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Reactive Flows in Deformable, Complex Media

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Abstract. Many processes of highest actuality in the real life are described through systems of equations posed in complex domains. Of particular interest is the situation when the domain is variable, undergoing deformations that depend on the unknown quantities of the model. Such kind of problems are encountered as mathematical models in the subsurface, or biological systems. Such models include various processes at different scales, and the key issue is to integrate the domain deformation in the multi-scale context. Having this as the background theme, this workshop focused on novel techniques and ideas in the analysis, the numerical discretization and the upscaling of such problems, as well as on applications of major societal relevance today.

Mathematics Subject Classification (2010): 35, 65, 74, 76.

Introduction by the Organisers

The focus of this meeting was on mathematical models, the analysis and discretization of flow and reactive transport models in deformable and complex (porous) media. It aimed at identifying relevant mathematical challenges connected with such issues and the underlying applications. This required the active participation of scientists with various expertise, willing to collaborate and exchange ideas in a common mathematical language. Therefore the participants had a broad and heterogeneous expertise, covering fields of mathematics (analysis, numerical methods), (geo-)physics, and environmental engineering.

The workshop was attended by 48 scientists from 10 countries, including 5 young scientists supported by the "Oberwolfach Leibniz Graduate Students" Programme. One of the participants, Prof. Todd Arbogast, was awarded the Simons Visiting

Professorship. This supported his visits to the universities in München (TU), Bergen and Eindhoven.

The programme included 28 lectures on the mathematical analysis, upscaling, numerical simulation and scientific computing of processes in complex (porous) media, some of them having a survey character. The talks addressed the workshop theme from various viewpoints:

- Mathematical methods, with subtopics in homogenization and multiscale analysis;
- Discrete representations, including (mixed and conformal) finite elements and finite volume methods, in a multi-scale context;
- Heterogeneous solvers, including domain decomposition methods and multilevel solvers;
- Advanced applications, dealing with subsurface processes and biological systems.

The organizers would like to acknowledge the involvement of Florin Adrian Radu (Bergen), who initiated the organisation of this workshop. The meeting atmosphere was very inspiring and collegial, with many discussions and promising initiatives. Needless to say, in achieving this the professional support offered kindly by the MFO was invaluable. All participants have experienced the hospitality and the wonderful conditions offered in Oberwolfach, and expressed the wish to come back. Next to them, the organizers are expressing the gratitude for this fantastic opportunity.

Acknowledgement: The MFO and the workshop organizers would like to thank the National Science Foundation for supporting the participation of junior researchers in the workshop by the grant DMS-1049268, "US Junior Oberwolfach Fellows". Moreover, the MFO and the workshop organizers would like to thank the Simons Foundation for supporting Todd Arbogast in the "Simons Visiting Professors" program at the MFO.

Workshop: Reactive Flows in Deformable, Complex Media

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Abstracts

Modeling of reactive flow through deformable porous media using homogenization

Andro Mikelić

Our goal is to derive the quasi-static Biot equations with Young moduli depending on the concentration of the transported species. They are posed in a porous medium Ω and read

$$-\text{ Div }\{A^H(c_1^0)e(\mathbf{u})-\alpha p\}=\rho\mathbf{F}, \tag{1}$$

$$\partial_t\Big(Mp+\text{ div }\big(\alpha\mathbf{u}\big)\Big)+\text{ div }\{\frac{K}{\eta}(\rho_f\mathbf{F}-\nabla p)\}=0. \tag{2}$$

We start from the first principles fluid/structure pore level interaction and use the the Lagrange formulation for the solid skeleton and a particular ALE (Arbitrary Lagrangian Eulerian) formulation for pore space filled by a fluid. Next, we concentrate to the characteristic times corresponding to a flow regime (contrary to the vibrational regime of Biot-Allard equations from [1], [2], [3] and [12]) and suppose small deformations, small fluid compressibility and small Reynolds numbers. It allows linearization of the coupling conditions at the fluid/solid interface Γ and the fluid-structure equations become linear in the reference configuration.

The fluid structure interaction is coupled with a reactive transport. A change of the concentration c_1 implies a change in the 4th order tensor A, containing the elasticity coefficients of the solid skeleton. We suppose that A changes continuously as a function of a Volterra integral operator in time applied to c_1 (see [6] and [5] for details).

It is supposed that there are two connected phases, a solid Ω_s and a fluid Ω_f one. A representative example of such geometry is the *periodic* porous medium with connected fluid and solid phases. After identifying the characteristic pore size $\varepsilon=\ell/L$ (the ratio between two length scales) as the small parameter, the technique of homogenization can be applied.

The rigorous homogenization of the fluid-structure problem in space and in time variables was undertaken in [1], [2] and [3]. In these references the slow and fast scales separation was performed, which allowed reducing the two-scale homogenized equations to the Biot equations from [12]. In [3] and [1], Biot's equations were justified using the two-scale convergence and the tensorial viscodynamic operator, linked to the dynamic permeability (see [10]), was calculated.

Furthermore, the result depends on the choice of the time scale T. If it is superior or equal to Terzaghi's time $T_c=\eta/(\Lambda\varepsilon^2)$, where Λ is the characteristic Young moduli and η the dynamic viscosity, then in [11] the quasistatic equations (1)-(2) were derived.

Therefore the effective behavior is described by the effective solid phase displacement $\mathbf{u}$ and the effective pressure p. They are defined at **every point** of Ω and we do not distinguish the solid and fluid phases any more. In the case of a

poroelastic medium with small thickness in one direction, these equations simplify to the poroelastic plate model (see [7]).

Concerning the approximation, it is proved in [11] that

$$\sqrt{\rho_f}\chi_{\Omega_f}(\mathbf{u}_f - \mathbf{u}_f^0(x, \frac{x}{\varepsilon}, t)) + \sqrt{\rho_s}(\mathbf{u}_s - \mathbf{u})\chi_{\Omega_s} \to 0 \text{ in } C([0,T]; L^2(\Omega)^3),$$

as $\varepsilon = \dfrac{\ell}{L} \to 0$.

We notice that for the geophysical applications, the ratio between the diffusion time L^2/D and Terzaghi time is large and the deformation would already finish, before the diffusion starts. In the applications to the living tissue, these times seem to be comparable (see [6] and [5] for details).

The link between the quasistatic Biot system and the pore scale fluid-structure problem was also considered in [4].

The system (1)-(2) is solved using specific splitting methods and we refer to [9] and [8] for more details.

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Upscaling flow and transport in an evolving porous medium with general interaction potentials

Nadja Ray
(joint work with Peter Knabner)

Introduction. Recently, two aspects have attracted an increased interest in upscaling flow and transport in porous media: the integration of electrostatics [1, 2, 3, 6, 8, 9] and an evolving porous matrix [4, 5, 7, 10]. In this research, we consider, similar to [7], a general interaction potential as transport mechanism, account for the evolving solid-liquid interface, and carry out the models upscaling.

Pore-scale model. At the pore-scale, we consider Stokes' equations for the fluid velocity v_ε and pressure p_ε, a transport equation including a general potential Φ_ε (drift) for the concentration c_ε. The level set equation for the level set L_ε characterizes the evolving solid-liquid interface Γ_ε of the saturated porous medium $\Omega_\varepsilon \subset \Omega$, at which boundary conditions are derived from conservation laws taking into account surface reactions f [7, 10]. Due to the multi-scale framework, the scale parameter ε is introduced; the parameter ρ denotes the constant density of the solid and the parameter α, β refer to volume change.

$$
\begin{aligned}
-\varepsilon^2 \Delta v_\varepsilon + \nabla p_\varepsilon &= -c_\varepsilon \nabla \Phi_\varepsilon && \text{in } \Omega_\varepsilon(t),\\
\nabla \cdot v_\varepsilon &= 0 && \text{in } \Omega_\varepsilon(t),\\
v_\varepsilon &= -\varepsilon \beta \alpha f(c_\varepsilon, \rho)\nu_\varepsilon && \text{on } \Gamma_\varepsilon(t),\\
\partial_t c_\varepsilon - \nabla \cdot (-v_\varepsilon c_\varepsilon + \nabla c_\varepsilon + c_\varepsilon \nabla \Phi_\varepsilon) &= 0 && \text{in } \Omega_\varepsilon(t),\\
(-v_\varepsilon c_\varepsilon + \nabla c_\varepsilon + c_\varepsilon \nabla \Phi_\varepsilon) \cdot \nu_\varepsilon &= \varepsilon \alpha f(c_\varepsilon, \rho)(c_\varepsilon - \rho) && \text{on } \Gamma_\varepsilon(t),\\
\partial_t L_\varepsilon - \varepsilon \alpha f(c_\varepsilon, \rho)|\nabla L_\varepsilon| &= 0 && \text{in } \Omega.
\end{aligned}
$$

Upscaled model. As a result of the averaging procedure by formal two-scale asymptotic expansion in a level set framework [10], we maintain a fully coupled two-scale model. In other words, we obtain a coupled system of partial differential equations consisting of Darcy's law and an upscaled transport equation defined in (new) macroscopic variables $\overline{v}_0 := \int_{Y_l} v_0 \, dy, \tilde{p}_0 := p_0 - c_0, u_0 := e^{\Phi_0} c_0$ (macro level), and a level set equation in L_0 (micro-macro level). Moreover, time- and space-dependent coefficient functions are defined by supplementary, fully coupled cell problems (micro level).

$$
\begin{aligned}
\overline{v}_0 &= -K^1(t,x)\nabla_x \tilde{p}_0 - K^2(t,x)\nabla_x u_0 && \text{in } \Omega\\
\nabla_x \cdot \overline{v}_0 &= \int_{\Gamma_0(t,x)} \beta f(c_0)\, do_y && \text{in } \Omega\\
\partial_t (A u_0) + \nabla_x \cdot (D^1 \nabla_x \tilde{p}_0 + D^2 \nabla_x u_0) &= -\int_{\Gamma_0(t,x)} f(e^{-\Phi_0} u_0, \rho)\, do_y && \text{in } \Omega\\
\partial_t L_0 - \alpha f(e^{-\Phi_0} u_0, \rho)|\nabla_y L_0| &= 0 && \text{in } Y \times \Omega.
\end{aligned}
$$

with permeability tensors K^i defined by integrating the solutions w_j^i, effective porosity $A := \int_{Y_{l,0}(t,x)} e^{-\Phi_0}\, dy$, and diffusion tensors D^i defined by the integrating the fluxes of the corresponding cell problems in ζ_j^i for $j = 1, 2$, $i = 1, 2$:

$$
\begin{aligned}
-\Delta_y w_j^1 + \nabla_y \tilde{\pi}_j^1 + e^{-\Phi_0}\nabla_y \zeta_j^1 &= -e_j && \text{in } Y_{l,0}(t,x),\\
\nabla_y \cdot w_j^1 &= 0 && \text{in } Y_{l,0}(t,x),\\
-\Delta_y w_j^2 + \nabla_y \tilde{\pi}_j^2 + e^{-\Phi_0}\nabla_y \zeta_j^2 &= -e^{-\Phi_0} e_j && \text{in } Y_{l,0}(t,x),\\
\nabla_y \cdot w_j^2 &= 0 && \text{in } Y_{l,0}(t,x),\\
w_j^i &= 0 && \text{on } \Gamma_0(t,x),\\
-\nabla_y \cdot (e^{-\Phi_0}\nabla_y \zeta_j^1) &= \nabla_y \cdot (e^{-\Phi_0} w_j^1 u_0) && \text{in } Y_{l,0}(t,x),\\
(e^{-\Phi_0}\nabla_y \zeta_j^1)\cdot \nu_0 &= -e^{-\Phi_0} w_j^1 u_0 \cdot \nu_0 && \text{on } \Gamma_0(t,x),\\
-\nabla_y \cdot (e^{-\Phi_0}\nabla_y \zeta_j^2) &= \nabla_y \cdot (e^{-\Phi_0} w_j^2 u_0 + e^{-\Phi_0} e_j) && \text{in } Y_{l,0}(t,x),\\
(e^{-\Phi_0}\nabla_y \zeta_j^2)\cdot \nu_0 &= -(e^{-\Phi_0} w_j^2 u_0 + e^{-\Phi_0} e_j)\cdot \nu_0 && \text{on } \Gamma_0(t,x),\\
w_j^i, \tilde{\pi}_j^2, \zeta_j^i \text{ periodic in } y, \quad & \frac{1}{|Y|}\int_{Y_{l,0}} \zeta_j^i\, dy = 0.
\end{aligned}
$$

Outlook. Due to the micro-macro coupling and degenerating coefficients, the upscaled model's analytical investigation is still an open question - even for simplified (sub-)problems.

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A multi-scale model for mass transport in arteries and tissue

Tobias Köppl
(joint work with Barbara Wohlmuth)

Mathematical models have become more and more important in many applications from medicine and biology. Quite often the resulting system of equations is complex, highly nonlinear and cannot be solved analytically. Thus stable and robust numerical simulation methods play an important role in understanding phenomena like the regulatory mechanisms of the heart or the balancing of metabolic supply and demand in the Cerebral Blood Flow (CBF). By these non invasive techniques, physiological processes in the human body can be examined and understood with less effort and less danger for a patient. As a consequence scientists can get more insight into the inherent mechanisms and improve their diagnosis techniques. Moreover quantitative prediction of the distribution of a chemical compound in living tissues, which provide important contributions to the development of new medical products [1], will be possible by the help of numerical simulation. In addition to that the impact on organs suffering from a reduced supply of oxygen can be predicted by the help of computational methods. A well known problem in this field is, e.g., to estimate the risk of ischemia caused by a stenosis [2]. Our aim is to give a reliable prediction of the distribution of certain chemicals like oxygen, carbon dioxide or lactate during the transport in blood vessels and human tissue.

Since blood flow within the network is fast compared to the flow within the tissue, we apply a domain decomposition in such a way that we separate the vessel network and the porous tissue and assign different models to them [1]. Blood flow and transport processes within the porous medium are governed by Darcy's equation and a convection diffusion equation in 3D. To model the network flow and transport, 1D reduced models and 0D lumped parameter models are used, which are given by transport equation systems or ODE-systems, respectively [1, 2, 3, 5]. Quite often three-dimensional (3D) models for blood flow, based on the incompressible Navier-Stokes equations are too expensive in order to simulate the blood flow through a large network. The reduced 1D models presented in [1] are derived from the Navier-Stokes equations, having the section area A and the mass flux Q as primary variables [3]. Providing a computional complexity that is several orders of magnitude lower than that of multidimensional models, these simplified models give a good description of the pressure and velocity propagation in blood vessels and allow the simulation of the whole circulatory system. Similar to the Navier-Stokes equations the convection-diffusion equation which models the mass transport can be simplified to a single transport equation having the averaged concentration Γ as a primary variable [1]. By means of this model, which has A, Q and Γ as primary variables, we are able to take into account at the same time blood flow and the transport of chemicals (oxygen, carbon dioxide, lactate, etc.) in blood. Up to now this model was only applied to a single artery. In this talk, we focus on the modelling of mass transport at a bifurcation. To do so we use a

domain decomposition approach, i.e., the branching vessel is split up into three single vessels. On each vessel, we solve a hyperbolic PDE system. The global solution is computed by coupling these PDE systems by an algebraic system of nine unknowns. For the variables A and Q, we use the already existing equations proposed in [1, 5]. The three remaining equations for the averaged concentration Γ are added in such a way that the number of particles which are transported through the bifurcation by the fluid is conserved [3].

