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Computational Multiscale Methods

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Abstract. Almost all processes in engineering and the sciences are characterised by the complicated relation of features on a large range of non-separable spatial and time scales. The workshop concerned the computer-aided simulation of such processes, the underlying numerical algorithms and the mathematics behind them to foresee their performance in practical applications.

Mathematics Subject Classification (2010): 65, 35B, 74Q, 70F, 76A, 76M.

Introduction by the Organisers

Many processes in geophysics, material sciences, biology and quantum mechanics are multiscale in nature and it is the complex interplay of effects at a large range of non-separable scales in space and time that characterises their relevant and surprising properties. Since this complex interplay is intractable analytically, their understanding and control is intrinsically tied to numerical simulation. However, in many interesting applications, computers are not able to resolve all details on all relevant scales. In the foreseeable future, the observation and prediction of physical phenomena from multiscale models will require sophisticated numerical techniques for the effective representation of unresolved scales, i.e., computational multiscale methods.

Computational multiscale methods are a systematic approach to the modelling and simulation of multiscale problems that includes the derivation of detailed models (fine scale discretisation) adapted to all relevant scales, the derivation of reduced models of feasible computational complexity, e.g. the compression/filtering

to coarse scales of interest while still maintaining its essential features (upscaling/homogenisation/coarse graining), the reconstruction of fines scale information from coarse scale computations (downscaling), and the fast simulation of the detailed/reduced model by iterative up- and downscaling (multilevel method) or concurrent coupling.

This workshop concerned the design of such efficient numerical algorithms and the mathematics behind them to foresee and assess their performance in engineering and scientific applications. For this purpose, the workshop broad together researchers with very different scientific backgrounds including numerical analysis, mathematical modelling, scientific computing, and computational mechanics. Amongst the particular trends of the workshop were numerical homogenization, discrete multiscale mathematical modelling, the coupling or blending of mathematical models on different scales, and the impact of randomness on models and numerical methods.

Computational homogenization refers to a class of numerical methods for partial differential equations with multiscale data aiming at the determination of macroscopic (effective) approximations that account for the complexity of the microstructure. While many approaches are empirically successful and robust for certain multiscale problems, there is an extremely high current interest for rigorous numerical analysis of those methods. This interest was reflected, e.g., by the lectures of Abdulle, Arbogast, Efendiev, Frederick, Hackbusch, Målqvist and Owhadi in the context of linear and non-linear problems. We have seen the high efficiency of numerical methods when structural knowledge of the problem is available but also the added value of computational homogenization when compared with classical analytical techniques, i.e., its applicability, reliability, and accuracy in the absence of strong assumptions such as periodicity and scale separation.

Multilevel approaches for the acceleration of the numerical solution of detailed models were addressed by Spillane for a linear model problem and also by Cancès and Henning in the context of the Kohn-Sham and the non-linear Schrödinger equation. The presentations of Gorb and Tsai presented network-type approaches to the effective numerical modelling of multiphase media. The lectures of Berlyand, van Brummelen, Heitzinger, Schmuck and Wheeler discussed the multiscale mathematical and numerical modelling of various multiscale and multiphysics problems. The estimation of modelling errors was addressed by Szepessy in the context of molecular dynamics simulations.

A major difficulty in multiscale problems is when fine scales and coarse scale are described by different equations. The lecture of Bochev and Luskin discussed the coupling of molecular and continuum models, Gunzburger and Lipton presented the intermediate model of peridynamics. Stochastic aspects and uncertainty quantification were also included in many lectures; Legoll addressed random homogenization, Bal studied the propagation of stochasticity in numerical homogenization, and Samaey discussed variance reduction methods for kinetic equations.

Most of the research presented during the week was motivated by applications such as the mechanical analysis of composite and multifunctional materials, transport processes in porous media, e.g. reservoir modelling or the transport of charged species in microfluidic devices, motility in biosystems, as well as the simulation of quantum mechanical systems. The range of related mathematical models included the minimisation of convex and non-convex energy functionals, inverse problems, non-linearly coupled systems as well as linear and non-linear eigenvalue problems. The large variety of applications and mathematical problems clearly demonstrated that the field of Computational Multiscale Methods is very active. Many promising results were presented and it is clear that in the future challenging multiscale problems and more general multiphysics applications will be investigated.

This workshop was well attended with 46 participants from 14 different countries (15 participants from the United States, 14 from Germany, 3 from France, 3 from Sweden, 2 from Switzerland, and respectively 1 from Austria, Belgium, Chile, China, England, Korea, Netherlands, Norway and Scotland). 26% of the participants were students or young postdocs (less than 3 years after their PhD).

The organizers would like to thank the institute and in particular its staff members for their hospitality and the great support before and during the workshop.

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Workshop: Computational Multiscale Methods

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Abstracts

Numerical methods for multiscale parabolic and hyperbolic problems

Assyr Abdulle

In this report we summarize some recent developments of numerical homogenization methods for nonlinear parabolic equations and wave equations in heterogeneous medium.

Monotone parabolic problems. Let $\Omega \subset \mathbb{R}^d$, $d \leq 3$ be a convex polygonal domain. Consider for $T > 0$, $f \in L^2(\Omega)$ the following nonlinear parabolic problem

$$\begin{aligned} \partial_t u^\varepsilon - \nabla \cdot (\mathcal{A}^\varepsilon(x, \nabla u^\varepsilon)) &= f \qquad \text{in } \Omega \times (0,T), \\ u^\varepsilon|_{\partial\Omega\times(0,T)} = 0, \qquad u^\varepsilon|_{t=0} &= g \qquad \text{in } \Omega. \end{aligned} \tag{1}$$

Assumptions:

- there exists $C_0 > 0$ such that $|\mathcal{A}^\varepsilon(x,0)| \leq C_0$ for a.e. $x \in \Omega$;
- Lipschitz continuity: $|\mathcal{A}^\varepsilon(x,\xi) - \mathcal{A}^\varepsilon(x,\eta)| \leq L|\xi - \eta| \quad \forall \xi, \eta \in \mathbb{R}^d$, a.e. $x \in \Omega$;
- Strong monotonicity: $[\mathcal{A}^\varepsilon(x,\xi) - \mathcal{A}^\varepsilon(x,\eta)] \cdot (\xi - \eta) \geq \lambda|\xi - \eta|^2 \quad \forall \xi, \eta \in \mathbb{R}^d$, a.e. $x \in \Omega$.

Under theses assumptions (1) has a unique solution $u^\varepsilon \in E$, where

$$E = \{v \in L^2(0,T; H_0^1(\Omega)) \,|\, \partial_t v \in L^2(0,T; H^{-1}(\Omega))\},$$

and $\{u^\varepsilon\}$ is a bounded sequence in E which weakly converges (up to extracting a subsequence) to a function $u^0 \in E$ that is solution of a homogenized problem that takes a form similar to (1) with $\mathcal{A}^\varepsilon(x, \nabla u^\varepsilon)$ replaced by $\mathcal{A}^0(x, \nabla u^0(x,t))$ (see e.g. [10]). As $\mathcal{A}^0(x, \nabla u^0(x,t))$ is usually not explicitly known in closed form, it must be approximated numerically.

Multiscale methods. Let the time interval $(0,T)$ be uniformly divided into N subintervals of length $\Delta t = T/N$ and define $t_n = n\Delta t$ for $0 \leq n \leq N$ and $N \in \mathbb{N}_{>0}$. Let $u_0^H \in S_0^1(\Omega, \mathcal{T}_H) = \{v^H \in H_0^1(\Omega) \,|\, v^H|_K \in \mathcal{P}^1(K), \forall\, K \in \mathcal{T}_H\}$ be a given approximation of the initial condition $g(x)$.

Fully nonlinear method. Consider the multiscale method given by the recursion: for $0 \leq n \leq N-1$, find $u_{n+1}^H \in S_0^1(\Omega, \mathcal{T}_H)$ such that

$$\int_\Omega \frac{u_{n+1}^H - u_n^H}{\Delta t}\, w^H dx + B_H(u_{n+1}^H; w^H) = \int_\Omega f\, w^H dx, \qquad \forall\, w^H \in S_0^1(\Omega, \mathcal{T}_H), \tag{2}$$

with the nonlinear macro map B_H given by

$$B_H(v^H; w^H) = \sum_{K \in \mathcal{T}_H} \frac{|K|}{|K_\delta|} \int_{K_\delta} \mathcal{A}^\varepsilon(x, \nabla v_K^h) dx \cdot \nabla w^H(x_K), \quad v^H, w^H \in S_0^1(\Omega, \mathcal{T}_H), \tag{3}$$

where $K_\delta \subset K$ are sampling domains of size δ (proportional to ε) and v_K^h solve the constrained micro problems: find $v_K^h - v^H \in S^1(K_\delta, \mathcal{T}_h)$ such that

$$\int_{K_\delta} \mathcal{A}^\varepsilon(x, \nabla v_K^h) \cdot \nabla z^h dx = 0, \qquad \forall\, z^h \in S^1(K_\delta, \mathcal{T}_h). \tag{4}$$

Here $S^1(K_\delta, \mathcal{T}_h)$ denotes a microscopic finite element subspace of $W^1_{per}(K_\delta) = \{v \in H^1_{per}(K_\delta) \mid \int_{K_\delta} v\, dx = 0\}$ or $H^1_0(K_\delta)$ and $\mathcal{T}_h$ is a partition of K_δ with micromesh size $h = \max_{T\in\mathcal{T}_h} \mathrm{diam} T$.

Linearized method. We next describe a method that relies only on *linear micro problems* and has the same computational cost than a numerical homogenization method for linear parabolic homogenization problems. Assume $\mathcal{A}^\varepsilon(x,\xi) = a^\varepsilon(x,\xi)\xi$. Define $\mathcal{S}^{H,h} = S^1_0(\Omega, \mathcal{T}_H) \times \prod_{K\in\mathcal{T}_H} S^1(K_\delta, \mathcal{T}_h)$, and the map $\hat{u}_n \mapsto \hat{u}_{n+1} = (u^H_{n+1}, \{u^h_{n+1,K}\}) \in \mathcal{S}^{H,h}$ given by the fully discrete space-time scheme

(1) evolution of the macroscopic state: find $u^H_{n+1} \in S^1_0(\Omega, \mathcal{T}_H)$ solution of the linear problem

$$\int_\Omega \frac{1}{\Delta t}(u^H_{n+1} - u^H_n)\, w^H dx + B_H(\hat{u}_n; u^H_{n+1}, w^H) = \int_\Omega f w^H dx;$$

(2) update the micro states: $\hat{u}_{n+1} = u^H_{n+1} + u^h_{n+1,K}$, where for $K \in \mathcal{T}_H$, $u^h_{n+1,K}$ satisfies $u^h_{n+1,K} - u^H_{n+1} \in S^1_h$ and

$$\int_{K_\delta} a^\varepsilon(\nabla \hat{u}^h_{n,K}) \nabla \hat{u}^h_{n+1,K} \cdot \nabla z^h dx = 0 \qquad \forall\, z^h \in S^1(K_\delta, \mathcal{T}_h).$$

A fully discrete space time analysis (including micro, macro and resonance errors) has been given in [4] and [5] for both methods under appropriate smoothness assumptions. We note that a new (linear) elliptic projection has been introduced in [4]. We note that for single scale problems, a nonlinear projection has been used with non-optimal L^2 convergence rates for low order finite elements [7]. Optimal convergence rates were obtained using weighted norm techniques for nonlinear problems [8]. Such weighted norm techniques are avoided in our analysis.

Multiscale wave problems. Let $\Omega \subset \mathbb{R}^d$, $d \le 3$ be a convex polygonal domain. Consider for $T > 0$, $f \in L^2(\Omega)$ the following wave equation with appropriate initial and boundary conditions

$$\partial_{tt} u^\varepsilon - \nabla \cdot (a^\varepsilon \nabla u^\varepsilon) = f \qquad \text{in } \Omega \times (0,T), \tag{5}$$

where $a^\varepsilon(x)$ is a rapidly varying tensor that is assumed to be uniformly elliptic and bounded. As for the parabolic problem, homogenisation theory ensures that $u_\varepsilon \rightharpoonup u_0$ weakly* in $L^\infty(0,T; H^1_0(\Omega))$, $\partial_t u_\varepsilon \rightharpoonup \partial_t u_0$ weakly* in $L^\infty(0,T; L^2(\Omega))$, where u_0 is the solution of a homogenized problem similar to (5) with $a^\varepsilon(x)$ replaced by and effective tensor $a^0(x)$ independent of the smallest scales [6].

Multiscale methods. Find $u^H \in [0,T] \to S^1_0(\Omega, \mathcal{T}_H)$ such that for $f \in L^2(\Omega)$

$$(\partial_{tt} u^H, v^H) + B_H(u^H, v^H) = (f, v^H)\ \forall v^H \in S^1_0(\Omega, \mathcal{T}_H) \tag{6}$$

with appropriate projection of the true initial conditions, where $B_H(u^H, v^H) = \sum_{K\in\mathcal{T}_H} \frac{|K|}{|K_\delta|} \int_{K_\delta} a^\varepsilon(x)\nabla u_K^h \cdot \nabla v_K^h dx$ and u_K^h (respectively v_K^h) are solutions of the following micro problems: for $K \in \mathcal{T}_H$ find $(u_K^h - u^H) \in S^1(K_\delta, \mathcal{T}_h)$ such that

$$\int_{K_\delta} a^\varepsilon(x)\nabla u_K^h \cdot \nabla z^h dx = 0, \qquad \forall z^h \in S^1(K_\delta, \mathcal{T}_h), \tag{7}$$

where $S^1(K_{\delta_j}, \mathcal{T}_h)$ is similar as defined before. Optimal convergence rates towards the homogenized solution has been proved in [1] for a generalized version of the method presented above (continuous in time fully discrete in space) allowing for arbitrary macro and micro polynomial degrees and time dependent right-hand side.

For limited time the propagation of waves in a highly oscillatory medium is well-described by the classical homogenized wave equation. With increasing time, however, the true solution, u^ε, deviates from the classical homogenization limit, u^0, as dispersive effects develop [11, 9]. In [3],[2] we proposed a new multiscale method based on (6) but with a modified L^2 scalar product $(\partial_{tt} u^H, v^H)$. The method is proved to be consistent with the homogenized solution and is shown to capture (for one-dimensional problems) dispersive effects that appear in the true solution with increasing time but are not present in the homogenized model. Moreover, the computational cost of the new method is *identical* to the cost of the method (6).

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Aspects of discontinuous multiscale flow approximations on transport and a two-level mortar preconditioner

Todd Arbogast

(joint work with Hailong Xiao, Zhen Tao)

The equations governing fluid flow are generally of elliptic or parabolic type, such as the equation governing single-phase flow in a porous medium:

$$\nabla \cdot u = f \quad \text{and} \quad u = -a\nabla p.$$

Because porous media are notoriously heterogeneous, the permeability coefficient a varies greatly on very small scales, and so the velocity u and pressure p must be approximated by multiscale techniques. Often in practical applications, u transports some chemical species governed by another equation of nearly hyperbolic type. We study the use of multiscale numerical techniques for flow and their effect on the combined flow and transport system.

