MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Mini-Workshop: Numerical Upscaling for Flow Problems: Theory and Applications

Organised by
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ABSTRACT. The objective of this workshop was to bring together researchers working in multiscale simulations with emphasis on multigrid methods and multiscale finite element methods, aiming at chieving of better understanding and synergy between these methods. The goal of multiscale finite element methods, as upscaling methods, is to compute coarse scale solutions of the underlying equations as accurately as possible. On the other hand, multigrid methods attempt to solve fine-scale equations rapidly using a hierarchy of coarse spaces. Multigrid methods need "good" coarse scale spaces for their efficiency. The discussions of this workshop partly focused on approximation properties of coarse scale spaces and multigrid convergence. Some other presentations were on upscaling, domain decomposition methods and nonlinear multiscale methods. Some researchers discussed applications of these methods to reservoir simulations, as well as to simulations of filtration, insulating materials, and turbulence

Introduction by the Organisers

The workshop *Numerical Upscaling for Flow Problems: Theory and Applications*, organized by Achi Brandt (Rehovot), Yalchin Efendiev (College Station), and Oleg Iliev (Kaiserslautern) was held March 1st–March 7th, 2009. This meeting was attended by 16 participants with broad geographic representation from around the world. The workshop blended leading scientist whose essential contribution have shaped the field of numerical upscaling with enthusiastic young researchers.

Apart from many fruitful discussions, the workshop succeeded in illuminating the link between multiscale and multigrid methods, one of its major goals. While it has long been recognized that there are similarities and these areas can benefit from each other substantially, the many blackboard discussions and brainstorming sessions helped the participants understand the emerging problems in the field from a multifaceted perspective.

Mini-Workshop: Numerical Upscaling for Flow Problems: Theory and Applications

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Abstracts

The Mixed Variational Multiscale Method and Aspects of Convergence for Heterogeneous Porous Media

Todd Arbogast

The Variational Multiscale Method (VMM) [11, 12, 7, 6, 3] is a technique for separating fine and coarse scales in variational problems. An important application is to the problem of flow in heterogeneous porous media, in which the *permeability* K varies on a small scale ϵ. This system is governed by an elliptic problem written in variational form as: Find $p \in W$ and $\mathbf{u} \in \mathbf{V}$ such that

(1) $\qquad (K^{-1}\mathbf{u}, \mathbf{v}) = (p, \nabla \cdot \mathbf{v}) \qquad \forall\, \mathbf{v} \in \mathbf{V} \qquad$ (Darcy's law),

(2) $\qquad (\nabla \cdot \mathbf{u}, w) = (f, w) \qquad \forall\, w \in W \qquad$ (conservation of mass),

where

$$W = L^2/\mathbf{R} \quad \text{and} \quad \mathbf{V} = H(\mathrm{div}) = \{\mathbf{v} \in (L^2)^3 : \nabla \cdot \mathbf{v} \in L^2, \ \mathbf{v} \cdot \nu = 0 \text{ on } \partial\Omega\}.$$

The idea of the VMM is to separate scales through a Hilbert space decomposition. We define a coarse computational grid on Ω, and let $W = \bar{W} \oplus W'$, where the coarse pressure space is

$$\bar{W} = \{\bar{w} \in W : \bar{w} \text{ is constant } \forall \text{ coarse elements } E\}$$

and the fine scales are $W' = \bar{W}^\perp$. The space $\mathbf{V}$ of velocities is decomposed more interestingly as $\mathbf{V} = \bar{\mathbf{V}} \oplus \mathbf{V}'$, where

$$\bar{\mathbf{V}} = \{\mathbf{v} \in \mathbf{V} : \nabla \cdot \mathbf{v} \in \bar{W}\},$$
$$\mathbf{V}' = \{\mathbf{v}' \in \mathbf{V} : \nabla \cdot \mathbf{v}' \in W', \ \mathbf{v}' \cdot \nu = 0 \text{ on } \partial E \ \forall\, E\},$$

so that $\mathbf{V}'$ is localized and conservation is maintained: $\nabla \cdot \bar{\mathbf{V}} = \bar{W}$ and $\nabla \cdot \mathbf{V}' = W'$.

By separating coarse and fine scales, we see that the full solution is

$$p = \bar{p} + p' \quad \text{and} \quad \mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'.$$

Separating scales in the test functions, we obtain a coupled set of equations that respect the scales in the problem. In fact, given the coarse solution $(\bar{\mathbf{u}}, \bar{p})$—actually, only $\bar{\mathbf{u}}$ is needed for the simple problem considered—we can solve for the fine part as an *affine* operator, so we have the relation

(3) $\qquad\qquad p = \bar{p} + p'(\bar{u}) \quad \text{and} \quad \mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'(\bar{u}),$

which is posed entirely on the coarse scale. In this way, we can remove the fine scales from the coarse equations, which can be solved for $(\bar{\mathbf{u}}, \bar{p})$, and (3) gives the full solution. The modified course problem is an elliptic system, with *antidiffusive* fine-scale correction terms.

Finite element approximation proceeds by replacing $\bar{W} \times \bar{\mathbf{V}}$ by the lowest order Raviart-Thomas (RT0) [14] or BDM1 [8] mixed spaces $\bar{W}_h \times \bar{\mathbf{V}}_h$ (and solving the local problems for $(p'(\bar{\mathbf{v}}), \mathbf{u}'(\bar{\mathbf{v}})$ in some way—we assume this is done exactly here,

since there is no scaling issue involved in solving these small local problems). The space

$$\hat{\mathbf{V}}_h = \{\bar{\mathbf{v}}_h + \hat{\mathbf{u}}'(\bar{\mathbf{v}}_h) \, : \, \bar{\mathbf{v}}_h \in \bar{\mathbf{V}}_h\},$$

where $\hat{\mathbf{u}}'$ is the linear part of the operator $\mathbf{u}'$, may be viewed as a multiscale finite element space [10, 9, 5], which uses the original, rather than the fine-scale modified, variational formulation. That is, we can view the fine scales as modifying the coarse equations, and solve for the coarse part of the solution, or we can modify the finite element spaces and solve for the full solution directly.

On a rectangular coarse grid, the multiscale finite elements that result from RT have one degree of freedom associated with each edge e of the grid. Let E_e be the two coarse edges containing e; then the basis function $\mathbf{v}_e$ solves the local problems

$$(4) \qquad\qquad\qquad \mathbf{v}_e = -K\nabla\phi_e \quad \text{in } E,$$

$$(5) \qquad\qquad\qquad \nabla \cdot \mathbf{v}_e = \pm|e|/|E| \quad \text{in } E,$$

$$(6) \qquad\qquad\qquad \mathbf{v}_e \cdot \nu = \begin{cases} 0 & \text{on } \partial E \setminus e, \\ 1 & \text{on } e, \end{cases}$$

which is solved on the two elements $E \subset E_e$ and adjoined. This element is known to converge optimally [4], and with respect to the heterogeneity scale ϵ [9, 5].

A finite element due to Aarnes et al. [1, 2] is defined by solving on all of the dual-support domain E_e:

$$(7) \qquad\qquad\qquad \mathbf{v}_e = -K\nabla\phi_e \quad \text{in } E_e,$$

$$(8) \qquad\qquad\qquad \nabla \cdot \mathbf{v}_e = \pm|e|/|E| \quad \text{in } E \subset E_e,$$

$$(9) \qquad\qquad\qquad \mathbf{v}_e \cdot \nu = 0 \qquad\qquad \text{on } \partial E_e.$$

Even though numerical tests show that this is a useful element in practical cases of interest, it does not reproduce constants when K exhibits anisotropy, and it so cannot converge in any reasonable sense.

A simplified proof of convergence with respect to the heterogeneity scale ϵ of the standard multiscale finite elements was developed. It is based on the microstructure theory of homogenization [13], which gives a smooth approximation to $(\mathbf{u}, p)$ and a higher order corrector. Using the simplified proof, the place where the Aarnes element fails was noted. A modified element based on the homogenization microstructure was used to define a similar dual-support element that does not have the same convergence problem.

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Principles of Systematic Upscaling

ACHI BRANDT

General. Systematic upscaling (SU) is a comprehensive methodology for the accurate derivation of equations (or statistical relations) that govern a given physical system at increasingly larger scales. Starting at a fine (e.g., atomistic) scale where first-principle laws (e.g., differential equations) are known, SU advances, scale after scale, to obtain suitable variables and operational rules for simulating the system at any large scale of interest. SU combines the complementary advantages of two major multilevel computational paradigms that have emerged over the last 35 years: multigrid in applied mathematics and renormalization group in theoretical physics. It includes systematic procedures to iterate back and forth between all the scales of the physical problem, with a general criterion for choosing appropriate variables that operate at each level, and general techniques to derive their operational rules. Indefinitely large systems can in this way be simulated, with computation at each level being needed only within certain rather small windows, so the computations are also free of the slowdowns usually associated with

the simulations of very large systems. No scale separation is assumed; unlike conventional ad-hoc multiscale modelling, SU is in principle generally applicable and bears fully-controlled accuracy.