On simulating the transport of oxygen in blood during one heart cycle, it can be observed that the oxygen concentration has steep gradients. Therefore we are interested in numerical schemes that provide approximations of transport problems with high accuracy on the one hand and without non physical oscillations in the vicinity of steep gradients or discontinuities on the other hand. To tackle these problems, we use a stabilized discontinuous Galerkin method originally introduced for a linear transport problem and generalize it to our transport equation systems [6].

The coupling conditions between the porous medium and the reduced models are not standard, since they involve the computation of average values and the usage of Delta measures [1].To understand the basic coupling concepts between 1D and 3D models we introduce them by taking the example of stationary diffusion-reaction models, before we derive in the next step a model for the dynamics of network flow and transport processes within a porous medium. The diffusion-reaction models are given by elliptic PDE systems, where the single equations depend on each other by some exchange terms. Such types of systems are much simpler to analyze than the time dependent systems coupling 1D transport equations and dynamic 3D models. By this mean, one can obtain a better insight into the mathematical and numerical difficulties associated with coupled 1D-3D systems [4] [1][Chapter 6].

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Porosity and pressure evolution in the presence of discontinuous reaction

Anna Scotti
(joint work with Abramo Agosti, Bianca Giovanardi)

Overpressures, i.e. pressures larger than hydrostatic, are usually found in sedimentary basins. Their prediction is crucial, for instance, for the simulation of hydrocarbons generation and migration and for drilling safety. However, overpressures are not completely ascribable to mechanical compaction and their link with diagenesis is still not clear. In this work we first analyze the coupled problem of compaction, flow and geochemical reactions by means of a simplified one-dimensional model that is able to describe the deposition of different sedimentary layers [1]. We then focus our attention on two diagenetic processes that can, combined with mechanical compaction, affect the porosity: oil generation, and mineral dissolution/precipitation. In the case of oil generation the solid organic matter, called kerogen, reacts forming liquid or gaseous hydrocarbons. These fluids can be partially retained, up to a certain threshold, by nanopores present in the source rock. From the mathematical point of view this behavior results in a set of ODEs with discontinuous right hand side, with a discountinuity that depends on the solution itself. On the other hand if we consider the process of mineral dissolution/precipitation, the dissolution rate, suitably scaled, can be represented as a Heaviside function of the concentration [2]. In both cases Filippov theory can be applied to prove existence and to determine the solution behavior at the discontinuities. From the numerical point of view, tailored numerical schemes are needed to guarantee positivity, mass conservation and accuracy. In particular, we rely on an event-driven approach such that, if the trajectory crosses a discontinuity, the transition point is exactly localized and integration is restarted accordingly [3]. This approach yields sharper results compared to the regularization of the right hand side, and does not introduce artificial stiffness in the system. Another relevant issue in the simulation of geochemical compaction is the nonlinear coupling among the equations. We observed that a naive iterative splitting can fail to converge for low permeabilities, while a full Newton approach is more robust but unpractical in most cases.

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Homogenization of a variational inequality with nonlinear restriction for the flux on the boundary of tiny holes

Maria Neuss-Radu
(joint work with Willi Jäger, Tatiana Shaposhnikova)

In this paper, we are considering variational inequalities arising e.g. in modeling diffusion of substances in a domain with inclusions. It is assumed that nonlinear adsorption is taking place at the boundary of these inclusions. Here, we are interested in the case of *tiny holes*, where the distribution of inclusions is periodic with period ε, and the size of each inclusion is very small of order ε^α.

The problem considered in the present paper, a variational inequality for the Laplace operator with nonlinear third type boundary conditions, is a generalization of the problems treated in [2], and [3], where the corresponding equation with nonlinear third type boundary condition was considered. Here, we use a similar approach to [3], see also [4]. Especially, we further generalize the test functions used in [3], in order to deal with nonlinear inequalities.

We are assuming balls as inclusions and we concentrate on developing methods needed for the derivation of the effective model, and of corrector results. More general shapes of inclusions are covered in a following investigation.

We consider a bounded domain Ω in $\mathbb{R}^n$, $n \geq 3$, with a smooth boundary $\partial\Omega$. We denote by G_0 the ball of radius 1 with its center in the origin of coordinates, and by $G_\varepsilon^j = a_\varepsilon G_0 + \varepsilon j$, $j \in \mathbb{Z}^n$. Here, $a_\varepsilon = C_0\varepsilon^\alpha$, with $\alpha \in (1, n/(n-2)]$, and C_0 a positive constant. Then, the domain perforated by tiny holes is $\Omega_\varepsilon = \Omega \setminus \overline{\bigcup G_\varepsilon^j}$, where just holes which do not touch the boundary $\partial\Omega$ are removed from Ω. The boundary of the perforations is denoted by S_ε.

In Ω_ε, we consider the following problem: Find $u_\varepsilon \in K_\varepsilon$, such that the following variational inequality is satisfied for all $v \in K_\varepsilon$:

$$\int_{\Omega_\varepsilon} \nabla u_\varepsilon \nabla(v - u_\varepsilon)dx + \varepsilon^{-\gamma} \int_{S_\varepsilon} \sigma(x, u_\varepsilon)(v - u_\varepsilon)ds \geq \int_{\Omega_\varepsilon} f(v - u_\varepsilon)dx. \tag{1}$$

Here, $f \in L^2(\Omega)$, and the set K_ε is defined by $K_\varepsilon = \{g \in H^1(\Omega_\varepsilon, \partial\Omega) : g \geq 0 \text{ a.e. on } S_\varepsilon\}$. Furthermore, we suppose that $\sigma(x, u)$ is continuously differentiable, monotone with respect to u, and $\sigma(x, 0) = 0$. Setting in (1) as test-function $v = 0$, we get the estimate $\|u_\varepsilon\|_{H^1(\Omega_\varepsilon)} \leq C$. Thus, for the $H^1(\Omega)$-extension $\widetilde{u}_\varepsilon$, constructed e.g. in [1], there exists a subsequence, such that for $\varepsilon \to 0$, we have

$$\widetilde{u}_\varepsilon \rightharpoonup u \text{ weakly in } H_0^1(\Omega), \text{ and } \widetilde{u}_\varepsilon \to u \text{ strongly in } L^2(\Omega). \tag{2}$$

Our aim now is to derive the problem satisfied by the limit function u, together with corrector results. It turns out that we have to distinguish between the following two cases.

1. The case $\alpha \in (1, n/(n-2))$, $\gamma = \alpha(n-1) - n$. In this case, the nonlinearity in the sink/source term has the same form as the nonlinearity in the boundary condition of the ε-problem. We obtain the following results:

Theorem 1. *Let $\alpha \in (1, n/(n-2))$, and $\gamma = \alpha(n-1) - n$, $n \geq 3$. Then the limit function u given by (2) is a weak solution of the following problem: find $u \in K_0$ such that the following variational inequality is satisfied for all $v \in K_0$:*

$$\int_\Omega \nabla u \nabla(v-u)dx + \mathcal{B}_n \int_\Omega \sigma(x,u)(v-u)dx \geq \int_\Omega f(v-u)dx, \tag{3}$$

where $\mathcal{B}_n = C_0^{n-1}\omega_n$, ω_n is the area of the unit sphere in $\mathbb{R}^n$, and the set K_0 is defined by $K_0 = \{g \in H_0^1(\Omega) : g \geq 0 \text{ a.e. in } \Omega\}$. Furthermore, the following strong convergence result for the approximation error holds:

$$\lim_{\varepsilon\to 0} \|u - u_\varepsilon\|_{H^1(\Omega_\varepsilon)} = 0, \quad \lim_{\varepsilon\to 0} \varepsilon^{-\gamma/2}\|u_\varepsilon - u\|_{L_2(S_\varepsilon)} = 0.$$

2. The case $\alpha = \frac{n}{n-2}$, $\gamma = \alpha(n-1) - n = \frac{n}{n-2} = \alpha$. This case is the more interesting one, since the nonlinearity in the sink/source term appearing in the effective equation has a different form from the nonlinearity in the ε-problem, and has to be determined as a solution of a functional equation.

Theorem 2. *Let $\alpha = n/(n-2)$, $n \geq 3$. Then the limit function u given by (2) is a weak solution of the following problem*

$$-\Delta u + \mathcal{A}_n\Big(H(x,u^+) + u^-\Big) = f, \text{ in } \Omega, \quad u = 0, \text{ on } \partial\Omega, \tag{4}$$

where $\mathcal{A}_n = (n-2)C_0^{n-2}\omega_n$, ω_n is the area of the unit sphere in $\mathbb{R}^n$, and for every $(x,\tau) \in \Omega \times \mathbb{R}$, $H(x,\tau)$ is the solution of the functional equation

$$\frac{(n-2)}{C_0} H = \sigma(x, \tau - H). \tag{5}$$

If we assume that u has the additional regularity $u \in W^{1,\infty}(\Omega)$, then for $\varepsilon \to 0$, we have the following corrector result:

$$\|u_\varepsilon - u^+ + W_\varepsilon H(x,u^+) - (1 - W_\varepsilon)u^-\|_{H^1(\Omega_\varepsilon)} \to 0,$$

and

$$\varepsilon^{-\alpha/2}\|u_\varepsilon - u^+ + H(x,u^+)\|_{L_2(S_\varepsilon)} \to 0.$$

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A Four-Species Diffuse-Interface Tumor-Growth Model of Gradient-Flow Type

Kristoffer G. van der Zee
(joint work with Andrea Hawkins-Daarud, J. Tinsley Oden, Serge Prudhomme)

1. Introduction: Diffuse-interface tumor growth

In this contribution, we consider a Cahn–Hilliard reaction–diffusion system arising in tumor-growth modeling. Let $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$ denote a Lipschitz domain, and $[0, T]$ the time interval of interest. The PDE system for the phase variables $\boldsymbol{u} := (u_1, u_2)$ and chemical potentials $\boldsymbol{\mu} := (\mu_1, \mu_2)$ is given by:

$$\left.\begin{aligned} \partial_t u_1 &= \operatorname{div}(m_1 \nabla \mu_1) + k(\mu_2 - \mu_1) \\ \partial_t u_2 &= \operatorname{div}(m_2 \nabla \mu_2) - k(\mu_2 - \mu_1) \end{aligned}\right\} \quad \text{in } (0,T] \times \Omega\,, \tag{1a}$$

$$\left.\begin{aligned} \mu_1 &= \partial_{u_1} f(\boldsymbol{u}) - \varepsilon \Delta u_1 \\ \mu_2 &= \partial_{u_2} f(\boldsymbol{u}) \end{aligned}\right\} \quad \text{in } (0,T] \times \Omega\,, \tag{1b}$$

where m_1, m_2, and k are nonnegative and may depend on $\boldsymbol{u}$ (suppressed for convenience), f is a sufficiently smooth nonconvex, double-well function with respect to u_1 and convex with respect to u_2, and $\varepsilon > 0$. We subject system (1a)–(1b) to:

$$\boldsymbol{u} = \boldsymbol{u}_0 \quad \text{on } \{t = 0\} \times \Omega\,, \qquad \varepsilon\, \partial_n u_1 = 0 \quad \text{on } [0,T] \times \partial\Omega\,, \tag{1c}$$

$$m_1\, \partial_n \mu_1 = m_2\, \partial_n \mu_2 = 0 \quad \text{on } [0,T] \times \partial\Omega\,. \tag{1d}$$

With u_1 and u_2 identified as the tumor and nutrient phase, respectively, the above model represents a four-species mixture with two saturation constraints, which captures the boundary of a nutrient-consuming evolving tumor as a *diffuse interface* [5]. The sharp-interface limit $\varepsilon \searrow 0$ has recently been identified with a suitable moving boundary problem [6], with the choice $m_1 = 1$, $m_2 = \delta$, $k = \varepsilon^{-1}\delta\, p(u_1)$ and $f(\boldsymbol{u}) = \varepsilon^{-1}\varphi(u_1) + u_2^2/(2\delta)$. Diffuse-interface tumor-growth models were originally proposed in [2].

2. Main result: Gradient-flow structure

Theorem 1 (Gradient-flow structure) *The PDE system* (1a)–(1d) *is a generalized gradient flow:* $\boxed{\partial_t \boldsymbol{u} = -K\boldsymbol{\mu} \quad \text{and} \quad \boldsymbol{\mu} = \nabla \mathcal{E}(\boldsymbol{u})}$, *for the driving functional* $\mathcal{E} : U \to \mathbb{R}$ *given by (total free energy)*

$$\mathcal{E}(\boldsymbol{u}) := \int_\Omega \left(f(\boldsymbol{u}) + \frac{\varepsilon}{2} |\nabla u_1|^2 \right) \mathrm{d}\Omega\,, \tag{2}$$

and positive-definite operator $K : H \to H^\star$ *given by*

$$K := \begin{bmatrix} -\operatorname{div}\left(m_1 \nabla(\cdot)\right) & 0 \\ 0 & -\operatorname{div}\left(m_2 \nabla(\cdot)\right) \end{bmatrix} + k \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \tag{3}$$

subject to initial conditions $\boldsymbol{u}(0) = \boldsymbol{u}_0$ *and, additionally,* $\varepsilon\, \partial_n u_1 = 0$ *on* $[0,T] \times \partial\Omega$.

If f has at most quadratic growth, $m \leq \{m_1, m_2\} \leq M$ for $m, M > 0$, and $k \geq 0$, then suitable spaces are $U = H^1(\Omega) \times L^2(\Omega)$ and $H = H^1(\Omega) \times H^1(\Omega)$. □

Corollary 2 (Free-energy dissipation) *Let the gradient-flow problem in Theorem 1 be well-posed. Then, its solution satisfies:*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(\boldsymbol{u})(t) = -\mathcal{D}(\boldsymbol{\mu}) \leq 0 \qquad \text{a.e. } t \in (0,T]\,.$$

where $\mathcal{D} : H \to \mathbb{R}$ is the quadratic form given by (total dissipation)

$$\mathcal{D}(\boldsymbol{\mu}) := \big\langle K\boldsymbol{\mu}, \boldsymbol{\mu}\big\rangle_{H^\star,H} = \int_\Omega \Big(m_1|\nabla\mu_1|^2| + m_2|\nabla\mu_2|^2 + k(\mu_1-\mu_2)^2\Big)\,.$$

In other words, the total free energy (sum of homogeneous free-energy and surface energy) is dissipated by means of three mechanisms: phase separation of u_1, diffusion of u_2, and reactions between u_1 and u_2 (tumor growth). □

The proof of Theorem 1 and Corollary 2 are stated in Section 4, following the description of a suitable gradient-flow setting in Section 3.