Because mass conservation is critical for most flow and transport problems, we concentrate on mixed methods for the elliptic flow problem. We consider three similar multiscale methods for flow problems, the mixed multiscale finite element method (MsFEM) [7, 10, 9], the variational multiscale method (VMM) [11, 3, 8], and the domain decomposition multiscale mortar mixed method [4]. MsFEM uses the original variational form but modifies the finite elements, whereas VMM uses standard finite elements but modifies the variational form. Modification of the variational form can be viewed as the original variational form with modified elements. In fact, the modified elements are standard multiscale elements, and so these two approaches are essentially the same [2].

The mortar domain decomposition method approximates the trace of the pressure λ on the interfaces Γ between the subdomains in a mortar space M. For a given $\lambda \in M$, one can easily solve the subdomain problems in parallel for $u(\lambda)$ and $p(\lambda)$, using λ as a boundary condition. The Schur complement system is

$$d(\lambda, \mu) = b(\mu) \quad \forall \mu \in M,$$

where $d(\lambda,\mu)-b(\mu) = \langle u(\lambda)\cdot\nu, \mu\rangle_\Gamma$ represents the weak form of the normal velocity flux jump on Γ. The method is efficient in parallel if M is not large.

Each mortar basis function $\lambda_i \in M$ gives rise to a multiscale finite element $\big(u(\lambda_i), p(\lambda_i)\big)$, and so the method can be viewed in terms of MsFEM or VMM. The resulting multiscale elements are very unusual, and have greater flexibility in approximating the pressure and velocity. However, it results in a velocity field that is merely weakly continuous in the direction normal to the subdomain interfaces.

Multiscale error analysis for a two-scale, locally periodic permeability coefficient suggests that the MsFEM has serious resonance error, which can be mitigated by using higher order elements [1]. The same is true of the mortar methods if

one uses polynomials to approximate the mortar pressure λ. However, one can develop a multiscale mortar approximation based on homogenization theory [5], and error analysis shows that the approximation is less sensitive to resonance. Numerical tests of highly heterogeneous media, including channelized media, can be conducted to compare the solution to the fine-scale reference solution. Results of the L^2-norm of the velocity error suggest that the mortar methods are superior to the MsFEM, even when polynomial mortar approximations are used, and that the homogenization-based mortars perform best of all.

The picture changes dramatically when the flow velocity u is used with a transport problem. We considered two-phase flow in a porous medium, which splits into an elliptic flow problem and a parabolic (but nearly hyperbolic) transport problem. Numerical tests show that the discontinuities in the mortar velocity (since it is only *weakly* continuous in the normal direction) produce internal sources and sinks that render the results unacceptable. Oversampled MsFE's also have discontinuities, and so should suffer the same fate. MsFE's that have a continuous normal velocity show no such internal sources and sinks. However, because the mortar velocity is overall more accurate in L^2, it does provide a very accurate approximation to the transport plume compared to the fine-scale solution. The MsFE's have difficulty reproducing the plume shape, and so are not sufficiently accurate.

One could postprocess the mortar velocity to obtain a continuous normal velocity [12, 14]; however, such an approach is likely to result in numerical diffusion, smearing the details of the flow. A more significant question is "Have we picked up all the relevant scales?" One might answer this using a-posteriori error estimation and grid addaptivity [4, 13]. However, this will result in a larger coarse mortar problem, and reduced parallel efficiency. Instead, we developed an iterative method that results in the fine-scale solution, which therefore picks up all relevant scales and produces a velocity with a continuous normal component. It is a two-level preconditioner for the fine-scale system [6].

Our new approach can be viewed as an example of VMM. Let M denote the fine-scale mortar space, for which the solution of the problem would result in the fine-scale velocity and pressure. We decompose the mortar space into $M = M_{\mathrm{c}} \oplus M_{\mathrm{f}}$, where M_{c} is the coarse component and the rest of the scales are M_{f}. Then $\lambda = \lambda_{\mathrm{c}} + \lambda_{\mathrm{f}}$ and the Schur complement system decomposes as

$$d(\lambda_{\mathrm{f}} + \lambda_{\mathrm{c}}, \mu_{\mathrm{c}}) = b(\mu_{\mathrm{c}}) \quad \forall \mu_{\mathrm{c}} \in M_{\mathrm{c}},$$
$$d(\lambda_{\mathrm{f}} + \lambda_{\mathrm{c}}, \mu_{\mathrm{f}}) = b(\mu_{\mathrm{f}}) \quad \forall \mu_{\mathrm{f}} \in M_{\mathrm{f}}.$$

In the VMM, one normally solves the second equation for the fine scale λ_{f} in terms of λ_{c}, and modifies the first equation to develop the coarse problem

$$d(\lambda_{\mathrm{f}}(\lambda_{\mathrm{c}}) + \lambda_{\mathrm{c}}, \mu_{\mathrm{c}}) = b(\mu_{\mathrm{c}}) \quad \forall \mu \in M_{\mathrm{c}}.$$

However, the second, finer scale problem for λ_{f} is nonlocal, and so VMM applied directly is inefficient. Instead, we solve this fine problem approximately using a local smoother. The local smoothing preconditioner is based on block Jacobi, using blocks defined by the interfaces between pairs of subdomains. We use restrictive

smoothing domains that are smaller normal to the interfaces, and overlapping in the directions tangential to the interfaces. Given the smoothed λ_{f}, the coarse problem can be solved efficiently, and so defines a coarse preconditioner. Combined, we have a two-level iterative scheme for the fine-scale velocity and pressure.

The prolongation operator of the coarse mortar to the fine is defined uniquely by the condition that the L^2-projection of a coarse mortar agrees with its projection onto the space of normal velocity fluxes, i.e., no energy is introduced when changing mortar scales. In the simplest case, the condition number of the preconditioned interface operator is bounded by a multiple of $(\log(1 + H/h))^2$, where H is the maximal diameter of the subdomains and h is the mesh diameter. Numerical examples involving strongly heterogeneous porous media demonstrate the efficiency and robustness of the scheme (it requires only about 20-60 iterations). It is often desirable, and sometimes necessary, to use a piecewise linear or better coarse mortar space to achieve good convergence for heterogeneous problems.

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Propagation of Stochasticity in PDEs with random coefficients

Guillaume Bal

We consider equations with highly oscillatory random coefficients and aim to understand macroscopic properties of the stochasticity of their solutions. Homogenization is a well-known theory showing that randomness is averaged out to provide an effective medium model in a appropriate limit. Understanding the residual stochasticity of solutions in such a setting in an important practical question. This talk presents recent results on such aspects of propagation of stochasticity and describe applications in multiscale algorithms as well as parameter estimations.

Coarse-graining in multiscale PDE models of motility in biosystems

Leonid Berlyand

We present a review of our work on modeling, analysis and computations of collective motion of microswimmers (e.g., bacteria). Since the number of bacteria is quite large and the collective nature of the motion results in rise of new scales, this problem presents a serious computational challenge and requires special coarse-graining (homogenization) techniques.

First, a stochastic PDE model is introduced for a dilute suspension of self-propelled bacteria. Using this model, an explicit asymptotic formula for the effective viscosity (EV) is obtained that explains the mechanisms of the drastic reduction of EV [1].

Next, we introduce a model with pairwise interactions and excluded volume constraints. We compute EV analytically and numerically and analyze the onset of collective motion in bacterial suspensions by developing a PDE/ODE model that captures the appearance of a *collective scale* [2]-[3]. Numerical analysis of this work is challenging due to the (i) large number of bacteria, (ii) uncertainty (randomness) in initial data and (iii) strong interactions. Well-known methods such as the fast multipole method (FMM) efficiently apply in a deterministic setting, but become very costly in a random setting, also the classical Mean Field (MF) approach does not capture correlations.

To address the challenges (i)-(iii) simultaneously, a novel computational approach for the time evolution of a system of a large number N of interacting particles, which goes beyond MF has been introduced in [4]. It is based on a derivation of a closed PDE system for one- and two-point probability distributions for particle locations. This system is obtained by a special choice of a truncation for the BBGKY hierarchy, which is a system of N coupled conservation law type PDEs (whose direct solution is prohibitively expensive even for not very large N). Finally we provide examples that show how to solve this nonlinear and non-local system numerically.

Collaborators: S. Ryan, B. Haines, M. Potomkin (PSU students/postdocs); I. Aronson, A. Sokolov, D. Karpeev (Argonne); P.-E. Jabin (Maryland).

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An Optimization-Based Atomistic-to-Continuum Coupling Method

Pavel Bochev

(joint work with Derek Olson, Mitchell Luskin, Alexander V. Shapeev)

Atomistic-to-Continuum (AtC) coupling methods are a novel means of computing the properties of a discrete crystal structure, such as those containing defects, that combine the accuracy of an atomistic (fully discrete) model with the efficiency of a continuum model. In this talk we extend the optimization-based AtC, formulated in [11] for linear, one-dimensional problems to multi-dimensional settings and arbitrary interatomic potentials.

Introduction

Solid materials have atomic configurations which are arranged as a crystalline lattice, and the properties of these materials are derived from the underlying structure of the lattice. Specifically, defects in the regular, repeating arrangement of atoms such as a dislocation, or an extra plane of atoms, determine fundamental mechanisms such as plastic slip. The presence of defects invalidate the central hypotheses of continuum mechanics so models that recognize the discrete nature of the material on the atomic scale must be used. Such methods can vary in their complexity ranging from quantum mechanical models which incorporate nuclear and electronic forces to empirical potential models that assume the existence of a potential energy which is a function of the nuclear positions only. The latter allows atoms to be considered as classical mechanical particles. Throughout this note, we assume that the exact mathematical problem we wish to solve is that of minimizing the global potential energy of a set of N atoms or, equivalently, of equilibrating the internal and external forces on the atoms.

The outstanding issue with empirical atomistic models is the complexity involved in their applications. In even the smallest problems of material interest on the nanoscale, there will be at least 10^9 and up to 10^{15} atoms meaning the number of degrees of freedom in an atomistic model is often far outside the scope of any current computational feasibility. A novel attempt at solving this problem has been to keep the atomistic model only in a small region near the defect, while employing a continuum model such as elasticity in the bulk of the material away

from the defect. Continuum models are well understood and can numerically be solved in an efficient manner using finite elements. In effect, the atomistic model provides a constitutive relation near the defect where the constitutive relation of the continuum model fails to hold.

These so called atomistic-to-continuum (AtC) coupling methods have seen a surge of interest in the last two decades, especially with the introduction of the quasicontinuum method in [12]. The problem introduced in these AtC methods is how to combine, or *couple*, the two different models. An informal way of carrying this out is to divide the computational domain, say Ω, into an atomistic region, Ω_{a}, and a continuum region, Ω_{c}. Then, a global hybrid energy or hybrid force field is constructed from the atomistic and continuum models on Ω_{a} and Ω_{c}. The resulting hybrid energy is then minimized, or alternatively, the internal and external forces are equilibrated to find the equilibrium configuration of Ω.

In this note we continue the development of the optimization-based AtC approach commenced in [11]. The core idea is to pose independent atomistic and continuum subproblems on overlapping domains Ω_{a} and Ω_{c} and then couple the models by minimizing an objective functional, which measures the difference between the strains of the atomistic and continuum states on $\Omega_{\mathrm{a}} \cap \Omega_{\mathrm{c}}$. In so doing, our approach combines ideas from *blending AtC* methods [8, 1, 3, 7, 2, 9, 10] with the optimization-based domain-decomposition approach for PDEs in [6, 5].

The resulting optimization-based AtC method differs substantially from current energy or force-based methods, and to the best of our knowledge [11] is the first instance of using an objective functional of this form to effect atomistic-to-continuum coupling. Conceptually, our AtC approach is similar to the heterogeneous domain decomposition method for PDEs developed in [4] with the important distinction that we couple two fundamentally different material models rather than PDEs.

The main focus of this talk is on the formulation of an optimization-based AtC method for modeling material defects in two and three dimensions, while allowing for arbitrary many-body terms in the potential energy.

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Multiscale problems in electronic structure calculation

Eric Cancès

Electronic structure calculation has a wide variety of applications in physics, chemistry, molecular biology, materials science, and nano-sciences. We discussed some of the multiscale features of the N -body electronic Schrödinger equation and of the main models used to approximate the solutions of this equation, with an emphasis on the Kohn-Sham model. A first multiscale problem is the mathematical derivation of the Born-Oppenheimer dynamics, using the mass ratio between electrons and nuclei as a small parameter. A second problem is concerned with thermodynamic limits and the derivation of macroscopic properties of materials from first-principle quantum mechanics, letting the number of particles go to infinity. A third source of multiscale problems is the interplay between many-body effects, the Pauli principle, and Colomb screening, which leads to a wide range of characteristic energies covering 10 orders of magnitude, even though no explicit small (or large) parameter is present in the equation.

Generalized Multiscale Finite Element Methods and Applications

Yalchin Efendiev

Many application problems have multiscale nature. Due to disparity of scales, the simulations of these problems are prohibitively expensive. Some types of upscaling or model reduction techniques are needed to solve many multiscale problems. In the talk, we discuss a few known techniques that are used for problems with scale separation and focus on Generalized Multiscale Finite Element Method (GMsFEM) that has been recently proposed in [5] for solving problems with non-separable scales and high contrast. The main objective of the method is to provide local reduced-order approximations for linear and nonlinear PDEs via multiscale spaces on a coarse computational grid.

The Generalized Multiscale Finite Element Method (GMsFEM) is a flexible framework that, by systematically enriching the coarse spaces, takes into account small scale information and complex input spaces. This approach divides the

computation into two stages: offline and online. In the offline stage, a small dimensional space is constructed that can be efficiently used in the online stage to construct multiscale basis functions. These multiscale basis functions can be re-used for any input parameter to solve the problem on a coarse grid. The main idea behind the construction of offline and online spaces is the selection of local spectral problems and the selection of the snapshot space.

We briefly discuss how the method can be used within different global finite element discretizations (e.g., Discontinuous Galerkin [6] or mixed finite element [2]) and the applications to various problems (e.g., two-phase flow in porous media [2] or wave equations [3]). We also discuss some issues such as adaptivity in GMsFEM [4] and the applications to nonlinear problems [1].

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Methods for multiscale inverse problems

Christina Frederick

We consider inverse problems governed by multiscale partial differential equations of the form

$$-\nabla \cdot (a^\epsilon \nabla u^\epsilon) + b^\epsilon u^\epsilon = f. \tag{1}$$

Here, the goal is to determine the coefficients in the equation from given data of the solution at the boundary. The constant $0 < \epsilon \ll 1$ represents the ratio of scales in the problem, and a^ϵ and b^ϵ contain microscopic variations on the $\epsilon-$scale.