Classical multigrid. For linear or mildly nonlinear systems, SU can use the nonlinear multigrid (FAS multigrid) and algebraic multigrid (AMG) methods, which are based on coarse-to-fine interpolation (including the new adaptive ways for deriving interpolation, such as Bootstrap AMG [1,§17.2]). This can in particular serve as a very effective general method for numerical homogenization. This approach allows for increasingly finer levels to be confined to progressively more specialized subdomains where they are needed (as in [2,§§7–9]). It also permits transitions between widely different physical formulations, e.g., from atomistic fine level to finite elements at the next coarser level (as in the quasi-continuum method used in materials science, a first version of which had actually appeared already in [3, §1.1]).

Current SU. For highly nonlinear and discrete-state systems, however, it turned out that interpolation-based methods can no longer be efficient (see [1, §13.1]). So instead, the more general SU approach employs the following multiscale principles.

(1) *The simulation at each level* is a sequence of local steps, such as Gauss-Seidel relaxation in energy-minimization problems, or Monte Carlo simulation in equilibrium calculations, or explicit time steps, etc.

(2) *Coarse variables* can each represent an average of several neighboring variables of the next finer level, or a count of the number of (next-finer-level) particles in a cell of a given lattice, and/or the average kinetic energy of those particles, etc. The choice of adequate variables is governed by the criterion below (see #4).

(3) *Coarse-to-fine transition* is generally based on "*compatible simulations*", i.e., simulations at the fine level such that keep the coarse variables unchanged. This process (completely missed in classical renormalization group methods) is very essential for choosing the coarse variables (see #4) and for coarse-to-fine acceleration (as in multigrid) and/or for confining the fine simulations to small windows (see #7).

(4) *General criterion of adequacy of the set of coarse variables* consists of requiring fast convergence (or equilibration, etc.) of the compatible simulation. This criterion (already extensively used in AMG [4]) is easy to apply and very effective in searching for good coarse variables. It ensures fast coarse-to-fine transitions and the feasibility of the following processes.

(5) *Derivation of coarse operational rules* (equations, or a governing energy or Hamiltonian functional) is based on requiring simulations at he coarse level to yield the same averages as simulations at the next finer level, for a given set of "observables". A general fast iterative method to achieve this has been developed (see [6], or [1, §§14.5–14.7] and [5], for example).

(6) *Error estimates* are obtained in terms of comparing averages at coarse and fine simulations, for a new set of observables. If large coarse-vs.-fine

discrepancy is detected, it directly leads to corrections (e.g., via adding terms to the governing functional).

(7) *Multiscale windows.* Each fine level is only simulated in some restricted "windows" (subdomains of the domains on which the next coarser level is defined). Around the boundary of each window the fine level is kept compatible with the coarse (see #3). the fine simulations supply the operational rules to the next coarser level (see #5), while that coarser level accelerates the simulations and determines where and when new fine-level windows should be opened. If the scale ratio between each pair of successive levels is kept suitably bounded, these inter-level iterative interactions should quickly settle into overall consistency (like the fast convergence of multigrid cycles). The number and size of windows at each level does not depend on the overall (macroscopic) size of the studied system.

See [6] for more details.

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Towards Physics-Oriented Algebraic Multigrid for Systems of Partial Differential Equations

TANJA CLEES

(joint work with SAMG Team at SCAI (Klaus Stüben), Herman and Johan Deconinck, Leonhard Ganzer, Stephan Matthäi, Mary Wheeler)

Classical AMG (for a history and a detailed introduction, see [1]) is known to provide efficient and robust hierarchical solvers or preconditioners for large classes of systems of linear equations (matrix problems) $Av = b$, an important one being the class of (sparse) linear systems with matrices A which are "close" to being M-matrices. Problems like this widely occur in connection with discretized scalar elliptic PDEs. In such cases, classical AMG is very mature and can handle millions of variables much more efficiently than any one-level method. Since explicit information on the geometry is not needed, AMG is especially suited for unstructured grids both in 2D and 3D. The coarsening process is directly based on the

connectivity pattern reflected by the matrix (and its weighted and directed graph), and interpolation is constructed based on the matrix entries. Restriction is simply defined to be the transpose of interpolation, regardless whether the matrix to be solved is symmetric or not. The Galerkin coarse-level matrix A_{n+1} for level $n+1$ is computed as

$$A_{n+1} := I_n^{n+1} A_n I_{n+1}^n$$

with I_{n+1}^n being the interpolation from level $n+1$ to n, and $I_n^{n+1} := I_{n+1}^n$ the restriction from level n to $n+1$, starting from level 1 which represents the original matrix equation $Av = b$.

However, more than just straightforward extensions of these "scalar" AMG methods are required to efficiently solve linear systems stemming from most practically important systems of PDEs involving two or more scalar functions. For instance, this is the case for semiconductor device simulation and, even more, for coupled circuit and device simulation. Clees [2] developed a flexible framework especially for constructing so-called "point-based" AMG (PAMG) approaches suitable for various types of strongly coupled PDE systems. This framework is integrated into the (parallel) linear solver library SAMG [3]. Although a reasonable choice of components depends on the class of applications at hand, considerable progress has been made during the last years to develop robust solution strategies. A brief summary is given below.

Detailed results for industrial applications in semiconductor simulation have been presented in [4, 2], showing that the usage of PAMG preconditioners can yield efficient solution processes for three very different types of PDE systems, namely linear elasticity (stress analysis), reaction-diffusion and drift-diffusion equations. A first physics-oriented concept for setting up the AMG hierarchy has been developed there.

Work [5, 6] on automatic and adaptive solver- and parameter-switching strategies (α-SAMG) has considerably extended robustness and efficiency of SAMG, in particular for mixed hyperbolic-elliptic PDE systems. The smoothing (or hybrid smoothing and solving) strategy developed in [5] already exploited physical properties of the systems to some extent ("surfing on characteristics" for convective parts).

The very recent [7] demonstrates the effectiveness of a new adaptive physics-oriented smoothing framework (α-smoothing), integrated into α-SAMG, particularly for PD(A)E systems with drift and diffusion terms and network equations. First benchmarks with α-SAMG integrated into the coupled circuit and device simulator MECS show the potential of the resulting package. More details shall be published in [8]. Ongoing investigations deal with extentions of α-smoothing as well as a strengthened connection with and/or influence on the coarsening and interpolation strategy.

Regarding comparisons to "standard" linear solvers, employed in industrial environments, α-SAMG outperforms, for instance, the efficient direct linear solver

PARDISO [9] as well as standard iterative one-level solvers, as for instance described in [10, 11], for many problems of relevant size and physical complexity, not restricted to the applications mentioned above.

The first part of the talk concentrated on an introduction into classical AMG, in particular, its coarsening and interpolation strategies for setting up the coarse-level systems along with transfer operators. The second part introduced and discussed the PAMG framework, α-SAMG and the very recently developed first α-smoothing.

A coarse-level system created by means of an AMG method can be seen as an upscaled linear system of equations, and, hence, AMG as a numerical upscaling technique. Further research shall concentrate on numerical and "physical" properties of the resulting coarse-level systems, depending on and/or compared with goals of a concrete upscaling task.

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Experience with Systematic Upscaling of Two-Dimensional Vortical Flows

BORIS DISKIN

(joint work with Achi Brandt)

This abstract summarizes recent experiences with Systematic Upscaling schemes for simulating vortical flows described by extended 2D Navier-Stokes equations:

$$
\begin{aligned}
&W_t + UW_x + VW_y - \nu\Delta W - \mu\Psi = 0, \\
&\Delta\Psi - W = 0, \\
&U_x + V_y = 0, \\
&U_y - V_x - W = 0,
\end{aligned}
$$
(1)

with periodic boundary conditions. Here, W is the vorticity, U and V are the velocity components, Ψ is the stream function, ν is the physical viscosity coefficient, and μ is the hypoviscosity coefficient. Hypoviscosity is introduced to take energy from large (smooth) vortexes and, thus, prevent inverse cascading. In all tests considered, $\mu = 0$.