We note that Corollary 2 was first obtained in [5] without resorting to a gradient structure, but in the context of consistency with the second law of thermodynamics. The gradient structure is fundamental in the recent study of well-posedness of diffuse-interface tumor growth models [1, 3], as well as in the derivation of stable numerical schemes [11]. Closely related to the above main result is the gradient structure of other reaction–diffusion systems in [4, 8, 7]. The extension to general N-species reactive Cahn–Hilliard systems is an open problem.

3. Abstract generalized gradient flows

While very general gradient flows have been studied before (see, e.g., [10, Ch. 23]), we restrict ourselves to a gradient system $\{(U,\mathcal{E}),(H,K)\}$ in which:

- U is a Banach space, $U \subset L \equiv L^\star \subset U^\star$ (dense, continuous embeddings), L being a (pivot) Hilbert space, and U has the trace property [9, Ch. 6.7] (i.e., a generalized Green's formula holds with $\partial_U(\cdot)$ and $\gamma_U(\cdot)$ denoting the generalized Neumann and Dirichlet operator);
- $\mathcal{E} : U \to \mathbb{R}$ is a bounded differentiable functional, with derivative $\mathcal{E}'(\boldsymbol{u})(\boldsymbol{v}) = \big(\nabla\mathcal{E}(\boldsymbol{u}), \boldsymbol{v}\big)_L + \big\langle \partial_U\boldsymbol{u}, \gamma_U\boldsymbol{v}\big\rangle_{\partial\Omega}$ for all $\boldsymbol{v} \in U$, $\boldsymbol{u} \in U$ and $\nabla\mathcal{E}(\boldsymbol{u}) \in L$;
- H is a Banach space, $H \subset L \equiv L^\star \subset H^\star$ (dense, continuous embeddings);
- $K(\boldsymbol{u}) : H \to H^\star$ is a positive-definite operator for all $\boldsymbol{u} \in U$.

The gradient flow is then given by the evolution equation: $\partial_t\boldsymbol{u} = -K(\boldsymbol{u})\nabla\mathcal{E}(\boldsymbol{u})$ in $H^\star$, for a.e. $t \in (0,T]$, with $\boldsymbol{u}$ a member of the evolution space

$$\mathcal{U} := \big\{\boldsymbol{u} \in L^\infty(0,T;U)\,,\ \nabla\mathcal{E}(\boldsymbol{u}) \in L^2(0,T;H)\,,\ \partial_t\boldsymbol{u} \in L^2(0,T;H^\star)\,,$$
$$\partial_U\boldsymbol{u} = \boldsymbol{0} \text{ on } [0,T]\times\partial\Omega\,,\ \boldsymbol{u}(0) = \boldsymbol{u}_0\big\}\,.$$

Granted well-posedness, it easily follows that for a.e. t,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(\boldsymbol{u})(t) = \big\langle \partial_t\boldsymbol{u}, \nabla\mathcal{E}(\boldsymbol{u})\big\rangle_{H^\star,H} = -\big\langle K(\boldsymbol{u})\nabla\mathcal{E}(\boldsymbol{u}), \nabla\mathcal{E}(\boldsymbol{u})\big\rangle_{H^\star,H} \leq 0\,. \tag{4}$$

4. Proof of main result

To proof Theorem 1, first note that, for $\mathcal{E}$ defined in (2),

$$\mathcal{E}'(\boldsymbol{u})(\boldsymbol{v}) = \int_\Omega \Big((\partial_{u_1} f(\boldsymbol{u}) - \varepsilon \Delta u_1)\, v_1 + \partial_{u_2} f(\boldsymbol{u})\, v_2 \Big) + \big\langle \varepsilon\, \partial_n u_1, v_1 \big\rangle_{\partial\Omega}\,,$$

in other words, recalling (1b), $\nabla \mathcal{E}(\boldsymbol{u}) = (\mu_1, \mu_2)$. Under the assumption on f stated in Theorem 1, this is justified for $(u_1, u_2) \in U := H^1(\Omega) \times L^2(\Omega)$ and $(\mu_1, \mu_2) \in L := L^2(\Omega) \times L^2(\Omega)$, so that $\varepsilon\, \partial_n u_1 \in H^{-1/2}(\partial\Omega)$ and $v_1 \in H^{1/2}(\partial\Omega)$.

Next, note that the equation $\partial_t \boldsymbol{u} = -K\boldsymbol{\mu}$ in $H^\star$ is equivalent to

$$\big\langle \partial_t \boldsymbol{u}, \boldsymbol{v} \big\rangle_{H^\star, H} = -\int_\Omega \Big(m_1 \nabla\mu_1 \cdot \nabla v_1 + m_2 \nabla\mu_2 \cdot \nabla v_2 + k(\mu_1 - \mu_2)(v_1 - v_2) \Big)$$

for all $\boldsymbol{v} \in H$, which is a weak form of (1a) and (1d). Under the assumptions on m_1, m_2 and k stated in Theorem 1, this is justified for $(\mu_1, \mu_2) \in H := H^1(\Omega) \times H^1(\Omega)$. In particular, $\langle K\boldsymbol{\mu}, \boldsymbol{\mu} \rangle_{H^\star, H} \geq 0$. This completes the proof of Theorem 1.

Finally, note that we have now fully specified a gradient system $\{(U, \mathcal{E}), (H, K)\}$ as defined in Section 3, so Corollary 2 follows directly from (4).

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Modeling, analysis, and simulation of processes in evolving porous media in applications to methane hydrate and biofilm modeling

Malgorzata Peszynska
(joint work with Ralph Showalter, Anna Trykozko)

In the talk we overview mathematical and computational challenges for two applications in evolving porescale geometries. The applications are i) methane hydrates in subsurface, and ii) biofilm formation. Both involve clogging of pore space which has to be coupled to hydrodynamics, and (eventually) to poromechanics. Our computational models for both applications have been built with semismooth Newton solvers implementing Nonlinear Complementarity Constraints, and are based on finite volume discretizations; the time stepping ranges from fully implicit to sequential through semi-implicit formulations.

Modeling at porescale complements imaging techniques such as tomography and SEM which can provide detailed information about processes at porescale but are too expensive for real-time imaging. An alternative is to build mathematical and computational models and use tomography-based porescale geometries [8]. This is especially useful for those substances which are difficult to image. In particular, methane hydrates are unstable in standard conditions, while biofilms are difficult to distinguish from the bulk liquid phase.

Methane hydrates are an ice-like substance present in deep subsea sediments and arctic regions whenever pressure is high enough and the temperature is low enough. They are a potential energy source but also pose substantial risk during drilling. Dissociation of hydrates due to increased temperature is a potential "smoking gun" that can be triggered during climate change. Methane hydrate models at Darcy scale involve coupled systems of PDEs for methane and salt components, coupled to pressure and energy equations and delicate phase behavior [5, 6]. Hydrate evolution is a free boundary problem where a free boundary separates the region with hydrate and that without, similar to a precipitation front. Our analysis of hydrates in [4] accounts for diffusive transport, and recent results [7] extend these to advection fluxes. More work on well-posedness and numerical analysis is underway.

At porescale, hydrate formation leads to decreased permeability and is associated with the change of other constitutive properties including the phase behavior in an increasingly confined void space. We have considered several hydrate models ranging from complex phase field formulations to simple "down-scaled" continuum models which can be useful as surrogates of the former. Work is in progress on a comprehensive model which involves fracture formation.

Biofilms are complex communities of microorganisms attached to surfaces or associated with interfaces. Among other applications, researchers study the use of biofilms as biocements to plug leaks and fractures and for use in green building. The microbial cells growing in a biofilm region attached to rock are distinct from planktonic cells of the same organism which are single-cells that may float or swim in a fluid region. The biofilm cells are frequently embedded within a self-produced

matrix of extracellular polymeric substance (EPS) which offers protection and strucural integrity to the cells, and the crux of biofilm modeling is in how to account for the fluid and biofilm domains and their interface [10, 2, 1, 11, 3]. We recently proposed and implemented a comprehensive and efficient model [9, 12] that is coupled to hydrodynamics and improves on the degenerate and singular diffusion-reaction model [1] using variational inequalities.

In summary, **mathematical and computational challenges** are in the construction of the porescale models and in their scale-up. While homogenization and other upscaling techniques have been well studied for linear or mildly nonlinear stationary problems, significant challenges remain as concerns scale-up of nonlinear coupled dynamical processes such as reactive transport and phase transitions in evolving and deforming porous media.

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Perspectives of Granular Dynamics and Lattice Boltzmann Methods in Porous Media Applications

Ulrich Rüde

(joint work with R. Ammer, D. Bartuschat, S. Bogner, E. Fattahi, C. Godenschwager, S. Mohanty, K. Pickl, T. Preclik, F. Schornbaum, B. Wohlmuth)

The rapid growth of compute power makes it possible to use simulation methods resolving all physically relevant scales without averaging or homogenization. For example, such a *direct numerical simulation* of a representative sample of $1cm^3$ of a porous medium with pore sizes of $50\mu m$ will typically require a resolution with grid cells of $10\mu m$ or smaller. This in turn results in the need to store $1000^3 = 10^9$ mesh cells and to update them in each time step. While this is too large for a personal computer, it is nowadays easily within reach provided that efficient parallel algorithms and scalable data structures are used and that these are implemented appropriately [6].

This work is focussed on using the Lattice Boltzmann method (LBM) since it has been particularly successful as an alternative to Navier-Stokes-based solvers for simulating the flow in complex geometries or around moving objects [1, 4]. The pore-scale-resolved simulations are realised within waLBerla [5], a software framework enabling the massively parallel simulation of fluid flow.

Structurally, the LBM is similar to an explicit time stepping scheme that can be parallelised with high efficiency even on many processors. The largest computations to date have been performed with in excess of 10^{12} mesh cells for the simulation of blood flow in a coronary artery tree [6]. On the Juqueen supercomputer, an update rate of more that 2×10^{12} cells per second can be achieved.

For simulations involving the interaction of fluids and rigid bodies [7], waLBerla can be coupled with the *pe* physics engine [8, 9]. The *pe* computes the dynamics of particle-systems by integrating their equations of motion in a Lagrangian framework. It incorporates efficient parallel algorithms for detecting collisions between particles and computing frictional collision responses. The collection of all contact constraints forms a system of non-linear (non-smooth) equations that must be solved in each time step. With the *pe*, the particles of a porous medium can be represented as fully resolved geometric objects.

Beyond this simple use, the *pe* is also designed so that it can be coupled dynamically to the LBM method in waLBerla and to enable the parallel simulation of moving particles in the flow. This uses a compatible domain partitioning for the two software frameworks, including mechanisms for migrating particles between processors. In combination, the interaction between Eulerian flow and Lagrangian particle dynamics uses a so-called four-way coupling, as developed in [7] based on the momentum exchange method [10, 11].

The methodology outlined above can for example be used to study the flow over porous media as illustrated in Fig. 1 to derive new closure relations in the form of drag correlations of fluid-solid systems as in [2]. To this end, arrangements with spheres that are embedded in the flow are generated randomly while the Reynolds

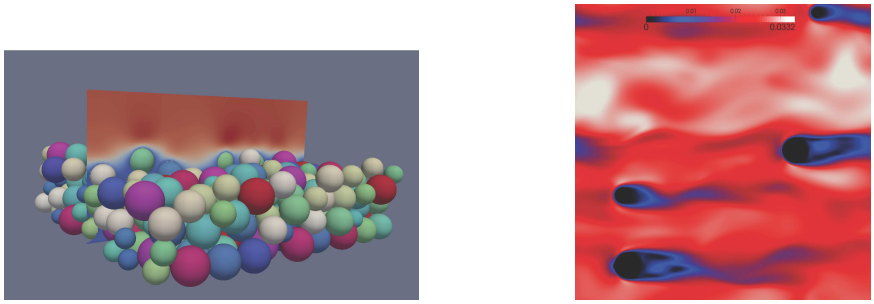

FIGURE 1. Example porous structure generated with the *pe* and vorticity in a vertical cut plane of a dilute porous medium as in a computation used for [3]

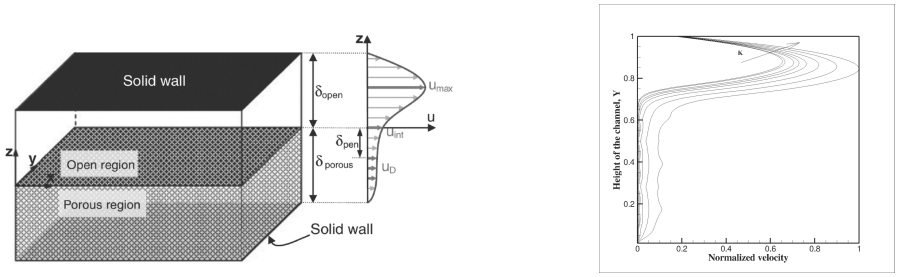

FIGURE 2. Flow over a porous medium and normalized velocity for various permeabilities

number and the volume fraction are varied systematically varied. In each such scenario, a direct numerical simulation is used to compute the drag. The values from several runs are then averaged and The collection of all simulation data can finally be used to derive a new and improved drag correlation [3].

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High-performance Computing for Flows in Porous Media

Peter Bastian

Simulation of flow and transport processes in porous media provides a formidable challenge and application field for high-performance computing. Relevant continuum-scale models include partial differential equations of elliptic, parabolic and hyperbolic type which are coupled through highly nonlinear coefficient functions. The multi-scale character and uncertainties in the parameters constitute an additional level of complexity but provide also opportunities for high-performance computing.

This talk will focus on the efficient solution of single and two-phase flow with discontinuous Galerkin methods. These schemes are comparable in efficiency (measured in accuracy per computation time) to simple cell-centered schemes but offer the opportunity to increase arithmetic intensity substantially in the assemble as well as the solve phase. For high-order schemes we exploit the tensor product structure using sum factorization which renders the work per degree of freedom almost independent of the polynomial degree. For the fast solution of the arising linear systems in the elliptic case a hybrid preconditioner based on subspace correction in the conforming finite element subspace is employed. Scalability and robustness of this preconditioner for the elliptic model problem and the full two-phase problem is investigated on a moderate number of processors including the Intel Phi architecture.