Multiscale inverse problems pose a challenge in both the mathematical formulation and the numerical modeling, which is hard even for forward computations.

The problem in its full generality is typically ill-posed; different sequences a^ϵ, b^ϵ produce the same limiting equations as $\epsilon \to 0$. One approach is to reduce the dimension of the original problem by just considering the inverse of an effective equation without microscale ϵ.

Homogenization theory [4] provides the form of the effective problem corresponding to (1); as $\epsilon \to 0$, $u^\epsilon \rightharpoonup U$, where U solves

$$-\nabla \cdot (A\nabla U) + \overline{b}U = f, \tag{2}$$

and the theory gives a constructive definition of A and $\overline{b}$. Inversion of the effective model results in a lower computational cost and is therefore attractive for use in practical applications.

Our approach is to assume some prior knowledge of the microstructure in the form of an accurate parameterization $m \to a^\epsilon(m)$, where m is low dimensional function and independent of ϵ. We prove that the problem of determining $a^\epsilon(m)$ using boundary data from the homogenized solution is a well-posed inverse conductivity problem when certain monotonicity conditions are met (as in [2]). We also demonstrate that this approach in many cases is better than first determining A and then in a second stage determining a^ϵ.

A severe drawback is that the explicit form of the homogenized coefficient corresponding to a^ϵ is generally not known. This issue is addressed with the implementation of the heterogeneous multiscale method, or HMM, introduced by E and Engquist [1, 5]. HMM provides a framework for the design of methods that capture macroscale properties of a system using microscale information. Using HMM forward solvers increases the accuracy in the inversion process while benefiting from the low computational cost of a macroscale solver. Numerical examples indicate how the technique can be applied to imaging problems in biology and exploration seismology.

We extend the study of multiscale methods to include a discussion of how to overcome the main computational challenge of direct simulation by using specific grids that are used in methods such as HMM. In direct simulation, the smallest important scales must be resolved over the length of the largest scales. Even the basic cost can be understood from the viewpoint of information theory. The classical sampling theorem [7] states that bandlimited functions are uniquely determined from uniform samples when at least two function values per wavelength are known. Applied to numerical grids, this implies that if the size of the computational domain is 1 and $0 < \epsilon \ll 1$ is the smallest important wavelength, then at least $2\epsilon^{-1}$ unknowns are required.

If this is too much for the available computational resources, then special features of the original problem must be exploited. Scale separation is assumed in homogenization theory, in our inverse problem above and in convergence analysis of HMM. The functions involved are typically of the form

$$f^\epsilon(x) = f(x, x/\epsilon) \qquad \text{where } f(x,y) \text{ is periodic in } y, \quad 0 < \epsilon \ll 1.$$

With equidistant sampling points, the sampling rate must still be the same as above, $O(\epsilon^{-1})$ in order to ensure full recovery. An alternative approach is to use

nonuniform sampling schemes to achieve a lower sampling rate [3] by taking advantage of the special structure of functions that have large spectral gaps. We relate these ideas to the design of grids used in multiscale computation, and prove that the resulting grids form stable sampling sets for a class of bandlimited functions.

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Review of Network Approximation Methods for Capturing Singular Phenomena in High Contrast Concentrated Composites

Yuliya Gorb

In computational mechanics one distinguishes between the two types of approximation: *structural* vs. *numerical*. The numerical approximation is characterized by a discretization scale, or mesh size, adjustable depending on the desired precision and includes finite difference, finite volume, finite element methods among others. On the other hand, the structural approximation is based on "physical discretization", where the discretization scale is intrinsically built into the problem through the size of particles and distances between them. Structural discretization typically leads to finite-dimensional problems on graphs, called *network models*, and normally reduces to an algebraic system of much smaller dimension than the corresponding numerical discretization. Moreover, the obtained via structural discretization finite-dimensional model can also be viewed as a simplified analog of the original continuum problem, hence, makes physics of the problem transparent.

For an arbitrary continuum problem one may not expect this approximation would work since it is based on specific features of the original problem, namely, the heterogeneous medium has to be described by a *high contrast rapidly varying function*. "High contrast" means that mechanical properties of composite constituents are vastly different, and is a physical condition. "Rapidly varying" means that this function fluctuates on a length scale that is much smaller than the size the domain occupied by the composite, and is a geometric condition. Exactly

these two conditions are the reason due to which the corresponding numerical approximation is prohibitively expensive.

This talk will provide a comprehensive overview of *discrete network approximation techniques* that have been demonstrated to be an elegant and powerful approach for deriving and justifying asymptotic formulas for (1) effective properties, (2) electric field, and (3) Dirichlet to Neumann map of high contrast disordered composites with particles close to touching.

More specifically, we present results of the following studies.

(1) *Blow Up of Effective Properties*
The first observation is that the effective properties of such composites exhibit blow up as the typical interparticle distance δ gets small. Two mathematical formulations will be explored: *scalar* and *vectorial* ones. The scalar problem represents densely spaced infinitely conducting particles in a medium of finite conductivity, while the vectorial problem describes the motion of an irregular array of highly packed solid particles in an incompressible Newtonian fluid. An application of discrete network approximation models will be presented as an effective tool in capturing singular behavior of the *effective conductivity*, see [1], and the *effective viscosity*, see [2], of the corresponding composites. Rigorous justification of the obtained asymptotics as $\delta \ll 1$ will be discussed. Such approximations will lead to an accurate and cost-effective numerical method for simulating of the properties of the corresponding heterogeneous media.

(2) *Blow Up of Electric Field*
Besides the effective properties of aforementioned composites the electric field described by the solution gradient also exhibits blow up at the points of the closest distance between neighboring particles. We note that the uniform estimates for solution gradient was a subject of numerous studies in the last decade with only upper and lower bounds for it being constructed. However, the *exact* asymptotics has not been captured yet. It will be demonstrated how the network models can be utilized to derive such asymptotics *precisely*, see [4]. It is also important to mention that previous contributions on the subject that provided only bounds for the gradients blow up, had their limitations, e.g. some of them use methods that work only in two dimensions, some deal with inhomogeneities of spherical shape only, and all of them were designed to treat *linear* problems only, with no direct extension to a nonlinear case. In contrast, techniques developed and adapted in the methodology based on network models work for any number of particles of arbitrary shape in any dimension, and allow for a straightforward generalization to a *nonlinear* case, such as p-Laplacian, see [5].

(3) *Asymptotic Approximation of the Dirichlet to Neumann map*
An asymptotic study of the Dirichlet to Neumann (DtN) map of high contrast composite media with perfectly conducting inclusions that are close

to touching will also be presented. The DtN operator maps the boundary trace of the solution to its normal derivative at the boundary, and is used in non-overlapping domain decomposition methods for solving numerically the equations, and elsewhere. It is determined by the quadratic form that represent the systems energy, however, the analysis of the DtN map is much more involved than that of the energy, because of the arbitrary boundary conditions in this case. It will be shown that the network approximation allows for an explicit characterization of the map in the asymptotic limit of the typical distance δ between the particles tending to zero, see [3].

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A multi scale mono-model for mechanics

Max Gunzburger

We define two requirements of any model, including a material mechanics model: validity and tractability: a valid model is one that provides a faithful description of the physics whereas a tractable model is one for which useful information can be extracted, e.g., through discretization, at a manageable cost. These two requirements allows us to define a multiscale model as one that is valid and tractable over a wide range of scales. A common approach towards developing a multiscale mechanics model couples two or more well-known models, e.g., molecular dynamics (MD) and classical elasticity (CE), each of which is useful at a different scale, thus creating a multiscale *multi*-model or *composite* model. Alternately, one can look for a single model for mechanics that remains valid and useful over a wide range of scales, thus acting as a multiscale *mono*-model. Many of the shortcomings of composite methods stem from the attempt to couple a *nonlocal* atomistic model to a local continuum model.

We study the use of the *peridynamics* (PD) model for solid mechanics, developed in [1, 2], as a multsicale mono-model for mechanics. Although a relatively

recent development, the effectiveness of PD has already been demonstrated in several sophisticated applications, including fracture and failure of composites, crack instability, fracture of polycrystals, and nanofiber networks.

Our interest in peridynamics includes developing, analyzing, implementing, and applying finite element methods, analyzing well-posedeness issues, justifying the phenomenological aspects, and ultimately, build a multiscale mechanics simulation capability that can handle defects. Why peridynamics? At "small" scales, PD behaves like the *nonlocal* MD model. At "large" scales, PD behaves like the *local* CE model. In between, PD can "smoothly" effect the transition between nonlocal and local behaviors.

PD is a phenomenological model for mechanics having the following features: it is a *continuum* model that is free of spatial derivatives and involves nonlocal interactions. These features result in the following desirable properties of solutions: mathematically speaking, spatial solution operators are less smoothing than classical elliptic operators, indeed, there need not be smoothing at all; solutions with jump discontinuities are admissible; the nucleation and propagation of cracks and other defects can automatically be accounted for; and in many practical settings, discontinuous Galerkin methods are conforming. PD models have the form

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{B}} \mathbf{k}\left(\mathbf{u}' - \mathbf{u}, \mathbf{x}', \mathbf{x}\right)\, d\mathbf{x}' + \mathbf{b}(\mathbf{x},t) \quad \forall\, \mathbf{x} \in \mathcal{B} \subset \mathbb{R}^3,\ t \in (0,T)$$

where $\mathbf{x}$ = material point in the reference configuration, $\mathcal{B}$ = the body in the reference configuration, $\mathbf{u}(\mathbf{x},t)$ = displacement of the material point $\mathbf{x}$, $\boldsymbol{\eta}(\mathbf{x},t) = \mathbf{x} + \mathbf{u}(\mathbf{x},t)$ = position of the material point $\mathbf{x}$ in the deformed configuration, $\mathbf{u}' = \mathbf{u}(\mathbf{x}',t)$, $\boldsymbol{\eta}' = \boldsymbol{\eta}(\mathbf{x}',t)$, $\rho(\mathbf{x})$ = mass density, and $\mathbf{b}(\mathbf{x},\mathbf{t})$ = external body force density. The kernel $\mathbf{k}(\cdot,\cdot,\cdot)$ contains the constitutive information about the material being considered. A constitutive assumption in PD is that the extent of nonlocal interactions is finite, i.e., there exists a *horizon parameter* δ such that

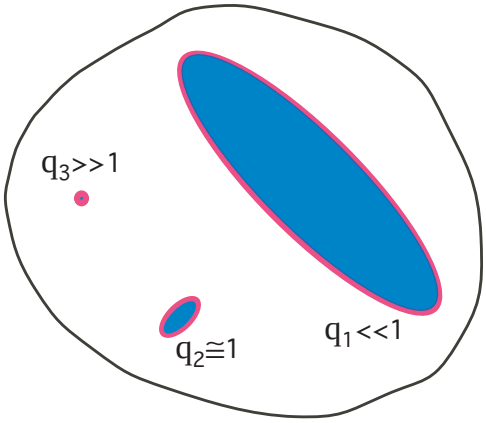
$$\mathbf{k}\left(\mathbf{u}' - \mathbf{u}, \mathbf{x}', \mathbf{x}\right) = \mathbf{0} \qquad \text{if} \qquad |\mathbf{x}' - \mathbf{x}| > \delta.$$

Two points within a distance δ of each other are said to be bonded. Damage in the peridynamics setting is effected by another constitutive assumption which, in simplified form, looks like: if $|\boldsymbol{\eta}(\mathbf{x}') - \boldsymbol{\eta}(\mathbf{x})| > s$, then the bond between $\mathbf{x}'$ and $\mathbf{x}$ is broken, i.e., $\mathbf{x}'$ and $\mathbf{x}$ no longer interact; s is called the *stretch parameter*.

We now describe in more detail the multiscale nature of the PD model. We partition the body $\mathcal{B}$ into a collection of non-overlapping covering subdomains Ω_j, i.e., $\cup_{j=1}^n \overline{\Omega}_j = \overline{\mathcal{B}}$ and $\Omega_j \cap \Omega_{j'} = \emptyset$ for $j \neq j'$. We assume that $|\mathcal{B}|$, the volume of $\mathcal{B}$, is sufficiently large so that MD is not tractable on $\mathcal{B}$. Given the PD horizon $\delta > 0$ and the subdomain Ω_j, let $\mathcal{B}_j^\delta$ denote points in $\mathcal{B}$ outside of Ω_j that are within a distance δ of Ω_j, i.e., $\mathcal{B}_j^\delta = \{\mathbf{x}' \in \mathcal{B}/\Omega_j : |\mathbf{x}' - \mathbf{x}| < \delta, \mathbf{x} \in \Omega_j\}$ and let $\mathcal{B}_j^*$ denote points in $\mathcal{B}$ outside of both Ω_j and $\mathcal{B}_j^\delta$, i.e., $\mathcal{B}_j^\delta = \mathcal{B} \setminus (\Omega_j \cap \mathcal{B}_j^\delta)$. Only points in $\mathcal{B}_j^\delta$ interact with points in Ω_j. Let $h_j = \text{diam}(\Omega_j)$ and $|\mathcal{B}_j^\delta|$ = volume of $\mathcal{B}_j^\delta$. Then, $|\mathcal{B}_j^\delta| = O(h_j^2\delta + h_j\delta^2 + \delta^3)$. Suppose that Ω_j is "nicely shaped", i.e., $|\Omega_j| = O(h_j^3)$ so that $\gamma_j = \frac{|\mathcal{B}_j^\delta|}{|\Omega_j|} = O\left(\frac{\delta}{h_j} + \frac{\delta^2}{h_j^2} + \frac{\delta^3}{h_j^3}\right)$. γ_j is an indicator of the

nonlocality of force for Ω_j; because δ is a fixed material parameter, γ_j decreases (resp. increases) as $|\Omega_j|$ increases (resp. decreases).

If $\delta \ll h_1$, then $q_1 = O(\delta/h_1) \ll 1$ and the internal force acting on Ω_1 is *local*, emanating from a very thin (relative to the size of Ω_1) layer of material points surrounding Ω_1. If $\delta \gg h_3$, then $q_3 = O(\delta^3/h_3^3) \gg 1$ and the internal force acting on Ω_3 is *nonlocal*, emanating from a very thick (relative to the size of Ω_3) layer of material points surrounding Ω_3. If $\delta = O(h_2)$, then $q_2 = O(1)$ and the internal force acting on Ω_2 is again ůnonlocal but now emanates from a layer of material points having roughly the same size as Ω_2. Thus, PD automatically changes its character *from nonlocal to local* as the "viewing window" changes in size from very small to very large relative to the horizon δ.



blue: Ω_j *purple:* $\mathcal{B}_j^\delta$

all three magenta rings have the same thickness δ

How do we use the multiscale nature of PD to construct a computational multiscale mono-model? Let $\cup_{j=1}^n \Omega_j$ denote a finite element grid and discretize the PD equation of motion using a finite element method; for kernels of practical interest discontinuous Galerkin methods are conforming. Let h_j denote the diameter of Ω_j. In regions where defects occur, we choose $h_j < \delta$; in this case PD is a nonlocal model and discretized PD with discontinuous Galerkin FEM discretizations can be shown to reduce to MD so that it can effectively account for defects. In regions where no defects occur, we choose $h_j > \delta$; in this case PD becomes a local model and discretized PD with continuous Galerkin FEM discretizations can be shown to reduce to discretized CE so that it can efficiently approximate in regions without defects. Thus, just by varying the grid size h relative to the horizon δ and using continuous FE in regions with no defects and discontinuous FE in regions with defects, discretized PD is automatically a computational multiscale mono-model.