The Systematic Upscaling process starts at the viscous scale, at which discretized Navier-Stokes equations provide an accurate flow description. Increasingly coarser-scale equations are derived recursively, employing at each scale simulations in relatively small computational windows. The fine-scale variables and governing equations are assumed given and accurate. A pair of (not far) separated fine and coarse scales is considered in a time. Typically, the coarser grid has about the same number of grid nodes as the finer grid and, with doubled mesh spacing, covers a larger domain (bigger computational window). Generally in Systematic Upscaling, the set of coarse variables is a reduced set of quantities (degrees of freedom) derived from fine-grid solutions. An example of coarse variables is averages of certain components of the fine-grid solutions. The set of coarse variables is considered adequate if there is an efficient reconstruction procedure that allows reconstructing the fine-grid flow from its set of coarse variables over few time steps, or at least satisfactorily approximating it. The demonstration of the success of such a procedure is called a compatibility test. Coarse-scale equations are derived to provide accurate and efficiently solvable laws for adequate coarse-scale variables.

Major advances

Methodology to choose an adequate set of coarse-level variables has been developed and tested. Specifically, adequate sets of coarse-level variables and corresponding compatibility tests have been shown for vortical flows at different regimes. In the case of algebraic systems of equations (such as steady-state flow problems), the fast recovery is achieved by "compatible relaxation". For the case of time-dependent problems, we have developed a compatibility test based on several compatibilization time steps. These tests proved invaluable in identifying adequate variables to compute flows at very coarse scales.

The desired timestep-to-meshsize scale ratio for efficient compatibilization has been identified.

Adequate coarse variables for sufficiently smooth flows on the scale of the coarse grid can be obtained simply in terms of vorticity averages. The developed compatibility tests showed that with these coarse variables the relative difference between the reference and reconstructed fine-grid solutions is bounded by the interpolation errors.

Adequate coarse variables for non-smooth flows are more complicated. It was shown that vorticity averages alone are not adequate to represent flows with strong small vortexes on coarse scales. On the (coarse) scales, where the velocity vector (its direction, in particular) changes much per meshsize or per time step, an adequate set of coarse variables is obtained by separating the flow into a sum of idealized vortexes and a background flow. An idealized vortex can in principle be any local solution to the steady-state Euler equations. For two-dimensional (2D) inviscid calculations, each idealized vortex can be described by a delta-function vorticity. For 2D viscous (including high-Reynolds) flows, each idealized vortex is described by a one-dimensional (1D) radial function. The complete set of coarse variables consists of idealized vortexes and vorticity averages of the background flow. It was demonstrated that with these coarse variables the reference and reconstructed fine-grid flows are indistinguishable after many hundreds of time steps.

Equations for separated flows have been derived, including equations for motion and radial-shape evolution of idealized vortexes and their interactions with the background flow. The accuracy of the equations has been verified on a sequence of increasingly larger domains employing progressively coarser grids, by comparing on each domain two calculations using two different resolutions. As an example, the (complicated) motion of the vortex centers has been monitored in fine and coarse-scale simulations. After several hundred time steps, a typical deviation in the center positions was smaller than the fine-scale resolution.

Improved accuracy of the separated-flow models has been demonstrated. Even on levels where vortexes are still well resolved, the new discretization that explicitly separates vortexes at high-vorticity regions is much more accurate than semi-Lagrangian calculations, suffering much less from numerical viscosity. The reason is that each idealized vortex is accurately moving (accurately resting) in its own field of velocities, and is also accurately modified by the viscosity. In addition (although less important), advecting other vorticity values (and in particular other idealized vortexes) in the velocity field of an idealized vortex can accurately be made along its circular streamlines. So the most violently changing velocity vectors are accurately accounted for, free of numerical viscosity.

Limitations of the obtained results

Only 2D flows were studied. Experimenting on sufficiently large three-dimensional (3D) grids would be too expensive, cumbersome, and time consuming; so we have decided to work with 2D models as long as we can learn much from them

concerning basic concepts of flow upscaling. Real 3D flows would of course require more elaborate shapes of idealized separated vortexes (cylindrical instead of radial, described by 2D instead of 1D functions).

Artificial vortex generation. While in 3D turbulence vortexes are naturally generated by the energy cascade, in our 2D models we had to generate them artificially, e.g., by introducing them in the initial conditions.

Separated vortex distortion. Current models of evolution of idealized separated vortexes in the background flow do not account for vortex distortion because of the difference in the background-flow velocity at the center and at the periphery of a separated vortex.

Only deterministic flows were studied. Our studies remained strictly in the realm of deterministic flows. Solution bifurcations (typical in 3D turbulence), and their upscaling in terms of stochastic terms in the vortex interactions, have not been investigated yet.

Too small scales. Our upscaling procedures have not yet dealt with such large scales at which the numerical grids no longer resolve the inter-vortical distances. In particular, we have not reached the very large scales at which there are many multiscale vortexes per meshsize, so that upscaling equations at those scales should combine small-vortex statistics with large-vortex resolution. However, the systematic approach developed for deterministic steady-state and time-dependent systems, together with our upscaling approaches for equilibrium statistics developed earlier, surely provide very useful tools for treatment of those larger-scale challenges.

Multiscale Problems and Upscaling.Simulation of multiscale filtration processes

OLEG ILIEV

(joint work with Z.Lakdawala, J.Willems, V.Starikovicius,P.Popov)

In the first part of the talk, general issues of the multiscale problems and upscaling are discussed. In particular, an attempt is done to classify the multiscale problems with respect to the upscaling goals and the upscaling costs. This preliminary classification looks as follows:

• Approaches for problems with separable scales (fine-to-coarse, coarse solution is the target):

homogenization+MG (most efficient); renormalization; volume averaging; heterogeneous multiscale method (HMM); MsFEM;

Costs to solve: coarse scale (cheap) + 1 cell problem at fine scale (cheap)

• Approaches for problems with unseparable scales (fine scale solution needed):

MG, AMG, Multilevel Domain Decomposition, (also as preconditioners for Krylov subspace methods)

Costs to solve: fine scale: expensive, but optimal with above methods (O(n))

• Approaches for problems with unseparable scales (coarse scale solution needed + approximation to the fine scale one):

- MsFEM; MSFV, subgrid, grain coarsening and related methods, Numerical upscaling (with iterations between scales can recover full fine scale solution)
Costs to solve: intermediate (compared to above, but still O(n))
• Approaches for problems with unseparable scales (coarse scale solution needed, plus approximation to the fine scale one where necessary)
- Systematic upscaling (with clever choice of variables and/or with windowing), MSFV with adaptivity, MsFEM with adaptivity,
Costs to solve: intermediate (less than O(n))
• Approaches for problems with unseparable scales (coarse scale solution needed)
- Formal homogenization plus statistics (if it works)
Costs to solve: intermediate (cheap + statistics)
- Systematic upscaling (when nothing else works)
Costs to solve: depends on the qualification.
Note: all the above may need to be reconsidered in the case of uncertainty.

In the second part of the talk, certain approaches for solving multiscale filtration problems are discussed.These are a subgrid approach, and coupling of microscale and macroscale filtration simulations.

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

Coupling of microscale and macroscale filtration simulations is a real challenge. The filtration is an essentially multiscale problem. The particles to be filtrated

might be of nano- or micron size, the assembled filter elements might be of centimeter or meter size. A team from Fraunhofer ITWM has developed algorithms and software for solving filtration problems at microscale, i.e., at the level of pores, fibers, and dirt particles. Stokes problem is solved to determine the velocity at pore scale, while stochastic ODE is solved to account for particles transport and capturing at pore level. For more details, see www.geodict.com, and references therein. At macroscale, Navier-Stokes-Brinkman system of equations, together with equation for concentration of particles, have to be solved in order to simulate the flow and particle transport at the level of a filter element. An algorithm for coupling microscale and macroscale simulations is developed, where the microscale problem is solved only in selected windows. The capturing of the particles computed at microscale allows to calculate the capturing rate needed in macroscopic concentration equation, as well as the change of the permeability. The macroscopic solution, from the other side, provides the inlet velocity in front of the selected filter media windows, as well as the concentration of the particles there.

Multiscale finite element methods for flows in heterogeneous porous media

YALCHIN EFENDIEV

(joint work with Lijian Jiang, Joerg Aarnes)

The modeling of multiphase flow in porous formations is important for both environmental remediation and the management of petroleum reservoirs. Practical situations involving multiphase flow include the dispersal of a non-aqueous phase liquid in an aquifer or the displacement of a non-aqueous phase liquid by water. In the subsurface, these processes are complicated by the effects of permeability heterogeneity on the flow and transport. Simulation models, if they are to provide realistic predictions, must accurately account for these effects. However, because permeability heterogeneity occurs at many different length scales, numerical flow models cannot in general resolve all of the scales of variation. Therefore, approaches are needed for representing the effects of subgrid scale variations on larger scale flow results.