Gravity fingering effects in unsaturated porous media — play-type and Prandtl-Ishlinskii hysteresis

Ben Schweizer
(joint work with A. Rätz)

We are interested in the flow of water in an unsaturated porous medium. Denoting spatial variables by $x \in \Omega \subset \mathbb{R}^n$ and time by $t \in [0,T)$, the evolution of the system is usually described with a saturation $s : \Omega \times [0,T) \to \mathbb{R}$ and a pressure $p : \Omega \times [0,T) \to \mathbb{R}$. Darcy's law imposes that the flux is proportional to the

force $-\nabla p + g$, where g denotes external forces, usually only gravity. Denoting the (saturation dependent) permeability factor by $k = k(s)$, mass conservation provides (after a normalization) the *Richards equation*

$$\partial_t s = \nabla \cdot (k(s)[\nabla p - g]) \,. \tag{1}$$

While there is little doubt about the validity of this law, it is much less clear how the system should be closed: We have to define a relation between saturation s and pressure p. The simplest approach is to demand an algebraic relation between the two quantities: For some characteristic function $p_c = p_c(s)$ of the medium, one demands $p = p_c(s)$. We note that in our notation (where s is the fluid content and p is the *fluid* pressure), the law p_c is monotonically *increasing.*

The algebraic capillary pressure relation does not take into account the well-known hysteresis effects of porous media: the p_c-law of an imbibition process ($\partial_t s > 0$) is different from the p_c-law of a drainage process ($\partial_t s < 0$). A model that takes into account hysteresis (parameter $\gamma > 0$) and non-equilibrium effects (parameter $\tau > 0$) has been developed in [2, 4]. In its simplest form, it reads (for some given monotonically increasing coefficient function p_c):

$$p \in p_c(s) + \gamma \operatorname{sign}(\partial_t s) + \tau \partial_t s \,. \tag{2}$$

Here, the sign-function is multivalued: $\operatorname{sign}(\xi) = \pm 1$ for $\pm\xi > 0$ and $\operatorname{sign}(0) = [-1, 1]$. We therefore have to consider an inclusion in (2), even if the law p_c is single-valued.

Well-posedness and numerical schemes for system (1)–(2) (and its two-phase flow variant) have been studied in a series of papers: [6] investigates non-degenerate coefficient functions k and p_c, [9] concerns non-degenerate k and degenerate p_c, [5] treats the non-degenerate two-phase flow system. While the standard Richards system (with algebraic pressure-saturation relation) has no potential to describe gravity fingering (compare [15]), the model with static hysteresis has the potential to describe gravity fingering in dry media (compare [8]): the Richards equation with static hysteresis has an instability mechanism which prevents it from defining an L^1-contraction.

Physically, in a system without static hysteresis, a finger will always smear out with time: The saturation is higher in the finger than in the lateral neighborhood (this defines the finger). If the higher saturation is necessarily connected to a higher pressure, then the pressure gradient induces lateral flow, which leads to an increasing finger width. In this sense, it is clear that static hysteresis ($\gamma > 0$) is essential for fingering effects. The connection to the non-equilibrium term ($\tau > 0$) was made clear in [7]: The τ-term induces a saturation maximum in the finger-tip of a travelling finger (compare [3, 13, 14]) and, as a result, a drainage process occurs behind the finger tip; the static hysteresis effect becomes important and allows a lower pressure (during imbibition, it had to be close to $p_c(s) + \gamma$, now it can be as low as $p_c(s) - \gamma$).

The papers [5, 6, 7] contain numerical results of A. Rätz. The results show the fingering effect in two space dimensions for single-phase (unsaturated) and for

two-phase flow. They prove that the simple hysteresis law (2) can explain the fingering instability.

An extension to Prandtl-Ishlinskii hysteresis

There is no doubt that hysteresis is important in the description of porous media. At the same time, it is not clear which hysteresis model should be used (for a Preisach model see [1]). We favor the play-type hysteresis model of (2) as a starting point. Our physical argument is essentially based on the well-known bottle-neck effect, the corresponding reasoning was mathematically developed in [10, 12]: The pressure for imbibition and drainage are different and, for constant saturation ($\partial_t s = 0$), every pressure between the two extremal values can be attained. These facts are modeled with the sign-function in (2).

On the other hand, measurements of secondary imbibition or drainage curves do not provide vertical scanning curves in the s-p-diagram. This fact can be regarded as an argument against (2). Our answer to this critisism is based on the analysis of [11]. In that paper we studied, using homogenization theory, a medium with play-type hysteresis, but now the parameter γ takes different values in different points x of the domain. We assumed a periodic distribution and derived the averaged hysteresis law. We find that the play-type hysteresis law is replaced by a Prandtl-Ishlinskii hysteresis law. The latter does not have vertical scanning curves. We can therefore argue as follows: Locally, play-type hysteresis describes a porous material. But, since different parameters appear in natural media, experiments on macroscopic domains show the averaged behavior — which is of Prandtl-Ishlinskii type.

We conclude with a description of this averaged model in a simple case (we remark that the homogenization process was made precise only for a linear law $s \mapsto p_c(s)$ and that, from its derivation, w was originally a pressure variable). We use a new independent variable $y \in [0,1]$. We can imagine that, e.g. $y = 0.231$ indicates that we are interested in those parts of the porous medium, where the value of γ happens to be 0.231. The saturation variable is enriched: We use, as a new unknown of the system, a function $w : \Omega \times [0,1] \times [0,T]$. The value $w(x, 0.231, t)$ stands for the saturation in the material part with the label $y = 0.231$.

The unknowns of the system are $p(x,t)$ and $w(x,y,t)$. The saturation s is reconstructed by averaging as

$$s(x,t) = \int_0^1 w(x,y,t)\,dy \tag{3}$$

for every (x,t). The saturation s must satisfy the Richards equation (1). The evolution of w is given by the local play-type laws

$$p(x,t) \in p_c(w(x,y,t)) + y\,\mathrm{sign}(\partial_t w(x,y,t)) \tag{4}$$

for every (x,y,t). The system must be complemented with a boundary condition for p and with an initial condition for w. We mention that, of course, several variants are be of interest: (i) the interval $[0,1]$ for the y-variable can be replaced

by a larger interval. (ii) different p_c-laws can be used for different y-values. (iii) a weight function $\psi(y)$ with $\int_0^1 \psi(y)\,dy = 1$ could be included in (3) in order to account for different volume fractions of the different materials. (iv) the τ-term can be included in (4).

Almost nothing is known for the Prandtl-Ishlinskii-Richards model given by (1), (3), and (4). We emphasize that the underlying partial differential equation has not been changed by introducing w: no derivatives of w are used. Instead, w acts only pointwise and moderates the law between $s(x,.)$ and $p(x,.)$. The function $w(x,.,t)$ records essential informations about the wetting history in the point x up to time t. Nevertheless, no analysis has been performed yet: No results on well-posedness are known and no numerical results are available. A central question is: Does the Prandtl-Ishlinskii-Richards model also show the fingering effect?

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Approximation of transport using Eulerian-Lagrangian techniques

Todd Arbogast
(joint work with Chieh-Sen Huang, Jianxian Qiu, Chen-Hui Hung, Jamie Pool, Wenhao Wang)

As computers become bigger but not faster, numerical modelers should perhaps use algorithms that emphasize many local operations with few data transfers. Explicit and high order methods may be preferred, as well as methods for transient problems that avoid any artificial CFL time step stability constraint. We wish to simulate transport processes over very long time periods, which requires algorithms that are also locally mass conservative, produce no or minimal numerical diffusion, no over/under-shoots, and obtain accuracy on coarse meshes. Our approach is to use Eulerian-Lagrangian methods, because they have these desired properties. However, the caveat is that we need to be able to implement these ideas appropriately in a practical setting.

Specifically, we consider the advection-diffusion-reaction governing equation

$$\frac{\partial(\phi c)}{\partial t} + \nabla\cdot(c\mathbf{u} - D\nabla c) = q_c(c) + R(c), \tag{1}$$

where c is the unknown tracer concentration(s), ϕ is the porosity (although we take $\phi = 1$ for simplicity), $\mathbf{u}$ is the bulk fluid (Darcy) velocity, D is diffusion/dispersion tensor, q_c is the source/sink of c, and R models the reactions. If diffusion is small, it is natural to operator split the diffusion from the advection and reactions. Then an appropriate method can be used to approximate the diffusion part of the equation. Moreover, if one follows the advection in Lagrangian coordinates, then reactions occur along the trace-lines, and so can be solved independently of the advection using an appropriate ordinary differential equation solver. We are left to solve

$$\frac{\partial(\phi c)}{\partial t} + \nabla\cdot(c\mathbf{u}) = q_c(c).$$

In Lagrangian coordinates, the trace-lines are defined by tracing a particle at $(\mathbf{x}, t^{n+1})$ as it evolves backward in time within a velocity field $\mathbf{v}$ to the trace-back point $(\check{\mathbf{x}}, t^n)$. The velocity $\mathbf{v}$ may be the particle velocity $\mathbf{u}(c)$ or the characteristic velocity $\partial[c\mathbf{u}(c)]/\partial c$. Starting from a fixed (Eulerian) mesh element E, particles sweep out a space-time region $\mathcal{E}$ which has a top side E at time $t = t^{n+1}$, a bottom $\check{E}$ at $t = t^n$, and space-time sides $\mathcal{S}$. Application of the divergence theorem over $\mathcal{E}$ provides the basis of the approximation scheme. Assuming that c is approximated as a constant in each element E, one has that

$$c_E^{n+1}|E| = \int_{\check{E}} \mathcal{R}(c_h^n)\,dx + \iint_{\mathcal{E}} q_{c_h^n}\,dx\,dt - \mathcal{A}\Big(\int_{\mathcal{S}} c_h^n(\mathbf{u},1)\cdot\nu\,d\sigma\Big), \tag{2}$$

wherein $\mathcal{R}$ is a reconstruction operator and some approximation $\mathcal{A}$ of the side normal flux must be computed.

In the linear case $\mathbf{u}$ is independent of c and we can take $\mathbf{v} = \mathbf{u}$, and then no side flux correction is needed. In multiple dimensions, $\check{E}$ must be approximated by a polygonal or other simple shape, leading to a local volume error. A simple

and accurate volume correction was proposed in [1], and proofs of stability and accuracy were given in [2, 3]. Numerical tests show good results on relatively coarse meshes for highly complex, heterogeneous velocity fields. Solutions are locally mass conservative, produce little numerical diffusion, have no over/undershoots on, and use time steps well above the CFL limit (10-20 times greater).

The volume correction is difficult to code and computationally expensive, so we turned to a combination of simple Strang splitting by space dimension compensated by high order WENO reconstructions for the operator $\mathcal{R}$. The linear scheme describing the computation of the mass integral over $\check{E}$ is given in [4]. Formal fifth order accuracy is achieved for smooth problems using long time steps.

For nonlinear problems, $\mathbf{u}(c)$ is unknown for tracing, and so some approximation $\mathbf{v} \approx \mathbf{u}(c)$ is required, and the flux correction integral over $\mathcal{S}$ in (2) must be treated. We use the decomposition

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x}(vc) + \frac{\partial}{\partial x}\big(u(c)c - vc\big) = 0, \tag{3}$$

and treat the first two terms as in the linear case. The flux integral applies to the remaining terms, which are handled adapting Eulerian ideas [6] to Lagrangian coordinates. The key advance is to be able to perform WENO reconstruction at an arbitrary trace-back point, which we accomplish by using a re-averaging technique [5]. Numerical results again show good qualitative and convergence properties for the scheme. Applications include two-phase flow in porous media and the system of Euler equations in gas dynamics.

Open problems include handling multi-dimensional problems without Strang splitting, better handling of systems, and the choice of the trace velocity $\mathbf{v}$.

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Multiscale domain decomposition methods for flow and mechanics problems

Ivan Yotov

This research project focuses on the development of a computational framework for modeling multiphysics systems of coupled flow and mechanics problems with multiscale input parameters. The research approach is based on a multiblock domain decomposition methodology. The simulation domain is decomposed into a union of subdomains, each one associated with a physical, mathematical, and numerical model. Physically meaningful interface conditions are imposed on the discrete level via mortar finite elements or Nitsche's coupling. The formulation provides great flexibility for multiphysics and multinumerics couplings. Furthermore, this domain decomposition approach, combined with coarse scale mortar elements, provides a multiscale approximation and an efficient way to solve the coarse grid problem in parallel. Topics of interest include 1) Mathematically rigorous and physically meaningful multiphysics models; 2) Robust, accurate and efficient multiscale discretization techniques; 3) Efficient multiscale parallel domain decomposition solvers and preconditioners.

We study variational formulations of systems of partial differential equations coupling free and porous media fluid flows with deformations of the porous solids. These formulations couple through physically meaningful interface conditions free fluid models such as Stokes, Brinkman, or Navier-Stokes equations with single phase or multiphase Darcy flow. In regions involving deformable porous media the Darcy flow is coupled with elasticity and modeled by the Biot system of poroelasticity. We study well posedness of the variational formulations [4] and develop stable and accurate multiscale mortar discretization methods for these multiphysics variational formulations [3, 4, 5, 6, 8, 10, 11, 12, 13, 14]. We employ suitable mixed finite element, finite volume, and continuous or discontinuous Galerkin finite element methods for the discretization of the subdomain equations on a fine scale. A mortar finite element space is utilized to impose interface conditions on a coarse scale. We carry out a priori multiscale error analysis for these methods. We also develop efficient parallel non-overlapping domain decomposition algorithms for the solution of the resulting algebraic systems by reducing the coupled global multiscale problem to a coarse scale interface problem. We analyze the condition number of the interface operator and develop efficient preconditioners for speeding up the interface iteration [7, 9].

We also consider Nitsche's coupling formulations for Stokes/Brinkman flows coupled with the Biot system of poroelasticity [1]. We study stability and accuracy of the spatial discretizations and loosely coupled non-iterative time split formulations. We investigate the use of the loosely coupled scheme as a preconditioner for the monolithic scheme and establish a spectral equivalence of the two formulations.

The computational framework has been applied to geoscience and biomedical problems, including coupled surface and groundwater flows [4, 5, 7, 8], flows in fractured deformable reservoirs [1], and arterial flows [1, 2].

This work has been done in collaboration with Pu Song and ChangQing Wang (University of Pittsburgh), Vivette Girault (Paris VI) and Danail Vassilev (Cobham), Martina Bukac, Rana Zakerzadeh, and Paolo Zunino (University of Pittsburgh), Mary F. Wheeler (University of Texas at Austin), Guangri Xue (Shell), Ruijie Liu (British Petroleum), and Ilona Ambartsumyan and Eldar Khattatov (University of Pittsburgh).

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A Two-Scale Approach to Precipitation and Dissolution in Porous Media using Phase-Field Modelling

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(joint work with Iuliu Sorin Pop, Magnus Redeker)

We consider a porous medium with a pore space that is completely filled by three different species: (1) an incompressible fluid (e.g. water) which can contain a dissolved solid (e.g. salt), (2) a crystalline solid phase, and (3) another immiscible, incompressible fluid that does not support solid dissolution (e.g. oil). For this setting we consider the physical process of dissolution of solids into the water fluid from the crystalline phase, and vice versa the attachment to this phase by precipitation. The ultimate goal of the study is a mathematical model that allows the efficient numerical simulation of the solid concentration on a homogenized Darcy scale.