The implementation of a multiscale finite element discretization of peridynamics has the following components:

1. detection of the elements that contain discontinuities;
2. grid refinement near or at discontinuities;
3. for elements containing discontinuities, discontinuous finite element basis functions are used;
4. for the remaining elements away from the discontinuity, continuous finite element basis functions are used;
5. quadrature rules that work for any δ, h combination are used; and

6. further away from the discontinuity, standard finite element/partial differential equation discretizations are used.

These are all relatively simple to do in 1D (except for 5 for which one has to deal with singular integrands), but difficulties arise in higher dimensions. The latter is the subject of current efforts. In 1D we have shown how to do adaptive grid refinement to identify the locations of discontinuities in the displacement, and how to refine the grid at those locations. Using discontinuous Galerkin methods near the discontinuity, we also have shown how one can do abrupt grid refinement, i.e., have and element of size $O(h^4)$ surrounding the discontinuity and having all other elements be of size $O(h)$ with the result that, using piecewise linear elements, we obtain $O(h^2)$ accuracy with respect to L^2 norms and, if we omit the element containing the discontinuity, we also obtain $O(h^2)$ accuracy in the L^∞ norm.

Background for the materials discussed above may be found in [3, 4, 5].

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Incomplete Evaluation of the Inverse

Wolfgang Hackbusch

1. Underlying Ideas

Let $Ax = b$ be a large system of equations. In the standard treatment one is used to consider only the (complete) solution vector $x \in \mathbb{R}^I$ as the solution of the system. Similarly, only the (full) inverse matrix $A^{-1} \in \mathbb{R}^{I\times I}$ seems to be the answer for the inverse mapping.

However, if $Ax = b$ is the discretisation of an elliptic boundary value problem $Lu = f$ in Ω with suitable boundary data, one is really not interested in $u(\xi)$ at *all* $\xi \in \Omega$. Instead, often certain functionals are of interest. Examples of functionals may be the boundary data $\partial u/\partial n$ at $\Gamma = \partial\Omega$ in the case of given Dirichlet data or only one integral $\int_{\Gamma_0} \partial u/\partial n \, d\Gamma$ along a part $\Gamma_0 \subset \Gamma$ describing the flux through Γ_0, or u at a fixed point $\xi_0 \in \Omega$ or at several points.

A particular situation originates from differential operators $L = \operatorname{div} a(\cdot) \operatorname{grad}$ with strongly oscillatory coefficients (or coefficients with other small-scale behaviour or xomplicated domains). Since also the solution is strongly oscillatory,

one is usually not interested in the exact solution with all its details, but only in local mean values $\bar{u}$ representing the makroscopic behaviour. In the case of periodic coefficients $a(\cdot)$ one can apply homogenisation techniques leading to an approximation of $\bar{u}$. If the presuppositions for this technique do not hold, a numerical homogenisation is of interest.

The algorithm is not primarily aiming at the solution x of $Ax = b$, but at (an approximation of) a restriction $B := RA^{-1}$ of the inverse (i.e., R has much less row than columns). Correspondingly, the computational work for B should be considerably smaller than for A^{-1}.

2. Domain decomposition based algorithm

We consider the boundary value problem $Lu_\Omega = f_\Omega$ in $\Omega \subset \mathbb{R}^d$ with Dirichlet boundary condition $u_\Omega|_\Gamma = g_\Gamma$ on $\partial\Omega$, discretised by a finite element method with triangulation. Next we construct a binary domain decomposition tree T_Ω by nested dissection: Ω is the root, the sons of Ω are two subdomains ω_1 and ω_2 with interior boundary $\gamma(\Omega) \subset \Omega$, i.e. $\overline{\gamma(\Omega)} = \partial\omega_1 \cap \partial\omega_2$. The subdomains ω_i are recursively devided in the same manner until the last subdomains coincide with elements of the triangulation.

For each subdomain $\omega \in T_\Omega$, the differential equation can be restricted to ω: $Lu_\omega = f_\omega$ in ω with boundary data $u_\omega|_{\partial\omega} = g_{\partial\omega}$ on $\partial\omega$. Let $f_h(\omega)$ be the restriction of the finite element function f_h, while $g_h(\partial\omega)$ contains the nodal value of $g_{\partial\omega}$ on $\partial\omega$. The corresponding finite element solution is denoted by $u_h(\omega)$. This allows to define the trace mapping

$$\Phi_\omega : (f_h(\omega), g_h(\partial\omega)) \mapsto u_h(\omega)|_{\gamma(\omega)}$$

onto the interior boundary data $\gamma(\omega)$, provided that Φ_ω is given for all $\omega \in T_\Omega$ except the leaves. Then the recursive evaluation of Φ_ω starting from the root yields the complete solution $u_h = u_h(\Omega)$.

The computation of Φ_ω requires the auxiliary operator, which can be computed together with Φ_ω in a recursion from the leaves to the root of T_Ω.

In the *definition phase*, we determine the mappings Φ_ω for all domains $\omega \in T_\Omega$. Afterwards, the *evaluation phase* can be applied once or many times to different data $f_h(\Omega), g_h(\partial\Omega)$. This part starts at the root Ω and terminates at the leaves.

The linear mappings Φ_ω are described by full matrices. In order to reach a complexity of $O(n \log^* n)$, the exact arithmetic is replaced by the arithmetic of *hierarchical matrices* (cf. [2], [4]).

3. Homogenisation aspects, partial evaluation, functionals

Now we assume that the differential equation contains coefficients with small-scale behaviour. For instance, the coefficient is highly oscillating. We assume a fine grid resolution h, which is small enough to resolve all details. However, for the presentation of the solution one is often interested only in data of a coarser grid, say with size $H \gg h$. Define a domain decomposition $T_\Omega^{\text{coarse}} \subset T_\Omega$ such that the leaves of T_Ω^{coarse} are subdomains of size H. Note that the mappings Φ_ω need to be

stored only for $\omega \in T_\Omega^{\text{coarse}}$. Performing the evaluation phase in the tree T_Ω^{coarse} we get the solution data on the boundaries of the leaves ω of T_Ω^{coarse} (size H) without any further errors related to the H.

Here, it is essential that the technique of hierarchical matrices works equally well for highly oscillatory coefficients (cf. [1]). Details of the algorithm are described in [5] and in chapter 12 of the monograph [4]. A preversion for the two-dimensional case is investigated in [6]. Numerical examples and comparisons can be found in [5] and [3].

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Transport through confined structures as a multiscale problem

Clemens Heitzinger

(joint work with Amirreza Khodadadian, Christian Ringhofer)

1. Introduction

It is well-known that the random walk of a particle converges toward a Wiener process, which in turn corresponds to a diffusion equation. It is also well-known that the drift-diffusion equations can be derived from the Boltzmann transport equation.

This raises the question if and how the movement of particles in a confined structure can be described by a diffusion-like equation. It is obvious that the bulk diffusion coefficient will not be a correct description of particle behavior inside the confined structure; at the same time, it is expected that the effective diffusion coefficient depends on the confinement potential. The natural starting point for the derivation of such an equation, if possible at all, is the Boltzmann equation.

In [1, 2], it was shown that it is indeed possible to derive a diffusion-like equation for a given confinement potential and—quite surprisingly—that the coefficients in the equation can be given in explicit form if the confinement potential is harmonic, i.e., a quadratic function of position. The independent variables in the equation are position along the confined structure and local energy.

In addition to its theoretic meaning, this result also has the computational significance that the (6+1)-dimensional Boltzmann equation is reduced to a (2+1)-dimensional diffusion equation. This makes it possible to calculate the current through a confined structure quickly, which is a considerable advantage compared to other methods.

There are two multiscale problems inherent in this kind of problems: There are two different time scales and the confined structures are much longer than wide so that we are interested in the case where the aspect ratio goes to zero.

Realizations of this mathematical model are ion channels (in biology) and nanopores (in engineering).

2. The transport equation for confined structures

The starting point is the Boltzmann transport equation in the form

$$\partial_t f + \{E, f\}_{XP} + \mathcal{Q}[f] = 0, \tag{1}$$

where the Poisson bracket is defined as

$$\{g, f\}_{XP} := \nabla_P g \cdot \nabla_X f - \nabla_X g \cdot \nabla_P f. \tag{2}$$

Here $f(X, P, t)$ is the kinetic particle density, $X \in \mathbb{R}^3$ is position, $P \in \mathbb{R}^3$ is momentum, t is time, $E(X, P)$ is the energy, and $\mathcal{Q}$ is the scattering operator. The energy is given by

$$E(X, P) := V(X) + \frac{|P|^2}{2m}$$

and the scattering operator $\mathcal{Q}$ is determined by the physical properties of the confined structures. The potential V determines the geometry of the structure and it has the form

$$V(x, y) = V_0(x) + V_1(x, y).$$

V_1 is the confinement potential and V_0 is an applied potential driving particles through the structure. We are interested in the scaling

$$y_s := \frac{y}{\epsilon},$$

where $\epsilon \ll 1$ is the aspect ratio of the confined structure.

It was found that dramatic simplifications are possible when the confinement potential $V_1(x, y)$ is harmonic (or quadratic) in y for each x, i.e., when it is of the form

$$V_1(x, y) = \frac{1}{2}\big(y - b(x)\big)^\top B(x)\big(y - b(x)\big), \tag{3}$$

where $y, b \in \mathbb{R}^2$ and $B(x)$ is a diagonal matrix

$$B(x) = \begin{pmatrix} B_1(x) & 0 \\ 0 & B_2(x) \end{pmatrix}.$$

In summary, the conservation law

$$\partial_t \rho(x, \eta, t) + \partial_x F^x(x, \eta, t) + \partial_\eta F^\eta(x, \eta, t) = 0 \tag{4}$$

with the fluxes F^x and F^η given by

$$F^x(x,\eta,t) = -\frac{4\pi^2 kT\tau\eta}{\sqrt{B_1B_2}}T_1 - \frac{\pi^2 kT\tau\eta^2}{\sqrt{B_1B_2}}\big(\partial_x(\ln B_1) + \partial_x(\ln B_2)\big)T_2 \tag{5}$$

and

$$\begin{aligned} F^\eta(x,\eta,t) = &-\frac{\pi^2 kT\tau\eta^2}{\sqrt{B_1B_2}}\big(\partial_x(\ln B_1) + \partial_x(\ln B_2)\big)T_1 \\ &-\frac{\pi^2 kT\tau\eta^2}{6\sqrt{B_1B_2}}\bigg(\frac{12mB_1(\partial_x b_1)^2}{m+\tau^2B_1} + \frac{12mB_2(\partial_x b_2)^2}{m+\tau^2B_2} \\ &\quad + 2\eta\partial_x(\ln B_1)\partial_x(\ln B_2) \\ &\quad + \frac{\eta(3m+8\tau^2B_1)(\partial_x(\ln B_1))^2}{m+4\tau^2B_1} \\ &\quad + \frac{\eta(3m+8\tau^2B_2)(\partial_x(\ln B_2))^2}{m+4\tau^2B_2}\bigg)T_2, \end{aligned} \tag{6}$$

where

$$\begin{aligned} T_1 &:= \mathrm{e}^{-V_0/(kT)}\nabla_x\big(\mathrm{e}^{V_0/(kT)}\frac{\rho}{N}\big), \\ T_2 &:= \mathrm{e}^{-\eta/(kT)}\partial_\eta\big(\mathrm{e}^{\eta/(kT)}\frac{\rho}{N}\big), \end{aligned}$$

can be derived. The independent variable x denotes position along the confined structure and η denotes the local energy.

3. Numerical Results

After validation of the numerical results by comparison with measured currents through three types of channels, namely Gramicidin A, the KcsA channel, and the OprP porin, we have also calculated sodium currents through artificial potassium channels. The selectivity filter of the natural KcsA channel contains four rings of oxygen atoms. In our simulations, we have investigated virtual channels that have shorter and longer selectivity filters. The results are shown in Figure 1: For selectivity filters longer than the natural one, the sodium current is nearly constant, while it increases as the filter length decreases. This can be interpreted by noting that longer filters would not be advantageous compared to the natural one, but they would be harder to assemble and stabilize, while shorter filters would have the disadvantage of allowing larger sodium currents, diminishing the physiological purpose of the KcsA channel.

4. Conclusions

A diffusion-like equation was derived from the Boltzmann transport equation for the description of transport through confined structures such as nanopores and ion channels. Current work focuses on the extension of this mathematical approach to multiple species and their interactions.

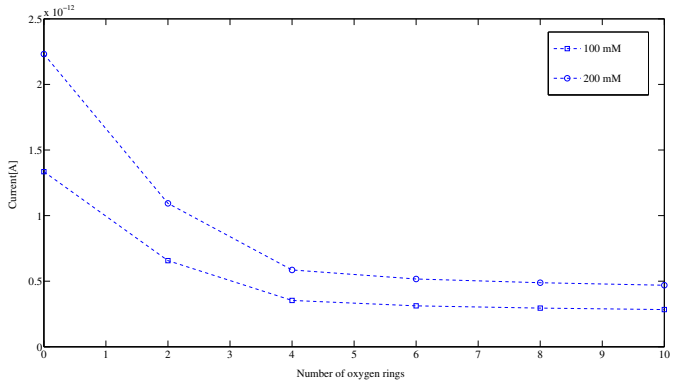

FIGURE 1. The sodium current as a function of the number of oxygen rings in virtual KcsA channels. The natural KcsA channel has four oxygen rings.