On the fine (fully resolved) scale, the subsurface flow and transport of N components can be described in terms of an elliptic (for incompressible systems) pressure equation coupled to a sequence of $N - 1$ hyperbolic (in the absence of dispersive and capillary pressure effects) conservation laws. In this abstract we address the upscaling of both pressure and saturation equations.

Traditional approaches for scale up of pressure equations generally involve the calculation of effective media properties. In these approaches the fine scale information is built into the effective media parameters, and then the problem on the coarse scale is solved. We refer to [3] for more discussion on upscaled modeling in multiphase flows. Recently, a number of approaches have been introduced where the coupling of small scale information is performed through a numerical

formulation of the global problem by incorporating the fine features of the problem into basis elements. In the presentation, I discussed multiscale finite element methods that share similar concept. Because of their conservative features, mixed finite methods are often preferred in the applications, such as flow in porous media. Our methodology is similar to the multiscale finite element methods [8]. We discuss numerical implementation, as well as some applications of our approach.

Though there are a number of technical issues associated with the subgrid models for the pressure equation, the lack of robustness of existing coarse-scale models is largely due to the treatment of the hyperbolic transport equations. Previous approaches for the coarse-scale modeling of transport in heterogeneous oil reservoirs include the use of pseudo-relative permeabilities, the application of nonuniform or flow-based coarse grids [2], and the use of volume averaging and higher moments [4]. Our methodology for subgrid upscaling of the hyperbolic (or convection dominated) equations uses volume averaging techniques and relies on unstructured grid. The grid is constructed such that the variation of the velocity is minimal. This yields unstructured grids.

In this talk, we mainly discussed a multiscale finite element approach in which the basis functions are constructed using the solution of the global fine-scale problem at the initial time (only). The heterogeneities of the porous media are typically well represented in the global fine-scale solutions. In particular, the connectivity of the media is properly embedded into the global fine-scale solution. Thus, for the porous media with channelized features (where the high/low permeability region has long-range connectivity), this type of approach is expected to work better. Indeed, our computations show that our modified approach performs better, for porous media with channelized structure, than the approaches in which the basis functions are constructed using only local information. Some analysis is presented to justify our numerical observations. In our numerical simulations, we have used cross-sections of recent benchmark permeability fields, such as the SPE comparative solution project, in which the porous media has a channelized structure and a large aspect ratio. The results are presented in [5].

These methods are also presented in the framework of mixed multiscale finite element methods. In particular, we present a general framework where multiple global information can be incorporated into the basis functions. In the talk, we discuss how to obtain the global information. Moreover, we discuss how one can approximate the limited global information in order to reduce the computational cost. Various approaches, such as the use of partial homogenization or the use MsFEM solutions are discussed.

We also discuss stochastic multiscale finite element methods. In this approach, the main idea to construct basis functions for the ensemble or a part of the ensemble. We discuss how the general approach of multiscale finite element methods using multiple limited global information can be used for this purpose. Numerical results are presented.

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Mathematical Modelling of Fractured Porous Media

ALFIO GRILLO

(joint work with Dimitry Logashenko, Gabriel Wittum)

This work deals with the study of transport processes in two-dimensional porous media interacting with a surrounding three-dimensional continuum. To this end, we employ an averaging procedure exposed in [1], and we compare our approach with the theory developed in [2][3]. Our preliminary results refer to the problem of predicting the diffusive and advective motion of a contaminant in a fractured porous medium.

In this contribution, we use the average-along-the-vertical technique [1] in order to describe the macroscopic transport of a solute in a medium that, because of its shape, can be regarded as a two-dimensional object embedded in a three-dimensional porous medium. The motivation of our work is given by the necessity of predicting the behaviour of contaminants in fractured rocks. In this context,

the two-dimensional object may be identified with a *fracture*. For simplicity, we consider the case in which the fracture is delimited by two parallel surfaces and a band-shaped lateral boundary, and its thickness is negligibly small as compared to characteristic size of the surrounding porous medium. Under these hypotheses, and the further assumption that the fracture is at rest, the method illustrated by Bear [1] leads to a mass balance equation for the solute in the fracture that is very similar to that found in [2] in modelling transport relations for surface integrals in the case of evolving fluid interfaces, i.e.

(1) $$\dot{C}_\sigma + C_\sigma \nabla_\sigma \cdot \mathbf{u}_{\tan} = \nabla_\sigma \cdot (D_\sigma C_\sigma) - [\![C(\mathbf{u} \cdot \mathbf{n} + \mathbf{j} \cdot \mathbf{n})]\!],$$

where C_σ is the surface concentration of the given contaminant, $\dot{C}_\sigma$ denotes the total time derivative derivative of C_σ (cf. [2]), ∇_σ is the surface divergence operator, $\mathbf{u}_{\tan}$ is the tangential of the fluid velocity along the surface, D_σ is the surface diffusivity coefficient, and the last term on the RHS denotes the jump of the overall normal mass flux computed on both sides of the surface. We notice that, if the fracture were moving with normal velocity V (cf. [2]), a term $-\kappa C_\sigma V$ (κ being the total curvature of the surface), and a term $[\![CV]\!]$ should be added to the LHS, and the RHS of Eq. (1), respectively, and the total derivatie $\dot{C}_\sigma$ should be replaced with the *migrationally* time derivative $\mathring{C}_\sigma$ [2].

Under the assumption of neglgible inertial terms and absence of pore-scale mass exchange terms between the fluid- and the solid-phase, the problem of fluid-flow and contaminant transport in a fractured porous medium is macroscopically governed by the mass balance laws for the contaminant and the fluid-phase as a whole. These equations must be written for both the porous medium and the fracture, i.e.

(2) $$\partial_m(\phi_m \rho_m) + \nabla \cdot (\phi_m \rho_m \mathbf{u}_m) = 0,$$
(3) $$\partial_t(\phi_m C_m) + \nabla \cdot (\phi_m C_m \mathbf{u}_m + \mathbf{j}_m) = 0,$$

and

(4) $$\partial_t(\phi_f \rho_f) + \nabla \cdot (\phi_f \rho_f \mathbf{u}_f) = 0,$$
(5) $$\partial_t(\phi_f C_f) + \nabla \cdot (\phi_f C_f \mathbf{u}_f + \mathbf{j}_f) = 0,$$

where ϕ_α, ρ_α, and $\mathbf{u}_\alpha$ (with $\alpha \in \{f, m\}$) are the fluid-phase volume fraction (porosity), mass density, and velocity, respectively, whereas C_α and $\mathbf{j}_\alpha$ (with $\alpha \in \{f, m\}$) are the concentration and diffusive flux of contaminant. In order to close the system of equations, it is assumed that mass density, ρ_α, is a given constitutive function of contaminant concentration, i.e. $\rho_\alpha = \hat{\rho}_\alpha(C_\alpha)$, and that fluid-phase velocity and contaminant diffusive flux are expressed through Darcy's and Fick's Laws, respectively, i.e.

(6) $$\phi_\alpha \mathbf{u}_\alpha = -\frac{k_\alpha}{\mu}[\nabla p_\alpha - \hat{\rho}_\alpha(C_\alpha)\mathbf{g}],$$
(7) $$\mathbf{j}_\alpha = -\phi_\alpha D_\alpha[1 - C_\alpha \hat{\gamma}_\alpha(C_\alpha)]\nabla C_\alpha,$$

where k_α, μ, p_α, $\mathbf{g}$, D_α and $\widehat{\gamma}_\alpha$ ($\alpha \in \{f, m\}$) denote permeability, fluid viscosity, pressure, gravity acceleration vector, diffusion coefficient, and fluid compressibility, respectively.

If porosity is constant both in the medium and in the fracture, the constitutive law $\widehat{\rho}_\alpha(C_\alpha) = A_\alpha + B_\alpha C_\alpha$ is assumed ($\alpha \in \{f, m\}$), and Eqs. (4) and (5) are averaged according to Bear's procedure [1], the problem of transport can be reformulated as

$$(8) \qquad\qquad \nabla \cdot (A_m \mathbf{q}_m - B_m \mathbf{j}_m) = 0,$$

$$(9) \qquad\qquad \phi_m \partial_t C_m + \nabla \cdot (C_m \mathbf{q}_m + \mathbf{j}_m) = 0,$$

and

$$(10) \qquad b\nabla_\sigma \cdot [A_f \langle \mathbf{q}_{f\sigma} \rangle - B_f \langle \mathbf{j}_{f\sigma} \rangle] + [\![A_f q_{fn} - B_\alpha j_{fn}]\!] = 0,$$

$$(11) \qquad \phi_f b \partial_t \langle C_f \rangle + \nabla_\sigma \cdot [b\langle C_f \rangle \langle \mathbf{q}_{f\sigma} \rangle + b\langle \mathbf{j}_{f\sigma} \rangle] + [\![C_f q_{fn} + j_{fn}]\!] = 0,$$

where $q_{\alpha n}$ and $j_{\alpha n}$ denote, respectively, the components of $\mathbf{q}_\alpha$ and $\mathbf{j}_\alpha$ normal to the fracture. In the limit in which the fracture width "shrinks", *excess quantities* [5] should be introduced.

