mathbf{v}_1^d \frac{\partial \varphi^0}{\partial x_1} = 0 \text{ in }]0, L[\tag{27}$$

$$\varphi^0(0) = 0 \quad , \quad \mathbf{A}_{11}^d \frac{\partial \varphi^0}{\partial x_1}(L) + (\mathbf{v}_1^d + \kappa)\varphi^0(L) = \kappa g^d \quad .$$

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Variational problems involving percolation

Andrea Braides

(joint work with Andrey Piatnitski)

In a recent paper [5] Braides and Piatnitski have studied the problem of describing the overall properties of a discrete membrane in which a random distribution of 'defects' is taken into account. The free energy of this two-dimensional discrete

membrane with a bounded open set $\Omega \subset \mathbb{R}^2$ as reference configuration is modelled by a functional

$$E_\varepsilon(u) = \frac{1}{2} \sum_{|i-j|=\varepsilon} \phi_{ij}^\varepsilon(u_i - u_j), \tag{1}$$

where $u : \varepsilon\mathbb{Z}^2 \cap \Omega \to \mathbb{R}$. The small positive parameter ε is introduced so that averaged properties of E_ε are described by its Γ-limit F (see e.g. [3, 1]).

The functions ϕ_{ij}^ε may take two forms:
(1) (*strong springs*) $\phi_{ij}^\varepsilon(z) = z^2$. If only strong springs are present E_ε is nothing but a finite-difference approximation of the *Dirichlet integral*, and $F(u) = \int_\Omega |\nabla u|^2\, dx$ is defined on $H^1(\Omega)$;
(1) (*weak springs*) $\phi_{ij}^\varepsilon(z) = \min\{z^2, \varepsilon\}$. In terms of the difference quotient we may write

$$\phi_{ij}^\varepsilon(u^i - u_j) = \varepsilon f\Big(\varepsilon\Big(\frac{u_i - u_j}{\varepsilon}\Big)^2\Big) = \begin{cases} (u_i - u_j)^2 & \text{if } \frac{u_i - u_j}{\varepsilon} \le \frac{1}{\sqrt{\varepsilon}} \\ 1 & \text{otherwise,} \end{cases} \tag{2}$$

where $f(w) = \min\{|w|, 1\}$.

The case when

$$\phi_{ij}^\varepsilon(z) = \begin{cases} \varepsilon f(\varepsilon z^2) & \text{with probability } p \\ z^2 & \text{with probability } 1-p \end{cases} \tag{3}$$

is considered. This can be done by introducing suitable i.i.d. random variables (see [5]) corresponding to a *bond-percolation model* (see e.g. [6]). With fixed a realization ω we will write E_ε^ω to highlight the fixed choice of ϕ_{ij}^ε in terms of ω, and F^ω the corresponding Γ-limit. The case $p < 1/2$ (subcritical regime) had been completely solved in [5] by showing that in that case the effect of the weak springs is almost surely negligible and the Γ-limit is simply the Dirichlet integral. The following theorem settles the supercritical case, improving the results in [5].

Theorem (Braides and Piatnitski). *If $p > 1/2$ then the limit is finite in the Ambrosio and De Giorgi's space of generalized special functions with bounded variation $GSBV(\Omega)$ (see [2]) and there exists $g_p \le c < +\infty$ such that almost surely*

$$F^\omega(u) = \int_\Omega |\nabla u|^2\, dx + \int_{S(u)} g_p(\nu)\, d\mathcal{H}^1 \tag{4}$$

for $u \in GSBV(\Omega)$. Here, $S(u)$ denotes the set of discontinuity points for u and ν its measure-theoretical normal.

Remark. (i) the definition of g_p is obtained as follows (we sketch the definition): with fixed a realization ω consider k, k' in the 'weak cluster', and for such pairs define the distance $d_\omega(k, k')$ as the minimal path within the weak cluster joining the two points. Then it can be proved that as $k, k' \to +\infty$ and $\frac{(k-k')}{|k-k'|} \to \nu$ the ratio $d_\omega(k, k')/|k - k'|$ converges to a limit $g_p(\nu)$, and g_p is almost surely independent of ω;

(ii) the main technical point to prove the theorem above is an 'optimality' lemma. Again loosely speaking, this asserts that almost surely if we have $k - k'$ large enough and we have a path joining the two points with length less than $(g_p((k-k')/|k-k'|) - \delta)|k-k'|$ then there exists a fixed proportion $L_\delta > 0$ such that the number of strong connections within that path exceeds $L_\delta|k-k'|$.

The theorem above was presented as a conjecture in [4], and will be included in an improved version of [5].

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Dispersion and localization in a damaging multi–phase medium

René de Borst

(joint work with Marie-Angèle Abellan)

For a fluid–saturated, one–dimensional continuum, the balances of momentum and mass read in an incremental format, e.g. [1] for a complete derivation:

$$\frac{\partial \dot{\sigma}_s}{\partial x} + n_f K^{-1}(\dot{v}_f - \dot{v}_s) - \rho_s \frac{\partial \dot{v}_s}{\partial t} - \rho_f \frac{\partial \dot{v}_f}{\partial t} = 0 \tag{1}$$

and

$$\alpha \frac{\partial^2 \dot{v}_s}{\partial x^2} + n_f \left(\frac{\partial^2 \dot{v}_f}{\partial x^2} - \frac{\partial^2 \dot{v}_s}{\partial x^2} \right) - n_f (KQ)^{-1} \left(\frac{\partial \dot{v}_f}{\partial t} - \frac{\partial \dot{v}_s}{\partial t} \right) = 0 \tag{2}$$

They are supplemented by the kinematic relation and the incremental stress–strain relation, which, after combination, read:

$$\dot{\sigma}_s = E^{tan} \frac{\partial \dot{u}_s}{\partial x} \tag{3}$$

with E^{tan} the tangential stiffness modulus of the solid.

To analyse the characteristics of wave propagation in the two–phase medium defined in the preceding section, a damped, harmonic wave is considered:

$$\begin{pmatrix} \delta \dot{u}_s \\ \delta \dot{u}_f \end{pmatrix} = \begin{pmatrix} A_s \\ A_f \end{pmatrix} \exp\left(\lambda_r t + \mathrm{i}(kx - \omega t)\right) \tag{4}$$

with λ_r representing the damping and ω the angular frequency. Substitution of this identity into eqs (1)–(2), using eq. (3), requiring that a non-trivial solution

can be found for the resulting set of homogeneous equations and decomposing into real and imaginary parts leads to:

$$8\lambda_r^3 + 8ak^2\lambda_r^2 + 2(a^2k^2 + b)k^2\lambda_r + (ab - c)k^4 = 0 \tag{5}$$

and

$$\omega^2 = 3\lambda_r^2 + 2ak^2\lambda_r + bk^2 \tag{6}$$

with

$$a = \frac{KQ(\rho_s + (n_f - \alpha)\rho_f')}{\rho_s + \rho_f} \ , \ b = \frac{E^{tan} + \alpha Q}{\rho_s + \rho_f} \ , \ c = \frac{KQE^{tan}}{\rho_s + \rho_f} \tag{7}$$

Evidently, wave propagation is dispersive, since eq. (6) is such that the phase velocity $c_f = \omega/k$ is dependent on the wave number k, cf. [2, 3]. Taking the long wave–length limit in eq. (5), i.e. $k \to 0$, yields $\lambda_r \to 0$. According to eq. (6) and after substitution of eq. (7b), we obtain an explicit expression for the phase velocity:

$$c_f = \frac{\omega}{k} = \sqrt{\frac{E^{tan} + \alpha Q}{\rho_s + \rho_f}} \tag{8}$$

Using Cardano's formulas, eq. (5) can be solved explicitly. For the short wave-length limit, i.e. when $k \to \infty$, we obtain that the discriminant $D \to 0$, which identifies the existence of three real roots for λ_r in this limiting case, two of them being equal. For the single root we obtain that $\lambda_r \to 0$. This implies that this solution has no damping properties and, therefore, gives no regularization. For the double root we find that $\lambda_r \sim -k^2$. From eq. (6) the expression for the phase velocity then becomes proportional to the wave number, $c_f \sim k$ (please note that for strain softening c_f will normally be imaginary). In view of eq. (4) and in analogy with a single–phase rate–dependent medium [4], an internal length scale can be defined as:

$$\ell = \lim_{k\to\infty} \left(-\frac{c_f}{\lambda_r} \right) \sim \lim_{k\to\infty} k^{-1} = 0 \tag{9}$$

which indicates that the internal length scale ℓ vanishes in the short wave–length limit.

1. NUMERICAL EXAMPLES

To verify and elucidate the theoretical results of the preceding section, a finite difference analysis has been carried out. The spatial derivatives in eqs (1) and (2) have been approximated with a second–order accurate finite difference scheme. Explicit forward finite differences have been used to approximate the temporal derivatives, which is first-order accurate. The choice for a fully explicit time integration scheme was motivated by the analysis of Benallal and Comi [3], in which they showed that in this case no numerical length scale was introduced in the

analysis, apart from the grid spacing. As implied in eqs (1) and (2) the velocities v_s and v_f of the solid skeleton and the fluid have been taken as fundamental unknowns and the displacements have been obtained by integration.

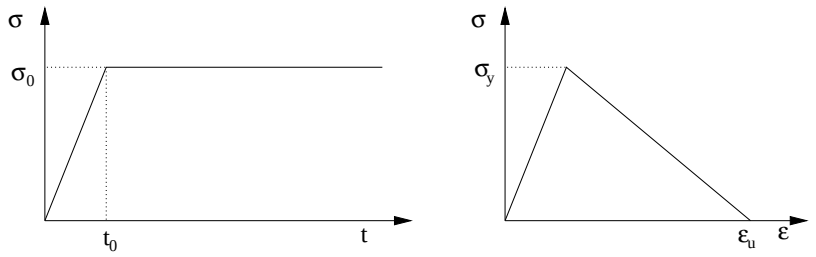

FIGURE 1. Applied stress as function of time (left) and local stress–strain diagram (right)

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All calculations have been carried out for a bar with a length $L = 100\ m$. For the solid material, a Young's modulus $E = 20\ GPa$ and an absolute mass density $\rho_s' = 2000\ kg/m^3$ have been assumed. For the fluid, an absolute mass density $\rho_f' = 1000\ kg/m^3$ was adopted and a compressibility modulus $Q = 5\ GPa$ was assumed. As regards the porosity, a value $n_f = 0.3$ was adopted and in the reference calculations $\alpha = 0.6$ and the permeability $K = 10^{-10}\ m^3/Ns$. In all cases, the external compressive stress was applied according to the scheme shown in Figure 1, with a rise time $t_0 = 0.05\ s$ to reach the peak level $\sigma_0 = 1.5\ MPa$. A time step $\Delta t = 0.5 \cdot 10^{-3}\ s$ was adopted, which is about half the critical time step for this explicit scheme.

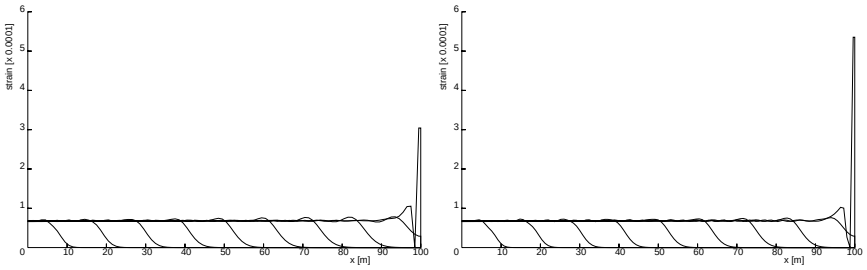

FIGURE 2. Strain profiles along the bar for 101 (left) and 126 (right) grid points and time step $\Delta t = 0.5 \cdot 10^{-3}\ s$

.

Upon reflection at the right boundary, the stress intensity doubles and the stress in the solid exceeds the yield strength $\sigma_y = 2.5\ MPa$ and enters a linear descending branch with an ultimate strain $\epsilon_u = 1.125 \cdot 10^{-3}$, see Figure 1. Figure 2 (left) shows that a Dirac–like strain distribution develops immediately upon wave reflection.

This is logical, since a standard two–phase medium does not have regularizing properties. To further strengthen this observation the analysis was repeated with a slightly refined mesh (126 grid points), which resulted in a marked increase of the localized strain (Figure 2 – right), which has been plotted on the same scale as the results of the original discretization in Figure 2. In [1] it has been shown that also the time step strongly influences the results, cf. [3].

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Gaseous Flows with Multicomponent Transport and Complex Chemistry

Vincent Giovangigli

Multicomponent reactive flows with complex chemistry and detailed transport phenomena arise in various engineering applications such as combustion, crystal growth, atmospheric reentry, or chemical reactors. This is a strong motivation for investigating the corresponding governing equations and analyzing their mathematical structure and properties [7].

We discuss the governing equations for multicomponent reactive flows as obtained from the kinetic theory of gases [4, 7]. These equations can be split into conservation equations, expressions transport fluxes, transport coefficients, and thermochemistry. The evaluation of transport coefficients—which are not explicitly given by the kinetic theory—requires solving transport linear systems. The mathematical structure of the transport linear systems has been investigated and has led to fast and accurate iterative solutions as well as direct inversions [3, 7]. A powerful library of computer programs for evaluating multicomponent transport coefficients is available at the Authors's web site for academic purposes. The mathematical properties of the transport coefficients can also be obtained from that of the transport linear systems [11, 6, 9].

We next investigate the Cauchy problem and obtain global existence theorems around constant equilibrium states as well as asymptotic stability and decay estimates [13, 11]. The system of partial differential equations is first symmetrized by using entropic variables and then rewritten in normal form, that is, in the form of a hyperbolic–parabolic composite system. All normal forms can also be characterized when the nullspace naturally associated with dissipation matrices is invariant.

Global existence in then obtained by using entropic estimates and local dissipativity properties of linearized equations. In particular, the linearized normal form is strictly dissipative and the chemistry source terms are locally stable.