The standard approach on the pore scale consists of a sharp interface model, where the domains occupied by the three species are separated by sharp hypersurfaces. It is however not clear how to perform the upscaling for the corresponding free boundary value problem with discontinuous concentration fields (but see [4] for a recent contribution). Therefore we develop a phase field approach that accounts for the time-dependent –and then smooth– spatial distribution of the three species and the overall concentration of the solid particles.

For the sake of brevity we present here a simplified version. Let the open set $\mathcal{P} \subset \mathbb{R}^d$ be the pore domain. For final time $T > 0$ we search for the concentration $u : (0,T) \times \mathcal{P} \to [0,1]$ and the phase-field vector $\Phi = (\phi_1, \phi_2, \phi_3) : (0,T) \times \mathcal{P} \to [0,1]^3$ (one component for corresponding species) such that

$$(*) \qquad \begin{aligned} \partial_t((\phi_1+\delta)u) - D\nabla\cdot((\phi_1+\delta)\nabla u) - g(\Phi)\partial_t\phi_1 &= 0, \\ \alpha\xi^2\partial_t\phi_i - \xi^2\Delta\phi_i + \textstyle\sum_{j\neq i}(W_{\phi_i}(\Phi) - W_{\phi_j}(\Phi)) &= -f_i(\Phi,u) \end{aligned}$$

hold in $(0,T)\times\mathcal{P}$ for $i = 1,2,3$. Initial and boundary conditions have to be added. In $(*)$ we denote by $\alpha > 0$ a relaxation parameter, by $\xi > 0$ the phase field parameter which controls the interfacial width, and by $D > 0$ the diffusion constant. Finally, $\delta > 0$ is a threshold parameter which suppresses the degeneration of the system for small phase field values of ϕ_1. Furthermore

$$W(\Phi) = \sum_{i=1,2,3} \phi_i^2(1-\phi_i)^2, \quad f_1(\Phi,u) = \alpha\xi h(\Phi) f(u), \quad f_2(\Phi,u) = 0$$

and $f_3(\Phi,u) = -f_1(\Phi,u)$. The function f controls the precipitation rate at the interface and g, h are interpolation functions for switching on/off precipitation. Note that the concentration of u is supposed to be driven solely by diffusion and that the evolution of the three phase domains are governed via the phase field functions by Allen-Cahn dynamics. This model can be seen as generalization of the models in [1, 3, 2], for details see [6]. Note that previous models were restricted to the two-phase case.

By homogenization (using formal asymptotics for some standard periodicity assumptions and appropriate order relations between pore size and the parameters for $(*)_2$) we deduce for a domain $\Omega \subset \mathbb{R}^d$ the following new two-scale model which uses the advantages of the diffuse interface approach to couple the Darcy scale solid concentration with phase field type equations on the pore scale.

Find (skipping again the initial/boundary conditions) the macroscopic concentration $u : (0,T) \times \Omega \to [0,1]$ satisfying

$$\partial_t \left(\overline{\phi_1 + \delta}^{\mathcal{P}} u \right) - D\nabla_x \cdot (K \nabla_x u) - \overline{g(\Phi)\partial_t \phi_1}^{\mathcal{P}} = 0 \text{ in } (0,T) \times \Omega,$$

Here $K = K[\phi_1, w_1, \ldots, w_d] \in \mathbb{R}^{d \times d}$ is an effective diffusion matrix and $\overline{z}^{\mathcal{P}}$ denotes integration of a pore-scale quantity $z = z(t,x,y)$ with respect to $y \in \mathcal{P}$. The pore space phase fields $\phi_i = \phi_i(t,x,y)$ and the functions $w_1(t,x,y), \ldots, w_d(t,x,y)$ are determined for every $x \in \Omega$ by

$$\begin{aligned} \alpha\xi^2 \partial_t \phi_i - \xi^2 \Delta_y \phi_i + \textstyle\sum_{j \neq i} (W_{\phi_i}(\Phi) - W_{\phi_j}(\Phi)) &= -f_i(\Phi, u), \\ -D\nabla_y \cdot ((\phi_1 + \delta)\nabla_y w_j) &= D\nabla_y \phi_1 \cdot e_j \end{aligned}$$

in $(0,T) \times \mathcal{P}$, $i = 1,2,3$, $j = 1, \ldots, d$.
This approach allows the construction of an efficient numerical scheme on the basis of the multiscale adaptive algorithm in [5].

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Multipoint Flux Mixed Finite Element Methods for Coupling Multiphase Flow, Reactive Transport, and Geomechanics in Porous Media on General Hexahedral Mesh

Mary Wheeler

(joint work with C. Yuan, M. Delshad, K. Kumar, G. Pencheva, and G. Singh)

In this work we discuss the Multipoint Flux Mixed Finite Element (MFMFE) algorithms for modeling two important porous media applications that involve the coupling of flow, reactive transport and geomechanics in porous media on general hexahedral meshes: The specific problems we address include two phase chemical enhanced oil recovery (EOR) and an equation of state (EOS) compositional flow model. The accurate simulation of chemical EOR including polymer flooding and alkaline/surfactant/polymer flooding (ASP) is vital for reliable recovery predictions of hydrocarbons. This tertiary recovery technique targets remaining oil after employing conventional recovery methods. These EOR techniques reduce the water mobility and the interfacial tension (IFT) of water/oil interface. An efficient numerical scheme for obtaining simulations in complex geometry is essential to obtain a reliable predictive model. Important challenges arise in resolving the complicated processes taking place in complex reservoir geometries. We have developed a MFMFE method in combination with an operator splitting based algorithm that provides a) computational efficiency of using general hexahedral geometry giving a high fidelity to the complex reservoir geometry, b) local mass conservation and accurate pressures and fluxes inside the element and on faces on general grids, and c) reliable numerical schemes to solve the resulting system of reactive transport model. This is particularly important in the case of natural and induced fractures that are non-planar, intersecting and may have bifurcations. The MFMFE deals with full tensorial permeability and allows for complex geometry including non-planar fractures, barriers, faults and pinch-outs A comprehensive framework for chemical EOR processes has been implemented in our in-house research simulator IPARS. In particular, we have developed a parallel chemical flooding module, using bricks as a mesh grid, including extensive rheological models for viscoelastic polymers, simplified two-phase surfactant phase behavior, relative permeability as a function of trapping number, generation of soap by the reactions of alkaline with acidic crude oil, ion exchange and other aqueous chemical reactions. Our novel surfactant model captures the low IFT of Type III phase behavior without introducing a third middle micro-emulsion phase for computational efficiency without sacrificing the accuracy. Our numerical simulations have been validated using UTCHEM for simple geometries. Moreover, we have conducted several tests including field studies and scenario studies for assessing the efficacy of these processes. These results have been extended to hexahedral grids using MFMFE for flow and transport. We have considered different complex geometries with non-planar layered reservoirs, faults and barriers with the grids conforming to these complexities. Compositional flow modeling has been used for simulating oil recovery processes using gas injection, CO2 sequestration and

contaminant plume migration studies. We present an iteratively coupled reservoir fracture flow model using MFMFE. The general hexahedral elements capture complex reservoir geometries and features without requiring substantial adjustment of associated petrophysical properties. An iteratively coupled, implicit pressure explicit concentration (IMPEC) formulation is used for solving component conservation equations. This solution algorithmic approach allows for di fferent time-step sizes in the reservoir and fracture domain This reduces computational costs associated with taking smaller time-steps over then entire domain while preserving accuracy. A Peng-Robinson equation of state (PR-EOS) is used to model hydrocarbon phases along with slightly compressible water phase. A number of numerical experiments including a field case are presented to validate and demonstrate the capabilities of the approach presented here. The MFMFE approach can be considered a mimetic method and is equivalent to the O method introduced by I. Aavatsmark.

Adaptive inexact Newton methods and their application to multi-phase flows

Martin Vohralík

(joint work with Clément Cancès, Daniele A. Di Pietro, Alexandre Ern, Eric Flauraud, Iuliu Sorin Pop, Mary F. Wheeler, Soleiman Yousef)

We present novel adaptive algorithms for the solution of large systems of nonlinear algebraic equations and show their application to real-life multi-phase (multi-component) porous media flows.

We first describe the adaptive inexact Newton method of [3]. Herein, to solve a nonlinear algebraic system arising from a numerical discretization of a steady nonlinear partial differential equation, we consider an iterative linearization (for example the Newton or the fixed-point ones), and, on its each step, an iterative algebraic solver (for example the conjugate gradients or GMRes). We derive adaptive stopping criteria for both these iterative solvers. Our criteria are based on an a posteriori error estimate which distinguishes the different error components, namely the discretization error, the linearization error, and the algebraic error. We stop the iterations whenever the corresponding error does no longer affect the overall error significantly. Our estimates hinge on equilibrated flux reconstructions. They yield a guaranteed upper bound on the overall error measured by the dual norm of the residual augmented by a jump nonconformity term. Our estimates are valid at each step of the nonlinear and linear solvers. Importantly, we prove their (local) efficiency and robustness with respect to the size of the nonlinearity.

We then apply this methodology to challenging porous media problems. We develop, following [4, 1, 2] a general abstract framework for a posteriori estimates for (im)miscible (in)compressible multi-phase (multi-component) flows in porous media, described by systems of strongly coupled unsteady nonlinear partial differential and algebraic equations. We always measure the error by the dual norm of

the residual. For nonconforming discretizations, the possible departure of the approximate solution from the correct functional space is additionally evaluated via a proper nonconformity error measure. In the immiscible incompressible two-phase case, the concept of global and complementary pressures is used to characterize in a mathematically proper way the unique weak solution. In this case, and for conforming discretizations, we also prove that the dual norm of the residual is an upper bound on the $L^2((0,T);H^{-1}(\Omega))$ difference between the exact and approximate saturations, the $L^2((0,T);H_0^1(\Omega))$ error in the global pressure, and the $L^2(\Omega\times(0,T))$ error in the Kirchhoff transform of the nonwetting phase saturation, see [1]. Even in the considered complex setting, we can derive a guaranteed upper bound on our error measure and estimate separately the different error components, namely the spatial discretization error, the temporal discretization error, the linearization or the iterative coupling error, and the algebraic solver error. We then design a fully adaptive algorithm with tailored stopping and balancing criteria. The framework covers fully implicit, implicit pressure–explicit saturation, or iterative coupling formulations; conforming spatial discretization schemes such as the vertex-centered finite volume method or the finite element method, and nonconforming spatial discretization schemes such as the cell-centered finite volume method, the mixed finite element method, or the discontinuous Galerkin method; linearizations such as the Newton or the fixed-point one; and general linear solvers. Important computational savings (speed-ups by a factor between 10 and 20 in terms of the number of total linear solver iterations already on fixed meshes) are illustrated on numerical experiments from [4, 2] for vertex- and cell-centered finite volume discretizations.

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Robust Numerical Upscaling at High Contrast

Robert Scheichl

(joint work with Daniel Peterseim)

Diffusion processes in heterogeneous porous media are notoriously difficult to approximate accurately if the permeability $\alpha(x)$ of the medium varies over many orders of magnitude and on multiple scales, particularly if the medium undergoes deformations. Modern areas of interest such as hydraulic fracturing, enhanced oil

recovery or uncertainty quantification help to compound this problem. Classical homogenisation only works when there is some scale separation, periodicity or ergodicity which rarely is the case in applications. Accurate predictions of flow through such media (with standard discretisation techniques) require the resolution of all major small-scale features. Alternatively, sub grid-scale features need to be taken into account in more costly multiscale schemes. Whether the former or the latter approach is chosen depends on how many simulations need to be carried out through the same medium or through a possibly slightly deformed/modified one (e.g. in a time-dependent multi-phase flow simulation or an optimisation loop).

However, both approaches need robust and efficient coarsening strategies. In the former case, they are needed as the coarse component in multilevel preconditioners that are essential for any scalable and efficient solution of the large-scale linear algebra problems that arise when all features are resolved by the grid. In the latter case, they are needed because standard FE methods will not converge unless the mesh size h is larger than the frequency ε at which the coefficient oscillates. The methodologies that have been developed and analysed are similar, but the difficulties are not entirely the same. Nevertheless, the two research areas have seen a fruitful interaction in recent years with the emergence of new multilevel preconditioners with multiscale coarse spaces lifted from the upscaling literature (e.g. [2]) and novel numerical upscaling techniques based on coarsening strategies from multilevel preconditioners (e.g. [5, 1]). There have even been two very successful Oberwolfach mini-workshops (#0910a and #1307a) on this interaction.

In this talk we consider a promising new numerical upscaling technique, the localisable orthogonal decomposition (LOD) method [4], applied to

$$a(u,v) := \int_\Omega \alpha \nabla u \cdot \nabla v \mathrm{d}x = \int_\Omega g v \mathrm{d}x =: G(v), \quad \text{for all } \ v \in H_0^1(\Omega), \tag{1}$$

with arbitrary heterogeneous coefficient $\alpha_{\min} \leq \alpha(x) \leq \alpha_{\max}$, without any periodicity or scale separation assumptions. It is a variational multiscale method [3] that uses a selectable quasi-interpolation operator to decompose the solution into a low-dimensional coarse space and a high-dimensional remainder space. The coarse space is spanned by computable basis functions with local support. The localisation is rigorously justified in [4] due to the exponential decay of the "correctors" w.r.t. the standard hat functions. This avoids any artifical localisation boundary conditions, typical for other multiscale methods. For moderate contrast and arbitrary oscillatory coefficients this methodology yields approximations that converge to the true solution at the optimal rate (with respect to the coarse mesh size) without any pre-asymptotic effects.

The promising numerical results in [4] for high-contrast model coefficients are not reflected by the theoretical results for localized bases in that reference, because the physical contrast $\alpha_{\max}/\alpha_{\min}$ enters the error analysis via norm equivalences between energy norm and H^1-seminorm. These equivalences are heavily used to connect variational techniques such as Galerkin orthogonality with approximation properties of standard (coefficient-independent) quasi-interpolation operators. In an upcoming paper [6], we circumvent the critical norm equivalences by using

coefficient-dependent quasi-interpolation operators, similar to those in [8], which enjoy optimal approximation properties in α-weighted Sobolev spaces.

Definition. Let $\mathcal{I}_H : V_h \to V_H$ be a linear, continuous interpolation operator from a fine to a coarse piecewise linear FE space, with $h < H$, such that

(QI1) the restriction of $\mathcal{I}_H$ to V_H is an isomorphism,

(QI2) there exists a generic constant C_2, such that for all $v_h \in V_h$ and all $T \in \mathcal{T}_H$,

$$H^{-1}\|\alpha^{1/2}(v_h - \mathcal{I}_H v_h)\|_{L^2(T)} + \|\alpha^{1/2}\nabla(v_h - \mathcal{I}_H v_h)\|_{L^2(T)} \leq C_2\|\alpha^{1/2}\nabla v_h\|_{L^2(\omega_T)}$$

with $\omega_T := \operatorname{int}\big(\bigcup\{K \in \mathcal{T}_H | \, \overline{K} \cap \overline{T} \neq \emptyset\}\big)$.