The system of Eqs. (8)–(11) was solved numerically by using the software packages UG and d3f. Results are shown in Figure 1, where the fluid velocity, and concentration of the solute both in the fracture and the surrounding porous medium are shown at a given time step. Figures 1a and 1b show the asymmetry in fluid velocity and concentration in the medium due to the particularly chosen orientation of the fracture.

If the identifications $C_\sigma = \phi_f b \langle C_f \rangle$, $\mathbf{u}_{\text{tan}} = \langle \mathbf{q}_{f\sigma} \rangle$, $\mathbf{u} \cdot \mathbf{n} = q_{fz}$, and $\mathbf{j} \cdot \mathbf{n} = \langle j_{fz} \rangle$ are made, our Eq. (11) resembles Eq. (1) given in [2]. To the best of our understanding, the main difference between these two models lies in the fact that the model presented in Eq. (1) is *a priori* two-dimensional, while our model obtains the transport equation in a two-dimensional medium through an averaging procedure. This difference becomes evident in the definition of the Fick's current for the fracture. Indeed, due to the constitutive law imposed on the fluid-phase mass density, the averaging procedure leads to the following averaged tangential Fickean flux

$$(12) \qquad\qquad \langle \mathbf{j}_{f\sigma} \rangle = -\phi_f D_f \left\langle \frac{\alpha}{\alpha + BC_f} \nabla C_f \right\rangle,$$

where the diffusion coefficient, D_f, has been assumed to be constant. This result is due to the fact that Fick's law and the definition of the fluid mass density as a function of solute concentration has been introduced before accomplishing the averaging procedure. Our next step is the comparison of the present results with those provided by the application of the theory proposed by Gray [6].

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Time 10.001 year (no. 201)

Velocity in the medium

Concentration in the medium
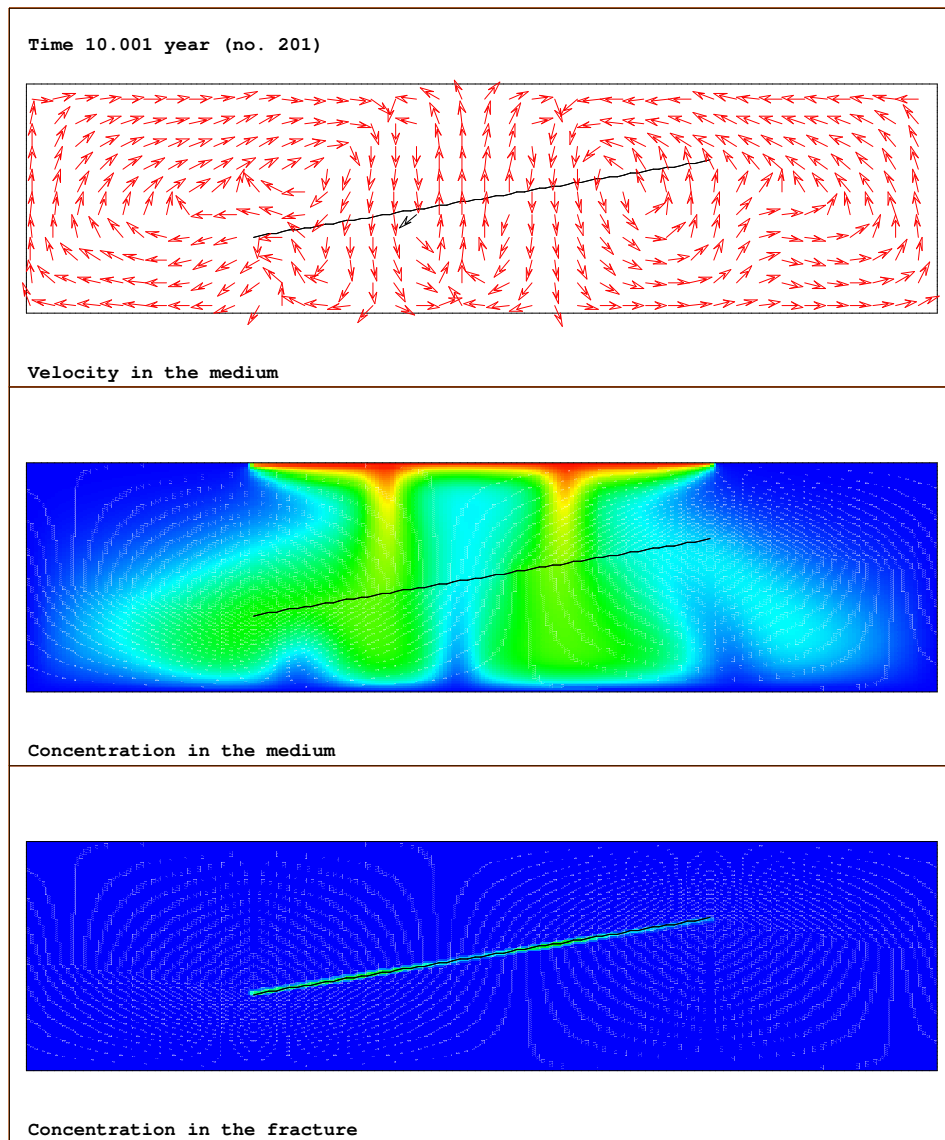

Concentration in the fracture

FIGURE 1. Velocity, concentration in the medium, and concentration of the fracture at time step $t = 10.001$ year.

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On the Adaptivity of Multiscale Methods for Flow and Transport

PATRICK JENNY

(joint work with Giuseppe Bonfigli and Hadi Hajibeygi)

Flow and transport problems arise in many areas of engineering and natural science, e.g. in hydrology, oil reservoir simulation and CO_2 sequestration. In order to perform accurate and efficient calculations, the simulation algorithms and codes have to cope with the typically large problems, which often involve highly heterogeneous permeability fields with complex spatial correlation structures. Due to computational limitations, it is in general not possible to resolve all relevant scales and therefore, from early on, upscaling techniques have been developed and are still applied with considerable success [3]. However, in particular if multi-phase flow is considered, it is difficult to obtain accurate results with upscaled models, in which the fine scale variability of the solution is disregarded. This shortcoming has been addressed with multi-scale methods by including a reconstruction step, i.e. such methods target fine scale solutions of the flow and transport problems. Several techniques have been developed and most of them can be categorized as multi-scale finite element methods (MsFEM) [5], multi-scale mixed finite element methods (MsMFEM) [1], or multi-scale finite-volume (MSFV) methods [6]. All these methods have in common that they rely on basis functions, which are numerically computed on local domains, where the fine-scale permeability field of the original problem is employed. Fine scale pressure and/or velocity solutions are approximated by superpositions of these basis functions and the coefficients are computed by solving a coarse system. The only approximation compared to a direct solution of the problem consists in the local boundary conditions, which are required in order to compute the basis functions on their local domains independent of the global solution. Different are the three multi-scale approaches with respect to the number of degrees of freedom (dof) of the resulting coarse problems and with respect to the reconstructed fine-scale velocity fields. There exists one dof in the coarse problems of MsFEM and MSFV methods. In MsMFEM on the other hand, dof not only include coarse pressure values, but also mean velocities at all coarse cell faces. A disadvantage of the MsFEM compared to the other two approaches is their inability to provide a conservative fine-scale velocity reconstruction, which is important if also transport equations have to be solved.

All these methods have been applied for a large variety of elliptic problems and in order to reduce the rate of recomputing the basis functions as e.g. the mobility evolves, an adaptive strategy was introduced, and in order to apply large time steps, a sequentially implicit solution algorithm based on Schwarz overalp for transport was devised. Later, the MSFV framework was extended for compressible multi-phase flow [8] and the introduction of correction functions [9] allowed to include gravity, capillary pressure and complex wells [11, 7]. An important development is a recently published iterative MSFV (iMSFV) method, which allows to use the multi-scale framework as an efficient linear solver [4]. This is achieved by iteratively improving the localization boundary conditions based on the previous

MSFV solution. In algebraic form, the iMSFV method can be interpreted as a particular two level domain decomposition or multi-grid method [10]. This is of interest, since it allows more easily to apply multi-scale methods in combination with general unstructured grids. An attractive aspect of the iMSFV method is that it can be applied anywhere between the original MSFV method an a fine-scale linear solver and that the resulting velocity field is always conservative. Moreover, it was shown that infrequent updates of the localization conditions is sufficient, thus in practice the iMSFV method is not significantly more expensive than the original MSFV method.