On the other hand, traveling waves in inert or reactive flows can be classified into deflagration and detonation waves [16]. In the context of combustion—which does not decrease the generality of the problem but makes things more explicit—weak deflagration corresponds to plane laminar flames. The anchored flame problem has been investigated with complex chemistry and detailed transport by using entropic estimates and the Leray–Schauder topological degree theory [6]. A key point is that entropy production estimates associated with multicomponent diffusion typically yields estimates of concentration gradients squared divided by concentrations. An important tool is also the exponential decay of entropy production residuals close to equilibrium [6].

These reactive flow models can also be used to describe gas mixtures in full vibrational disequilibrium when each vibrational quantum level is treated as a separate "chemical species" allowing detailed state-to-state relaxation models [11]. When the vibrational quantum levels are partially at equilibrium between them but not at equilibrium with the translational/rotational states—allowing the definition of a vibrational temperature—a different structure is obtained

The case of infinitely fast chemistry, that is, the case of equilibrium flows can also be embedded in the same framework [7]. In this situation, one has to solve the momentum and energy equations together with equations expressing the conservation of atomic elements These results have recently be extended to the situation of partial chemical equilibrium [12]. Note, however, that the mathematical structure of numerous simplified chemistry methods is still obscure at variance with partial equilibrium.

The system of partial differential equations modeling reactive ambipolar plasmas can also be embedded in this framework [8]. The ambipolar—or zero current—model is obtained from general plasmas equations in the limit of vanishing debye length. In this model, the electric field is expressed as a linear combination of macroscopic variable gradients and the resulting system can be recast into a symmetric hyperbolic-parabolic composite form. Asymptotic stability of equilibrium states, decay estimates, and continuous dependence of global solutions with respect to vanishing electron mass are then established [8].

We have further studied a system of partial differential equations modeling ionized magnetized reactive gas mixtures. In this model, dissipative fluxes are anisotropic linear combinations of fluid variable gradients and also include zeroth order contributions modeling the direct effect of electromagnetic forces. There are also gradient dependent source terms like the conduction current in the Maxwell-Ampere equation. We have introduced the notion of partial symmetrizability and that of entropy for such systems of partial differential equations and recast the systems into a partially normal form, that is, in the form of a quasilinear partially symmetric hyperbolic-parabolic system. Using a result of Vol'Pert and Hudjaev, we have proved local existence and uniqueness of a bounded smooth solution [9].

Global existence of solutions and asymptotic stability is an open problem for such nonisotropic systems.

Finally, numerical simulation of compressible flows is a very difficult task that has been the subject of numerous textbooks and requires a solid background in fluid mechanics and numerical analysis. The nature of compressible flows may be very complex, with features such as shock fronts, boundary layers, turbulence, acoustic waves, or instabilities. Taking into account chemical reactions dramatically increases the difficulties, especially when detailed chemical and transport models are considered. Interactions between chemistry and fluid mechanics are especially complex in reentry problems, combustion phenomena, or chemical vapor deposition reactors.

An important aspect of complex chemistry flows is the presence of multiple time scales. Indeed, chemical characteristic times can range typically from 10^{-8} seconds up to several second and there are also acoustic waves. In the presence of multiple time scales, implicit methods are advantageous, since otherwise explicit schemes would be limited by the smallest time scale [1, 2, 5, 7, 14, 15]. A second potential difficulty associated with the multicomponent aspect is the presence of multiple space scales. In combustion applications, for instance, the flame fronts are very thin and typically require space steps of 10^{-3} cm whereas typical flow scales may be of 10 cm. The multiple scales can only be solved by using adaptive grids obtained by successive refinements or by moving grids for unsteady problems [1, 2, 15]. Nonlinear discrete equations can be solved by using Newton's method or any generalization. The resulting large sparse linear systems must then be solved by using a Krylov-type method, such as GMRES and More sophisticated methods involve coupled Newton–Krylov techniques. Evaluating aerothermochemistry quantities is computationally expensive since they involve multiple sums and products. Optimal evaluation requires a low-level parallelization, e.g., by using vector capabilities of computers, depending on the problem granularity.

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Uniqueness of weak solutions for a fluid-structure interaction problem

Giovanna Guidoboni
(joint work with Mariarosaria Padula)

Fluid-structure interaction problems arise in many fields of science, such as aeroelasticity problems, fluttering of wings, dynamics of offshore structures subjected to the cyclic sea currents and fluid flow in compliant conduits. The main difficulty in the mathematical theory of fluid-structure interaction problems is associated to the control of the regularity of the deformable boundary whose evolution is an unknown of the problem. Few results are available in literature concerning the existence of solutions to fluid-structure interaction problems [1, 2, 3, 4, 5].

The goal of the present work is to prove uniqueness of weak solutions for a two-dimensional problem, where a layer of viscous incompressible fluid is confined between a rigid plane and a deformable structure. Periodicity is assumed in the horizontal direction and the structure is described as a linear viscoelastic beam. Existence of weak solutions for this problem was proved in [5].

The classical proof of uniqueness starts by assuming that there exists two different solutions corresponding to the same initial data. Then, energy estimates are derived for the difference between these two solutions and uniqueness follows from Gronwall's lemma. In fluid-structure interaction problems, the two solutions are defined in different domains which are unknowns of the problem as well. Therefore the classical steps of the proof need to be modified in order to give meaning to the difference between the two solutions.

Let $\mathcal{S}_1 = (\mathbf{u}_1, \eta_1)$ and $\mathcal{S}_2 = (\mathbf{u}_2, \eta_2)$ be two solutions corresponding to the same initial data, where $\mathbf{u}$ is the velocity field of the fluid and η is the curve describing the deformable boundary. The domains in which $\mathcal{S}_1$ and $\mathcal{S}_2$ are defined are

$$\Omega_{\eta_1}(t) = \{Z = (X, Y) \in \mathbb{R}^2 \,|\, X \in \Sigma,\, 0 < Y < \eta_1(x, t)\},$$

$$\Omega_{\eta_2}(t) = \{z = (x, y) \in \mathbb{R}^2 \,|\, x \in \Sigma,\, 0 < y < \eta_2(x, t)\},$$

respectively, where Σ is the horizontal periodicity cell. A time-dependent change of coordinates is introduced to map $\Omega_{\eta_1}(t)$ onto $\Omega_{\eta_2}(t)$:

$$\begin{array}{rccl} \phi_t: & \Omega_{\eta_1}(t) & \to & \Omega_{\eta_2}(t) \\ & Z & \to & z = \begin{cases} x = X \\ y = Y\frac{\eta_2}{\eta_1}. \end{cases} \end{array}$$

Therefore, every function $f(x, Y, t)$ defined on $\Omega_{\eta_1}(t)$ is transformed in the function $\hat{f}(x, Y, t) = f(x, \frac{\eta_1}{\eta_2}y, t)$ defined on $\Omega_{\eta_2}(t)$. The transformed velocity field is not solenoidal, but the vector field $\mathbf{v}_1 = J\mathbf{J}^{-1}\hat{\mathbf{u}}_1$, where $\mathbf{J}$ is the Jacobian matrix of the transformation and J its determinant, is divergence free.

Now the difference between $\mathcal{S}_1$ and $\mathcal{S}_2$ can be defined on the same domain $\Omega_{\eta_2}(t)$ and the difference in the velocity fields will be taken as $\mathbf{u}_2 - J\mathbf{J}^{-1}\hat{\mathbf{u}}_1$ to preserve solenoidality. The regularity of the change of coordinates allows to obtain the energy estimates for the difference and uniqueness follows from Gronwall's lemma.

By introducing a slight modification in the definition of the change of coordinates, this result, as well as the existence theorem in [5], can be proved also in the case of a fluid layer contained between two deformable boundaries. This project is strongly motivated by the modeling of blood flow in large arteries, and therefore the next step is the study of existence and uniqueness of weak solutions when a time-dependent pressure drop is present.

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Laboratory scale capillarity without capillary pressure

R. Hilfer

The accepted mathematical model for simultaneous flow of two immiscible Newtonian fluids inside a rigid porous medium has serious shortcomings concerning the correct incorporation of capillary forces, hysteresis and residual saturations. Mathematicians in applied analysis have attempted to overcome this problem using homogenization of pore scale equations [1]. Here, an alternative formulation is given that is based on the distinction between percolating and nonpercolating fluid regions [2, 3]. The formulation does not require capillary pressure as an input function thereby challenging the physical basis of the traditional model [4, 5].

The equations in the residual decoupling approximation read

$$\begin{aligned}
\frac{\partial S_1}{\partial t} &- \nabla\left[R_1^{-1}\phi S_1^2\left(\Pi_b\nabla S_3^{-\beta}+\delta P_4^*\nabla S_4^{\delta-1}+(\rho_o-\rho_w)g\right)\right]\\
&= \eta_2\phi\rho_w\left(\frac{S_2-S_2^*(\partial S_w/\partial t)}{S_w^*(\partial S_w/\partial t)-S_w}\right)\frac{\partial S_w}{\partial t}\\
\frac{\partial S_2}{\partial t} &= -\eta_2\phi\rho_w\left(\frac{S_2-S_2^*(\partial S_w/\partial t)}{S_w^*(\partial S_w/\partial t)-S_w}\right)\frac{\partial S_w}{\partial t}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial S_3}{\partial t} &- \nabla\left[R_3^{-1}\phi S_3^2\left(\Pi_a\nabla S_1^{-\alpha}+\gamma P_2^*\nabla S_2^{\gamma-1}+(\rho_w-\rho_o)g\right)\right]\\
&= \eta_4\phi\rho_o\left(\frac{S_4-S_4^*(\partial S_w/\partial t)}{1-S_w^*(\partial S_w/\partial t)-S_o}\right)\frac{\partial S_w}{\partial t}\\
\frac{\partial S_4}{\partial t} &= -\eta_4\phi\rho_o\left(\frac{S_4-S_4^*(\partial S_w/\partial t)}{1-S_w^*(\partial S_w/\partial t)-S_o}\right)\frac{\partial S_w}{\partial t}
\end{aligned}$$

for the unknown saturations $0 \le S_1(x,t), S_2(x,t), S_3(x,t), S_4(x,t) \le 1$ of the percolating (resp. nonpercolating) wetting (resp. nonwetting) fluids, and $x \in \mathbb{S} \subset \mathbb{R}^3$, $t \in \mathbb{R}_+$. The saturations fulfill $\sum_{i=1}^4 S_i = 1$ and $S_w = S_1 + S_2$ (resp. $S_o = S_3 + S_4$) are the wetting (resp. nonwetting) saturation. In these equations ϕ denotes porosity, R_1^{-1}, R_3^{-1} are the inverses of viscous resistance coefficient matrices. The scalar parameters $\Pi_a, \Pi_b, \alpha, \beta, \gamma, \eta_2, \eta_4$ can be determined from experiment. The fluid densities are ρ_o for the nonwetting fluid and ρ_w for the wetting fluid. The nonlinear functionals $S_2^*(\partial S_w/\partial t)$, $S_4^*(\partial S_w/\partial t)$ and $S_w^*(\partial S_w/\partial t)$ describe the breakup and coalescence of fluids analogous to a chemical reaction. A preliminary analysis of these equations indicates that, under certain conditions, their solutions can reproduce all quasistatic phenomena of capillary hysteresis observed in experiment.

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Riemann solvers for two-phase flow through a change in rock type

Jérôme Jaffré
(joint work with Adimurthi, Siddhartha, Veerappa Gowda)

The purpose of this communication is to show how to extend the Godunov numerical flux to the case with a change of rock type which results in a discontinuity in space for the flux function of the phase conservation law. In addition we claim that in this case cell-centered finite volume schemes using the upstream mobility flux do not converge to the entropy satisfying solution.

Homogeneous two-phase flow

Under the assumptions that capillary effects are neglected, two-phase flow in a porous medium is modeled by a nonlinear hyperbolic equation:

$$\phi \frac{\partial S}{\partial t} + \frac{\partial f}{\partial x} = 0$$

where ϕ is the porosity of the rock, $S = S_1$ is the saturation of phase 1 which lies in a bounded interval $[0, 1]$. The flux function f is the Darcy velocity φ_1 of phase 1 and has the form

$$f = \varphi_1 = \frac{\lambda_1}{\lambda_1 + \lambda_2}[q + (g_1 - g_2)\lambda_2]. \tag{1}$$

Here $q = \varphi_1 + \varphi_2$ denotes the total Darcy velocity where $\varphi_\ell, \ell = 1, 2$, denotes the Darcy velocity of phase ℓ with, for the second phase,

$$\varphi_2 = \frac{\lambda_2}{\lambda_1 + \lambda_2}[q + (g_2 - g_1)\lambda_1].$$

Since the flow is assumed to be incompressible, the total Darcy velocity q is independent of the space variable x.

The quantities λ_ℓ, $\ell = 1, 2$ are the effective mobilities. They are products of the absolute permeability K by the mobilities k_ℓ : $\lambda_\ell = K k_\ell$, $\ell = 1, 2$. The absolute permeability K may depend on x and the quantities k_ℓ and λ_ℓ are functions of S which satisfy the following properties :

$$\begin{aligned} &k_1 \text{ and } \lambda_1 \text{ are increasing functions of } S,\ k_1(0) = \lambda_1(0) = 0, \\ &k_2 \text{ and } \lambda_2 \text{ are decreasing functions of } S,\ k_2(1) = \lambda_2(1) = 0. \end{aligned}$$

We also shall assume that these functions are smooth functions of the saturation S and so is the flux function f.

The gravity constants g_ℓ, $\ell = 1, 2$ of the phases are $g_\ell = g\rho_\ell \dfrac{dx}{dz}$, $\ell = 1, 2$, with g the acceleration due to gravity, ρ_ℓ the density of phase ℓ and z is the vertical position of the point of abscissa x.

Observe that with the above hypothesis, f is a function with at most one maxima and no minima in $[0, 1]$ with $f(0) = 0$ and $f(1) = q$ respectively.

We restrict ourselves to one-dimensional finite volume methods and we focus on the flux calculation which must be done at the intercell interfaces. In the multidimensional case, most numerical methods still use the one-dimensional flux calculation in the direction normal to the boundaries of the discretization cells.