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Two-level discretization for the Gross-Pitaevskii eigenvalue problem with a rough potential

PATRICK HENNING

(joint work with Axel Målqvist, Daniel Peterseim)

This contribution considers the Gross-Pitaevskii eigenvalue problem, which describes for instance the formation of ground states and excited states of Bose-Einstein condensates. In the following we restrict our considerations to the ground state eigenvalues. In strong formulation, the problem reads: find the minimal eigenvalue λ and a corresponding eigenfunction $u \in H^1_0(\Omega)$ with $\|u\|_{L^2(\Omega)} = 1$ and

$$-\operatorname{div} A\nabla u + bu + \beta|u|^2 u = \lambda u \quad \text{in } \Omega, \quad \text{and} \quad u = 0 \quad \text{on } \partial\Omega.$$

We assume that $\Omega \subset \mathbb{R}^d$ (for $d = 1, 2, 3$) is a bounded Lipschitz domain with a polygonal boundary; $A \in L^\infty(\Omega, \mathbb{R}^{d\times d}_{sym})$ is a symmetric matrix-valued function with $A(x)\xi \cdot \xi \geq \alpha|\xi|^2$ for all $\xi \in \mathbb{R}^d$ and for some fixed $\alpha > 0$; $b \in L^2(\Omega)$ with $b(x) \geq 0$ and $\beta \in \mathbb{R}_{\geq 0}$. We implicitly assume that b describes a rough potential, i.e. that it does not provide more regularity than $L^2(\Omega)$. The energy is described by the functional $E\colon H^1_0(\Omega) \to \mathbb{R}$ with

$$E(\phi) := \frac{1}{2}\int_\Omega A\nabla\phi \cdot \nabla\phi \, dx + \frac{1}{2}\int_\Omega b\phi^2 \, dx + \frac{1}{4}\int_\Omega \beta|\phi|^4 \, dx \quad \text{for } \phi \in H^1_0(\Omega).$$

Using the above notation, the weak formulation of the Gross-Pitaevskii problem is to find the positive, L^2-normalized minimizer of the energy functional E, i.e. find $u \in H_0^1(\Omega)$ such that $u \geq 0$ a.e. in Ω, $\|u\|_{L^2(\Omega)} = 1$, and

$$E(u) = \inf_{\substack{v \in H_0^1(\Omega) \\ \|v\|_{L^2(\Omega)}=1}} E(v).$$

This problem has a unique solution (cf. [4]). The corresponding ground state eigenvalue is $\lambda := 2E(u) + 2^{-1}\beta\|u\|_{L^4(\Omega)}^4$.

In order to find the minimizer of the energy functional numerically, iterative schemes are required. Starting from a given initial value, the energy of the functional E shall be diminished in each iteration step. Possible approaches involve gradient-flow methods (cf. [1]), methods based on a direct minimization of the energy functional (cf. [2]), explicit imaginary-time marching (cf. [9]), the DIIS method (direct inversion in the iterated subspace, cf. [6]), or the Optimal Damping Algorithm (cf. [5, 3]). However, in order to use such an iterative algorithm, the space $H_0^1(\Omega)$ needs to be first replaced by a finite-dimensional space. Obvious choices for such a space are Lagrange-spaces (in the context of finite element methods) or Fourier-spaces. A general a priori error analysis on the approximation properties of these spaces with respect to the ground state eigenvalue u was presented by Cancès, Chakir and Maday [4]. Typically, Fourier-spaces yield good approximations with low computational costs. However, this requires regularity of the potential b, which might be not available in some cases. For instance if b describes an array of quantum wells to investigate Josephson oscillations and macroscopic quantum self-trapping of Bose-Einstein condensates. In such extreme cases, finite element spaces are required. But this might come we a new issue: in order to resolve all relevant structures of the data functions, the underlying computational grid can become quite fine and hence the dimension of the discrete FEM space quite large. In each step of the iterative algorithm, a linear problem needs to be solved in this space. If a lot of iterations are required (depending on the size of the gaps between the eigenvalues) and if the computations have to be repeated for various choices of β (which typically describes the number and the type of the particles), then the computational cost can become enormous. In this contribution we therefore propose the construction of a **low** dimensional solution space (in which we minimize the energy functional E) which has very high approximation properties (cf. [7]).

In order to describe the construction of the discrete space, we let $\mathcal{T}_H$ denote a regular simplicial partition of Ω, we denote by $H := \max_{T \in \mathcal{T}_H}\{\mathrm{diam}(T)\}$ the mesh size and the corresponding conforming $P1$ finite element space by

$$V_H := \{v \in H_0^1(\Omega) \mid \forall T \in \mathcal{T}_H, v|_T \text{ is a polynomial of total degree} \leq 1\}.$$

Next, we let $P_H : H_0^1(\Omega) \to V_H$ denote the L^2-projection on V_H and define the kernel of the projection by V^{f}, i.e. $V^{\mathrm{f}} := \{v \in H_0^1(\Omega) \,|P_H(v) = 0\}$. This yields the splitting $H_0^1(\Omega) = V_H \oplus V^{\mathrm{f}}$, where $V_H \perp_{L^2} V^{\mathrm{f}}$. In the next step, we define the scalar product $a(\cdot,\cdot)$ on $H_0^1(\Omega)$ by $a(v,w) := (A\nabla v, \nabla w)_{L^2(\Omega)} + (bv, w)_{L^2(\Omega)}$.

This scalar product describes the linear part of the Gross-Pitaevskii equation. We are now interested in the $a(\cdot,\cdot)$-orthogonal complement of V^{f} (recall that V_H is the L^2-orthogonal complement). For that purpose, define the a-orthogonal projection $P^{\mathrm{f}} : H_0^1(\Omega) \to V^{\mathrm{f}}$ by $a(P^{\mathrm{f}}(v), w) = a(v, w)$ for all $w \in V^{\mathrm{f}}$ and set $V^{\mathrm{c}} := \mathrm{kern}(P^{\mathrm{f}}|_{V_H})$. This yields the new splitting $H_0^1(\Omega) = V^{\mathrm{c}} \oplus V^{\mathrm{f}}$, where $V^{\mathrm{c}} \perp_{a(\cdot,\cdot)} V^{\mathrm{f}}$. This orthogonal decomposition was originally proposed in [8]. Observe that the dimension of V^{c} is the same as the dimension of V_H. However, we can show that V^{c} yields much better convergence rates for Galerkin approximations. We can hence solve the Gross-Pitaevskii in V^{c}.

Definition 1 (Pre-processed approximation)**.**
We call $u_H^{\mathrm{c}} \in V^{\mathrm{c}}$ a V^{c}-approximation of u if it fulfills $(u_H^{\mathrm{c}}, 1) \geq 0$, $\|u_H^{\mathrm{c}}\|_{L^2(\Omega)} = 1$ and

$$E(u_H^{\mathrm{c}}) = \inf_{\substack{v^{\mathrm{c}} \in V^{\mathrm{c}} \\ \|v^{\mathrm{c}}\|_{L^2(\Omega)}=1}} E(v^{\mathrm{c}}).$$

The corresponding eigenvalue in V^{c} is given by $\lambda_H^{\mathrm{c}} := 2E(u_H^{\mathrm{c}}) + 2^{-1}\beta\|u_H^{\mathrm{c}}\|_{L^4(\Omega)}^4$.

For u_H^{c} we proved the following a-priori error estimate that can be found in [7].

Theorem 1 (Error estimates for the pre-processed approximation)**.** *For $u \in H_0^1(\Omega)$ and $u_H^{\mathrm{c}} \in V^{\mathrm{c}}$ as above (i.e. they are the minimizers of E in $H_0^1(\Omega)$ and V^{c} respectively) it holds*

$$H^{-1}\|u - u_H^{\mathrm{c}}\|_{H^1(\Omega)} + |\lambda - \lambda_H^{\mathrm{c}}| + \|u - u_H^{\mathrm{c}}\|_{L^2(\Omega)} \leq CH^3.$$

Here, C denotes a constant that is independent of the mesh size H.

For a fully discretized and localized version of V^{c}, we refer to our paper [7]. It also makes sense to solve an additional linear elliptic problem (in a standard finite element space) to further improve the approximations. In the above discussed semi-discrete setting, this 'post-processing step' can be described as follows.

Problem 2 (Post-processed approximation)**.** *We call $u^{\mathrm{c}} \in H_0^1(\Omega)$ the post-processed approximation if it solves*

$$a(u^{\mathrm{c}}, v) = \lambda_H^{\mathrm{c}} \int_\Omega u_H^{\mathrm{c}} v \, dx - \int_\Omega \beta |u_H^{\mathrm{c}}|^2 u_H^{\mathrm{c}} v \, dx$$

for all $v \in H_0^1(\Omega)$. We finally define $\lambda^{\mathrm{c}} := (2E(u^{\mathrm{c}}) + 2^{-1}\beta\|u^{\mathrm{c}}\|_{L^4(\Omega)}^4)\|u^{\mathrm{c}}\|_{L^2(\Omega)}^{-2}$.

The post-processed approximation boosts the convergence rates even further.

Theorem 2 (Error estimates for the post-processed approximation)**.**
The post-processed approximation u^{c} and the post-processed eigenvalue λ^{c} satisfy

$$H^{-1}\|u - u^{\mathrm{c}}\|_{H^1(\Omega)} + |\lambda - \lambda^{\mathrm{c}}| + \|u - u^{\mathrm{c}}\|_{L^2(\Omega)} \leq CH^4.$$

Again, C denotes a constant that is independent of the mesh size H.

For a proof and further details we refer to [7]. The convergence rates of up to fourth order show that only very coarse grids $\mathcal{T}_H$ are required to obtain very accurate approximations. Hence, the dimension of V^c can be very small and the computations become cheap. In [7], we also present numerical experiments which indicate that our high convergence rates might still be pessimistic.

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A parameter identification problem in random homogenization

Frederic Legoll

(joint work with William Minvielle, Amael Obliger and Marielle Simon)

Computing the homogenized properties of a random heterogeneous material, e.g. modelled by the equation

$$-\mathrm{div}\left(A\left(\frac{x}{\varepsilon},\omega\right)\nabla u^\varepsilon\right) = f \ \text{ in } \mathcal{D}, \quad u^\varepsilon = 0 \ \text{ on } \partial\mathcal{D},$$

for a random stationary matrix A, is very expensive. These properties are indeed defined from the so-called corrector function, that solves an auxiliary PDE set on the entire space (see e.g. [1, 2, 5]). A standard approximation (see e.g. [4]) is to consider a truncated version of that corrector problem (complemented with appropriate boundary conditions), from which apparent effective properties can be computed. As a result of truncation, these effective properties are random. To

compute their expectation, one can resort to a direct Monte Carlo approach, or to more elaborated approaches, based on variance reduction techniques (see e.g. [3]).

In the above computations, we have assumed that we have a complete knowledge of the microstructure of the material. In practice, this is not always the case. In this talk, we consider a related parameter identification problem. Knowing the homogenized quantities, is it possible to recover some features of the microstructure properties? Obviously, since homogenization is an averaging procedure, not everything can be recovered from macroscopic quantities. A realistic situation is the case when we assume a functional form of the probability distribution of the microscopic properties, but with some unknown parameters that we would like to determine. Using a least-square approach, we show (see [6] for details) how one can determine the unknown parameters of the microscopic distribution on the basis of macroscopic (e.g. homogenized) quantities.

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The dynamics of unstable mesoscopic interactions and their connection to macroscopic simulations of dynamic brittle fracture

Robert Lipton

The dynamic fracture of brittle solids is a particularly challenging problem for computational modeling. It involves collective interaction connecting both large and small length scales. Apply enough stress or strain to a sample of brittle material and one eventually snaps bonds at the atomistic scale leading to fracture of the macroscopic specimen. With these ideas in mind we investigate a new class of models for solving problems of free crack propagation described by the peridynamic formulation [2]. In the peridynamic formulation material points interact through short-range forces acting over a prescribed horizon. The formulation allows for both continuous and discontinuous deformations associated with cracks.

We introduce a peridynamic model for which the short-range forces between material points are unstable and soften beyond a critical relative displacement [1]. This model is used to represent the dynamics at mesoscopic length scales and for the simulation of free crack propagation. Analysis shows that the resulting mesoscopic dynamics is well posed [1].

In this research we show how this computational model is able to capture the dynamics of brittle fracture mechanics as seen at macroscopic length scales. We provide a suitable scaling technique that relates the mesoscopic dynamics to the macroscopic dynamics as viewed across coarser length scales. This scaling is associated with the radius of the horizon and potential energy of the peridynamic motion. An analysis is provided that shows that peridyamic evolutions associated with suitably scaled peridynamic energies are close in norm to macroscopic evolutions that have bounded energy given by the bulk and surface energies of classic brittle fracture mechanics. The macroscopic free crack evolution corresponds to the simultaneous evolution of the fracture surface and linear elastic displacement away from the crack set. The elastic moduli, wave speed, and energy release rate for the macroscopic evolution are explicitly determined by moments of the peridynamic potential energy. This delivers a rigorous connection between motions associated with suitably scaled peridyamic energies and dynamic free crack evolution inside a brittle medium as observed at the macroscopic scale.

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An Analysis of Transition State Theory Rates upon Spatial Coarse-Graining

Mitchell Luskin

(joint work with Andrew Binder, Danny Perez, Art Voter)

Molecular dynamics (MD) – the direct integration of atomistic equations of motion – provides a powerful tool for the study of chemical and material processes. Such an approach accurately captures the physics at the atomic scale and, in principle, enables the accurate modeling of a wide range of atomistic systems. However, despite the high speed of modern computers, MD simulations still struggle to access wildly disparate length and time scales required in many applications. To partially overcome this diffculty, multiscale methods that bridge the length-scales from the nano- to the meso-scales have been proposed. While such methods are certainly promising, relatively little is known of the effect of spatial coarse-graining on the quality of the dynamics. Improving our understanding of these issues is necessary in order to expand upon the range of problems that can be modeled using such an approach.

Our lecture concerned itself with spatial multiscale processes for which the critical atomistic behaviors are localized yet strongly coupled to the environment through long-range elastic effects. Probably the most well known numerical method to treat such systems is the quasicontinuum (QC) method. Specifically, the QC method aims to solve molecular statics (i.e., molecular dynamics at zero temperature) problems in such cases [1, 9, 10, 11, 15]. In the QC method, the localized region of interest is treated atomistically in order to preserve a high degree of accuracy, while the behavior of the remainder of the system is approximated using continuum mechanics. This coupling between the length scales is meant to allow for an elastic coupling of the two regions, ensuring proper boundary conditions for the atomistic region. The number of degrees of freedom necessary to describe the system is significantly reduced through the use of the Cauchy-Born approximation and a coarsening of the continuum region via the finite element method (FEM). This greatly reduces its computational cost compared to a fully atomistic solution. Recently, finite temperature versions of the quasicontinuum method, so-called hot-QC methods [4, 14], have been developed in order to extend the QC approach to finite-temperature molecular dynamics. Hot-QC was designed to simulate systems held at a constant temperature, which permits an analysis from a thermodynamic perspective. Mathematical approaches to finite temperature equilibrium and dynamics have been given in [2, 3, 5, 6, 8]. Hot-QC aims at preserving any thermodynamic quantity that depends only on a (small) subset of all degrees of freedom. It has recently been pointed out that this property implies that transition state theory (TST) rates between metastable states of the system should be well reproduced insofar as the system's constituents that are essential to the the transitions are approximately local to the fully-resolved atomistic region. This property has been exploited in an extension of these methods – the hyper-QC method [7] -which seeks to effciently and accurately simulate state-to-state dynamics of spatially coarse-grained rare-event systems through the use of accelerated molecular dynamics [12].