A further topic is multi-scale modeling of transport, which becomes more relevant as the cost for the flow computations is significantly reduced. A successful strategy consists in adaptively switching between coarse and fine transport equations depending on the local saturation/concetration variation. However, efficient and accurate treatment of transport in heterogeneous porous media remains a challenging research topic with many open questions.

Finally, such multi-scale methods have a great potential for multi-physics applications, e.g. for coupled systems, where different sub-domains are governed either by the Navier-Stokes equations or Darcy's law [2].

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Homogenisation and Numerical Simulation of Flow Problems in Geometries with Textile Microstructures

MARGRIT KLITZ

(joint work with Michael Griebel, Bart Verleye, Dirk Roose and Stepan Vladimirovitch Lomov)

New materials with textile microstructures are used in an increasing number of high-performance products such as aerospace components, boat hulls and racing car bodies, since they combine strength and stiffness with lightness and corrosion-resistance. In order to manufacture these composite materials, Liquid Composite Moulding (LCM) processes are used. One of the LCM techniques is Resin Transfer Moulding (RTM), which is the injection of resin into a closed cavity filled with fibre preforms. Here, practical experiments aim at the enhancement of resin flow through the fibre preform to reduce voids, bubbles and injection time. This is however very costly, since flow in RTM is highly dependent on the tooling geometry and often requires the building of many sets of expensive prototypes to test the process. An alternative is offered by the numerical simulation of fluid flow in the fibre preforms which allows for the virtual testing of different mold designs in the computer. In this talk we aim at the prediction of textile permeability, since the existing tools that simulate the injection stage of Resin Transfer Moulding require the permeability at different positions in the preform model.

Textile reinforcements are hierachically structured materials, which may involve microstructures on several length scales. Pictures with examples from different scales are given in Figure 1. On the microscale individual strands of fibres are bundled and create the fibre tows or yarns. A fibre unit cell consists of an arrangement of fibres which repeated periodically into space gives the yarn. The yarns are woven or knitted together and create a porous network with inter-yarn and intra-yarn spaces, which form the mesoscopic length scale. The macroscopic length scale describes the molded composite part as a whole. In this structural hierarchy the manufactured composite part is one hundred times larger than the mesoscale fabric unit cell, which again is one hundred times larger than the microscale fibre unit cell.

In most cases, the large discrepancy between the involved length scales renders a direct numerical simulation of flow through textiles by solving the Stokes equations in the pore microstructure impossible due to computational complexity. The required resolution of the textile's microstructure calls for very fine grids, which draw heavily on the capacities of existing computer architectures. A way to deal with this problem is to upscale the analytical equations of fluid mechanics that hold on the microscale to laws on the macroscale by e.g. averaging [3] or analytical homogenisation methods (cf. [2, 3, 5]).

The so derived macroscopic equations take the microscale only effectively into account and are thus numerically easier to handle for simulation purposes. For
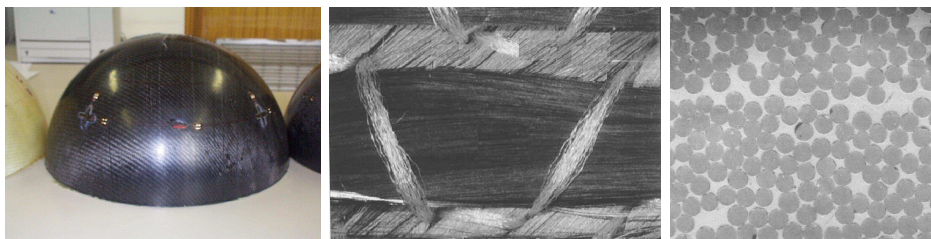
FIGURE 1. A hierarchy of textile structures from left to right: the composite part (1 m), the fabric (0.01 m), the fibres (0.0001 m). [Pictures: S. Lomov].

instance the homogenisation of the Stokes equations yields Darcy's law:

$$\boldsymbol{u} = \frac{1}{\mu}\boldsymbol{K}(\boldsymbol{f} - \nabla p) \quad \text{in } \Omega$$

(1)

$$\nabla \cdot \boldsymbol{u} = 0 \quad \text{in } \Omega$$

on the macroscale. Here, $\Omega \subset \mathbb{R}^n$, $n = 2,3$ denotes an open, bounded and connected set with a smooth boundary of class C^1, $\boldsymbol{u}$ denotes the velocity field, p the pressure, $\boldsymbol{f}$ denotes volume forces and μ the viscosity. A different scaling of the volume fraction results in another filtration law which is Brinkman's equation

$$-\mu\Delta\boldsymbol{u} + \nabla p + \frac{\mu}{\sigma^2}\boldsymbol{M}^{-1}\boldsymbol{u} = \boldsymbol{f} \quad \text{in } \Omega$$

(2)

$$\nabla \cdot \boldsymbol{u} = 0 \quad \text{in } \Omega$$

where σ is the limit of a scaling factor responsible for the derivation of the different equations on the macroscale. In both equations the permeability tensor $\boldsymbol{K}$ or $\boldsymbol{M}$ is the only property in which information about the complicated microscopic textile geometry is still kept as a measure of its ability to transmit fluids. Both tensors are defined by the solution of a different set of unit cell problems in homogenisation theory.

Two different situations have to be considered on the textile mesoscale. On the one hand, the textile yarns can be approximated as impermeable. Then, the homogenisation of the Stokes equations yields Darcy's law [4]. On the other hand, if the yarns are permeable, the fabric consists of both fluid parts as well as of the porous fibre bundles. In this case, the Stokes equations in the fluid domain Ω_f have to be coupled with Darcy's Law or Brinkman's equation in the porous part Ω_p with appropriate interface conditions between the porous and fluid medium. In order to explicitly avoid complicated interface conditions, we employ the so-called Stokes/Brinkman equations

$$-\tilde{\mu}\Delta\boldsymbol{u} + \nabla p + \mu\boldsymbol{K}^{-1}\boldsymbol{u} = \boldsymbol{f} \quad \text{in } \Omega$$

(3)

$$\nabla \cdot \boldsymbol{u} = 0 \quad \text{in } \Omega$$

with

$$(4) \qquad \boldsymbol{K} = \begin{cases} \boldsymbol{K}_f \to \infty & \text{in } \Omega_f \\ \boldsymbol{K}_p & \text{in } \Omega_p \end{cases}$$

in the whole domain $\Omega = \Omega_f \cup \Lambda \cup \Omega_p$. Here, $\tilde{\mu}$ denotes an effective viscosity. In these equations the permeability tensor $\boldsymbol{K}$ takes its specific value in the porous part and goes to infinity in the fluid domain as a penalization of the Stokes equations [1].

The contribution of this talk is as follows. First, we discuss the application of homogenisation theory in textile geometries (since most works consider disconnected grains as porous media only). Second, for a simple test geometry, we numerically solve the unit cell problems and the Stokes/Brinkman equations in three dimensions and compare the results to a direct numerical simulation of the Stokes equations on the microscale. Third, we present the prediction of textile permeability and validate our numerical permeability results against experimental data. Here, the presented method is successfully applied to several classes of industrial textile reinforcements.

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Multiscale Modeling and Simulation of Fluid Flows in Deformable Porous Media

PETER POPOV

(joint work with Yalchin Efendiev, Yulia Gorb and Oleg Iliev)

In this work we consider a Multiscale Finite Element framework for modelling flows in highly deformable porous media. The physical processes under consideration spans two length-scales. On the macroscopic level, one has fluid, diffusing through a nonlinear porous solid. At the microscale the solid has a complex pore geometry and interacts with a Stokes flow. We assume good scale separation, with the usual small parameter ε being the ratio of the fine to the coarse length

scales. We denote the fine scale domain by Ω_ε^0, which contains two subdomains - a fluid part $\mathcal{F}_\varepsilon^0$ and solid part $\mathcal{S}_\varepsilon^0$. The superscript 0 indicates the reference, or undeformed configuration of the body. The interface between the solid and fluid domains is denoted by $\Gamma_\varepsilon^0 = \partial\mathcal{F}_\varepsilon^0 \cap \partial\mathcal{S}_\varepsilon^0$. The physics is described by the strongly coupled, stationary fluid structure interaction problem [3]: *Find the interface Γ_ε, velocity $\mathbf{v}$, pressure p and displacements $\mathbf{u}$ such that:*

$$(1) \qquad \Gamma_\varepsilon = \left\{ \mathbf{X} + \mathbf{u}_\varepsilon(\mathbf{X}) | \ \forall \ \mathbf{X} \in \Gamma^0 \right\},$$

the Stokes and Elasticity equations are satisfied:

$$(2) \qquad -\nabla p_\varepsilon + \mu\Delta\mathbf{v}_\varepsilon + \mathbf{f} = 0, \qquad \nabla \cdot \mathbf{v}_\varepsilon = 0 \qquad in \ \mathcal{F}_\varepsilon$$

$$(3) \qquad -\nabla \cdot \mathbf{S}_\varepsilon(\mathbf{E}) = \mathbf{f} \qquad in \ \mathcal{S}_\varepsilon^0$$

with the interface condition

$$(4) \quad \det(\nabla\mathbf{u}_\varepsilon + \mathbf{I})(-p\mathbf{I} + 2\mu\mathbf{D}(\mathbf{x}(\mathbf{X}))) \left(\nabla\mathbf{u}_\varepsilon + \mathbf{I}\right)^{-T} \mathbf{n}_0 = \mathbf{S}_\varepsilon(\mathbf{E})\mathbf{n}_0 \qquad on \ \Gamma^0.$$