Two numerical flux calculations are under consideration, the Godunov flux and the upstream mobility numerical flux, the latter being widely used among hydrogeologists and petroleum reservoir engineers.

For the Godunov flux, taking into account the particular shape of the two-phase flow flux function (1)– it has just one global and local extremum –,a new formula was recently introduced:

$$F^G(a,b) = \min\{f(\min\{a,\theta\}), f(\max\{\theta,b\})\}, \tag{2}$$

where a and b are the left and right values of the saturation and θ is the point where f reaches its maximum. The advantage of this formula, compared to the standard one, is that it can be readily extended to the case with a change of rock type, that is when the flux function is changing because of a rock heterogeneity.

The upstream mobility flux is defined by the formulas

$$\begin{aligned} F^{UM}(a,b) = \quad & \varphi_1 = \frac{\lambda_1^*}{\lambda_1^* + \lambda_2^*}[q + (g_1 - g_2)\lambda_2^*], \\ & \varphi_2 = \frac{\lambda_2^*}{\lambda_1^* + \lambda_2^*}[q + (g_2 - g_1)\lambda_1^*], \end{aligned} \tag{3}$$

with the phase mobilities λ^* calculated with the values which are upstream with respect to the corresponding phase flow:

$$\lambda_\ell^* = \begin{cases} \lambda_\ell(a) & \text{if } \varphi_\ell > 0, \\ \lambda_\ell(b) & \text{if } \varphi_\ell \leq 0. \end{cases}$$

This numerical flux is the favorite flux calculation among hydrogeologists and petroleum reservoir engineers.

Cell-centered finite volume methods using either the Godunov flux or the upstream mobility flux are proven to calculate a solution converging to the entropy satisfying solution in the homogeneous case [1].

The case with a change of rock type

In many applications, the porous medium is not homogenous. Let us consider a point where the rock type is changing. At this point the porosity and the mobilities are changing, and so does the flux function f, and the question is now to define a suitable numerical flux calculation.

To distinguish the rock types, we introduce the upper indices I and II respectively for the left and right rock types.

Using formula (2) the Godunov flux can be easily extended to this case as

$$\overline{F}^G(a,b) = \min\{f^{\mathrm{I}}(\min\{a,\theta^{\mathrm{I}}\}), f^{\mathrm{II}}(\max\{\theta^{\mathrm{II}},b\})\}.$$

A complete analysis of the associated finite volume scheme is carried out in [2]. This includes definition of an entropy condition and proof of convergence to the

entropy satisfying solution. It also includes existence and uniqueness of the continuous problem.

To extend the upstream mobility flux is also straightforward:

$$\overline{F}^{UM}(a,b) = \begin{array}{ll} \varphi_1 = \dfrac{\lambda_1^*}{\lambda_1^*+\lambda_2^*}[q+(g_1-g_2)\lambda_2^*], \\ \varphi_2 = \dfrac{\lambda_2^*}{\lambda_1^*+\lambda_2^*}[q+(g_2-g_1)\lambda_1^*] \end{array}$$

with $\lambda_\ell^* = \begin{cases} \lambda_\ell^{\mathrm{I}}(a) & \text{if } \varphi_\ell > 0, \\ \lambda_\ell^{\mathrm{II}}(b) & \text{if } \varphi_\ell \le 0. \end{cases}$

For this numerical flux it is only possible to prove convergence to a weak solution, and in [3] one can see examples where the method does not find the entropy solution. Therefore it si not possible to prove convergence to the entropy satisfying solution.

This was not observed before by engineers because completely wrong solution are calculated with the upstream mobility flux only in certain configurations of f^{I} and f^{II}.

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Numerical Methods for Chemistry and for Coupling Transport with Chemistry in Porous Media

Michel Kern

(joint work with Jocelyne Erhel)

The simulation of multispecies reacting systems in porous media is of importance in several different fields: for computing the near field in nuclear waste simulations, in the treatment of bio-remediation, and in the evaluation of underground water quality.

Multi-species chemistry involves the solution of ordinary differential equations (if the reactions are kinetic) or nonlinear algebraic equations (if we assume local equilibrium). When simulating a coupled system, these equations have to be solved at each (grid) point, and at every time (step), leading to a huge coupled non-linear system. As has been observed several times, it is essential to use efficient numerical methods so as to be able to handle the size of systems occurring in the applications.

Methods for solving the chemical system

As we stated above, and assuming local equilibrium, a batch chemical system is modeled by mass action laws, and mass conservation equations, leading to a set of non-linear algebraic equations.

A (closed) chemical system involving N_r equilibrium reactions can be rewritten so that each reaction expresses the formation of a single *secondary species* in terms of several *component species*. Each reaction gives rise to a mass action law

$$x_i = K_i \prod_{j=1}^{N_c} x_j^{r_{ij}}, \quad i = 1, \ldots, N_r, \tag{1}$$

where c_j (resp. x_i) is the *concentration* of the ith component (resp. secondary species, mineral species), and where r_{ij} and are stoichiometric coefficients.

Precipitation–dissolution reactions introduces additional difficulties, as these are reactions with a threshold: they only take place if the solubility product reaches 1. For each mineral, the mass action law (1) has to be replaced by

$$\begin{cases} p_k = 0 & \text{if } \Pi_k < 1 \\ \Pi_k = 1 & \text{otherwise ,} \end{cases} \tag{2}$$

where the *solubility product* Π_k is defined by

$$\Pi_k = K_k^p \prod_{j=1}^{N_c} c_k^{d_{jk}}, \quad , j = 1, \ldots, N_p. \tag{3}$$

We also write a mass conservation equation for each component:

$$T_j = c_j + \sum_{i=1}^{N_r} r_{ij} x_i + \sum_{k=1}^{N_p} d_{kj} p_k, \quad j = 1, \ldots, N_c \tag{4}$$

Equations (4) and (1) together form a system of nonlinear algebraic equations. In a complex system with several mineral species, it may not be easy to guess which species will actually precipitate (or dissolve), and the procedure most often used by practitioners involve a expensive (a non-linear system has to be solved each time), and potentially hazardous (it might theoretically enter a cycle) combinatorial procedure.

We propose to reformulate the problem as a non-linear complementarity problem, leading to a system similar to the KKT equations in inequality constrained optimization. A possibility for solving this system is to relax the complementarity constraint, and to use interior points methods to solve the system. At each iteration, the Newton direction has to be modified to ensure that the iterates remain "sufficiently positive", and the relaxation parameters tends to 0. The advantage of the method is that it converges to the solution of the original problem without having to specify a priori which minerals will or will not precipitate. The main drawback is that the system to be solved is larger than the original one, and that intermediate linear systems may become very ill-conditioned. See [1], [2].

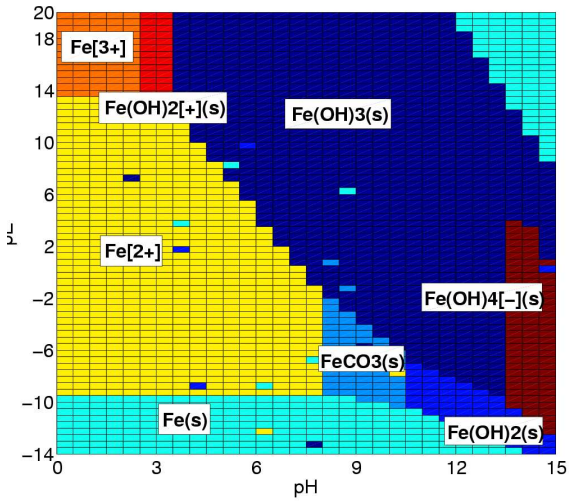

FIGURE 1. Equilibrium diagram for iron. For each value of the pH and pE, an equilibrium system involving 9 aqueous and 4 mineral species is solved using the above method.

METHODS FOR COUPLING TRANSPORT WITH CHEMISTRY

When looking at a coupled system, we take into account sorption reactions between the porous matrix and the species in solution. The role of chemistry is simply to separate the species into mobile and immobile species (immobile species come from sorption, and are not subject to transport). In this work, we assume that the medium is saturated, and that surface reactions do not change the porosity. We have not yet taken into account precipitation dissolution reactions. For each species, we have to consider both its mobile and fixed concentration.

We formulate the coupled problem keeping as main unknowns both the mobile and fixed concentrations of all the component species, and also the total concentrations. If we again assume local equilibrium, then the coupled system may be written as a DAE. Since methods and software for solving DAEs have reached a high level of maturity (at least for small index system, which is the case here), it is natural to try and use this technology.

An advantage of this formulation, which is closely related to the Direct Substitution Approach used by the geochemists [3], [4], is that transport and chemistry are on the same level. At each time step, a single non-linear system has to be solved, and the Jacobian matrix couples both the transport matrix, and the chemistry Jacobian matrix.

We have implemented a first version using Matlab, for 1D models. An important implementation issue was the use of a sparse linear system solver. Comparisons on a simple model show efficiency gains up to 5 with respect to the usual block Gauss-Seidel method.

One important issue for solving more realistic models will the size of the system to be solved, as all chemical species at all grid points are coupled. For any realistic configuration, it will not be possible to form, let alone factor, the Jacobian matrix. A better solution is to use Newton–Krylov methods, where the linear system at each Newton iteration is solved by an iterative method. We can thus keep the fast convergence of Newton's method, while only requiring Jacobian matrix–vector products, and these can be approximated by finite differences.

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Viscous fluid flow in bifurcating channels and pipes

Michael Lenzinger

The study of fluid flow through branching structures is of special interest in many applications from different sciences, like e.g. biology, physiology or engineering. The arterial-venous system in the human body is a typical physiological example. Often, flux and pressure distributions in such networks are computed using simple one-dimensional models based on a linear flux-pressure relation and Kirchhoff's law of the balancing fluxes in each node point (cf. e.g. [4]). In contrast, our aim is to establish an effective approximation for the Navier-Stokes flow of a viscous Newtonian fluid in a bifurcation Ω^ϵ of thin three-dimensional pipes with a diameter-to-length ratio of order $O(\epsilon)$. Our model is based on the steady-state Navier-Stokes equations with pressure conditions on the outflow boundaries. Existence and local uniqueness is proven under the assumption of small data represented by a Reynolds number Re_ϵ of order $O(\epsilon)$. The presented results are elaborated in [2].
The aim is to construct an asymptotic expansion in powers of ϵ and Re_ϵ based on Poiseuille flow for the solution of this Navier-Stokes problem. Our approach extends the ideas developed in [3], analyzing the influence of the bifurcation geometry on the fluid flow by introducing local Stokes problems in the junction and establishing a formal method of computing the pressure drop and the flux in the pipes. Furthermore, we show that the solution of the Stokes problem in the junction of diameter $O(M)$ approximates the solution of the corresponding boundary layer problem in the infinite bifurcation (called "Leray's problem" in literature, cf. [1]) up to an error decaying exponentially in M. The construction of the approximation for the Navier-Stokes solution then is presented and its properties are discussed.

The approximation is based on the idea of a continuous matching of the Poiseuille velocity to the solution of the junction problem on each pipe-junction interface. The main result of our analysis is the derivation of error estimates for the approximation in powers of ϵ and Re_ϵ according to the designated approximation accuracy. The obtained results generalize and improve the existing ones in literature (cf. [3]). In addition, our results show that Kirchhoff's law has to be corrected in $O(\epsilon)$ in order to obtain an adequate error estimate for the gradient of velocity in $L^2(\Omega^\epsilon)$.

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Rigorous Justification of the Reynolds Equations for Gas Lubrication

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(joint work with Maja Starčević)

1. Introduction

Fluid film bearings are the machine elements consisting of two (in our case rigid) surfaces in relative motion and a thin gap between them filled by a fluid (lubricant).

We are interested in studying the equations governing that thin fluid film. In our model, one of those surfaces is rough and the shape of its asperities plays an important role in our study. Another important feature are the physical properties of the fluid. We are interested in case when the fluid is not a liquid but a gas, in most applications, a clean dry air. There are several differences in qualitative behavior of gases compared to liquids, mainly: compressibility and small viscosities.

In general, gas bearing operates with higher velocity and smaller clearance ratio than the liquid one. Although the gas viscosity is small (typically of order 10^{-5}) we rarely have to consider the turbulence. In fact, due to the small typical length (gap thickness smaller than $1\mu m$ is not uncommon) the Reynolds numbers are usually smaller than 100 (see e.g. [7]). The most common examples where the gas lubrication appears are computer hard discs, magnetic tapes and some high precision measuring devices. To fix the ideas we give some details in case of magnetic hard disc. The model describing such situation was formally derived in [2]. Two surfaces, in that case are the disc and the magnetic head. The hard disc surface is

artificially roughened in order to control the interfacial static force. In order to get higher recording density and, therefore, improve the performance of the recording device the gap between two surfaces (flying height) has been very small and for a present hard-disc the distance between the disc and the head ranges between 5 and 20 nanometers[1]. The typical speed of such device is between 5000 and 10000 rounds per minute (usually smaller for notebooks then for desktop computers). With disc radius of 5-10 cm it gives the characteristic velocity between 20 and 100 m/sec. Hard discs have a small pressure-equalization port keeping the internal pressure equal to the external so the characteristic pressure is between 1000 and 1020 m bar. The typical dry air density is 1.2 $[kg/m^3]$. Dry air viscosity equals $1.8 \cdot 10^{-5}$ $[kg/m \cdot sec.]$. Recommended operating temperature, for most drives is from 35 to 40 Celsius. In the above situation the Reynolds number[2] would be of order 10^{-2}, i.e., deeply in the laminar regime. In fact, in such circumstances it would be reasonable to neglect the effects of inertia.

As in the case of incompressible fluids, the lower dimensional model for describing the process of lubrication by compressible fluid, called the compressible Reynolds equation, has been first derived in the engineering literature, as for instance [1], [2], [3], [7].

However, no rigorous results of that kind for compressible fluids are known to us. The basic difficulty is that the weak convergence method used for compressible models does not pass directly here due to the nonlinearity of the continuity equation.