(QI3) there exists a generic constant C_3, such that for all $v_H \in V_H$ there exists $v_h \in V_h$ with the properties

$$\mathcal{I}_H v_h = v_H, \quad \operatorname{supp} v_h \subset \operatorname{supp} v_H \quad \text{and} \quad \|\alpha^{1/2}\nabla v_h\|_{L^2(\Omega)} \leq \; C_3\|\alpha^{1/2}\nabla v_H\|_{L^2(\Omega)}.$$

This operator gives rise to the L^2-orthogonal decomposition $V_h = V_H \oplus V^{\mathrm{fs}}$ where $V^{\mathrm{fs}} := \ker \mathcal{I}_H$. The key idea to a better approximation is to a-orthogonalise this decomposition. Consider the a-orthogonal projection $\mathcal{P}^{\mathrm{cs}} : V_h \to V^{\mathrm{fs}}$ that maps $v \in V_h$ to the unique solution of

$$a(\mathcal{P}^{\mathrm{cs}} v, w) = a(v, w), \quad \text{for all } w \in V^{\mathrm{fs}}, \tag{2}$$

and define $V^{\mathrm{cs}} := (1 - \mathcal{P}^{\mathrm{cs}})V_H$. Then $V_h = V^{\mathrm{cs}} \oplus V^{\mathrm{fs}}$ and $a(V^{\mathrm{cs}}, V^{\mathrm{fs}}) = 0$.

In practice, we solve localised approximations of the corrector problems (2) for the basis functions Φ_z of V_H, restricting the calculation to nodal patches $\omega_{z,k} \subset \Omega$, centred at the corresponding coarse grid vertex $z \in \mathcal{N}_H$ and $2k$ layers of coarse grid elements wide (see [4, 6] for details). This leads to an approximate multiscale coarse space $V_k^{\mathrm{cs}} \approx V^{\mathrm{cs}}$ with $\dim(V_k^{\mathrm{cs}}) = \dim(V_H)$ and to the upscaled equation

$$a(u_k^{\mathrm{cs}}, v) = G(v), \quad \text{for all } \; v \in V_k^{\mathrm{cs}}. \tag{3}$$

Main Theorem. *If (QI1)–(QI3) are satisfied with constants $C_2 = \mathcal{O}(1) = C_3$ independent of α, and provided $k \gtrsim \log\left(\frac{\alpha_{\max}}{H\,\alpha_{\min}}\right)$ and h is sufficiently small, then*

$$\|\alpha^{1/2}\nabla(u - u_k^{cs})\|_{L^2(\Omega)} \;\lesssim\; \alpha_{\min}^{-1/2}\|g\|_{L^2(\Omega)}\, H. \tag{4}$$

This result does not require any periodicity or scale separation assumptions on the coefficients, and the hidden constants are independent of the contrast $\alpha_{\max}/\alpha_{\min}$.

An example of a quasi-interpolation operator that satisfies assumptions (QI1)–(QI3) with constants $C_2 = \mathcal{O}(1) = C_3$ independent of $\alpha_{\max}/\alpha_{\min}$ for a special class of coefficients that are quasi-monotone on the coarse mesh scale is the quasi-interpolation operator analysed in [8] (or rather a slightly modified version of it. See [8] for a more precise discussion of the type of coefficients that is covered. The constants C_2 and C_3 in our analysis do unfortunately depend on H/ε, but this dependence is not evident in the numerical experiments (see [6]).

In our future work we expect to extend this work to wider classes of coefficients, using different initial coarse spaces, instead of the piecewise linear space V_H, such

as those proposed in [1, 7] that enjoy optimal approximation properties in α-weighted Sobolev spaces for arbitrary positive coefficients. The associated quasi-interpolation operators satisfy an assumption similar to (QI2), but it remains to be seen if the whole theory can readily be extended.

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Convergence of iterative schemes for coupled flow and geomechanics in a fractured reservoir

Kundan Kumar

(joint work with Vivette Girault, Tameem Almani, Mary Wheeler)

Coupling of geomechanics and flow in a poroelastic porous media has several applications including subsidence events, ground water remediation, hydrocarbon production, enhanced geothermal systems, solid waste disposal, hydraulic fracturing, biomedical modeling and geological carbon sequestration. The geomechanical effects account for the influence of deformations in the porous media caused due to the pore pressure whereas the changes in the pore structure due to mechanical stresses affect the flow field. The fact that the fractures in the porous media have strong influence on the flow profiles and the deformations are particularly significant in such reservoirs motivates studying the coupled geomechanics and flow problems in fractured reservoirs.

There are broadly two categories of schemes for coupling geomechanics and flow in a poroelastic medium: *fully implicit* and *fully explicit*. The fully implicit scheme allows one to take larger time steps and provides more stability but the coupled linear system is difficult to solve; in particular for multiphase flows there are different operators involved for geomechanics and flow problems. Also, the flexibilities are lost to an extent, as for example, the time steps for geomechanical response may be larger compared to the flow time steps; three, for practical reasons, the

implementation is much easier by considering these equations separately. On the other hand, an explicit coupling approach is simpler, however a *naive* explicit decoupling gives at best conditionally stable schemes! An elegant way to combine the advantages of two broad approaches is to consider an iterative scheme. The design of an appropriate iterative scheme demands careful considerations. We report here some of the developments in developing suitable iterative schemes and their analysis for fractured porous media.

Our work is inspired from the previous work of Mikelić and Wheeler [1] and extends their results for the fractured medium. The fractures are treated as an interface and our iterative scheme is an adaptation of classical fixed stress-splitting scheme. The analysis of these schemes relies on studying the equations satisfied by the difference of iterates and using Banach contraction argument to prove that the scheme is a contraction. Concerning the limitations, we assume linear equations for flow and mechanics and the nonlinear extensions remain open even though numerically we see that the scheme works well. Moreover, in our proof, we control the time derivative of fracture width (which provides the mechanical response of the fracture on the flow) by the time derivative of symmetrized gradients of displacement in the bulk domain (using Korn and trace inequalities) and only under an assumption of Lamé parameters and the compressibilities of the fluids are we able to obtain the contraction.

The model equation consists of flow equations (F):

$$\begin{aligned}
\frac{\partial}{\partial t}\left((\frac{1}{M}+c_f\phi_0)p+\alpha\nabla\cdot\boldsymbol{u}\right)-\nabla\cdot\left(\frac{1}{\mu_f}\boldsymbol{K}(\nabla p-\rho_{f,r}g\nabla\eta)\right)&=\tilde{q},\ \text{in}\ \Omega\setminus\mathcal{C},\\
c_{fc}\frac{\partial p_c}{\partial t}+\frac{\partial w}{\partial t}-\bar{\nabla}\cdot\left(\frac{\boldsymbol{K}_c}{\mu_f}(\bar{\nabla}p_c-\rho_{f,r}g\nabla\eta)\right)&=\tilde{q}_W-\tilde{q}_L,\\
[\frac{1}{\mu_f}\boldsymbol{K}(\nabla p-\rho_{f,r}g\nabla\eta)]_{\mathcal{C}}\cdot\boldsymbol{n}^+&=\tilde{q}_L,\ \text{on}\ \mathcal{C},
\end{aligned}$$

and the geomechanics equations (M)

$$\begin{aligned}
-\nabla\cdot\boldsymbol{\sigma}^{\text{por}}(\boldsymbol{u},p)&=\boldsymbol{f}\ \text{in}\ \Omega\setminus\mathcal{C},\\
\boldsymbol{\sigma}^{\text{por}}(\boldsymbol{u},p)&=\boldsymbol{\sigma}(\boldsymbol{u})-\alpha p\boldsymbol{I},\ \text{in}\ \Omega\setminus\mathcal{C},\\
\boldsymbol{\sigma}(\boldsymbol{u})&=\lambda(\nabla\cdot\boldsymbol{u})\boldsymbol{I}+2G\boldsymbol{\varepsilon}(\boldsymbol{u})\\
\boldsymbol{\sigma}^{\text{por}*}\boldsymbol{n}^*&=-p_c\boldsymbol{n}^*,*=+,-\ \text{on}\ \mathcal{C}.
\end{aligned}$$

The reservoir domain is Ω, the fracture surface is $\mathcal{C}$ and the unknowns are reservoir pressure p, fracture pressure p_c, and displacement $\boldsymbol{u}$. The fractures are modeled as a lower dimensional geometric object. The above system is simply a Biot's equation coupled to a flow model on the fracture and a separate flow equation allows us to explicitly resolve the fracture flow.

The iterative scheme follows the fixed stress splitting algorithm and adds a stabilization term $(\gamma(\partial_t p^{n+1}-\partial_t p^n),\gamma_c(\partial_t p_c^{n+1}-\partial_t p_c^n))$ for the mass balance equations in the flow equations (F). The question is to determine suitable coefficients γ,γ_c for which the scheme has geometric convergence. We obtain the following results:

(1) The iterative scheme is a contraction in an appropriate norm and the converged solution is a unique weak solution of the coupled problem. An appropriate choice for the regularization terms are $\gamma = \frac{\alpha^2}{\lambda}$ and $\gamma_c = \frac{Mc_f\alpha^2}{\lambda + Mc_f\phi_0}$. Moreover, the contraction coefficient is:

$$\max\left\{\frac{1/\lambda^2}{\left(\frac{1}{M\alpha^2}+\frac{c_f}{\alpha^2}\varphi_0+\frac{1}{\lambda}\right)^2}, \frac{\gamma_c}{(c_{fc}+\gamma_c)\,\lambda\left(\frac{1}{M\alpha^2}+\frac{c_f}{\alpha^2}\varphi_0+\frac{1}{\lambda}\right)}\right\}.$$

(2) The contraction argument is extended to the fully discrete case for both flow and geomechanics. For the flow, we have taken mixed fem spaces and conformal Galerkin for the displacement. Moreover, a multi rate strategy is adopted where finer time steps are used for the flow and coarser time steps for the geomechanics. We find that the contraction coefficient is independent of discretization parameters. For the multirate formulation, contraction is obtained under mild assumption on the fluxes.

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Greenhouse Gases: Engineering Solution (CO_2) and Source Characterization (CH_4)

Mike Celia

If the relentless increase in anthropogenic greenhouse gas emissions is to be mitigated, engineered solutions must be deployed on a very large scale. The two most important anthropogenic greenhouse gases are carbon dioxide and methane. For CO2 emissions, the only currently available technology that allows continued use of fossil fuels while reducing atmospheric emissions is Carbon Capture and Storage, or CCS. The idea is to capture the CO2 at large stationary sources like power plants, and to inject the captured CO2 into deep geological formations. For this to be a feasible solution, the long-term fate of the injected fluid needs to be understood, and the behavior of the overall subsurface system must be simulated. This includes estimates of the amount of fluid likely to leak upward into shallow drinking-water zones or ultimately back to the atmosphere. In places like North America, where more than a century of oil and gas drilling has left millions of abandoned wells, leakage along old wells is an important concern, and the associated risk of leakage needs to be quantified. The mathematical description of this system involves extreme spatial and temporal scales, with the relevant physical and chemical processes leading to a potentially large set of coupled nonlinear partial differential equations. In order to provide tractable solutions, we have developed a series of simplified models that capture the dominant physics of the system while

being extremely efficient. This allows for large numbers of Monte Carlo simulations, which are necessary because of the high uncertainty in the properties of leaky wells. When coupled with experiments to estimate the statistics of the properties of potentially leaky old wells, a quantitative risk assessment for leakage can be achieved. For an application in Alberta, Canada, the results show a low risk of significant leakage over 50 years of CO2 injection.

Old wells can also play a role in methane emissions to the atmosphere, constituting a here-to-fore unrecognized source of anthropogenic methane. A series of first-of-a-kind measurements of methane leakage rates for a set of old wells in the state of Pennsylvania, USA, allows for initial estimates of the amount of methane leaking from old wells. Our current results indicate that the methane leaking from old wells is on the order of 10% of the currently estimated total anthropogenic emissions for the state of Pennsylvania. This indicates that methane leakage from old wells is significant enough to include in methane emission inventories.

These two problems, coupled with related problems associated with hydraulic fracturing and the production of shale gas, offer many opportunities for mathematical model development that requires advanced computational tools. Such problem are computationally challenging while addressing grand challenge problems in energy and environment.

Modeling of colloid transport during transient two-phase flow in porous media

Majid Hassanizadeh
(joint work with Qiulan Zhang)

This research regards the study of transport of colloids during transient flow of two immiscible fluids in porous media. We present results of experiments carried out in a micro-model made of PDMS (a hydrophobic polymer) and the immiscible fluids were water and fluorinert-FC43. The micro-model had a pore network covered an area of 1mm–10mm. It contained around 90 pore bodies and 200 pore throats, with mean pore size of 30 microns, and porosity of 40%. Given that the micro-model was hydrophobic, fluorinert was the wetting phase and water was the non-wetting phase. We used hydrophilic fluorescent microspheres (dispersed in water) with mean diameter of 300nm. We directly observed colloid movement and fluids distribution within pores of the micro-model using a confocal laser scanning microscope. We also obtained concentration breakthrough curves by measuring the fluorescence intensity in the outlet of the micro-model. Zhang et al. (2013), performed colloid transport experiments during two-phase flow in a micro-model. Spikes in colloid concentration breakthrough curves were found each time the flow rate was changed, causing a change in saturation. In these experiments, during stage 1, steady-state flow of a non-wetting fluid phase was established while the saturation was kept constant; the non-wetting phase saturation were 100%, 60%, and 40% in experiments 1, 2, and 3, respectively. Then, for a finite duration, colloids were added to non-wetting phase flowing into the micro-model. The colloid

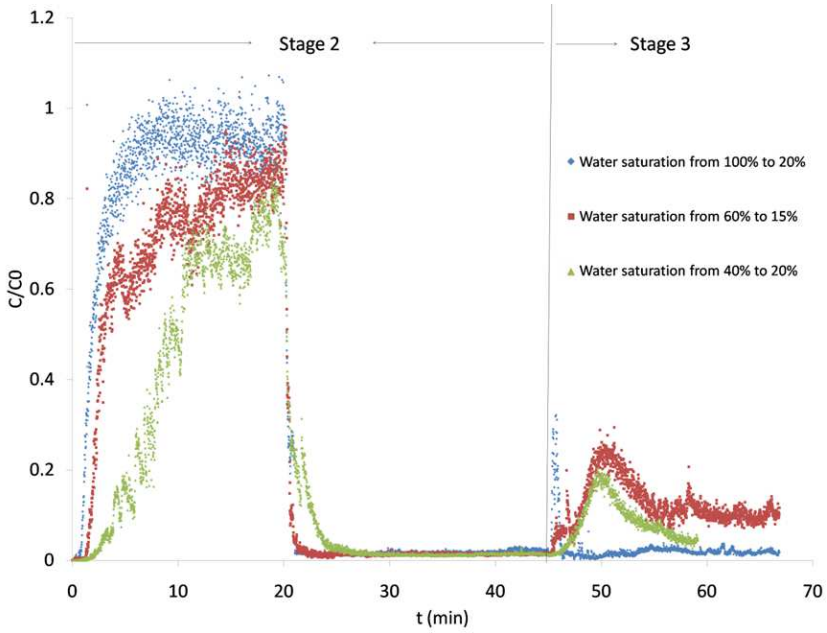

FIGURE 1. Influence of transient flow rate on colloid mobilization (upper set of data points is for 100%, middle set for 60%, lower set for 40%)