In our lecture, we study the error in transition rates introduced by coarsegraining the periphery of the system. In order to isolate this error, we consider the coarse-graining of an atomistic system according to the coarse-grained molecular dynamics (CGMD) formalism described in [13]. However, we note that our choice of coarse variables differ from that of conventional CGMD, as will be discussed below. CGMD and hot-QC share the same formal basis, but CGMD provides a closed-form expression to the coarse Hamiltonian, which enables a mathematical analysis. Further, it naturally handles the interface between the region to be treated with atomistic detail and the remainder of the system, in contrast to QC methods where so-called ghost forces pose additional challenges [10]. In order to obtain closed-form results, we considered transition rates computed within the purview of harmonic transition state theory (HTST) [16]. HTST is often the method of choice to approximate transition rates in hard materials. Our choice for the dividing surface between the two metastable regions and how the dividing surface is affected by the coarse-graining was discussed. Our error analysis for the

TST rate serves as confirmation of the validity of the approach and provide intuition for the types of error made in the coarsening process for spatial multiscale methods.

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Multiscale techniques for solving quadratic eigenvalue problems

Axel Målqvist
(joint work with Daniel Peterseim)

We consider numerical approximation of quadratic eigenvalue problems arising in structural mechanical systems with damping, using the Localized Orthogonal Decomposition (LOD) technique introduced in [5]. In this approach, a low dimensional generalized finite element space is constructed by solving localized (in space) independent linear stationary problems. The quadratic eigenvalue problem is then solved in the computed low dimensional space at a greatly reduced computational cost.

1. Problem formulation

The setting is as follows, let $V = \mathrm{H}^1_0(\Omega)$,

$$\begin{aligned} &\Omega \subset \mathbb{R}^d \text{ be a polyhedral domain,} \\ &0 < \kappa_0 \leq \kappa(\cdot) \leq \kappa_1 < \infty, \\ &c : V \times V \to \mathbf{R} \text{ bounded.} \end{aligned}$$

We seek $u \in V$ and $\lambda \in \mathbb{C}$ such that,

$$\langle \kappa \nabla u, \nabla w \rangle + \lambda\, c(u, w) + \lambda^2 \langle u, w \rangle = 0, \tag{1}$$

for all $w \in V$. A simple example of damping is the proportional damping where $c(u, w) = \langle \alpha\kappa\nabla u, \nabla w\rangle + \langle \beta u, w\rangle$ with $\alpha, \beta \in \mathbb{R}$. In this case the eigenmodes coincides with the eigenmodes of the linear generalized eigenvalue problem $\langle \kappa\nabla u, \nabla w\rangle = \lambda\langle u, w\rangle$ but with different eigenvalues. In a more realistic model α, β are allowed to vary in space. This corresponds to a system of proportionally damped components.

The analysis of quadratic eigenvalue problems is often done by linearization. This is achieved by introducing a new variable $v = \lambda u$ and rewriting the problem into a 2×2 system. The resulting linearized operator may or may not be compact and symmetric (depending of the damping), see [7]. Finite element convergence for these problems have been carefully studied e.g. in [1, 2] (compact operator) and [3, 4] (non-compact operator).

2. Generalized finite element approximation

We now present the LOD technique introduced in [5] and later applied to the linear eigenvalue problem in [6].

Let $\mathcal{T}_H$ denote a regular finite element mesh of Ω into closed simplices with mesh-size functions $0 < H \in L^\infty(\Omega)$. The first-order fine and coarse conforming finite element spaces are

$$V^{\mathrm{FE}}_{\mathrm{H}} := \{v \in V \mid \forall T \in \mathcal{T}_H, v|_T \text{ is polynomial of degree} \leq 1\}. \tag{2}$$

By $\mathcal{N}_H$ we denote the set of interior vertices of the mesh. For every vertex z, let ϕ_z denote the corresponding nodal basis function.

We apply a Clément-type interpolation operator $\mathcal{I}_H : V \to V_H$ defined in the following way. Given $v \in V$, $\mathcal{I}_H v := \sum_{z\in\mathcal{N}_H} (\mathcal{I}_H v)(z)\phi_z$ with $(\mathcal{I}_H v)(z) := \frac{(v,\phi_z)_{L^2(\Omega)}}{(1,\phi_z)_{L^2(\Omega)}}$ for $z \in \mathcal{N}_h$. This interpolation operator fulfills the usual interpolation and stability bounds.

We want to decompose V into a low dimensional part, with good approximation properties, and a remainder part. To this end we introduce the remainder space,

$$V_{\mathrm{f}} := \operatorname{kernel}\big(\mathcal{I}_H\big) \subset V,$$

representing the fine scales in the decomposition. The orthogonalization of the decomposition with respect to the scalar product $\langle\kappa\nabla\cdot,\nabla\cdot\rangle$ yields the definition of a modified coarse space $V_{\mathrm{H}}^{\mathrm{LOD}}$, that is the $\langle\kappa\nabla\cdot,\nabla\cdot\rangle$-orthogonal complement of V_{f} in V.

Given $v \in V$, define the orthogonal fine scale projection operator $\mathcal{P}_{\mathrm{f}} v \in V_{\mathrm{f}}$ by

$$\langle\kappa\nabla\mathcal{P}_{\mathrm{f}} v, \nabla w\rangle = \langle\kappa\nabla v, \nabla w\rangle \quad \text{for all } w \in V_{\mathrm{f}}.$$

Lemma 1 (Orthogonal two-scale decomposition)**.** *Any function $u \in V$ can be decomposed uniquely into $u = u_{\mathrm{c}} + u_{\mathrm{f}}$, where*

$$u_{\mathrm{c}} = \mathcal{P}_{\mathrm{c}} u := (1 - \mathcal{P}_{\mathrm{f}})u \in (1 - \mathcal{P}_{\mathrm{f}})V_H =: V_{\mathrm{H}}^{LOD}$$

and

$$u_{\mathrm{f}} := \mathcal{P}_{\mathrm{f}} u \in V_{\mathrm{f}} = \operatorname{kernel}\mathcal{I}_H.$$

The decomposition is orthogonal, $\langle\kappa\nabla u_{\mathrm{c}}, \nabla u_{\mathrm{f}}\rangle = 0$.

Proof. See [MaPe12]. □

We are now ready to present the LOD approximation of the quadratic eigenvalue problem. We seek for an approximation of equation (1) in the space $V_{\mathrm{H}}^{\mathrm{LOD}}$. Find eigenfunctions $u_H \in V_{\mathrm{H}}^{\mathrm{LOD}}$ with associated eigenvalues $\lambda_H \in \mathbb{C}$ such that,

$$\langle\kappa\nabla u_H, \nabla w\rangle + \lambda_H\, c(u_H, w) + \lambda_H^2\, \langle u_H, w\rangle = 0 \quad \text{for all } w \in V_{\mathrm{H}}^{\mathrm{LOD}}. \tag{3}$$

If we assume, for some $0 \le s < 1$ that,

$$|c(u, w)| \le C\|u\|_{H^s(\Omega)}\|w\|_{H^s(\Omega)},$$

for all $u, w \in V$, the corresponding linearized operator becomes compact and the analysis in [1] is available. By applying their abstract result with the constructed space $V_{\mathrm{H}}^{\mathrm{LOD}}$ we get the following result.

Theorem 2. *Let λ be an isolated eigenvalue of algebraic multiplicity n and let λ_H be the harmonic mean of the n discrete eigenvalues approximating λ. Under the assumptions above it holds,*

$$|\lambda - \lambda_H| \le CH^{2-2s}, \tag{4}$$

for sufficiently small H.

3. Numerical Experiments

We present two numerical experiments. In both cases we let $\Omega = [0,1]^2$ and κ be piecewise constant on a uniform 64×64 grid taking (uniformly distributed random) values between 0.003 and 1.0. In the first case the damping is $c(u,v) = \langle (1 + sin(10x))u, v\rangle$ and in the second case $c(u,v) = \langle (2 - x - y)\nabla u, \nabla v\rangle$. We let $h = 2^{-6}$ be the reference mesh and vary H form 2^{-1} to 2^{-5}. We plot the relative error in eigenvalue (compared to the reference solution) for the ten lowest eigenvalues versus degrees of freedom N_H, see Figure 3. We detect H^4 convergence

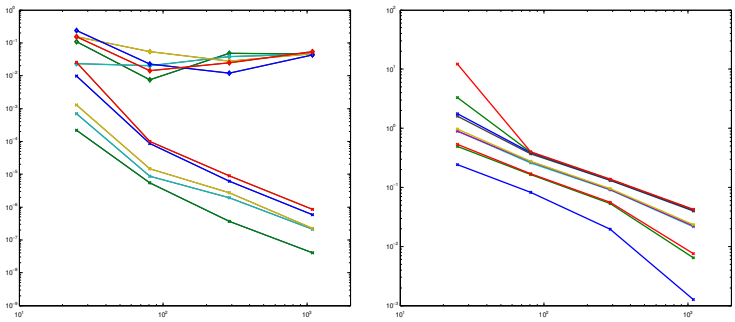

Figure 1. Relative error in the lowest eigenvalues for the two damping cases versus degrees of freedom N_H.

in the first case and H^2 in the second case. This is two orders better than our theoretical prediction. We believe this is because of the similarity between the first damping matrix and the mass matrix (for which the multiscale split is almost orthogonal) and the second damping matrix and the stiffness matrix for which the multiscale split is orthogonal.

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Bayesian Numerical Homogenization

Houman Owhadi

Numerical homogenization, i.e. the finite-dimensional approximation of solution spaces of PDEs with arbitrary rough coefficients, requires the identification of accurate basis elements. These basis elements are oftentimes found after a laborious process of scientific investigation and plain guesswork. Can this identification problem be facilitated? Is there a general recipe/decision framework for guiding the design of basis elements? We suggest that the answer to the above questions could be positive based on the reformulation of numerical homogenization as a Bayesian Inference problem in which a given PDE with rough coefficients (or multi-scale operator) is excited with noise (random right hand side/source term) and one tries to estimate the value of the solution at a given point based on a finite number of observations. We apply this reformulation to the identification of bases for the numerical homogenization of arbitrary integro-differential equations and show that these bases have optimal recovery properties. In particular we show how Rough Polyharmonic Splines can be re-discovered as the optimal solution of a Gaussian filtering problem.

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Multiscale variance reduction techniques for individual-based simulation of kinetic equations

Giovanni Samaey
(joint work with Annelies Lejon, Mathias Rousset)

We discuss variance reduced agent-based simulations using velocity-jump models, as they arise in biological applications. As a first problem, we consider a process in which the individual agents possess an internal state that allows the velocity-jump rate to depends on the memory of some chemoattractant concentration along their path of motion [1, 2]. We discuss a variance reduction technique that uses a coupling of this model with a simpler process in which the internal dynamics has been replaced by a direct gradient sensing of the chemoattractants concentrations. This coupling between paths of individual bacteria simulated by both models is achieved by using the same sets of random numbers in both simulations, and is used to construct a hybrid scheme with reduced variance. We first compute a deterministic solution of the kinetic density description of the direct gradient sensing model; the deviations due to the presence of internal dynamics are then evaluated via the coupled individual-based simulations. We show that the resulting variance reduction is asymptotic, in the sense that, in the diffusive asymptotics,

the difference between the two processes has a variance which vanishes according to the small parameter. In a second application, we consider a velocity-jump process with proliferation (allowing agents to reproduce), modeling tumor growth [3]. In this model, the internal state allows to model the evolution of an agent through its cell phase cycle; it hence influences directly the proliferation. Here, the variance reduction is obtained via a coupling with a model without internal state and without proliferation. The hybrid scheme then essentially computes the (space-dependent) proliferation rates, removing all variance related to the random motion of the agents.

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Effective Macroscopic Phase Field Equations in Strongly Heterogeneous Environments for General Homogeneous Free Energies

Markus Schmuck

(joint work with Marc Pradas, Grigorios A. Pavliotis, Serafim Kalliadasis)

Our analysis starts with the widely accepted diffuse-interface formulation describing the dynamics of interfaces between different phases in homogeneous domains. Diffuse interface approximations are highly versatile and due to increasing computational power also more and more feasible for highly complex problems. Its physical and thermodynamic foundation gives a strong basis for extension towards new and increasingly complex scientific and engineering applications such as more realistic descriptions for the computation of transport in porous media [1] which represents a high-dimensional multiscale problem with many numerical challenges.

Here, we restate the main results from [2] and hence refer the reader to the references therein:
"The physical basis of the diffuse interface formulation relies on the following class of abstract energy densities

$$e(\phi) := \frac{1}{\lambda} F(\phi) + \frac{\lambda}{2} |\nabla \phi|^2 \,. \tag{1}$$

The free energy density F defines equilibrium phases ϕ_i, $i = 1, 2, \ldots, M$ as $M \in \mathbb{N}$ local minima and the gradient term $\frac{\lambda}{2} |\nabla \phi|^2$ penalizes the interfacial area between these equilibrium phases. In thermodynamic contexts, F represents the (Helmholtz) free energy density $F(\phi) := U - TS$, where U is the internal energy, T is the temperature, and S is the entropy. Popular examples include the energy of regular solutions (also known as the Flory-Huggins energy. The regular

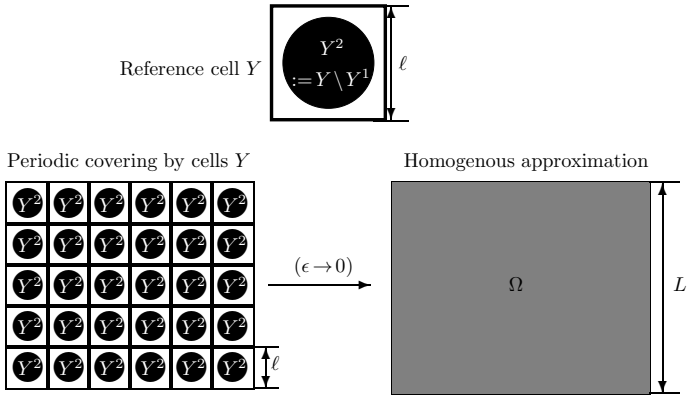

FIGURE 1. **Left:** Strongly heterogeneous/perforated material as a periodic covering of reference cells $Y := [0, \ell]^d$. **Top, middle:** Definition of the reference cell $Y = Y^1 \cup Y^2$ with $\ell = 1$. **Right:** The "homogenization limit" $\epsilon := \frac{\ell}{L} \to 0$ scales the perforated domain such that perforations become invisible on the macroscale.

solution theory plays a crucial role in many important applications. Also wetting phenomena, often studied using classical sharp-interface approximations are also described by phase-field equations which have been extended to include electric fields (so-called electrowetting).