The goal of this paper is to derive the isothermal Reynolds model for gas lubrication using the rigorous asymptotic analysis.

2. Position of the problem

To derive the model we start from equations of motion governing the compressible, stationary flow through a thin domain with thickness ε described by the shape function h:

$$\Omega_\varepsilon = \{x = (x', x_n) \in \mathbf{R}^n \ ; \ x' = (x_1, \cdots, x_{n-1}) \in \mathcal{O} \ , \ 0 < x_n < \varepsilon \ h(x') \ \} \ ,$$

where $\mathcal{O} \subset \mathbf{R}^{n-1}$ is a bounded smooth domain and $h : \overline{\mathcal{O}} \to \mathbf{R}$ is a smooth function such that there exist two constants $h_M, h_m > 0$ satisfying $h_m \leq h(x') \leq h_M$.

Let $\Gamma_\varepsilon = \{x = (x', x_n) \in \mathbf{R}^n \ ; \ x' = (x_1, \cdots, x_{n-1}) \in \partial\mathcal{O} \ , \ 0 < x_n < \varepsilon \ h(x') \ \}$ be the lateral boundary.

We shall also need rescaled domain and it's lateral boundary

$$\Omega = \{(x', y_n) \in \mathbf{R}^n \ ; \ x' = (x_1, \cdots, x_{n-1}) \in \mathcal{O} \ , \ 0 < y_n < \ h(x') \ \} \ ,$$
$$\Gamma = \{(x', y_n) \in \mathbf{R}^n \ ; \ x' = (x_1, \cdots, x_{n-1}) \in \partial\mathcal{O} \ , \ 0 < y_n < \ h(x') \ \}$$

The unknowns in the model are u^ε - the velocity , p^ε - the pressure , ρ^ε − the density. We suppose that the fluid is viscous and compressible and that the flow is

[1] 1000 to 5000 times thinner then a human hair

[2] the one obtained by taking the flying height as a characteristic distance

stationary. As usual, we use the ideal gas law $\rho = \frac{p}{R\,T}$ where T is the temperature [K] and R is the gas constant [J/kg K] (equals 287.05 for dry air).

Typically, in the engineering literature, the temperature variations in the thin film are treated as negligible (see e.g. [1], [3], [7]) and the temperature is supposed to be constant, i.e. equal to the ambiental temperature. Thus, we suppose that the flow is isothermal and, consequently, verifying the simple pressure-density relation $p^\varepsilon = a_\varepsilon\,\rho^\varepsilon$, where $a_\varepsilon = T_\varepsilon\,R > 0$ is a constant. To get the idea, on the room temperature (between 20 and 25 C^0) and the typical atmospheric pressure between 1000 and 1020 m bar, the value of a_ε would be of order 10^{-5}. We also neglect the inertial term, i.e. we assume that the Reynolds number $Re_\varepsilon \ll 1$. The total quantity of the fluid in the domain is prescribed and equal to $M_\varepsilon > 0$, i.e. $M_\varepsilon = \int_{\Omega_\varepsilon} \rho^\varepsilon(x)\,dx$.

The velocity of the relative motion of two surfaces is denoted by $\mathbf{V} \in H_0^1(\mathcal{O})^n$. Of course, we assume that $\mathbf{V} \perp \mathbf{e}_n$ with $\mathbf{e}_n = (0, \cdots, 0, 1)$. Our system then reads

$$-\mu\Delta u^\varepsilon - (\lambda+\mu)\nabla(\operatorname{div} u^\varepsilon) + \nabla p^\varepsilon = 0 \ , \ \operatorname{div}(\rho^\varepsilon\,u^\varepsilon) = 0 \ \text{ in } \ \Omega_\varepsilon \tag{1}$$

$$u^\varepsilon = 0 \ \text{ for } \ x_n = \varepsilon\,h(x') \ , \ u^\varepsilon = \mathbf{V} \ \text{ for } \ x_n = 0 \ , \ u^\varepsilon = 0 \ \text{ on } \ \Gamma_\varepsilon \ . \tag{2}$$

The problem is solvable and admits a solution $u^\varepsilon \in H^1(\Omega_\varepsilon)^n$, p^ε , $\rho^\varepsilon \in L^2(\Omega_\varepsilon)$ such that $\rho^\varepsilon \geq 0$ and $\int_{\Omega_\varepsilon} \rho^\varepsilon = M_\varepsilon$. The existence theorem for (1)-(2) can be found in [4], section 6.10, page 162 (except for the non-homogeneous boundary condition and the fact that we are dealing with a non-smooth domain but that can be handled). For our asymptotic analysis we need additional hypothesis $\lim_{\varepsilon\to 0} \varepsilon^2 a_\varepsilon \frac{M_\varepsilon}{|\Omega_\varepsilon|} = M$.

3. Asymptotic analysis

We first rewrite the problem on the fixed domain Ω by change of variables. We define

$$U^\varepsilon(x', y_n) = u^\varepsilon(x', \varepsilon\,y_n) \quad , \quad P^\varepsilon(x', y_n) = p^\varepsilon(x', \varepsilon\,y_n) \ . \tag{3}$$

We can then write the equation (1) in the form

$$-\mu\left(\frac{\partial^2 U_\alpha^\varepsilon}{\partial y_n^2} + \varepsilon^2\Delta_{x'}U_\alpha^\varepsilon\right) - (\lambda+\mu)\left(\varepsilon\,\frac{\partial^2 U_n^\varepsilon}{\partial y_n \partial x_\alpha} + \varepsilon^2\,\frac{\partial}{\partial x_\alpha}\operatorname{div}_{x'}U^\varepsilon\right) + \varepsilon^2\,\frac{\partial P^\varepsilon}{\partial x_\alpha} = 0, \qquad \alpha = 1, \ldots, n-1 \tag{4}$$

$$-\mu\left(\frac{\partial^2 U_n^\varepsilon}{\partial y_n^2} + \varepsilon^2\Delta_{x'}U_n^\varepsilon\right) - (\lambda+\mu)\left(\frac{\partial^2 U_n^\varepsilon}{\partial y_n^2} + \varepsilon\,\frac{\partial}{\partial y_n}\operatorname{div}_{x'}U^\varepsilon\right) + \varepsilon\,\frac{\partial P^\varepsilon}{\partial y_n} = 0 \tag{5}$$

$$\frac{\partial(P^\varepsilon\,U_n^\varepsilon)}{\partial y_n} + \varepsilon\operatorname{div}_{x'}(P^\varepsilon\,U^\varepsilon) = 0 \ \text{ in } \ \Omega \ , \tag{6}$$

We deduce by standard methods the following estimates for U^ε and P^ε
(7)

$$|U^\varepsilon|_{L^2(\Omega)} \leq C \ , \ \left|\frac{\partial U^\varepsilon}{\partial y_n}\right|_{L^2(\Omega)} \leq C \ , \ |\nabla_{x'} U^\varepsilon|_{L^2(\Omega)} \leq C\,\varepsilon^{-1} \ , \ \varepsilon^2\,|P^\varepsilon|_{L^2(\Omega)} \leq C \ .$$

3.1. **Passing to the limit.** Using the estimates (7), we conclude that there exist $U \in Y(\Omega) = \{W \in L^2(\Omega)\ ;\ \frac{\partial W}{\partial y_n} \in L^2(\Omega)\ \}$ and $P \in L^2(\mathcal{O})$ and a subsequences, denoted for simplicity by the same symbol $\{U^\varepsilon\}_{\varepsilon>0}$, $\{P^\varepsilon\}_{\varepsilon>0}$ such that

$$U^\varepsilon \rightharpoonup U \quad , \quad \frac{\partial U^\varepsilon}{\partial y_n} \rightharpoonup \frac{\partial U}{\partial y_n} \quad , \ \varepsilon^2\,P^\varepsilon \rightharpoonup P \ \text{ weakly in } \ L^2(\Omega) \ . \tag{8}$$

Furthermore

$$U(x',0) = \mathbf{V} \quad , \quad U(x',h(x')) = 0 \ . \tag{9}$$

With that we can only prove that the limit functions U and P satisfy the Reynolds equation

$$U = -\frac{1}{2\mu}\,y_n\,(h-y_n)\,\nabla_{x'}\,P + (1-\frac{y_n}{h(x')})\,\mathbf{V} \ . \tag{10}$$

Furthermore $P \in H^1(\mathcal{O})$. However to pass to the limit in the continuity equation we need a strong convergence either for the pressure or for the velocity. By decomposing the pressure $P^\varepsilon = \frac{1}{h}\int_0^h P^\varepsilon(x',y_n)\,dy_n + \Big(P^\varepsilon - \frac{1}{h}\int_0^h P^\varepsilon(x',y_n)\,dy_n\Big)$ we can prove that indeed

$$\varepsilon^2\,\frac{1}{h}\int_0^h P^\varepsilon dy_n \to P \quad \text{strongly in} \quad L^2(\mathcal{O}) \ .$$

We also get the estimate for the reminder in a norm worst then L^2 but better then H^{-1} :

$$\left|\,\varepsilon^2\int_\Omega (P^\varepsilon - \frac{1}{h}\int_0^h P^\varepsilon dy_n)\,\varphi\,\right| \leq C(\varepsilon\,|\varphi|_{L^2(\Omega)} + \varepsilon^3\,|\nabla_{x'}\,\varphi|_{L^2(\Omega)}\ ) \ , \ \varphi \in H_0^1(\Omega) \ .$$

It is sufficient to obtain the main result:

Theorem 2. *Let $(u^\varepsilon, p^\varepsilon)$ be the solution of the equations of motion (1)-(2) and let U^ε , P^ε be defined from it by change of variables (3). Then*

$$U^\varepsilon \ \to \ U \ \ \textit{weakly in} \ \ Y(\Omega) \tag{11}$$

$$\varepsilon^2 P^\varepsilon \ \to \ P \ \ \textit{strongly in} \ \ L^2(\Omega) \tag{12}$$

where (U,P) is a unique solution of the compressible Reynolds equations

$$U = -\frac{1}{2\mu}\,y_n\,(h-y_n)\,\nabla_{x'}\,P + (1-\frac{y_n}{h(x')})\,\mathbf{V} \tag{13}$$

$$\textit{div}_{x'}\,(P\,\overline{U}) = 0 \quad \textit{in} \ \ \mathcal{O} \ , \ \ P\,\overline{U}\cdot\mathbf{n} = 0 \ \ \textit{on} \ \ \partial\mathcal{O} \ , \ P \geq 0\,, \ \int_\Omega P = M\,|\Omega| \tag{14}$$

and $\overline{U}(x') = \int_0^{h(x')} U(x',\xi)\,d\xi$.

In case $n = 2$ Reynolds equation is an ODE and it can be solved explicitly. Assume that $V \geq 0$. We define the number $d = \frac{6\mu}{\int_0^1 h(t)dt} \int_0^1 h(t) \int_0^t \frac{V(s)\,ds}{h^2(s)}\ dt$. In case $M \geq d$ the solution has a form $P(x) = 6\mu \int_0^x \frac{V(s)\,ds}{h^2(s)} + M - d$. It is obviously smooth and strictly positive (except in case $M = d$, when $P(0) = 0$). In case $M < d$ we have a solution $P(x) = \begin{cases} 0 \text{ for } 0 \leq x \leq \overline{x} \\ 6\mu \int_0^x \frac{V(s)\,ds}{h^2(s)} + M - d \text{ for } x \geq \overline{x} \end{cases}$ where $\overline{x} \in]0,1[$ is the unique solution to the equation $\int_0^{\overline{x}} \frac{V(s)\,ds}{h^2(s)} = \frac{d-M}{6\mu}$. It is not smooth and equals zero on an interval.

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Computational Approaches for Flow through Stochastic Porous Media

Hermann G. Matthies

The flow through a porous medium is considered in a simple but prototypical setting. Knowledge about the conductivity of the soil, the magnitude of source-terms, or about the in- and out-flow boundary conditions is often very uncertain. These uncertainties inherent in the model result in uncertainties in the results of numerical simulations.

Stochastic methods are one way to model these uncertainties, and in our case we are concerned with spatially varying randomness, and model this by random fields [1, 75, 12]. If the physical system is described by a partial differential equation (PDE), then the combination with the stochastic model results in a stochastic partial differential equation (SPDE) [2]. The solution of the SPDE is again a random field, describing both the expected response and quantifying its uncertainty.

SPDEs can be interpreted mathematically in several ways. At the moment we concentrate on randomness in space. If evolution with stochastic input has to be

considered, one may combine the techniques described here with the already well established methods in that field [38]; for theoretical results, e.g. see [54].

One may distinguish—as in the case of stochastic ordinary differential equations (SDEs)—between additive and multiplicative noise. As is well known from SDEs, in the case of multiplicative noise one has to be more careful. A similar problem occurs here. Additive noise—particularly for linear problems—is well known and much simpler to deal with [40], even if the random fields are generalized to stochastic distributions. With multiplicative noise on the other hand the product of a random coefficient field and the solution may have no meaning [25]. As with SDEs, it is a modelling decision how this is resolved [38].

Additive noise corresponds to the case where the right hand side—the loading or the solution independent source term—is random, whereas when the operator is random, we have multiplicative noise. In the first case it is the external influences which are uncertain, in the latter it is the system under consideration itself. In general, both uncertainties are present.

In an engineering setting, these models have been considered in different fields, see for example [65, 15, 20, 24, 41, 42, 46, 48, 59]. Many different kinds of solution procedures have been tried, but mostly Monte Carlo methods have been used (e.g. [59, 15]). Alternatives to Monte Carlo methods, which first compute the solution and then the required statistic, have been developed in the field of stochastic mechanics—cf. [41, 42], for example perturbation methods, e.g. [37, 65, 46], methods based on Neumann-series, e.g. [3], or the spectral stochastic finite element-method (SSFEM), first proposed in [21]. The latter expands the input random fields in eigenfunctions of their covariance kernels, and obtains the solution by a Galerkin method in a space of stochastic ansatz functions. More information, references and reviews on stochastic finite elements can be found in [47, 66, 72, 67, 28, 52]. A somewhat specialized field is the area of structural reliability, e.g. see [14, 24].