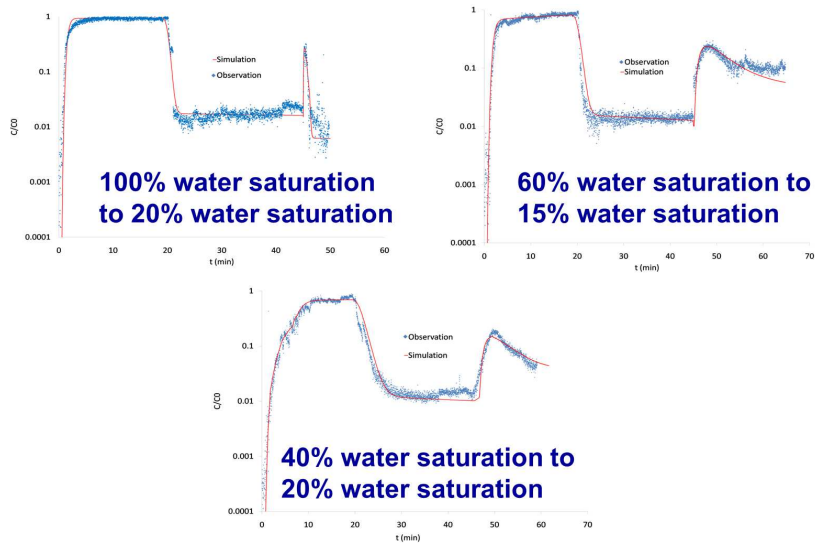

FIGURE 2. Comparison of simulation results (red lines) with experimental data (blue dots)

breakthrough curves were measured at the outlet until a long tail was established (see Stage 2 shown in Figure 1). Stage 3 of experiment started by stopping the flow of non-wetting phase and injecting the wetting phase, thereby causing the imbibition and reducing the non-wetting phase saturation to 20%, 15%, and 20% in experiments 1, 2, and 3, respectively. The saturation change was accompanied by a spike in colloid breakthrough concentration (see Stage 3 in Figure 1).

Generally, these remobilization effects have been attributed to the dynamics of fluid-fluid interfaces present in two-phase flow and the interplay of colloids with those interfaces (see e.g. [1, 2]. In this study, we developed a numerical model of coupled two-phase flow and colloid transport, wherein the variation of fluid-fluid interfacial area as a function of saturation was included. In this model, the detachment of adsorbed colloids was modelled as a function of the rate of change of saturation. We were able to simulate breakthrough curves successfully. Results are shown in Figure 2.

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Interfacial phenomena in porous media fracture, swelling, diffusiophoresis and diffusio-osmosis

Jacques Huyghe

(joint work with Kamyar Malakpoor, Sami Musa)

Because of the high interfacial area between constituents in a porous medium, interfacial effects are paramount in porous media. The usual concept of porous media researchers is that these effect are well understood on the pore scale. Understanding the porous medium on the macroscale amounts to upscaling the pore events to a macroscopic description of the medium. This report illustrates that even at the pore scale many questions remain open, while the upscaling to macroscopic level remains a challenging task, particularly in cases where localisation and ionisation play a primordial role. Particularly swelling and fracture are pinpointed as focal areas in the upscaling and diffusio-osmosis, and diffusiophoresis are pointed as important phenomena at the pore scale.

Swelling and fracture of living tissues has been mentioned as a key element in diagnostics of disease since antiquity. Concomitantly, geotechnical engineers see swelling and fracture in geomaterials as their prime enemies. In diapers, female pads and tampons swelling strain exceeds 1000 %. The challenges to simulate the swelling numerically are considerable. And so is the experimental challenge to measure the 3D swelling and associated fracture propagation. Surface instabilities typically occur as soon as the swelling strain is substantial. Exclusion zones developing around gels and tissues pushing away colloids hundred microns away from the surface are explained by means of diffusio-osmosis and diffusio-phoresis. The finite swelling of an electrically charged is described as a superimposition of four continua, one for the solid subject to finite deformation, one for the fluid, one for the counter-ions and one for the co-ions [4]. Conservation laws are formulated

for the four constituents and for the mixture as a whole. The second law of thermodynamics is used to obtain constitutive restrictions for the material laws. The constitutive restrictions require that the stress in the solid is the derivative of the free energy of the mixture as a whole per unit initial mixture volume with respect to the strain. Unlike a regular solid, this free energy depends on the local counter ion and co-ion concentration. This dependence is experimentally demonstrated [7] for cartilage and for hydrogel [13] and is referred to as chemical stress. The resulting set of partial differential equations are solved using a mixed hybrid finite element model [8, 12]. A Raviart-Thomas quadrilateral element is used. In 2D, for example, a quadrilateral element with displacement degrees of freedom of the corner nodes and fluid and ion fluxes across the sides. Lagrange multipliers, physically representing the electrochemical potential of the fluid and ions are introduced to enforce local mass conservation across the element interfaces. An analytical solution of 1D swelling and consolidation are compared to the numerical solutions to make sure the code actually solves the equation they are supposed to solve [11]. For complex 3D simulations a simplified version of the code in implemented into ABAQUS [9, 15] and used for predicting the mechanics of cartilage [16] the native intervertebral disc [14]. Detailed experimental verification for this model is needed. Three dimensional deformations are measured using optical tracking [5]. Radiotracer techniques measure ion concentrations in hydrogels [10]. Many of the swelling materials exhibit fracturing because of external mechanical load and internal stresses associated with gradients of osmolarity. Fractures are experimentally observed to open and close depending on the osmotic environment [17]. Fractures are simulated using xfem techniques [6]. At the interface between the gel and the fluid in the fracture exclusion zones are observed in which colloids are moving away from the surface of the gel. The mechanism of this phenomenon has been identified as diffusiophoresis and diffusio-osmosis [3]. Given these insights developed during this numerical-experimental analysis of swelling materials, design of an artificial intervertebral disc [1] has been worked out based on the insights of osmotic prestressing of the native intervertebral disc. The functioning of the prosthesis can be computed in a (swelling) finite element model of the gel-jacket-end-plate design [2].

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Reaction fronts in porous media

Marc A. Hesse
(joint work with Valentina Prigiobbe, Ashwin Venkatraman, Colin McNeece)

The theory of systems of hyperbolic partial differential equations (PDEs) provides a framework to understand multi-component reactive transport in porous media. Under the assumption of local chemical equilibrium and in the limit of negligible hydrodynamic dispersion, one-dimensional reactive transport is governed by the following system of n quasi-linear PDEs

$$(\mathbf{c} + \mathbf{z}(\mathbf{c}))_t + \mathbf{c}_x = 0,$$

where $\mathbf{z}(\mathbf{c})$ is the equilibrium constraint between the total concentrations of the components in the fluid, $\mathbf{c}$, and the total concentrations of the components in the solid, $\mathbf{z}$. In classical chromatography the equilibrium constraint is convex and the system is genuinely non-linear, which implies one reaction front per conservation equation, [1].

This analysis can be extended to the case of pH-dependent surface complexation reactions. These reactions involve the adsorption of protons and the consideration of electrostatic forces at the solid-liquid interface [2]. The proton conservation

equation must account for the dissociation of water so that the conserved variable, c, becomes the total acidity of the aqueous phase, given by

$$c = c' - k/c',$$

where c' is the proton concentration and k the dissociation constant of water. This added nonlinearity changes the nature of the reactive transport and introduces a non-convex equilibrium constraint, $z''(c) = 0$. This leads to the occurrence of composite shock-rarefaction waves in the non-genuinely non-linear characteristic field. This explains the composite waves that are observed in the elution profiles of column flood experiments with glass beads subjected to a change in the inflow pH [3].

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Reaction–diffusion systems on evolving domains: The fishy story of Turing patterns

Omar Lakkis
(joint work with A. Madzvamuse, A. Muntean, C. Venkataraman)

Introduction. In his seminal work [2], Alan Turing argued that certain development biology systems that under "noisy" perturbations experience instabilities that drive them to pattern creation. In mathematical parlance these systems are governed by time-dependent parabolic reaction–diffusion systems of equations (RDS) whereof the "patterns" are the stable steady states. Turing analyzes linear systems of equation by writing out explicit solutions on simple domains such as rectangles or spheres, but concludes his paper by advocating nonlinear equations as more accurate models and the use of "a digital computer". Thus, mathematical and computational biology were born and since then the literature on pattern formation in biology the subject has exploded as witnessed in [3]. One aspect that has remained until quite recently relatively unstudied is the *effect of domain evolution, that is when the domain upon which the RDS is defined undergoes change with respect to the time variable* and this is the object of our study. This objective is both exciting and challenging as the concept of steady state stops making sense, since, in contrast to Turing's equations, the PDE is not autonomous. Since pattern formation is most important in applications such as understanding the coloring patterns on an animal's skin our study is closely related to [4] which we will use for illustration as it answers an important question raised (and partially

answered) in [5]: *what are the models that take into account the movement of patterns as the animal grows?* The answer, as we shall see is that domain growth and curvature evolution, in addition to the classical Turing instability, are the main drivers in such pattern formation.

Reaction–diffusion systems on moving domains. Suppose $\Omega_t,\ t \in [0,T)$ with $0 < T \leq \infty$, is a parametric family of open subsets of $\mathbb{R}^d$, consider a vector of chemical concentrations $\boldsymbol{u}(\boldsymbol{x},t) = (u_1(\boldsymbol{x},t),\ldots,u_m(\boldsymbol{x},t))$ satisfying the following system of evolution PDE's

$$\begin{aligned} \partial_t u_i(t) - D_i \Delta u_i(t) + \nabla \cdot [\boldsymbol{a}(t) u_i(t)] &= f_i(\boldsymbol{u}(t)), \text{ in } \Omega_t, \\ \boldsymbol{n} \cdot \nabla u_i(t) &= 0, \text{ on } \partial\Omega_t \end{aligned} \tag{1}$$

for each $t \in (0,T)$ with the initial condition $u_i = u_i^0$ on Ω_0, where $\boldsymbol{f}$ accounts for nonlinear chemical reactions, $\boldsymbol{a}$ arises from the movement of Ω_t. This model was introduced by [5], from a phenomenological view-point, and first studied computationally by [6]. It was further studied in various situations by others cited in [7], where we gave a definitive analytic treatment by showing the problem is well-posed for isotropic evolution. The behavior of these systems with respect to various choices of $\boldsymbol{f}$, modeling biologically relevant systems, was studied computationally in [8, 9].

PDE and numerical analysis. Our strategy for a thorough analytic and numerical study of the RDS (1) is *Lagrangian*, i.e., we pull-back the equations onto a reference domain Ω via a time-dependent family of C^1-diffeomorphisms $\mathcal{A}_t : \Omega \to \Omega_t$ to obtain the RDS with space-time-dependent coefficients for $\hat{\boldsymbol{u}}$:

$$\begin{aligned} \partial_t \hat{u}_i - \frac{D_i}{J} \nabla \cdot (\boldsymbol{B} \nabla \hat{u}_i) + \hat{u}_i \nabla \cdot \hat{\boldsymbol{a}} &= f_i(\hat{\boldsymbol{u}}), \text{ on } \Omega \times (0,T], \\ \hat{\boldsymbol{n}} \cdot \boldsymbol{B} \nabla \hat{u}_i &= 0, \text{ on } \partial\Omega \times (0,T], \\ \hat{u}_i(\boldsymbol{\xi},0) &= \hat{u}_i^0(\boldsymbol{\xi}), \quad \boldsymbol{\xi} \in \Omega. \end{aligned} \tag{2}$$

Surprisingly the first studies of this type of equations on fixed domains dates back to [1] where structural assumptions are posed on $\boldsymbol{f}$ by postulating the existence of a Lyapunov function that guarantee global stability bounds. We extended this work to the moving domain framework in [7] and analyzed a Galerkin method in [8] where precise $\mathrm{L}_\infty(\Omega)$-bounds play a crucial role.

Fishy patterns. As mentioned, an application of (1) and our studies to developmental biology is the study of pattern formation and *pattern migration* on fish skin, such as the Amago trout studied in [4]. It was found there that evolution does produce patterns that could not be observed, nor even predicted by a Turing-instability type of analysis since, in our case, the bifurcation diagram is time-dependent, so to speak.

Outlook and open problems. Further effects observed in this study related to the curvature when we break-free from the flat-domain assumption. Although numerical analysis is still open, computations are feasible and show an interesting relationship between *Gaussian curvature* and the type of patterns observed: e.g., stripes versus spots, that could explain such variability in fishes. It is also interesting to understand the onset of patterns in multiscale settings when competing species coexist at the macroscopic level, also in non-biological systems such as corrosion [10, 11, 12, e.g.].

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Numerical techniques for differential equations with multiple scales in space or time

Assyr Abdulle

In this report we discuss recently developed numerical methods for multiscale problems in time (a numerical integrator for stiff advection-diffusion-reaction equations with or without noise) and multiscale problems in space (a numerical homogenization algorithm that combines different physics at different scales).

Numerical methods for stiff advection-diffusion-reaction equations with or without noise. Consider a system of (stochastic) ordinary differential equations originating from space discretized partial differential equations (PDEs)

$$\dot{y} = F(y) = F_D(y) + F_A(y) + F_R(y) + \sum_{j=1}^{m} F_G^j(y)\dot{\xi}_j, \qquad y(0) = y_0, \tag{1}$$

where $F_D(y), F_A(y), F_R(y), F_G^j \in \mathbb{R}^n$ and $\xi_j, j = 1, \ldots, m$ are independent one-dimensional Wiener processes. Here $F_D(y)$ represent a diffusion term with eigenvalues close to the negative real axis, $F_A(y)$ advection terms with eigenvalues close to the imaginary axis, $F_R(y)$ stiff (reaction) terms and F_G^j (stiff) noise terms, respectively. Classical numerical methods usually face the following issues

- a step size restriction for *explicit methods* due to the F_D term ("CFL-type" restriction), F_R term (multiple reaction rates that can vary over order of magnitudes) and F_G^j term ("stiff" mean-square stable problems) [2],[8];
- large nonlinear systems at each time steps when using *implicit methods* that can become quite involved, particularly for systems involving complicated nonlinear structure [9].