Here $\mathbf{X}$ is the material coordinate, μ is the fluid viscosity, $\mathbf{f}$ is the body force. Further, $\mathbf{S}$ is the Piola-Kirchhoff stress tensor in the solid, which may depend linearly or nonlinearly on the strain $\mathbf{E}(\mathbf{u}) = \frac{1}{2}\left(\nabla\mathbf{u}(\mathbf{X}) + \nabla\mathbf{u}(\mathbf{X})^T\right)$, $\mathbf{D}(\mathbf{v}) = \frac{1}{2}\left(\nabla\mathbf{v}(\mathbf{x}) + \nabla\mathbf{v}(\mathbf{x})^T\right)$ is the stretching tensor, and $\mathbf{n}_0$ is the normal to the interface in the reference configuration. The interface condition (4) introduces a nonlinearity in the problem, regardless of the constitutive form for $\mathbf{S}$.

Multilevel Algorithm. The difficulty in upscaling this problem arises when the $\mathcal{F}$ deforms substantially at the fine-scale, breaking the assumptions underlying classic homogenized models such as Darcy and Biot [1, 5, 4, 2]. To avoid this we use a standard asymptotic expansion [6] of the Stokes equation 2 in the *deformed* configuration for the velocity and pressure, which is not known apriori:

$$\mathbf{v}_\varepsilon(\mathbf{x}) = \varepsilon^2\mathbf{v}_0(\mathbf{x},\mathbf{y}) + \varepsilon^3\mathbf{v}_1(\mathbf{x},\mathbf{y}) + ..., \quad p_\varepsilon(\mathbf{x}) = p_0(\mathbf{x}) + \varepsilon p_1(\mathbf{x},\mathbf{y}) + ... \quad \mathbf{y} \in Y_\mathcal{F}.$$

Then, one is able to recast the FSI problem (1)-(4) as a cell problem in a Representative Element of Volume (REV), which connects the fine-scale quantities to the coarse level pressure p_0, displacement $\mathbf{u}_0$, and their gradients. Moreover, one can also justify a general second-order elliptic equations for the averaged flow and elasticity at the macroscale, which naturally linearized as:

$$(5) \qquad \nabla \cdot (\mathbf{K}^n(\mathbf{x})\nabla p_0^{n+1}) = \mathbf{f} \qquad \nabla \cdot (\mathcal{L}^n(\mathbf{x})\nabla\mathbf{u}_0^{n+1}) = \mathbf{g}.$$

One can then consider a general two-scale algorithm with a macroscopic discretization much coarser than fine-scale, that is $h >> \varepsilon$. After initializing the macroscopic variables p_0 and $\mathbf{u}_0$ one then iterates as follows:

(1) Given $p_0^{(n)}$, $\mathbf{u}_0^{(n)}$ solve for $\tilde{\mathbf{v}}_0^{(n)}$, $\tilde{p}_1^{(n)}$ and $\tilde{\Gamma}_\varepsilon^{(n)}$ which satisfy the corresponding cell problems in a REV at a particular macroscopic location.

(2) Freeze the fine-scale boundary $\tilde{\Gamma}_Y^{(n)}$ of the deformed REV at that location and find the corresponding permeability $\mathbf{K}^{(n)}$ and elasticity tensor $\mathcal{L}^{(n)}$.

(3) Using Eqn. (5) find new coarse pressure $p_0^{(n+1)}$ and displacement $\mathbf{u}_0^{(n+1)}$.

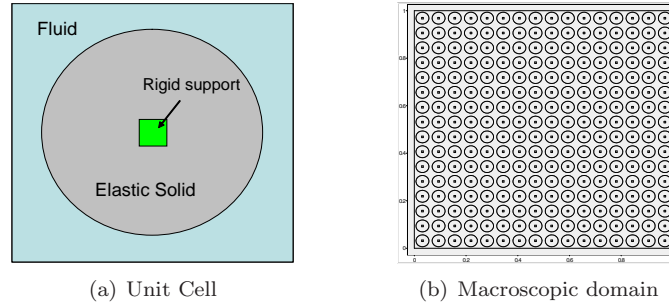(a) Unit Cell   (b) Macroscopic domain

FIGURE 1. Unit cell (a) and macroscopic domain (b) used in computations.

The key to this algorithm is the ability to solve the fine-scale FSI problem numerically (step 1). The numerical algorithm for that has been presented elsewhere [3]. It is based on successive solutions to fluid and solid subproblems: one starts with a guess for the fluid domain, solves the stokes equation there, and computes the fluid stress on the interface. This stress is then used to solve an elasticity problem, whose solution is then used to deform the fluid domain. The process is repeated until convergence. Given this scheme, one can further consider a variant of the above two-level algorithm, where in step 1, the FSI cell problem is not solved exactly, but only a few iterations are done, the extreme case being a single one.

Numerical Examples Several numerical examples were considered in order to test the proposed algorithms. The basic fine-scale domain is a 2D periodic arrangement of elastic obstacles (Figure 1). The unit cell (Figure 1(a)) consists of circular linear elastic material, surrounded by the fluid. The elastic media is supported rigidly in the center. The unit cell is arranged periodically to form the macroscopic domain. A series of macroscopic domains with $\varepsilon^{-1} = 4, 8, 16, 32$ were considered. Shown in Figure 1(b) is the fine-scale domain with $\varepsilon^{-1} = 16$.

First, we demonstrated numerically the convergence of the nonlinear iterative processes involved in our two-level algorithm. This was done by considering a set of boundary value problems (BVPs) in which a uniform pressure P_l is applies at the left side of the macroscopic domain. The pressure at the right side is 0 and no-flow boundary conditions are considered at the top and bottom sides of the domain. The two-level algorithms took 6 iterations to converge for $P_l = 0.1$ and 8 with $P_l = 0.2$, uniformly with respect to ε or the macroscopic mesh size h. Also, it proved insensitive to the number of iterations performed on the cell FSI problem in step 1, including the extreme case of a single one. Secondly, thanks to the simple geometry and boundary conditions, it was possible to obtain fine-scale solutions for the same set of BVPs via a direct numerical simulation (DNS). This allowed to demonstrate convergence with respect to ε of the fine-scale approximations obtained via our two-scale algorithm and the DNS results (Table 1).

A number of more complicated two-dimensional flows were also computed. Shown in Figure 2 is an example of corner point flow. The permeability field (Figure 2(b)) is strongly correlated with the macroscopic pressure. It is highest where

TABLE 1. Error in the fine-scale displacements when compared to DNS results

ϵ	$P_l = 0.1$				
	Iterations	L^∞ Error	L^∞ Rel. Error	L^2 Error	L^2 Rel. Error
1/4	6	1.23×10^{-3}	0.18	2.48×10^{-4}	0.23
1/8	6	3.18×10^{-4}	0.10	4.39×10^{-5}	0.13
1/16	6	8.07×10^{-5}	0.053	7.75×10^{-6}	0.069
1/32	6	2.03×10^{-5}	0.027	1.37×10^{-6}	0.0351
	$P_l = 0.2$				
	Iterations	L^∞ Error	L^∞ Rel. Error	L^2 Error	L^2 Rel. Error
1/4	8	2.96×10^{-3}	0.22	4.93×10^{-4}	0.22
1/8	8	7.94×10^{-4}	0.126	8.78×10^{-5}	0.127
1/16	8	2.06×10^{-4}	0.068	1.56×10^{-5}	0.067
1/32	8	5.25×10^{-5}	0.035	2.75×10^{-6}	0.034

(a) BCs and discretization   (b) K_{11} (c) Macroscopic pressure p_0
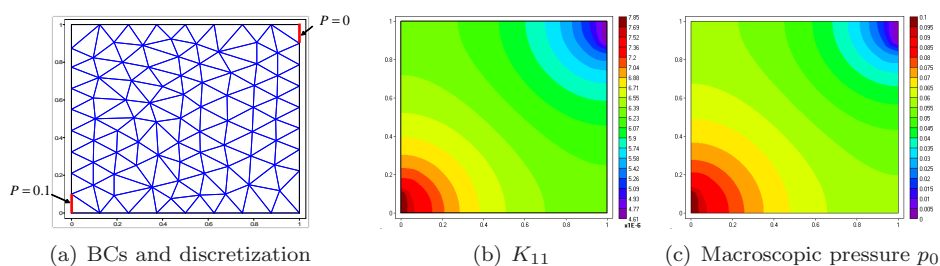
FIGURE 2. This 2D flow is driven by pressure specified at the bottom left and top right corners of the domain

the pressure is highest (lower left-corner) and lowest, where the pressure is lowest (upper-left corner). This example demonstrates that the proposed algorithms can be used for non-trivial problems and the resulting solutions are physically reasonable.