A theory of SPDEs where products between random fields are interpreted as Wick [26] products was developed in [25]. This allows highly irregular random fields as coefficients, and obtains the solution as a stochastic Kondratiev distribution. Its main shortcoming is that—e.g. for linear problems—higher statistical moments of system parameters do not influence the mean of the solution, a contradiction to the results of homogenization theory. Another problem is the required existence of strong solutions [25] to the PDE. These may be relaxed by a variational formulation [74, 48, 73], but nonetheless the Wick product seems not to be the right model for the problems that we aim at.

For products interpreted in the usual sense, stronger regularity is required for the coefficient random fields [10], still allowing the stochastic part of the solution to be a Kondratiev distribution. A general variational setting for general randomness has been given in [33, 53]. More restricted models have been considered in [13, 3, 4, 5].

One direction of numerical investigation focuses on computing the moments of the solution, e.g. [2, 68, 69]. These are very common, but specific response

descriptors. Often other functionals of the solution may be desired. Monte Carlo (MC) methods can be used directly for this, but they require a high computational effort [11]. Variance reduction techniques are employed to reduce this somewhat. Quasi Monte Carlo (QMC) methods [11, 55] may reduce the computational effort considerably without requiring much regularity. But often we have high regularity in the stochastic variables, and this is not exploited by QMC methods. The problem of computing such high-dimensional integrals comes up as a subtask also in the stochastic Galerkin method which we pursue. The integrands are often very smooth, and MC and QMC methods do not take much advantage out of this, although some results in that direction are in [6, 7, 8].

For this subtask, we propose sparse grid (Smolyak) quadrature methods as an efficient alternative. These have first been described in [71], and have found increasing attention in recent years, e.g. [56, 57, 17, 23, 58, 63, 61, 62, 34].

The stochastic Galerkin methods started from N. Wiener's *polynomial chaos*, a term coined in [76]. This has been used extensively in the theoretical *white noise analysis* in stochastics, e.g. [25, 26, 44]. This device may of course also be used in the *simulation* of random fields [70, 64]. Methods which are not based on polynomial chaos but other expansions under additional assumptions are given in [13, 3, 4, 5], where also convergence is addressed. In [27, 77, 78, 79], different bases for the random variables are explored.

In general, the stochastic Galerkin methods allow a *direct* representation of the solution. Following [21], where they have been proposed as a numerical device, stochastic Galerkin methods have been applied to various linear problems, e.g. [22, 18, 19, 60, 49, 50, 51, 29, 16, 27, 77, 78, 79, 31, 32, 35, 36], using a variety of numerical techniques to accelerate the solution. Recently, nonlinear problems with stochastic loads have been tackled, e.g. [78], and some first results of both a theoretical and numerical nature for nonlinear stochastic operators are in [30]. A convergence theory in has been started in [74, 9, 73], but we are very much at the beginning.

These Galerkin methods allow us to have an explicit functional relationship between the independent random variables and the solution—and this is contrast with usual Monte Carlo approaches, so that subsequent evaluations of functionals—statistics like the mean, covariance, or probabilities of exceedance—are very cheap. This may be seen as a way to systematically calculate more and more accurate "response surfaces" [39].

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Homogenization of thin porous layers and applications to ion transport through channels of biological membranes

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(joint work with Willi Jäger)

Ion transport trough membranes is an important mechanism in regulating the ion concentrations inside and outside living cells. Mathematical models and simulations have to be used in order to study the ion transport more quantitatively. However, so far models are formulated mainly phenomenologically and the geometries are simplified, using compartmental (i. e. spatially one-dimensional) concepts or reducing the processes in 3d to surfaces or curves. Reduction to a lower dimensional geometry may be justified only under special assumptions, which are not justified for diffusion and transport of ions in living cells, see [3].

In our contribution the macroscopic behavior of membranes including channels will be derived rigorously from microscale models using the theory of asymptotic analysis and homogenization. We extend the classic notions of two scale convergence and localization method to sequences of functions defined on thin porous layers and prove compactness results with respect to the extended notions.

We start with the following microscopic model: consider two domains $\Omega_\varepsilon^\pm \subset \mathbb{R}^n$ modelling the intracellular and extracellular space, separated by the membrane $\Omega_\varepsilon^M \subset \mathbb{R}^n$ perforated by channels placed in periodically distributed cells. The thickness of the membrane and the diameter of the cells are of order ε, see Fig.1.

The transport of ions is modelled by the Nernst-Planck equations, properly scaled in the channels. Thus the unknowns of our model are the ion concentration u_ε and the electric potential ϕ_ε. In the membrane channels we consider an additional concentration of charges v_ε, partially fixed to the channels, which model the selectivity and gating properties of the channels. The restrictions of functions

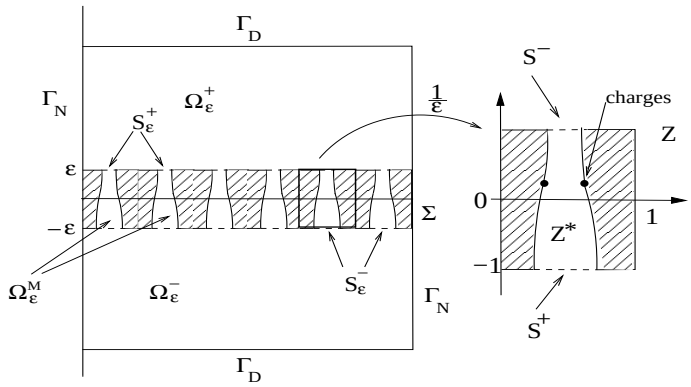

FIGURE 1. The domain Ω_ε and the standard cell Z.

defined on Ω to the subdomains Ω_ε^+, Ω_ε^-, and Ω_ε^M are denoted by the superscripts $+$, $-$, and M respectively. The equations modeling the ion transport are the following:

$$\begin{aligned}
\partial_t u_\varepsilon^\pm &= div\, j_\varepsilon^\pm && \text{in } (0,T)\times\Omega_\varepsilon^\pm\\
-div(\alpha^\pm \nabla\Phi_\varepsilon^\pm) &= z_u u_\varepsilon^\pm && \text{in } (0,T)\times\Omega_\varepsilon^\pm\\
j_\varepsilon^\pm\cdot\vec{\nu} &= 0 && \text{on } (0,T)\times(\partial\Omega^\varepsilon\setminus S_\varepsilon^\pm)\\
u_\varepsilon^\pm(0) &= u_0 && \text{on } \Omega_\varepsilon^\pm\\
\Phi_\varepsilon^\pm &= \Phi_D && \text{on } (0,T)\times\Gamma_D^\pm\\
\tfrac{\partial\Phi_\varepsilon^\pm}{\partial\vec{\nu}} &= 0 && \text{on } (0,T)\times(\partial\Omega^\varepsilon\setminus(\Gamma_D^\pm\cup S_\varepsilon^\pm))\\
\partial_t u_\varepsilon^M &= div\, j_\varepsilon^M && \text{in } (0,T)\times\Omega_\varepsilon^M\\
\partial_t v_\varepsilon^M &= div\, f_\varepsilon^M && \text{in } (0,T)\times\Omega_\varepsilon^M\\
-div(\varepsilon\alpha^M\nabla\Phi_\varepsilon^M) &= \tfrac{1}{\varepsilon}(z_u u_\varepsilon^M + z_v v_\varepsilon^M) && \text{in } (0,T)\times\Omega_\varepsilon^M\\
j_\varepsilon^M\cdot\vec{\nu} &= 0 && \text{on } (0,T)\times[\partial\Omega_M^\varepsilon\setminus(S_\varepsilon^+\cup S_\varepsilon^-)]\\
u_\varepsilon^M(0) &= u_0 && \text{on } \Omega_\varepsilon^M\\
\tfrac{\partial\Phi_\varepsilon^M}{\partial\vec{\nu}} &= 0 && \text{on } (0,T)\times[\partial\Omega_M^\varepsilon\setminus(S_\varepsilon^+\cup S_\varepsilon^-)]
\end{aligned}$$

The fluxes are defined as follows:

$$\begin{aligned}
j_\varepsilon^\pm &= -D^\pm(\nabla u_\varepsilon^\pm + \mu z_u\cdot u_\varepsilon^\pm\nabla\Phi_\varepsilon^\pm)\\
j_\varepsilon^M &= -\varepsilon D^M(\nabla u_\varepsilon^M + \mu z_u\cdot u_\varepsilon^M\nabla\Phi_\varepsilon^M)\\
f_\varepsilon^M &= -\varepsilon K^M(\nabla v_\varepsilon^M + \mu z_v\cdot v_\varepsilon^M\nabla\Phi_\varepsilon^M + v_\varepsilon^M\cdot\nabla\gamma_\varepsilon)
\end{aligned}$$

We see that the flux for v_ε contains an extra term modelling a retractive force (e.g. Hook-type law). For the ion concentrations u_ε and the potential Φ_ε we impose natural transmission conditions on S_ε^+ and S_ε^-.

In the limit $\varepsilon\to 0$ the membrane modeled by the thin porous layer Ω_ε^M reduces to the interface Σ between the intracellular and extracellular spaces Ω^+ and Ω^-

respectively and the important feature is to determine the appropriate transmission conditions for the limit concentrations across this interface. The first step in doing this is to prove a priori estimates of the solutions in properly chosen function spaces. Based on this a priori estimates and on the extensions of two scale convergence and localization method to thin porous layers, we can proof convergence for subsequences of $u_\varepsilon, \phi_\varepsilon, v_\varepsilon$ to limit functions u_0, ϕ_0, v_0 with respect to the adequate topology. Finally we can prove the main result of our paper:

Theorem 1. *The limit functions $\phi_0^\pm, u_0^\pm$ satisfy the Nernst-Planck-equations on the domains $\Omega^\pm$ together with the following effective transmission conditions on the interface Σ*

$$\begin{aligned}
[\Phi_0]_\Sigma := (\Phi_0^+ - \Phi_0^-)(t,\bar{x},0) &= \int_{Z^*} v_0(t,\bar{x},y)\eta(y)dy \\
&+ |Z^*|(\alpha^+\eta^+\partial_3\Phi_0^+(t,\bar{x},0) - \alpha^-\eta^-\partial_3\Phi_0^-(t,\bar{x},0)) \\
(\partial_3\Phi_0^+ - \partial_3\Phi_0^-)(t,\bar{x},0) &= -\int_{Z^*} v_0(t,\bar{x},y)dy
\end{aligned}$$

$$\begin{aligned}
(j_0^+\cdot\nu - j_0^-\cdot\nu)(t,\bar{x},0) &= 0 \quad \textit{i.e. the normal flux is continuous on } \Sigma \\
(j_0^M\cdot\nu)(t,\bar{x},y) &= c_j(j_0^+\cdot\nu)(t,\bar{x}) \quad \textit{for } y\in S^+\cup S^-
\end{aligned}$$

The values η^+ and η^- are the constant values on S^+ and S^- of the boundary layer function $\eta \in V = \left\{\varphi \in H^1(Z^*), \varphi = \textit{const on } S^+ \textit{and } S^-\right\}$, with zero mean value on Z^*, satisfying for all $\varphi \in V$

$$\int_{Z^*} \alpha^M \nabla\eta(y)\nabla\varphi(y)dy = \frac{1}{|S^+|}\int_{S^+}\varphi(y)ds - \frac{1}{|S^-|}\int_{S^-}\varphi(y)ds.$$

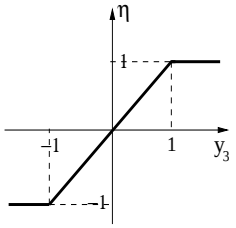

FIGURE 2. The boundary layer function η for Z^* of cylindrical shape.

The limit functions ϕ_0^M, u_0^M and v_0^M which enter the transmission conditions are the solutions of the following local problems:

$$\begin{aligned}
-\Delta_y\Phi_0^M(t,\bar{x},y) &= c_v^M v_0^M(t,\bar{x},y), \ \textit{in } [0,T]\times\Sigma\times Z^* \\
\Phi_0^M(t,\bar{x},y) &= \Phi_0^+(t,\bar{x}), \quad \textit{if } y\in S^+ \\
\Phi_0^M(t,\bar{x},y) &= \Phi_0^-(t,\bar{x}), \quad \textit{if } y\in S^- \\
(\nabla\Phi_0^M\cdot\nu)(t,\bar{x},y) &= 0, \ \textit{on } \partial Z^*\setminus(S^+\cup S^-)
\end{aligned}$$

$$\begin{aligned}
\nabla_y(D_u^M\nabla_y u_0^M + K_u^M u_0^M \nabla_y \Phi_0^M)(t,\bar{x},y) &= 0,\ in\ [0,T]\times\Sigma\times Z^* \\
u_0^M(t,\bar{x},y) &= u_0^+(t,\bar{x}), \quad if\, y\in S^+ \\
u_0^M(t,\bar{x},y) &= u_0^-(t,\bar{x}), \quad if\, y\in S^- \\
(\nabla u_0^M\cdot\nu)(t,\bar{x},y) &= 0,\ on\ \partial Z^*\setminus(S^+\cup S^-)
\end{aligned}$$

$$\begin{aligned}
\nabla_y(D_v^M\nabla_y v_0^M + K_v^M v_0^M\nabla_y\Phi_0^M + v_0^M\nabla_y\gamma) &= 0, \quad in\ [0,T]\times\Sigma\times Z^* \\
(D_v^M\nabla_y v_0^M + K_v^M v_0^M\nabla_y\Phi_0^M + v_0^M\nabla_y\gamma)\cdot\nu &= 0, \quad on\,\partial Z^*
\end{aligned}$$

$$\int_{Z*} v_0^M(y) = c \quad \textit{(conservation of charge)}$$

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A non-equilibrium statistical mechanics approach to effective theories of domain coarsening

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(joint work with A. Hönig, F. Otto, J. Velázquez)

Background. In Ostwald Ripening, a fundamental process in the aging of materials, many small particles of one phase embedded in another phase interact by diffusional exchange to reduce the total interfacial area of the particles. Experiments indicate that this process evolves after an initial transient time in a statistically self-similar universal manner.