In [6] we present a new partitioned implicit-explicit orthogonal Runge-Kutta (RK) method (PIROCK) for the time integration of (1). Due to the use of a *stabilized* explicit second order orthogonal RK Chebyshev method (ROCK2) [1] for the F_D term, the severe restriction of the CFL condition for explicit schemes can be relaxed. A second order singly diagonally implicit RK that is unconditionally stable is used for the F_R term and a third order explicit method (stable on a portion of the imaginary axis) is taken for the F_A term. Finally an explicit stabilized method is also used for the F_G^j terms following the methods developed in [2],[5].

Other implicit-explicit or partitioned method have been proposed for (1)[1], and we mention the implicit-explicit Runge-Kutta-Chebyshev method (IRKC) derived in [10] and the fully explicit partitioned Runge-Kutta-Chebyshev method (PRKC) proposed in [11] (see [10],[11],[6]) for a more comprehensive literature review. For problems with stiff reactions, the PIROCK method is more efficient than the IRKC method as the number of function evaluations of the reaction terms F_R (solved implicitly) is independent of the (possibly high) stage number used in the stabilized explicit method for the diffusion terms F_D (it has also a better behavior for advection dominated problems than IRKC). Compared to the PRKC method

[1]However, none of them have been developed for equations including (stiff) noise terms.

(that can only handle non stiff reaction terms) the PIROCK method has larger stability domains on both the real and the imaginary parts. PIROCK implemented in a single black-box FOTRAN code available at `http://anmc.epfl.ch`, is fully adaptive, provides a posteriori error estimators, and requires from the user solely the right-hand side of the differential equation.

An adaptive numerical homogenization method for a Stokes problem. Consider the Stokes problem in heterogeneous media with pore sizes ε that can be several orders of magnitude smaller than the macroscopic size of the computational domain of interest Ω. Then, a full Stokes solver over Ω is often too expensive. For such problems we propose in [7] an adaptive multiscale micro-macro homogenization method, using the framework of the finite element heterogeneous multiscale method (FE-HMM) [4] with an adaptive strategy [3]. The new method relies on adaptive mesh refinement on macro and micro problems and on rigorous residual-based a posteriori error estimates derived in [7]. We propose a strategy to adequately couple macro and micro error indicators (a challenging issue) in order to achieve a desired accuracy with minimal computational cost on both the macro and the micro scales.

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Formal Asymptotic Limit of a Diffuse-Interface Tumor-Growth Model

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(joint work with J. Kampmann, T.N. Nguyen & K.G. van der Zee)

We consider a diffuse-interface tumor-growth model which has the form of a phase-field system. We characterize the singular limit of this problem. More precisely, we formally prove that as the coefficient of the reaction term tends to infinity, the solution converges to the solution of a novel free boundary problem. We present numerical simulations which illustrate the convergence of the diffuse-interface model to the identified sharp-interface limit.

Diffuse-interface tumor-growth models have been studied recently in several articles. The basic model is composed of a fourth order parabolic equation for the tumor cell phase $u : \Omega \to \mathbb{R}$ coupled to an elliptic equation for the nutrient phase $\sigma : \Omega \to \mathbb{R}$:

$$u_t = \Delta(-\varepsilon^{-1} f(u) - \varepsilon \Delta u) + \varepsilon^{-1} p_0 \sigma u \tag{1a}$$

$$0 = \Delta\sigma - \varepsilon^{-1} p_0 \sigma u, \tag{1b}$$

where ε^2 is the diffusivity corresponding to the surface energy, the positive constant p_0 is a proliferation growth parameter, and f is a bistable function.

Introducing the chemical potential $\mu : \Omega \to \mathbb{R}$, given by

$$\mu := -\varepsilon^{-1} f(u) - \varepsilon \Delta u,$$

(1a)-(1b) becomes

$$u_t = \Delta\mu + \varepsilon^{-1} p_0 \sigma u, \tag{2a}$$

$$\mu = -\varepsilon^{-1} f(u) - \varepsilon \Delta u, \tag{2b}$$

$$0 = \Delta\sigma - \varepsilon^{-1} p_0 \sigma u. \tag{2c}$$

The above system models the evolution of the first stage of a growing tumor. In this stage a tumor grows because of the consumption of nutrients that diffuse through the surrounding tissue. This stage is referred to as avascular growth, as the tumor has not yet acquired its own blood supply to nurture itself. Consumption of nutrients is modeled in (2a) and (2c) via the reactive terms. To describe the evolution of the tumor boundary a diffuse-interface description is employed. This is classically modeled in (2a) with a diffusion via the chemical potential μ which depends in a nonlinear manner on u and contains the higher-order regularization $\varepsilon\Delta u$, see (2b).

Diffuse-interface tumor-growth models fall within the broader class of multiconstituent tumor-growth models based on continuum mixture theory. The derivation of diffuse-interface models within continuum mixture theory requires the set up of balance laws for each constituent as well as the specification of constraints on the constitutive choices imposed by the second law of thermodynamics. Typically, only the cellular and fluidic constituents of a tumor are modeled as parts of a mixture, while nutrients are considered separately. Recently however, a diffuse-interface tumor growth model has been proposed that incorporates all constituents

within the mixture and is proven to be thermodynamically consistent. The model proposed by Hawkins-Daarub van der Zee and Oden, which turns out to be a gradient flow, is a modification of (2). It is given by:

$$u_t = \Delta\mu + \varepsilon^{-1} p(u)(\sigma - \delta\mu) \tag{3a}$$

$$\mu = -\varepsilon^{-1} f(u) - \varepsilon\Delta u \tag{3b}$$

$$\sigma_t = \Delta\sigma - \varepsilon^{-1} p(u)(\sigma - \delta\mu) \tag{3c}$$

where $\delta > 0$ is a small regularization parameter, and the growth function $p(u)$ is defined by

$$p(u) := \begin{cases} 2p_0\sqrt{W(u)} & u \in [-1,1] \\ 0 & \text{elsewhere.} \end{cases} \tag{4}$$

Here $W(u) := -\int_{-1}^{u} f(s)\,ds$ is the classical Cahn–Hilliard double well free-energy density. We assume that the bistable function $f(u)$ has two stable roots ± 1, an unstable root 0 and zero mean. The above model has the following multi-constituent interpretation: a tumorous phase $u \approx 1$, a healthy cell phase $u \approx -1$, and nutrient-rich extracellular water phase $\sigma \geq 0$.

Note that, compared to (2a)-(2c), the reactive terms have been modified to be thermodynamically consistent. They include a regularization part $\delta\mu$ and they have been localized to the interface (since $p(u)$ is nonzero if $u \in (-1,1)$).

In this work, we formally study the singular limit $\varepsilon \downarrow 0$ of (3a)-(3c). We furthermore perform numerical simulations which validate the identified singular limit.

Modelling and Simulation of Gas Production from Methane-Hydrate Reservoirs

Shubhangi Gupta

(joint work with Barbara Wohlmuth, Rainer Helmig)

A methane hydrate formation is a fairly complex sub-surface system characterized by a large number of highly interdependent physical phenomena. The typical physical processes occuring in a stimulated hydrate reservoir include, for instance, hydrate dissociation/reformation; non-isothermal multi-phase, multi-component flow; and, mechanical deformation of the sediment; change in hydraulic as well as mechanical properties of the sediment, etc.

Phenomenological modeling and numerical simulation of these systems is vital for conducting studies and making predictions for mitigating bore-hole, local and regional slope stability hazards; for optimizing recovery techniques for extracting methane from hydrate bearing sediments; for sequestering carbon-dioxide in gas hydrate; and for evaluating role of gas hydrate in the global carbon cycle, etc.

In this talk a mathematical model was presented describing the various processes occuring in hydrate reservoirs. Special focus was laid on extending the

poroelasticity concept and the consolidation theory to hydrate systems. The validation of reaction kinetics model against experimental data from Yuhu B. et al [7], and Tang et al [5] was also presented. The hydro-mechanical coupling was verified using the Terzaghi 1-D consolidation problem [4], and the selected results were presented.

The mathematical model describing processes in hydrate reservoirs is highly coupled, complex and non-linear. This system can, in principle, be solved 'fully-coupled', the direct advantage being a more accurate and consistent feedback of deformation on flow processes. However, this fully coupled solution technique is very expensive in terms of computation time.

An alternative solution strategy is to reformulate the system of equations into equation-subsets which have weak interdependencies. This allows 'decoupling' of the complete system into smaller sub-models which can be solved separately. Besides decreasing the computational costs, the decoupled formulations also allow application of different discretization schemes for the different sub-models which lead to an increase in efficiency. The disadvantage is, however, a loss in interdependency of the physical system inherited from the decoupling process.

Another focus of this talk was to present a possible strategy for decoupling and solving a non isothermal hydro-geomechanical system in the context of sub-oceanic hydrate reservoirs. In this strategy, sub-models are defined based on the three major controlling 'physical' processes occuring in a typical hydrate reservoir under an external stimulus, viz. dissociation of hydrate; non-isothermal flow through porous sediment; and geo-mechanical deformation of the sediment. The discussion included the ideology and advantages of such a decoupling scheme and it's effects on the computation efficiency and coupling errors.

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Mixed hybrid finite element schemes for advection-diffusion-reaction problems

Fabian Brunner
(joint work with F. A. Radu, J. Fischer, M. Bause and P. Knabner)

We study approximations of the mixed advection-diffusion-reaction problem

$$\partial_t c + \nabla \cdot \boldsymbol{q} + Rc = f \ , \quad \boldsymbol{q} = -\boldsymbol{D}\nabla c + \boldsymbol{Q}c \tag{1}$$

using the Raviart-Thomas and the Brezzi-Douglas-Marini mixed finite elements of lowest order on a domain $\Omega \subset \mathbb{R}^2$, where $\boldsymbol{D}$ denotes a symmetric and uniformly-positive diffusion tensor, $\boldsymbol{Q}$ represents a given velocity field and R denotes a linear reaction rate.

When advection strongly dominates diffusion, the standard mixed method [1] typically fails to resolve steep gradients in the analytical solution and produces approximations that are polluted by spurious oscillations. To overcome this, we incorporate upwinding into the method by extending the classical scheme to obtain a new family of mixed hybrid schemes based on an Euler-implicit discretization in time and a hybrid mixed discretization in space. It relies on the fact that the Lagrange multipliers represent approximations of the scalar unknown on the interelement boundaries and uses them in the approximation of the advective fluxes.

1. Approximations with the RT_0 element

In the fully discrete mixed hybrid formulation of (1), on each time level $t = t^n$ we seek $(\boldsymbol{q}_h^n, c_h^n, \lambda_h^n) \in \tilde{\boldsymbol{V}}_h \times W_h \times \Lambda_h$ such that

$$(\boldsymbol{D}^{-1}\boldsymbol{q}_h^n, \boldsymbol{v}_h) - (\nabla \cdot \boldsymbol{v}_h, c_h^n) - (\boldsymbol{D}^{-1}\mathcal{B}(\lambda_h^n, c_h^n), \boldsymbol{v}_h) = -\sum_{K\in\mathcal{T}_h} \langle \lambda_h^n, \boldsymbol{v}_h \cdot \boldsymbol{n}\rangle_{\partial K} \ , \tag{2}$$

$$\frac{1}{\Delta t^n}(c_h^n - c_h^{n-1}, w_h) + (\nabla \cdot \boldsymbol{q}_h^n, w_h) + (Rc_h^n, w_h) = (f^n, w_h) \ , \tag{3}$$

$$\sum_{K\in\mathcal{T}_h} \langle \mu_h, \boldsymbol{q}_h^n \cdot \boldsymbol{n}\rangle_{\partial K} = 0 \tag{4}$$

for all $(\boldsymbol{v}_h, w_h, \mu_h) \in \tilde{\boldsymbol{V}}_h \times W_h \times \Lambda_h$, where the space W_h consists of piecewise polynomials on the triangular grid $\mathcal{T}_h$, $\tilde{\boldsymbol{V}}_h$ is the space of piecewise RT_0 functions on $\mathcal{T}_h$ and Λ_h represents the space of piecewise constant functions on the set of edges of $\mathcal{T}_h$. The operator $\mathcal{B}$ is defined elementwise by

$$\mathcal{B}(\lambda_h^n, c_h^n) = \sum_{K\in\mathcal{T}_h} \sum_{E\subset\partial K} Q_{KE}^n \mathcal{B}_{KE}(\lambda_E^n, c_K^n)\boldsymbol{v}_{KE} \ ,$$

where $\boldsymbol{v}_{KE}$ represents the basis function of the Raviart-Thomas space of lowest order associated with edge E on the triangle $K \in \mathcal{T}_h$, and the coefficients Q_{KE}^n represent the projection of $\boldsymbol{Q}^n$ in the space of Raviart-Thomas elements of lowest

order. The weights $\mathcal{B}_{KE}$ have to be specified to obtain one particular scheme. To obtain a full upwind-mixed hybrid scheme, for example, we define

$$\mathcal{B}_{KE}(\lambda_E^n, c_K^n) = \begin{cases} c_K^n & \text{if } Q_{KE}^n \geq 0 \ , \\ \lambda_E^n & \text{otherwise} \ . \end{cases}$$

The convergence analysis carried out in [3] shows that the method converges with first order in space and time if the condition

$$|\mathcal{B}_{KE}(\lambda_E^n, c_K^n) - c_K^n| \leq C|\lambda_E^n - c_K^n|$$

is satisfied for a constant $C > 0$. Since the definition of the weights $\mathcal{B}_{KE}$ involve only data from the element K, the equations (2) are fully local. Consequently, the number of global unknowns can be reduced by eliminating the flux and the scalar unknowns from the system, which is not possible if an upwind-mixed scheme is employed that involves information from neighbour elements in the definition of the upwind weights. Our numerical results indicate that the errors of the classical and our hybrid upwind-mixed schemes are of the same order of magnitude, while the CPU time was 50% lower for the hybrid method.

2. Approximation with the BDM_1 element

If the mixed problem (1) is approximated using the Brezzi-Douglas-Marini element, suboptimal first order of convergence for the flux variable occurs [2]. This may happen when the finite element spaces employed have a higher order for the flux variable than for the scalar variable. By using the Lagrange multipliers of the mixed-hybrid formulation it is possible to reestablish optimal second order convergence in space. More precisely, we use the operator

$$\mathcal{B} = \sum_{K \in \mathcal{T}_h} \sum_{E \subset \partial K} \sum_{i=1}^{2} \mathcal{B}_{KE_i}(\lambda_{E_1}^n, \lambda_{E_2}^n, c_K^n)$$

together with the weights

$$\mathcal{B}_{KE_i}(\lambda_{E_1}^n, \lambda_{E_2}^n, c_K^n) = Q_{KE_i}^n \frac{\lambda_{E_1}^n + \lambda_{E_2}^n + \lambda_{E_i}^n}{3} \boldsymbol{v}_{KE_i} \ , \quad i = 1, 2$$

in the discretization of the advective term. Numerical results for this scheme are contained in [4], the error analysis is ongoing work.

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