Here, we provide an upscaling for H^{-1}-gradient flows of *arbitrary free energy* densities based on a Taylor expansion of the free energy density at the effective upscaled solution. Before we can state our main result, we formulate the basic setting to study general interfacial dynamics.

(a) Homogeneous domains Ω. The total (Ginzburg-Landau/Cahn-Hilliard) energy is defined by $E(\phi) := \int_\Omega e(\phi)\, d\mathbf{x}$ with density (1) on a bounded domain $\Omega \subset \mathbb{R}^d$ with smooth boundary $\partial\Omega$ and $1 \le d \le 3$ denotes the spatial dimension. It is well accepted that thermodynamic equilibrium can be achieved by minimizing the energy E supplemented by a possible wetting boundary contribution $\int_{\partial\Omega} g(\mathbf{x})\, d\mathbf{x}$ for $g(\mathbf{x}) \in H^{3/2}(\partial\Omega)$. Mass conservation for this minimization can be generally achieved with a H^{-1}-gradient flow associated to $E(\phi)$, i.e.,

$$\text{(Homogeneous case)} \quad \frac{\partial}{\partial t}\phi = \operatorname{div}\left(\hat{\mathrm{M}}\nabla\left(\frac{1}{\lambda}f(\phi) - \lambda\Delta\phi\right)\right) \quad \text{in } \Omega_T\,, \tag{2}$$

together with the boundary conditions $\nabla_n\phi := \mathbf{n}\cdot\nabla\phi = g(\mathbf{x})$ on $\partial\Omega_T$, and $\nabla_n\Delta\phi = 0$ on $\partial\Omega_T$, where $\Omega_T := \Omega\times]0,T[$, $\partial\Omega_T := \partial\Omega\times]0,T[$, ϕ satisfies the initial condition $\phi(\mathbf{x},0) = \psi(\mathbf{x})$, and $\hat{\mathrm{M}} = \{\mathrm{m}_{ij}\}_{1\le i,j\le d}$ denotes a mobility tensor with real and bounded elements $\mathrm{m}_{ij} > 0$. This equation serves as a prototype for interfacial dynamics and phase transformation under homogeneous Neumann boundary conditions, i.e., $g = 0$, and free energy densities F.

(b) Heterogeneous/perforated domains Ω^ϵ. Our main focus concentrates on (1) in a perforated domain $\Omega^\epsilon \subset \mathbb{R}^d$ instead of a homogeneous $\Omega \subset \mathbb{R}^d$. The

parameter $\epsilon = \frac{\ell}{L} > 0$ is called heterogeneity where ℓ represents the characteristic pore size and L is the macroscopic length of the porous medium, see Figure 1. Herewith, we can define the porous medium by a reference pore/cell $Y := [0, \ell_1] \times [0, \ell_2] \times \cdots \times [0, \ell_d]$. For simplicity, we set $\ell_1 = \ell_2 = \cdots = \ell_d = 1$. The pore (Ω^ϵ) and the solid phase (B^ϵ) are defined by

$$\Omega^\epsilon := \bigcup_{\mathbf{z}\in\mathbb{Z}^d} \epsilon\left(Y^1 + \mathbf{z}\right) \cap \Omega\,, \qquad B^\epsilon := \bigcup_{\mathbf{z}\in\mathbb{Z}^d} \epsilon\left(Y^2 + \mathbf{z}\right) \cap \Omega = \Omega \setminus \Omega^\epsilon\,, \tag{3}$$

where the subsets Y^1, $Y^2 \subset Y$ are such that Ω^ϵ is a connected set. The set $Y^1 \subset Y$ represents the pore phase (e.g. liquid or gas phase in wetting problems), see Figure 1. Herewith, we can can rewrite (2) as the following microscopic porous media problem

$$\textbf{(Microscopic formulation)} \quad \begin{cases} \partial_t \phi_\epsilon = \operatorname{div}\left(\hat{\mathrm{M}}\nabla\left(-\lambda\Delta\phi_\epsilon + \frac{1}{\lambda} f(\phi_\epsilon)\right)\right) & \text{in } \Omega_T^\epsilon\,, \end{cases} \tag{4}$$

with the boundary ($\nabla_n \phi_\epsilon := \mathbf{n}\cdot\nabla\phi_\epsilon = 0 \quad \text{on } \partial\Omega_T^\epsilon$, $\nabla_n \Delta\phi_\epsilon = 0 \quad \text{on } \partial\Omega_T^\epsilon$) and initial ($\phi_\epsilon(\mathbf{x}, 0) = \psi(\mathbf{x}) \quad \text{on } \Omega^\epsilon$) conditions. Our main objective is the derivation of a systematic and reliable homogenized/upscaled phase field formulation valid for general energy densities (1) by passing to the limit $\epsilon \to 0$ in (4). We formally achieve this by asymptotic multiscale expansions.

1. Main results

Before we state our main result of effective macroscopic phase field equations (including the Cahn-Hilliard equation) which is valid for arbitrary energy densities (1), we introduce the following scale separation property of the chemical potential.

Definition 1. (Scale separation) *We say that the chemical potential is scale separated if and only if*

$$\frac{\partial\mu(\phi_0(\mathbf{x}))}{\partial x_k} = \begin{cases} 0 & \text{on the reference cell } Y\,, \\ \frac{\partial\mu(\phi_0(\mathbf{x}))}{\partial x_k} & \text{on the macroscale } \Omega\,, \end{cases}$$

where $\phi_0(\mathbf{x})$ is the upscaled/slow variable solving the upscaled phase field equation.

Remark 3. *Definition 1 accounts for the problem specific separation between the large (macroscopic) scale* $\mathbf{x}$ *with slow processes and the small (microscopic) scale* $\mathbf{y}$ *with fast processes.* ◇

In the homogenization/upscaling of nonlinear equations, Definition 1 appears naturally in the sense that it leads to the same class of equations on the macroscale as on the microscale and that it guarantees that resulting cell problems are well-posed [1]. These considerations together with the splitting strategy [1], which decouples 4-th order problems (4) into two 2-nd order equations, allow us to state our

Main Result: (Upscaled Cahn-Hilliard equations) *Suppose that $\psi(\mathbf{x}) \in H^2_E(\Omega)$. For scale separated chemical potentials $\mu_0 = \nabla_\phi E(\phi_0)$ (Definition 1), the microscopic porous media formulation (4) can be effectively and reliably approximated by the following macroscopic problem,*

$$\text{(Upscaled equation)} \begin{cases} \theta_1 \frac{\partial\phi_0}{\partial t} = \operatorname{div}\left(\hat{\mathrm{M}}_\phi/\lambda\nabla f(\phi_0)\right) + \frac{\lambda}{\theta_1}\operatorname{div}\left(\hat{\mathrm{M}}_w\nabla\left(\operatorname{div}\left(\hat{\mathrm{D}}\nabla\phi_0\right)\right)\right) & \text{in } \Omega_T\,, \end{cases} \tag{5}$$

with boundary ($\nabla_n\phi_0 = \mathbf{n}\cdot\nabla\phi_0 = 0$ *on* $\partial\Omega_T$, $\nabla_n\Delta\phi_0 = 0$ *on* $\partial\Omega_T$) *and initial* ($\phi_0(\mathbf{x},0) = \psi(\mathbf{x})$ *in* Ω) *conditions, where* $\theta_1 := \frac{|Y^1|}{|Y|}$ *is the porosity and the porous media correction tensors* $\hat{\mathrm{D}} := \{\mathrm{d}_{ik}\}_{1\le i,k\le d}$, $\hat{\mathrm{M}}_\phi = \left\{\mathrm{m}^{\phi}_{ik}\right\}_{1\le i,k\le d}$ *and* $\hat{\mathrm{M}}_w = \{\mathrm{m}^{w}_{ik}(\mathbf{x})\}_{1\le i,k\le d}$ *are defined by*

$$
\left\{\begin{array}{ll}
\mathrm{d}_{ik} & := \frac{1}{|Y|}\sum_{j=1}^{d}\int_{Y^1}\left(\delta_{ik}-\delta_{ij}\frac{\partial\xi^k_\phi}{\partial y_j}\right)d\mathbf{y}\,,\\
\mathrm{m}^{\phi}_{ik} & := \frac{1}{|Y|}\sum_{j=1}^{d}\int_{Y^1}\left(\mathrm{m}_{ik}-\mathrm{m}_{ij}\frac{\partial\xi^k_\phi}{\partial y_j}\right)d\mathbf{y}\,,\\
\mathrm{m}^{w}_{ik}(\mathbf{x}) & := \frac{1}{|Y|}\sum_{j=1}^{d}\int_{Y^1}\left(\mathrm{m}_{ik}-\mathrm{m}_{ij}\frac{\partial\xi^k_w}{\partial y_j}\right)d\mathbf{y}\,.
\end{array}\right. \tag{6}
$$

The corrector functions $\xi^k_\phi \in H^1_{per}(Y^1)$ *and* $\xi^k_w \in L^2(\Omega; H^1_{per}(Y^1))$ *for* $1\le k\le d$ *solve in the distributional sense the following reference cell problems*

(7)

$$
\xi^k_w:\begin{cases}
-\sum_{i,j,k=1}^{d}\frac{\partial}{\partial y_i}\left(\mathrm{m}_{ik}-\mathrm{m}_{ij}\frac{\partial\xi^k_w}{\partial y_j}\right) = -\sum_{k,i,j=1}^{d}\frac{\partial}{\partial y_i}\left(\mathrm{m}_{ik}-\mathrm{m}_{ij}\frac{\partial\xi^k_\phi}{\partial y_j}\right) & \text{in } Y^1\,,\\
\sum_{i,j,k=1}^{d}\mathrm{n}_i\Big(\left(\mathrm{m}_{ij}\frac{\partial\xi^k_w}{\partial y_j}-\mathrm{m}_{ik}\right)+\left(\mathrm{m}_{ik}-\mathrm{m}_{ij}\frac{\partial\xi^k_\phi}{\partial y_j}\right)\Big)=0 & \text{on } \partial Y^1_w\cap\partial Y^2_w\,,\\
\xi^k_w(\mathbf{y}) \text{ is } Y\text{-periodic and } \mathcal{M}_{Y^1}(\xi^k_w)=0,
\end{cases}
$$

$$
\xi^k_\phi:\begin{cases}
-\sum_{i,j=1}^{d}\frac{\partial}{\partial y_i}\left(\delta_{ik}-\delta_{ij}\frac{\partial\xi^k_\phi}{\partial y_j}\right)=0 & \text{in } Y^1\,,\\
\sum_{i,j=1}^{d}\mathrm{n}_i\left(\delta_{ij}\frac{\partial\xi^k_\phi}{\partial y_j}-\delta_{ik}\right)=0 & \text{on } \partial Y^1\,,\\
\xi^k_\phi(\mathbf{y}) \text{ is } Y\text{-periodic and } \mathcal{M}_{Y^1}(\xi^k_\phi)=0.
\end{cases}
$$

The expression $\nabla_\phi E(\phi)$ denotes the Fréchet derivative of E with respect to ϕ. The upscaled equations show the mathematically and physically convincing feature that they preserve the structure from the microscopic formulation except for the effective correction tensors (6). Recently, we also achieved a rigorous error quantification between solutions of this upscaled equations and the microscopic formulation (4).”

Acknowledgements

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How to make a domain decomposition method more robust

Nicole Spillane
(joint work with Victorita Dolean, Patrice Hauret, Frédéric Nataf, Clemens Pechstein, Daniel J. Rixen, Robert Scheichl)

When faced with the problem of solving a large linear system on a parallel architecture two families of solvers are available with optimized black box implementations: direct solvers and iterative solvers. Direct solvers are robust in the sense that it is guaranteed that they will find the solution in a given number of operations no matter how hard the problem. Their memory requirements however are such that they can become unreliable when the problem becomes too large. On the other hand iterative solvers are naturally parallel since they mostly use matrix vector products. The drawback is that they often lack robustness: for ill conditioned problems the use of a preconditioner becomes essential in order for convergence to be achieved and choosing the right preconditioner is an art in itself.

Domain decomposition methods can be viewed as hybrid methods: they solve the problem with an iterative solver within which local direct solvers on some subproblems are used to reformulate the original problem or to define the preconditioner (or both). The rationale is to get the advantages out of both families of methods: robustness and parallelizability.

Unfortunately classical domain decomposition methods (Additive Schwarz, FETI, BDD) often converge very slowly or not at all for hard problems such as multiscale problems. This situation is even worse if the partition into subdomains does not follow the heterogeneities. This lack of robustness can be explained by a lack of global communication between subdomains: during one iteration a subdomain only exchanges information with its neighbours or in some cases (preconditioned FETI and BDD) the neighbours of its neighbours. For this reason a remedy is to add a global communication mechanism to the algorithm. The idea is to use a direct solver not only in each of the subdomains but also on a subproblem which is shared by all subdomains: the coarse problem. The choice of the coarse space is of course crucial and we aim to propose one that guarantees convergence even for multiscale problems.

The fundamental idea on which this work is based is that within an iterative solver, by using well chosen projections, we can separate the problem into two parts: the first is solved with the classical domain decomposition (iterative) solver and a direct solver is applied to the second (this is the coarse solve). For this reason our main objective in defining an efficient coarse space is to identify the part of the solution space on which the iterative solver does a good job. The complementary of this space is responsible for slow convergence and we make it into the coarse space so that it is taken care of by a direct solver.

Due to these observations the strategy for the construction of the coarse space is the following: using the Abstract Schwarz framework the bottleneck estimate in the convergence proof is derived. Based on this a generalized eigenvalue problem

is identified which separates the vectors that are problematic and need to be in the coarse space from the others. This way we can guarantee convergence theoretically.

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Computational error estimates for molecular dynamics

Anders Szepessy

(joint work with Ashraful Kadir, Håkon Hoel, Petr Plechac, Mattias Sandberg)

We have three types of errors in molecular dynamics simulations: time discretization error, sampling error and modelling error. The time discretization error comes from approximating the differential equation for molecular dynamics with a numerical method, based on replacing time derivatives with difference quotients and time steps Δt. The sampling error is due to truncating the infinite τ and using a finite value of τ in determining a molecular dynamics observable $\int_0^\tau g(X_t)dt/\tau$. The modelling error originates from eliminating the electrons in the Schrödinger nuclei-electron system and replacing the nuclei dynamics with their classical paths; this approximation error was first analyzed by Born and Oppenheimer in their seminal paper 1927.