In the classical theory by Lifshitz, Slyozov and Wagner (LSW) [2] it is argued in the regime of low volume fraction that the particles interact only via a spatially constant mean-field u_∞ which is determined by the constraint that the volume fraction of particles is conserved. This approach yields a nonlocal evolution law for the particle radius distribution:

$$\partial_t f + \partial_R\Big(\frac{1}{R^2}(Ru_\infty - 1)\, f\Big) = 0,$$

where u_∞ is such that $\int R^3 f(R)\, dR = const$, that is $u_\infty = \frac{\int f(R)\, dR}{\int Rf(R)\, dR}$.

Self-similar solutions. The above non-local transport equation has indeed a one-parameter family of self-similar solutions with compact support. LSW predict in their classical theory that one particular of those profiles characterizes the large-time behavior of all solutions.

Disadvantages of mean-field theory. It has been shown, however, that the long-time behavior of the LSW-equation is not at all universal but depends very sensitively on the data [4]. Roughly speaking, the dynamics are determined by the details of the initial distribution of largest particles. Furthermore, a second problem within the classical LSW-theory is that all self-similar profiles and the corresponding coarsening rates do not well agree with experiments.

Higher order corrections. It is common belief that these inconsistencies of the LSW model can be resolved by taking the finiteness of the volume fraction of particles into account. In the LSW approach the underlying assumption is that each particle communicates in the same way with all other particles. This however neglects screening, which implies that a particle effectively only communicates with particles in a certain range, the screening length. The correction term due to this effect is of order $\phi^{1/2}$, the ratio between mean particle size and screening length. In [1] we develop an efficient method to identify first order corrections and derive a self-consistent theory in the framework of statistical mechanics which closes at the level of the two-particle distribution function. This analysis recovers a result by Marder [3] under natural assumptions on the data, whereas Marder makes an ad-hoc assumption on the solution of the system itself. However, it is presently not clear whether the resulting theory overcomes the weak selection problem of self-similar asymptotic states.

Are collisions relevant? A second mechanism which induces corrections to the mean-field model are collisions between particles. This effect was already considered in the original work [2], but a careful analysis of the order of size of the corresponding corrective terms has not been made. On a first glance, the effect of particle collisions is smaller than the corrections due to screening since the fraction of particles involved in collisions is proportional to ϕ. However, it turns out that the relative size of the corrective terms are not the same for all particles, but that they are larger for the largest particles in the system. Since those largest particles determine the coarsening dynamics for large times, this effect is crucial. In [5] it is conjectured that the effect of collisions between particles is the dominating effect which drives the particle system toward a unique self-similar state. This theory is thus somewhat similar in spirit to the Boltzmann equation for gas dynamics.

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Dissolution and precipitation processes in porous media: a pore scale model

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(joint work with C. J. van Duijn, V. M. Devigne)

We discuss a micro–scale model for precipitation and dissolution processes in a porous medium. The void region is occupied by a fluid in which cations and anions are dissolved. Under certain conditions, these ions can precipitate and form a crystalline solid, which is attached to the surface of the grains (the porous skeleton) and thus is immobile. The reverse reaction of dissolution is also possible.

This model is considered in [1] and represents the pore–scale analogue of the one proposed in [4]. It builds on several components: the Stokes flow in the pores, the transport of dissolved ions by convection and diffusion, and dissolution/precipitation reactions on the surface of the porous skeleton (grains).

General reactive porous media flow models, are surveyed, for example, in [3]. The particularity of the model considered here is in the description of the dissolution and precipitation processes taking place on the surface of the grains, involving a multi–valued dissolution rate function. In mathematical terms, this translates into a graph–type boundary condition that couples the convection–diffusion equation for the concentration of the ions to an ordinary differential equation defined only on the grain boundary and describing the concentration of the precipitate.

Our main interest is focused on the chemistry, this being the challenging part of the model. To be specific, we denote by Ω the void space of the porous medium. Its boundary has an internal part (Γ_G), which is the surface of the porous skeleton (the grains), and an external part $\Gamma_D \bigcup \Gamma_N$, which is the outer boundary of the domain.

Let $\vec{q}$ be the fluid velocity. We assume that the flow geometry, as well as the fluid properties are not affected by the chemical processes. Then $\vec{q}$ can be determined by solving the Stokes system, which is completely decoupled from the other components of the model. Having computed $\vec{q}$, we can determine c, the electric charge inside the fluid. This is defined as the linear combination of the concentrations of the two ions, the valences acting as coefficients. The reason for doing so is twofold. First, c satisfies a linear convection diffusion equation with standard boundary conditions. This equation depends only on $\vec{q}$, and therefore can be decoupled from the remaining part of the model. Next, once c is known, we can give up the - say - anion concentration, which can be easily obtained after the cation concentration u is determined. In this way we can restrict our investigations to the reduced set of equations modeling the chemistry:

$$\begin{cases} \partial_t u + \nabla \cdot (\vec{q}u - D\nabla u) = 0, & \text{in } (0,T)\times\Omega, \\ -D\vec{\nu}\cdot\nabla u = \varepsilon n \partial_t v, & \text{on } (0,T)\times\Gamma_G, \\ u = u_D, & \text{on } (0,T)\times\Gamma_D, \\ \vec{\nu}\cdot\nabla u = 0, & \text{on } (0,T)\times\Gamma_N, \\ u = u_I, & \text{in } \Omega, \text{ for } t=0, \end{cases}$$

for the ion transport, and

$$\begin{cases} \partial_t v &= Da(r(u,c)-w), & \text{on } (0,T)\times\Gamma_G,\\ w &\in H(v), & \text{on } (0,T)\times\Gamma_G,\\ v &= v_I, & \text{on } \Gamma_G, \text{ for } t=0, \end{cases}$$

for the precipitation and dissolution. Here v denotes the concentration of the precipitate, which is defined only on the interior boundary Γ_G. The precipitation rate r is a positive locally Lipschitz continuous function, increasing in u and decreasing in c. By H we mean the Heaviside graph, and w is the actual value of the dissolution rate.

All the quantities and variables in the above are dimensionless. D denotes the diffusion coefficient (the same for both ions) and n the cation valence. Da represents the ratio of the characteristic precipitation/dissolution time scale and the time scale related to the diffusion - the Damköhler number, which is assumed to be of moderate order. By ε we mean the ratio of the characteristic pore scale and the reference (macroscopic) length scale.

A first result is given for general domains. Using regularization techniques and a fixed point argument, we obtain the existence of a weak solution. This solution is positive in both components u and v, which are also essentially bounded. Moreover, assuming that the medium is ε–periodic, the estimates for energy are also ε independent.

Further results are obtained for a simple geometry, a strip. Assuming a parabolic flow profile, with dissolution and precipitation occurring at the lateral boundaries, we investigate the formation of dissolution and precipitation fronts. Any of such fronts is located at a free boundary separating a region where the precipitate is present from another one where no crystals are encountered. A detailed analysis is carried out for the undersaturated regime, where an initially in equilibrium system with crystals uniformly distributed on the grain boundary is perturbed by injecting an undersaturated fluid. Then a dissolution process is initiated, and after a waiting time t^* a dissolution front will start moving in the flow direction. The associated free boundary is continuous and strictly increasing at any time beyond t^*.

As a first step towards a rigorous justification of a macro–scale model we let the ratio between the thickness and the length of the strip go to 0. In the limit we end up with the upscaled transport–reaction model proposed in [4], for which we can prove the existence and uniqueness of a solution in one spatial dimension. In the same context we mention the rigorous analysis performed in [5], where the influence of some simpler chemical processes on the effective parameters is investigated in the transport dominated flow regime.

In [2] we continue investigating the model from a numerical point of view. To be specific, we analyze the convergence of a time discretization method for the coupled system given above. The scheme is of first order, implicit in u and explicit in v. Moreover, to overcome the difficulties posed by the multi–valued dissolution rate, we approximate this by a monotone continuous rate H_δ, where $\delta > 0$ is taken to be of order $\tau^{1/2}$. In this setting, if u^p and v^p are approximating $u(p\tau)$,

respectively $v(p\tau)$, and assuming u^{p-1} and v^{p-1} given, the scheme can be written formally as

$$\left\{\begin{array}{rcll} u^p - u^{p-1} & = & \tau D\triangle u^p - \tau\nabla(\vec{q}\,u^p) & \text{in } \Omega, \\ -\tau\vec{\nu}\cdot(D\nabla u^p) & = & \epsilon n(v^p - v^{p-1}) & \text{on } \Gamma_G, \\ v^p - v^{p-1} & = & \tau Da(r(u^p) - H_\delta(v^{p-1})) & \text{on } \Gamma_G \\ w^p & = & H_\delta(v^p) & \text{on } \Gamma_G \end{array}\right.$$

In [2] we show that the numerical scheme is stable in both the L^∞ and the energy norms. By compactness arguments we obtain convergence to a weak solution of the model.

Finally, we notice that at each time step we have to solve a nonlinear elliptic problem in u. In doing so we make use of a fixed point type linear iteration procedure

$$\left\{\begin{array}{rcll} u^{p,i} - u^{p-1} & = & \tau D\triangle u^{p,i} - \tau\nabla(\vec{q}\,u^{p,i}), & \text{in } \Omega, \\ -D\vec{\nu}\cdot\nabla u^{p,i} & + & L_r\varepsilon nDa\ u^{p,i} & \\ & = & \varepsilon nDa\left\{L_r u^{p,i-1} + r(u^{p,i-1}) - H_\delta(v^{p-1})\right\}, & \text{on } \Gamma_G. \end{array}\right.$$

This iteration has a linear convergence rate, but is unconditionally stable. Moreover, as i goes to infinity, $u^{p,i}$ approaches u^p regardless of the initial iteration.

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An efficient numerical scheme for precise time integration of a dissolution/precipitation chemical system

Jérome Pousin

(joint work with B. Faugeras)

The multi-species diffusion-dissolution/precipitation model takes the form of an initial-boundary value problem in which partial differential equations (PDEs) and ordinary differential equations (ODEs) are coupled through nonlinear discontinuous terms. The reader is referred to [6], [5] for the derivation of the model and its mathematical analysis. The system of equations for N_s species is formulated as follows. $\mathbf{C} = (C_i)_{i=1,\dots N_s}$ is the vector of chemical species concentrations in liquid phase and $\mathbf{S} = (S_i)_{i=1,\dots N_s}$ is the vector of chemical species concentrations in solid

phase. C_i^* are nonlinear functions of C representing saturation concentrations, α_i and D_i are strictly positive constants. The following notations are also used

$$\forall z \in \mathbb{R},\ z^+ = max(z,0) \text{ and } z^- = z^+ - z \geq 0,$$

and

$$sgn^+(z) = \begin{cases} 1 \text{ if } z > 0, \\ 0 \text{ otherwise.} \end{cases}$$

For $i = 1$ to N_s we have:

$$(1) \quad \begin{cases} \partial_t C_i = D_i \Delta C_i + sgn^+(S_i)\alpha_i(C_i^*(C) - C_i)^+ \\ \qquad\qquad -\alpha_i(C_i^*(C) - C_i)^- & \text{in } (0,T)\times\Omega, \\ \partial_t S_i = -sgn^+(S_i)\alpha_i(C_i^*(C) - C_i)^+ \\ \qquad\qquad +\alpha_i(C_i^*(C) - C_i)^- & \text{in } (0,T)\times\Omega, \\ C_i(0,x) = C_i^0(x) > 0,\ S_i(0,x) = S_i^0(x) > 0 & \text{in } \Omega, \\ C_i(t,x) = 0 & \text{in } (0,T)\times\partial\Omega. \end{cases}$$

The purpose of this talk is to present an efficient numerical scheme of order 2 in time to integrate systems such as system (1). We propose a scheme combining an operator splitting method [8], [7], and an event location algorithm using a dense output formula [4] which enables us to determine the switching times at which the discontinuities occur in the reaction terms with a desired accuracy. Throughout this talk we consider a semi-discretized system of equations. Indeed a difficulty appears in the fully continuous case, since the switching time, t_d, is an unknown function of x, the space variable. We thus consider that the chemical system is already discretized in space, using, for example, a finite difference or a finite element method. The system of ODEs we consider then reads

$$(2) \quad \begin{cases} \dfrac{d\mathbf{C}}{dt} = \mathbf{A}\mathbf{C} + \mathbf{F}(\mathbf{C},\mathbf{S}), \\ \dfrac{d\mathbf{S}}{dt} = -\mathbf{F}(\mathbf{C},\mathbf{S}), \\ \mathbf{C}(0) = \mathbf{C}_0,\ \mathbf{S}(0) = \mathbf{S}_0. \end{cases}$$

$\mathbf{C}$ and $\mathbf{S}$ are vectors of $\mathbb{R}^N$ and $\mathbf{A}$ is the $N \times N$ matrix resulting from the spatial discretization of the Δ operator which is symmetric negative definite. The nonlinear terms read

$$\mathbf{F}(\mathbf{C},\mathbf{S}) = (F_k(\mathbf{C},\mathbf{S}))_{k=0,\ldots N},$$

with

$$(3) \quad F_k(\mathbf{C},\mathbf{S}) = \begin{cases} G_k^1(\mathbf{C}), \text{ if } S_k > 0, \\ G_k^2(\mathbf{C}), \text{ if } S_k \leq 0. \end{cases}$$

We describe the scheme we propose, combining an operator splitting method analyzed in [1] for the following reaction diffusion system

$$(4) \quad \begin{cases} \dfrac{d\mathbf{C}}{dt} = \mathbf{A}\mathbf{C} + \mathbf{G}(\mathbf{C}),\ t > 0 \\ \mathbf{C}(0) = \mathbf{C}_0, \end{cases}$$

and an adaptation of the event location algorithm. We prove that the scheme is of order 2, and its effectiveness is illustrated numerically [3]. Let us mention that a similar case where the chemical reactions are at equilibrium have been considered in [2].

Let us illustrate our results by a numerical experiment with a simple test case. We consider the following system of equations :

$$\left\{\begin{array}{lll} \partial_t C = \Delta C + \alpha C(1-C) & \text{if } S > S_d \\ \quad\;\; = \Delta C + \beta C & \text{if } S \leq S_d \\ \partial_t S = -\alpha C(1-C) & \text{if } S > S_d \\ \quad\;\; = -\beta C & \text{if } S \leq S_d \end{array}\right. \tag{5}$$

where α, β and S_d are constants. Initial and boundary conditions for C are determined by the exact solution, $C = (1/1 + \exp(\sqrt{\frac{\alpha}{6}}x - \frac{5}{6}\alpha t))^2$ to Fisher's equation,

$$\partial_t C = \Delta C + \alpha C(1-C).$$

Initial conditions for S are given by $S(0,x) = 1 + \exp(-(x-1/2)^2)$. The diffusion operator is discretized using second order finite differences with a step size of 10^{-2} and its time integration is performed using the unconditionally stable second order Crank Nicolson scheme. Reaction terms are integrated with a second order explicit Runge-Kutta scheme. A reference solution is computed for the classical splitting method and for the method proposed in this paper with a time step $h_{ref} = \dfrac{0.1}{2^{14}}$. Solutions are computed using 5 different time steps, $h = \dfrac{0.1}{2^9}, \dfrac{0.1}{2^{10}}, \dfrac{0.1}{2^{11}}, \dfrac{0.1}{2^{12}}$ and $h = \dfrac{0.1}{2^{13}}$. For each solution the global errors

$$E_C = ||\mathbf{C}_h(T) - \mathbf{C}_{h_{ref}}(T)||,\ E_S = ||\mathbf{S}_h(T) - \mathbf{S}_{h_{ref}}(T)||,$$

are computed at $T = 0.1$. Figure 1 shows $-\log(E_C)$ and $-\log(E_S)$ versus $-\log(h)$ when the classical splitting method is used to compute the solution to problem (5). The convergence curve is very perturbed and the estimated order of the scheme is less then 1. This is not surprising since the method is not able to deal with the discontinuities correctly. On the other hand Figure 2 shows $-\log(E_C)$ and $-\log(E_S)$ versus $-\log(h)$ when the method proposed in this paper is used. The estimated order is about 2, which is in agreement with the theoretical result.

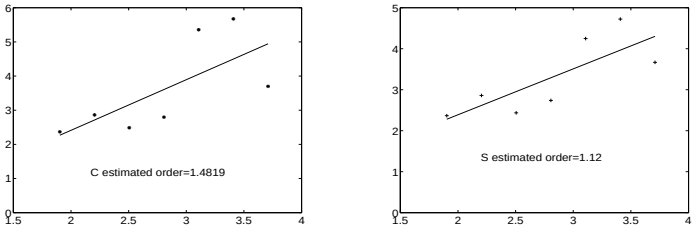

FIGURE 1. $-log(E)$ versus $-log(h)$. Convergence curve for the classical splitting (left C and right S).

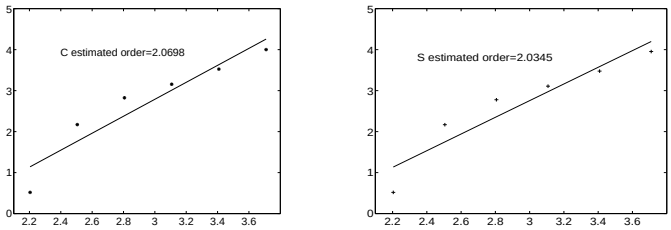

FIGURE 2. $-log(E)$ versus $-log(h)$. Convergence curve for the proposed scheme (left C and right S).

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On capillary hysteresis in porous media and the averaging of a play-type hysteresis model

BEN SCHWEIZER

1. PHYSICAL BACKGROUND ON CAPILLARY HYSTERESIS

We are interested in the description of partially saturated porous media. For definiteness, let us consider a medium filled with water and air, and let us assume that the air has a constant pressure. Our aim is to describe the flow of water in this medium. We include the well-known effect of capillary hysteresis.

The standard description of the macroscopic properties of the medium uses the two quantities water pressure and water saturation, $p(x,t)$ and $u(x,t)$. For the

velocity $v(x,t) \in \mathbb{R}^N$ one assumes the Darcy law in the form $v = -K\nabla p$, here we assume a linear relation. Conservation of mass then reads

$$\partial_t u = \nabla \cdot (K \nabla p). \tag{1}$$

To close the system we need a relation between p and u. Thinking of a porous medium whose pores are straight cylindrical tubes with different radii, one imposes a relation $p(x,t) = p_c(x, u(x,t))$ with a given monotone function $p_c(x,.) : [0,1] \to \mathbb{R}$. The physical reasoning is as follows: If an interface water-air is situated in a pore with radius d, then the interface is a spherical cap with radius R determined by d and the contact angle, R is increasing with d. The pressure jump between the two phases (and hence the pressure p) is proportional to the mean curvature $1/R$, hence a function of d. At a higher saturation, smaller pores must be filled (for a non-wetting fluid), hence $1/R$ increases.

The shortcoming of the above reasoning is the assumption of cylindrical pores. As soon as one considers e.g. ondulated tubes, the interfaces have different curvatures depending on the position in the pore. During imbibition ($\partial_t u(x,t) > 0$), the fronts spend most time at the bottle-necks and the pressure jump is large, instead, during drainage ($\partial_t u(x,t) < 0$), the fronts spend most time at positions of large diameter and the pressure jump is small. This effect is made precise in [4], [5], it leads to two distinct curves $p_c^{\pm}(x,.) : [0,1] \to \mathbb{R}$ describing the pressure-saturation relation in the two cases $\pm\partial_t u > 0$. For $\partial_t u = 0$ and for given u, the pressure $p(x,t)$ may take any value in the interval $[p_c^-(x,u), p_c^+(x,u)]$. The simplest model to describe this behavior is the play-type hysteresis [7], investigated by Beliaev in [2], [1],

$$p \in au + b + \gamma\,\mathrm{sign}(\partial_t u). \tag{2}$$

Here, the parameters a, b, and $\gamma > 0$ are scalars that may depend on the spatial variable x, and sign is the multivalued function $\mathrm{sign}(\xi) = \pm 1$ for $\pm\xi > 0$, $\mathrm{sign}(0) = [-1,1]$. The system must be closed with appropriate initial and boundary conditions.

From a physical point of view and for a constant coefficient γ, the above equations are not satisfactory since the *scanning curves* are vertical lines: One can, at constant saturation, increase or decrease the pressure. The process can be reversed and leads to identical points in the u-p-plane. We will see that a homogenization of the equations for highly oscillatory coefficients leads to different and more physical equations.

2. The averaged play-type hysteresis model

On the coefficients we assume the following: On each cube of the form $\varepsilon(q + (0,1)^N)$ with $q \in \mathbb{Z}^N$ the coefficient functions K, a, b, and γ are constant. The values on each cube are random variables and we assume for each coefficient that, on different cubes, the values are independent and identically distributed. We assume that K has a positive lower bound and, for simplicity, that the values of γ are uniformly distributed in $[0,1]$. For fixed ε, the solution to the above problem

is denoted by $(u^\varepsilon, p^\varepsilon)$ and we are interested in bulk equations describing a weak limit (u^0, p^0).

Let us try to guess a limiting equation. Our first goal is to find non-oscillating quantities. Since the gradient of the pressures p^ε is uniformly bounded in an L^2-space, the pressure can be considered as non-oscillating. The other quantities such as u^ε, $a^\varepsilon u^\varepsilon$, or $a^\varepsilon u^\varepsilon + b^\varepsilon$ are all oscillating. Still, the last quantity, we call it $w^\varepsilon := a^\varepsilon u^\varepsilon + b^\varepsilon$, has an interesting property. To begin with, assume that $\partial_t u^\varepsilon$ is negative all the time. In this case we have $w^\varepsilon = p^\varepsilon + \gamma^\varepsilon$, and the oscillations of w^ε are only due to the oscillations of γ^ε. If we plot the value of w^ε in a cell against the value of $y = \gamma^\varepsilon$ in the same cell, we find $w^\varepsilon(x, y, t) = p^\varepsilon(x, t) + y$.

Let us now assume that the situation is changed to imbibition, that is, to $\partial_t p^\varepsilon > 0$. Then, in cells with small value of $y = \gamma^\varepsilon$, the saturation must follow the evolution of the pressure. Therefore, in a vicinity of $y = 0$, the function w^ε satisfies $w^\varepsilon(x, y, t) = p^\varepsilon(x, t) - y$. In cells with values of γ^ε above some threshold $s(t)$, the pressure increase does not result in an increase of the saturation, hence w^ε remains at the previous level. The function w encodes the relevant information on the history of the process. A curve w as in Figure 1 is generated e.g. by a drainage process, followed by an imbibition process increasing the pressure by $2s(t)$.

Based on these considerations, we guess the averaged system to be as follows. We seek for functions $u(x, t)$, $p(x, t)$, $w(x, y, t)$ satisfying

$$u(x,t) = \int_0^1 \frac{w(x,y,t) - b^*}{a^*}\, dy \qquad \forall x \in \Omega, t \in (0,T), \tag{3}$$

$$\partial_t u = \nabla \cdot (K^* \nabla p), \tag{4}$$

$$p(x,t) \in w(x,y,t) + y\,\mathrm{sign}(\partial_t w(x,y,t)) \qquad \forall x \in \Omega, y \in [0,1], t \in (0,T). \tag{5}$$

Here, (3) expresses that we can recover the averaged saturation u from the values of w by averaging, using the expected values

$$a^* := \left\langle a^{-1} \right\rangle^{-1}, \quad b^* := \langle b \rangle .$$

Equation (4) is the standard homogenization limit of the original conservation equation where the matrix K^* can be found by solving a stochastic cell-problem [3]. Equation (5) expresses the algebraic side condition in the different cells. The following theorem is made precise and proved in [6].

Theorem. *Let a sequence of stochastic geometries be given and let $(u^\varepsilon, p^\varepsilon)$ be a strong solution of the ε-equations (1)–(2) with appropriate initial and boundary conditions. Let furthermore (u, p, w) be a strong solution of the limit system (3)–(5) with appropriate initial and boundary values. Then, for any sequence $\varepsilon \to 0$, almost surely we find*

$$p^\varepsilon \rightharpoonup p \text{ in } H^1((0,T), H^1(\Omega)),$$
$$u^\varepsilon \overset{*}{\rightharpoonup} u \text{ in } L^\infty((0,T), L^2(\Omega)).$$

The theorem verifies that the oscillations in the parameter γ introduce an additional independent and an additional dependent variable in the limit system. In

some sense, γ is replaced by the independent variable y in the system. In particular, the scanning curves are qualitatively different in the limit system: Increasing or decreasing the pressure instantaneously results in an increase or decrease of the saturation, hence the scanning curves are no longer straight lines. Furthermore, changing from imbibition to drainage, we never follow the original path. One effect of the hysteresis in the limit system is the irreversibility.

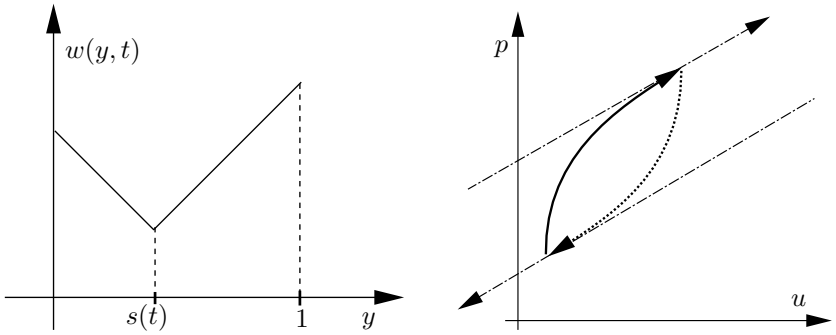

FIGURE 1. a) The function $w(., t)$ b) scanning curves of the limit system

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Front Propagation in Heterogeneous Media

ANGELA STEVENS
(joint work with Fathi Dkhil, Steffen Heinze, George Papanicolaou)

In [1] a variational characterization of front speeds for reaction-diffusion-advection equations in periodically varying heterogeneous media was given. This formulation allows to calculate sharp estimates for the speed explicitly and the method can be applied to any problem obeying a maximum principle. In examples the effects of the inhomogeneous medium on the speed can be analyzed in comparison to

the related homogeneous problem, thus for instance for shear flows in cylinders as they appear e.g. in the study of premixed flame propagation where an underlying flow field is given.

As a heuristic rule it is known that turbulence increases the effectiveness of combustion. In [1] it was rigorously proved that the introduction of a small amplitude drift coefficient always enhances the front speed. Also, an explicit speed estimate could be provided which is accurate in the small amplitude limit and the rapid oscillation limit.

For the discretized version of the Nagumo equation with an exact cubic reaction term is can be shown that a weaker coupling of the nerve cells in the model slows down the propagation of the action potential in comparison to the related continuous model. The expansion of the speed can be calculated explicitly up to second order.

Diffusion in heterogeneous media or multiscale problems is very common in applications and can frequently be described by its effective behavior. During an averaging or homogenization process the often complicated small scale structure of the problem is replaced by an asymptotically equivalent homogeneous structure. In [1] for reaction-diffusion models with general rapidly oscillating diffusion and drift coefficients the formal asymptotic expansion of the speed could be rigorously justified in the fast oscillation limit and the deviation of the speed in comparison to the homogenized problem could be calculated. In [3] a detailed look on specific problems was taken, since the speed of the wave can often not be clarified by its first order expansion in terms of space periodicity, especially not when the diffusion matrix is symmetric. Detailed examples are given where the effects of the symmetric and antisymmetric part on the wave speed are explored.