The time discretization and truncation error components are in some sense simple to handle by comparing simulations with different choices of Δt and τ, although it can, of course, be difficult to know that the behavior does not change with even smaller Δt and larger τ. The modelling error is more difficult to check since a direct approach requires the solution of the Schrödinger equation. Consequently the modelling error requires mathematical error analysis. The difference between the value of observables for the time-independent Schrödinger equation, with matrix valued potentials, and the values of observables for *ab initio* Born-Oppenheimer molecular dynamics, of the ground state, depends on the probability to be in excited states. In the presence of conical intersections or avoided crossings

of electron potential surfaces this probability can be large or small. An important question in classical molecular dynamics simulations is how to verify the accuracy computationally without solving a Schrödinger equation. In the literature there seems to be no error analysis that is precise, simple and constructive enough so that a molecular dynamics simulation can use it to assess the modeling error. To construct such an algorithm for the accuracy of molecular dynamics simulations one needs to know what to compare the simulation with and to derive the modeling error. Our alternative error estimate in [1], combining analysis and computations, is developed with the aim of accurately estimating the modeling error in molecular dynamics computations. Our analysis differs from previous ones by studying

- the time-independent Schrödinger equation as the reference model, including excited electron states with near crossing potential surfaces and the accuracy of observables as a function of the probability to be in excited states, using Egorov's theorem and assuming that space-time averages of the molecular dynamics observable converge in distributional sense with a rate related to the maximal Lyapunov exponent,
- stability analysis of a perturbed eigenvalue problem to estimate the probability to be in excited electron states, based on perturbations related to (Landau-Zener like) dynamic transition probabilities,
- Ehrenfest molecular dynamics to computationally estimate the dynamic transition probabilities.

The estimation method is tested on one and two dimensional problems. A perturbation p_E, in the dynamic transition probability for a time-dependent Schrödinger WKB-transport equation, yields through resonances a larger probability of the order $\mathcal{O}(p_E^{1/2})$ to be in an excited state for the time-independent Schrödinger equation, in the presence of crossing or nearly crossing electron potential surfaces. The stability analysis uses micro-local analysis based on Egorov's theorem and shows that the approximation error can be estimated in terms of nuclei-electron mass ration, M, and p_E provided the molecular dynamics has an ergodic limit which can be approximated with time averages over the period τ and a weak convergence rate depending on the Lyapunov exponent. Numerical simulations verify that the transition probability p_E can be determined from Ehrenfest molecular dynamics simulations, cf. Figure 1.

We have preliminary computational results for Car-Parrinello and Ehrenfest dynamics adaptive mass algorithms, based the algorithm in step (ii-iii) determining excitation probabilities in Ehrenfest dynamics related to Landau-Zener probabilities, see Figure 2.

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Multiscale coupling of pore-scale network models and porous media equations

Richard Tsai

We discussed a multiscale algorithm which extracts the effective properties of pore-scale networks by properly set up localized numerical simulations on the networks,

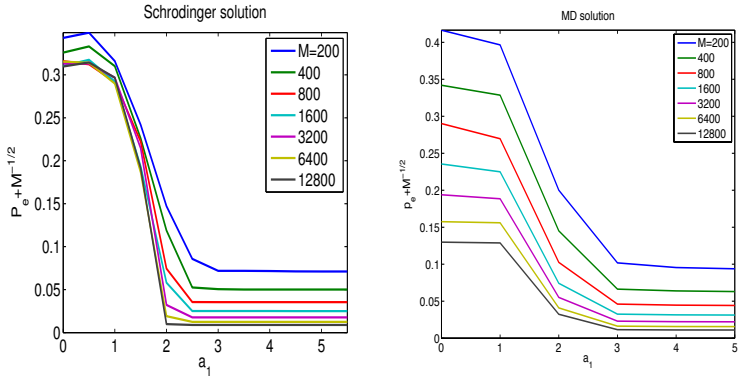

Figure 1. The minimal probability p_e to be in the excited state for the Schrödinger equation and the estimated minimal probability $\hat{p}_e$ to be in the excited state for an example of two dimensional ergodic molecular dynamics with a varying conical intersection center $(a_1, 0)$. The molecular dynamics method in the figure to the right is capable to roughly estimate the true probability to be in the excited state as determined by the Schrödinger equation in the figure to the left.

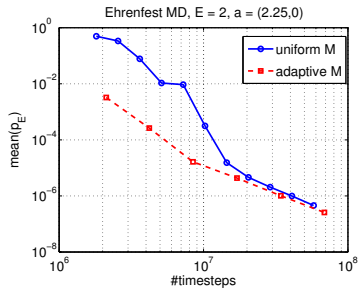

Figure 2. The mean excitation probability, p_E, as a function of computational work, i.e. number of total time-steps, for Ehrenfest dynamics with uniform mass and with adaptive mass for a model problem in 2D. For very small error (i.e. very small excitation probability p_E), the adaptive and uniform mass algorithms have the same efficiency while for larger excitation probability the adaptive method is more efficient. As the eigenvalue separation gets smaller the adaptive method becomes more and more advantageous.

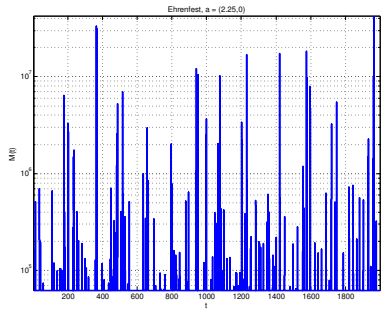

FIGURE 3. Adaptive mass as a function of time for Ehrenfest molecular dynamics, for a model problem in 2D. How well Ehrenfest dynamics follows the ground state eigenfunction depends on how far the electron eigenvalues are separated. If the separation is small it can be compensated by a larger mass which requires smaller time steps. If the separation is small only locally, as for instance for so called avoided potential crossings, the adaptive method is more efficient. The peaks with large mass corresponds to instances when the path is close to the conical intersection, which in this case is in the classical forbidden region.

and use the extracted data at a macroscopic scale for the evolution of two-phase fluid. We also discussed the connection to standard homogenization problems involving elliptic equations.

Hierarchical Multiscale Methods for the Boltzmann equation

HARALD VAN BRUMMELEN
(joint work with Michael Abdel Malik)

The Boltzmann equation (BE) poses a formidable challenge for numerical approximation methods, on account of its high dimensional phase-space setting: for a problem in N spatial dimensions, the single molecule phase-space is $2N$ dimensional. Away from the fluid dynamical regime numerical approximations of kinetic systems are predominantly based on particle methods, such as the Direct Simulation Monte Carlo (DSMC) method. However, the phase-space description of the system results in the prohibitive computational cost of DSMC in the fluid dynamical limit. Moreover, from an approximation perspective, DSMC can be inefficient since it is inherent to the Monte-Carlo process that the approximation error decays only as $n^{-\frac{1}{2}}$ for the number of simulation molecules n [5]. Hence, efficiently modeling gases in the transition regime between the free molecular flow and fluid dynamics remains difficult.

An alternative strategy to describe deviations from fluid dynamics is by means of moment-closure approximations [3, 7]. In moment-closure approximations, the

BE is projected onto a polynomial space, in the velocity dependence, and the system is closed by providing an approximation to the one-particle marginal based on the same polynomial space. This procedure can in fact be conceived of as a Galerkin approximation. The closure is chosen such that the structural properties of the BE are retained. From an adaptive approximation standpoint, the resulting hierarchical structure of the the moment closure system presents promising potential for rigorous model adaptivity. However, fundamental challenges remain to be addressed. This work applies the moment method onto a generic form of kinetic equations, given by Boltzmann's equation (BE), to simplify kinetic models of particle systems. This leads to a hierarchy of moment systems and the corresponding moment closure problem. Grad [3] conceived of moment closure approximations based on the expansion of the one-particle distribution in Hermite polynomials. However, Grad's moment systems are impaired by two essential deficiencies, viz., the potential occurrence of inadmissible locally negative phase-space distributions and potential loss of hyperbolicity [1, 8]. Levermore [7] has developed a moment-closure procedure based on constrained entropy minimization that leads to an exponential closure. Levermore's moment systems retain the fundamental structural properties of BE. Moreover, the moment systems form a hierarchy of symmetric hyperbolic systems and the corresponding distributions are non-negative. It was later shown by Junk [4], however, that Levermore's moment-closure procedure suffers from a realizability problem, in that there exist moments for which the minimum-entropy distribution is non-existent. Moreover, the fluxes in Levermore's moment systems can become arbitrarily large in the vicinity of (local) equilibrium when they exist on the boundary of the domain of realizable moments. Practically, the non-tractability of Levermore's moment-closure system poses a formidable challenge to numerical implementation.

In this work we consider alternative moment-closure relations for BE, based on non-negative approximations of the exponential function. We propose a generalization of the setting of the moment-closure problem from Kullback-Leibler divergence [6] (i.e relative entropy) to the class of φ-divergences [2]. The considered φ-divergences constitute an approximation to the Kullback-Leibler divergence in the vicinity of equilibrium. It will be shown that the approximate-exponential closure relation can be derived via constrained minimization of a corresponding φ-divergence. The proposed description encapsulates as special cases Grad's closure relation and Levermore's entropy-based closure. Moreover, the corresponding moment systems are symmetric hyperbolic, tractable and retain the fundamental properties of BE. Finally, numerical approximation of the moment system using discontinuous Galerkin finite elements and opportunities pertaining to goal-oriented adaptive modeling provided by the hierarchical structure of the moment equations will be discussed.

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Multiscale Modeling for Multiphase Flow in a Fractured Porous Medium

Mary F. Wheeler
(joint work with Gurpreet Singh)

Fractured shale and tight gas plays have two uniquely differentiable features: (1) shale, a high pore volume and low permeability feature and (2) fracture, a low pore volume and high permeability feature. It is pivotal for a fractured-reservoir flow model to capture these contrasting features in order to understand dominating flow mechanisms and also to develop an intuitive understanding of fracture flow behavior. The role of modeling choices, robust algorithms and simulations driven by rigorous mathematical derivations is of utmost importance for delivering high fidelity and reliable software. In this work, we develop a multiscale flow model where the fracture is treated as an interface and resides on the edges or faces of the grid elements. Complex reservoir and fracture geometries can be captured by general hexahedral elements owing to the choice of a multipoint flux mixed finite element method (MFMFE) [3] scheme for spatial discretization.

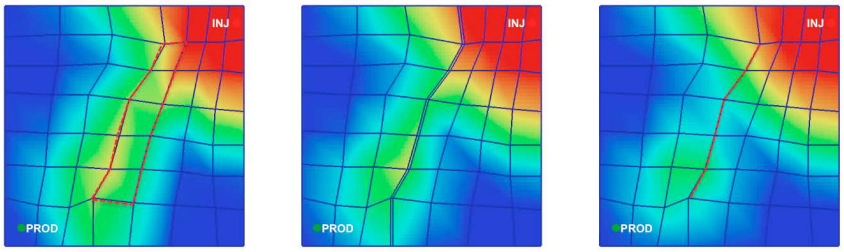

Figure 1. Understanding modeling choices: averaged (left), meshed-in (middle) and interface (right) approaches

Figure 1 shows results from three different choices and their effect on fluid mobilization and consequently recovery estimates. Fracture models which rely upon

permeability and porosity averaging lead to mobilization of additional reservoir fluids overestimating recovery predictions but have lower computational costs. A meshed-in approach is able to capture these contrasting features however, it runs into numerical difficulties leading to small time- step sizes thereby increasing computational cost. An interface based approach is able to strike balance between the advantages and disadvantages of the above two methods.

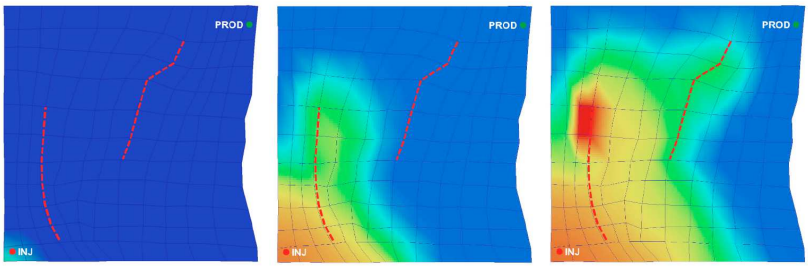

FIGURE 2. Understanding modeling choices: averaged (left), meshed-in (middle) and interface (right) approaches

Figure 2 shows the effect of fracture orientation on flow behavior. The fracture orthogonal to the line joining injector and producer acts as a screen to the pressure and fluid front thereby improving sweep whereas the one parallel to this line acts a channel reducing the sweep area. We intend to use this understanding to drive algorithmic and numerical choices, such as preconditioners and adaptivity, so as to extend the model to handle more complex fracture networks while maintaining accuracy.

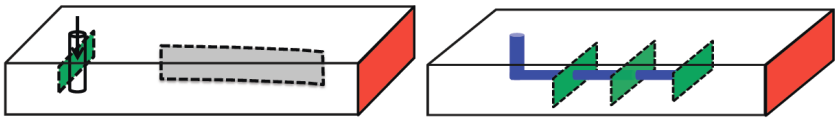

FIGURE 3. Understanding modeling choices: averaged (left), meshed-in (middle) and interface (right) approaches

We then turn our attention to understanding different kind of fracture interactions in a setting closer to the physical problem. Figure 3 shows the schematic of two numerical experiments to study the effect of boundary conditions, hydraulic-natural and hydraulic- hydraulic fracture interactions. Preliminary results [2] indicate an optimal fracture pattern (fracture shape, spacing, orientation and azimuth) can be identified for different fractured- reservoir scenarios to maximize recovery while reducing the number of stages. Further, we want to couple the flow model to a diffusive phase field fracture growth model [4]. Figure 4 shows a schematic

where a given hydraulic fracture pattern can be utilized for determining an optimal choice of fracture well placement in a naturally fractured reservoir. This will allow us to predict fracture patterns in complex reservoir settings and also to study the effect of reservoir features, such as barriers, faults, natural fractures and boundary conditions on fracture propagation.

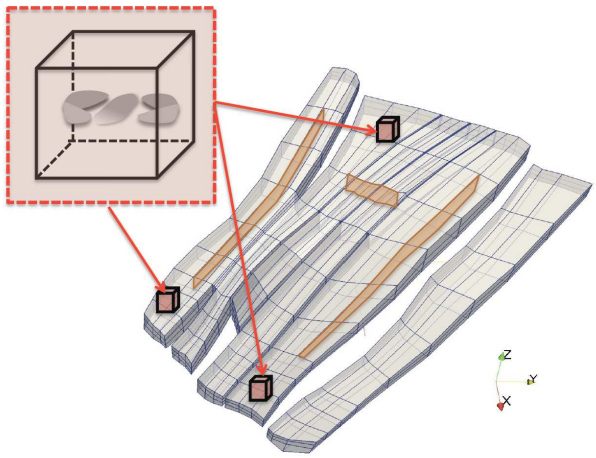

FIGURE 4. Understanding modeling choices: averaged (left), meshed-in (middle) and interface (right) approaches

Further of interest is coupled flow and reservoir geomechanics in the presence of fractures [1, 2]. The changes in stress field around a fractured well bore during injection and production stages will allow us to identify optimal scenarios for fracturing. We intend to develop a screening tool to classify reservoir candidates based upon available hydraulic fracturing choices.

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