In [2] a nonlocal integro-differential equation is considered for which unique stable traveling waves exist, as well as for the related classical reaction diffusion model and combinations of both, for certain bistable nonlinearities. It was shown how small perturbations with a nonlocal term affect the speed of the original reaction-diffusion problem. By deriving an asymptotic expansion for the wave speed and calculating the parameters in terms of the non-local part of the equation a discrimination of its effects on the wave speed becomes possible. For exact bistable nonlinearities explicit examples are given, which show, that if the non-local term has small support the absolute value of the wave speed of the mixed problem is slowed down and thus the non-local term has little effect in comparison with simple diffusion. On the other hand the wave speed is enhanced for nonlocal terms with support far away from zero. Thus in this case the effect of the non-local term is strong in comparison with simple diffusion.

Further important related literature is given in the reference lists of the below mentioned articles.

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Spectral Collocation for Partial Differential Equations with Random Coefficients

Raúl Tempone
(joint work with Ivo Babuska and Fabio Nobile)

This work proposes and analyzes a Stochastic-Collocation method to solve elliptic Partial Differential Equations with random coefficients and forcing terms depending on a finite number of random variables. The method consists in a Galerkin approximation in space and a collocation in the zeros of suitable tensor product orthogonal polynomials (Gauss points) in the probability space and naturally leads to the solution of uncoupled deterministic problems as in the Monte Carlo approach. It can be seen as a generalization of the Stochastic Galerkin method proposed in [1], yet allows one to treat easily a wider range of situations, such as: input data that depend non-linearly on the random variables, diffusivity coefficients with unbounded second moments, random variables that are correlated or have unbounded support. In what follows we present briefly the method and quote the rigorous convergence analysis developed in [2] which gives exponential convergence of the "probability error" with respect of the number of Gauss points in each direction in the probability space, under some regularity assumptions on the random input data.

Problem setting and notation Let D be a convex bounded polygonal domain in $\mathbb{R}^d$ and $(\Omega, \mathcal{F}, P)$ a complete probability space. Here Ω is the set of outcomes, $\mathcal{F} \subset 2^\Omega$ is the σ-algebra of events and $P : \mathcal{F} \to [0,1]$ is a probability measure. Consider the stochastic linear elliptic boundary value problem: find a random function, $u : \Omega \times \overline{D} \to \mathbb{R}$, such that P-almost everywhere in Ω, or in other words almost surely (a.s.), the following equation holds:

$$\begin{aligned} -\nabla \cdot (a(\omega,\cdot)\nabla u(\omega,\cdot)) &= f(\omega,\cdot) \quad \text{on} \quad D, \\ u(\omega,\cdot) &= 0 \quad \text{on} \quad \partial D. \end{aligned} \tag{1}$$

Here and in what follows the gradient notation ∇ always means differentiation with respect to $x \in D$, unless otherwise stated.

Then, equation (1) can be written in weak form as

$$\int_D E[a\nabla u \cdot \nabla v]\, dx = \int_D E[fv]dx, \quad \forall\, v \in L^2_P(\Omega) \otimes H^1_0(D). \tag{2}$$

To guarantee existence and uniqueness for the solution of (2) we assume that the diffusion coefficient a is uniformly coercive and that the load f is in $L^2_P(\Omega, L^2(D))$.

Finite Dimensional Noise Assumption. In many problems the source of the randomness can be approximated using just a small number of uncorrelated, sometimes independent, random variables.

This motivates us to assume that
$a(\omega, x) = a(Y_1(\omega), \ldots, Y_N(\omega), x)$ and $f(\omega, x) = f(Y_1(\omega), \ldots, Y_N(\omega), x)$ on $\Omega \times \overline{D}$, where $\{Y_n\}_{n=1}^N$ are real valued random variables with mean value zero and unit variance. Moreover, for $n = 1, \ldots, N$, we denote by Γ_n the image of Y_n and with ρ the (known) joint probability density for the random vector $\mathbf{Y} = [Y_1, \ldots, Y_N]$; $\rho : \Gamma \to \mathbb{R}^+$ with $\rho \in L^\infty(\Gamma)$. Observe that $\Gamma \equiv \Pi_{n=1}^N \Gamma_n \subset \mathbb{R}^N$ contains the support of such probability density. A possible way to build a stochastic filed $a(\omega, \cdot)$ which depends nonlinearly only on a finite number of uncorrelated random variables and is coercive consists in performing a truncated Karhunen-Loève expansion of $log(a - a_{min})$:

$$\log(a - a_{min}) = b_0(x) + \sum_{1 \le n \le N} b_n(x) Y_n. \tag{3}$$

After assuming that the coefficients depend on a finite number of random variables the solution u of the stochastic elliptic boundary value problem (2) can be described as a function of the same random variables, i.e. $u(\omega, x) = u(Y_1(\omega), \ldots, Y_N(\omega), x)$. Observe that the stochastic variational formulation (2) has a "deterministic" equivalent which is the following: find $u : \Gamma \to H_0^1(D)$ such that

$$\int_D a(y) \nabla u(y) \cdot \nabla \phi \, dx = \int_D f(y) \phi \, dx, \quad \forall \phi \in H_0^1(D), \ \ \rho\text{-a.e. in } \Gamma. \tag{4}$$

Spectral collocation approximation.

When the diffusion coefficient $a(x, Y)$ is not linear with respect to Y the system of linear equations that defines the stochastic Galerkin approximate solution cannot be decoupled by means of double orthogonal polynomials [1]. It is clear that nonlinear Y-dependence offers good control over the coercivity of $a(x, Y)$ and at the same time,we would like to avoid solving large coupled systems as much as possible. This motivates us to consider stochastic collocation. To this end, consider a tensor product space $V_{p,h} = \mathcal{P}_p(\Gamma) \otimes H_h(D)$ approximating $L^2_\rho(\Gamma) \otimes H_0^1(D)$, where $H_h(D) \subset H_0^1(D)$ is a standard finite element space with mesh spacing parameter $h > 0$, $\mathcal{P}_p(\Gamma) \subset L^2(\Gamma)$ is spanned by tensor product polynomials with degree at most $\mathbf{p} = (p_1, \ldots, p_N)$ i.e. $\mathcal{P}_p(\Gamma) = \bigotimes_{n=1}^N \mathcal{P}_{p_n}(\Gamma_n)$, with $\mathcal{P}_{p_n}(\Gamma_n)$ being spanned by one variable polynomials with degree at most p_n.

Obtain the semi-discrete approximation, $u_h : \Gamma \to H_h(D)$, by projecting equation (4) onto the subspace $H_h(D)$, for each $y \in \Gamma$, i.e.

$$\int_D a(y) \nabla u_h(y) \cdot \nabla \phi_h \, dx = \int_D f(y) \phi_h \, dx, \quad \forall \phi_h \in H_h(D), \ \text{ for a.e. } y \in \Gamma. \tag{5}$$

The next step consists in collocating equation (5) on the zeros of orthogonal polynomials and build the discrete solution $u_{h,p} \in \mathcal{P}_p(\Gamma) \otimes H_h(D)$ by interpolating in y the collocated solutions. To this end, we first introduce an auxiliary

probability density function $\hat{\rho} : \Gamma \to \mathbb{R}^+$ that can be seen as the joint probability of N independent random variables, i.e. it factorizes as $\hat{\rho}(y) = \prod_{n=1}^{N} \hat{\rho}_n(y_n)$, $\forall y \in \Gamma$, and is such that $\left\| \frac{\rho}{\hat{\rho}} \right\|_{L^\infty(\Gamma)} < \infty$. For each dimension $n = 1, \ldots, N$ let y_{n,k_n}, $1 \le k_n \le p_n + 1$ be the $p_n + 1$ roots of the orthogonal polynomial q_{p_n+1} with respect to the weight $\hat{\rho}_n$, which satisfies then $\int_{\Gamma_n} q_{p_n+1}(y) v(y) \hat{\rho}_n(y) dy = 0, \quad \forall v \in \mathcal{P}_{p_n}(\Gamma_n)$. Standard choices for $\hat{\rho}$, such as constant, Gaussian, etc., lead to well known roots of the polynomial q_{p_n+1}, which are tabulated to full accuracy and do not need to be computed. To any vector of indexes $[k_1, \ldots, k_N]$ we associate the global index $k = k_1 + p_1(k_2 - 1) + p_1 p_2(k_3 - 1) + \ldots$ and we denote by y_k the point $y_k = [y_{1,k_1}, y_{2,k_2}, \ldots, y_{N,k_N}] \in \Gamma$. We also introduce, for each $n = 1, 2, \ldots, N$, the Lagrange basis $\{l_{n,j}\}_{j=1}^{p_n+1}$ of the space $\mathcal{P}_{p_n}$: $l_{n,j} \in \mathcal{P}_{p_n}(\Gamma_n)$; $\quad l_{n,j}(y_{n,k}) = \delta_{jk}, \quad j, k = 1, \ldots, p_n + 1$ where δ_{jk} is the Kronecker symbol, and we set $l_k(y) = \prod_{n=1}^{N} l_{n,k_n}(y_n)$. Thus, the collocation approximation is $u_{h,p}(y, x) = \sum_{k=1}^{N_p} u_h(y_k, x) l_k(y)$, where $u_h(y_k, x)$ solves (5) with $y = y_k$. Equivalently, if we introduce the Lagrange interpolant operator $\mathcal{I}_p : C^0(\Gamma; H_0^1(D)) \to \mathcal{P}_p(\Gamma) \otimes H_0^1(D)$, such that $\mathcal{I}_p v(y) = \sum_{n=1}^{N} v(y_k) l_k(y)$, $\forall v \in C^0(\Gamma; H_0^1(D))$. Then we have $u_{h,p} = \mathcal{I}_p u_h$ and under mild regularity assumptions (see Section 3 of [2]) the main convergence result is

Theorem 1. *There exist positive constants r_n, $n = 1, \ldots, N$, and C, independent of h and p, such that*

$$\begin{aligned} \|u - u_{h,p}\|_{L^2_\rho \otimes H^1_0} \le & \frac{1}{\sqrt{a_{min}}} \inf_{v \in L^2_\rho \otimes H_h} \left(\int_{\Gamma \times D} \rho a |\nabla(u - v)|^2 \right)^{\frac{1}{2}} \\ & + C \sum_{n=1}^{N} \beta_n(p_n) \exp\{-r_n(p_n^{\theta_n})\} \end{aligned} \tag{6}$$

with $\theta_n = \beta_n = 1$ for Γ_n bounded and $\theta_n = 1/2$, $\beta_n = O(\sqrt{p_n})$ for Γ_n unbounded. The constants r_n do not depend on h and p and are defined rigorously in [2].

In particular, the convergence result given in Theorem 1 applies to the case of a stochastic diffusivity coefficient of the form (3).

Conclusions. This work [2] proposed a Collocation method for the solution of elliptic partial differential equations with random coefficients and forcing terms. This method has the advantages of leading to uncoupled deterministic problems –also in case of input data which depend non-linearly on the random variables–; treating efficiently the case of non independent random variables with the introduction of an auxiliary density $\hat{\rho}$; dealing easily with random variables with unbounded support – such as Gaussian or exponential ones–, dealing with no difficulty with a diffusivity coefficient a with unbounded second moment. The main result (exponential convergence) is given in Theorem 1 . See [2] for details. Numerical tests presented in [2] are in agreement with the theory. The method is both versatile and accurate for the class of problems considered (as accurate as the Stochastic

Galerkin approach). The extension of the analysis to other classes of linear and non-linear problems is an ongoing research. Besides, the use of tensor product polynomials suffers from the *curse of dimensionality* and it is efficient only for a small number of random variables. For a moderate or large dimensionality of the probability space one should use *sparse tensor product spaces*. This aspect will be investigated in a future work.

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Sparse Perturbation Algorithms for Elliptic Problems with Stochastic Data

Radu Alexandru Todor

We consider the moment problem for stochastic diffusion in a bounded physical domain $D \subset \mathbb{R}^d$,

$$-\mathrm{div}(a(\cdot,\omega)\nabla u(\cdot,\omega)) = f(\cdot,\omega) \quad \text{in } H^{-1}(D), P\text{-a.e. } \omega \in \Omega, \tag{1}$$

with homogeneous boundary conditions. Here (Ω, Σ, P) is a probability space modelling the data uncertainty.
For $k \in \mathbb{N}_+$ the moment of order k of u solution to (1) is defined on the kd-dimensional domain $D^k := D \times D \times \cdots \times D$ (k times) by

$$\mathcal{M}^k(u)(x_1, x_2, \cdots, x_k) = \int_\Omega u(x_1,\omega)u(x_2,\omega)\cdots u(x_k,\omega)\, dP(\omega). \tag{2}$$

For the moment computation of the stochastic solution u to (1) we develop perturbation algorithms which combine classical ideas with modern techniques for efficient data representation and complexity reduction: sparse tensor product spaces, wavelet preconditioning and best N-term approximation.

For example, if $\varepsilon > 0$ denotes the accuracy to be achieved in the moment computation using one of the three well-established methods (MC, PA, SG), the corresponding standard complexity estimates are expressed in the table below in terms of the number $N(\varepsilon)$ of *deterministic* model problems to be solved - intuitively, $N(\varepsilon)$ denotes the number of *samples*.

Method	$N(\varepsilon)$ as $\varepsilon \searrow 0$
Monte-Carlo Simulation	Quadratic: $N(\varepsilon) \sim \varepsilon^{-2})$
Perturbation Algorithms	Superalgebraic: $N(\varepsilon) > O(\varepsilon^{-n})\ \forall n$
Stochastic Galerkin Method	Superalgebraic: $N(\varepsilon) > O(\varepsilon^{-n})\ \forall n$

We prove that the new algorithms (which are of perturbation type), have *nearly optimal complexity*, that is

$$N(\varepsilon) \leq O(\varepsilon^{-o(1)}) \quad \text{as } \varepsilon \searrow 0, \tag{3}$$

under the assumption that the fluctuation in the stochastic diffusion coefficient a is piecewise analytic in the physical domain D. The central idea is a best N-term approximation of higher order moments (2) based on the Legendre/Karhunen-Loève expansion of the random fluctuation in the stochastic coefficient a. We conclude that the moment problem can be solved for the stochastic equation (1) in essentially the same complexity as one deterministic diffusion problem, as $\varepsilon \searrow 0$ (the number of needed samples is negligible compared to the effort needed to compute one sample).

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