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Domain Decomposition and Upscaling

ROBERT SCHEICHL

(joint work with Ivan Graham, Clemens Pechstein, Eero Vainikko, Jan Van lent)

In this talk we discuss the use of domain decomposition parallel iterative solvers for highly heterogeneous problems of flow in porous media, in both the deterministic and (Monte-Carlo simulated) stochastic cases. We are particularly interested in the case of highly unstructured coefficient variation where standard periodic or stochastic homogenisation theory is not applicable, and where there is no a priori scale separation. We will restrict attention to the important model elliptic problem

$$(1) \qquad\qquad -\nabla \cdot (K\nabla u) \;=\; f \;,$$

in a bounded polygonal or polyhedral domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, with suitable boundary data on the boundary $\partial\Omega$. The $d \times d$ coefficient tensor $K(x)$ is assumed symmetric positive definite, but may vary over many orders of magnitude in an unstructured way on Ω. Many examples arise in groundwater flow and oil reservoir modelling, e.g. in the context of the SPE10 benchmark or in Monte Carlo simulations of stochastic models for strong heteoregeneities (see Figure 1).
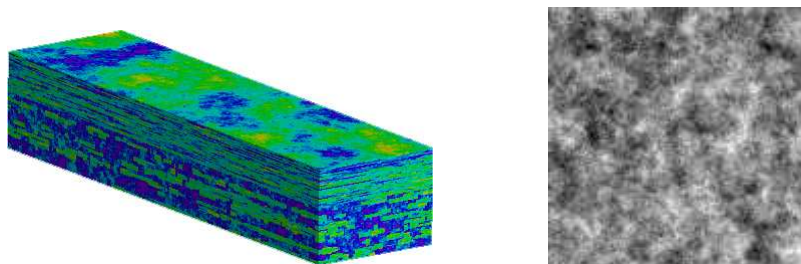
FIGURE 1.   Typical coefficients: Society of Petroleum Engineer benchmark SPE10 (left); lognormal random field (right).

Let $\mathcal{T}^h$ be a conforming shape-regular simplicial mesh on Ω. The finite element discretisation of (1) in the space $\mathcal{V}^h$ of continuous piecewise linear finite elements on $\mathcal{T}^h$ yields a linear system

$$(2) \qquad\qquad A\mathbf{u} = \mathbf{f} \;.$$

It is well-known that the size of this system grows like $\mathcal{O}(h^{-d})$, as $\mathcal{T}^h$ is refined, and that the condition number $\kappa(A)$ of A worsens like $\mathcal{O}(h^{-2})$. Moreover the conditioning of A also depends on the heterogeneity (characterised by the range and the variability of K) and on the anisotropy (characterised by the maximum ratio of the largest to the smallest eigenvalue of $K(x)$ at any point $x \in \Omega$). It is of interest to find solvers for (2) which are robust to changes in the mesh width h as well as to heterogeneity and anisotropy in K. For the remainder we assume that K is only "mildly" anisotropic, i.e. that the ratio of the largest to the smallest

eigenvalue of $K(x)$ is uniformly bounded from above by a benign constant of $\mathcal{O}(1)$, and concentrate on spatial heterogeneity in the coefficient tensor K.

When the smallest scale ε, at which the coefficient tensor $K(x)$ varies, is very small it may not be feasible to solve (1) on a mesh of size $h = \mathcal{O}(\varepsilon)$ with standard solvers, and it may be necessary to scale up the equation to a coarser computational grid of size $H \gg \varepsilon$. A large number of computational methods have been suggested over the years in the engineering literature on how to derive such an upscaled equation numerically (see e.g. the review [13]). More recently this area has also started to attract the attention of numerical analysts, who have started to analyse the approximation properties of such upscaling or multiscale techniques theoretically. Among the methods that have been suggested and analysed are the Variational Multiscale Method [6], the Multiscale Finite Element Method [5], and the Multiscale Finite Volume Method [7]. However, the existing theory is restricted to periodic fine scale variation or to ergodic random variation. No theory is yet available that gives a comprehensive analysis of the dependency of the accuracy of the upscaled solution on the coefficient variation in the general case.

Moreover, if the coefficient varies arbitrarily throughout Ω and there is no scale separation into a fine $\mathcal{O}(\varepsilon)$–scale variation and a coarse $\mathcal{O}(H)$–scale variation, then all these methods require the solution of $\mathcal{O}(H^{-d})$ local "cell" problems, each of size $\mathcal{O}((H/\varepsilon)^d)$. Thus, even if we assume that the local problems can be solved with optimal (linear) complexity, the total computational cost of the method is $\mathcal{O}(\varepsilon^{-d})$. In practice the complexity may actually be worse. A huge advantage is of course the fact that the cell problems are all completely independent from each other. This means that they can be solved very efficiently on a modern multiprocessor machine. This makes this method so attractive to scale up a physical problem, especially if the upscaled matrix can be used for several right hand sides, within a two-phase flow simulation, or for several time steps in a time-dependent simulation.

A viable alternative is the use of parallel multilevel iterative solvers, such as multigrid or domain decomposition, for the original fine scale problem (2) on the "subgrid" $\mathcal{T}^h$ where $h = \mathcal{O}(\varepsilon)$. These are known to lead to a similar overall computational complexity $\mathcal{O}(\varepsilon^{-d})$ and, especially in the case of domain decomposition, are designed to scale optimally on modern multiprocessor machines. That is, at (asymptotically) the same cost as using any of the above upscaling procedures, we can obtain the fine-scale solution with guaranteed and quantifiable approximation properties. However, previously no theory was available that guarantees the robustness of these multilevel iterative solvers to heterogeneities in the coefficients, and indeed most of these methods are not robust in their unmodified form with the number of iterations growing steeply as the heterogeneity worsens. The most successful, completely robust method for (2) is algebraic multigrid (AMG), originally introduced in [2]. Many different versions of AMG have emerged since, but unfortunately no theory exists that proves the (observed) robustness of any of these methods to arbitrary spatial variation of $K(x)$. The robustness of geometric multigrid for "layered media" in which discontinuities in K are simple interfaces that can be resolved by the coarsest mesh has recently been proved in [17]. Some

ideas towards a theory for more general coefficients can be found in [1]. Matrix-dependent multigrid coarsening strategies, such as the one in Dendy's BoxMG have also been used in the context of numerical upscaling (e.g. [8, 9, 10]).

The situation is different for domain decomposition methods. There are many papers (with rigorous theory) which solve (2) for "layered media" in which discontinuities in K are simple interfaces resolved by the subdomain partitioning/coarse mesh (see e.g. [15]). However, until recently there was no rigorously justified method for general heterogeneous media. In a series of papers [3, 4, 11, 12, 14, 16] we have started to develop new theoretical tools to analyse domain decomposition methods for (2) (which have inherent robustness with respect to h). This analysis indicates explicitly how subdomains and coarse solves should be designed in order to achieve robustness also with respect to heterogeneities. It does not require periodicity and does not appeal to homogenisation theory. Although the analysis in [11, 12] on nonoverlapping FETI-type methods is also of large current interest, in the talk we will focus on the theory for two-level overlapping Schwarz methods in [3, 4, 14, 16], since it gives a clearer picture of the synergies between domain decomposition and numerical upscaling. In particular, we will highlight the important concept of a certain energy minimising property of the coarse space which has yet got to be fully understood in the context of numerical upscaling.

To give a brief indication of the kind of results presented in [3, 4, 14, 16] let us assume that we have a finite overlapping covering of Ω by (open) subdomains $\{\Omega_i : i = 1, \ldots, s\}$. Let us assume that the diameter of a typical subdomain is of size $\mathcal{O}(H)$ and that the overlap with neighbouring subdomains is (uniformly) of size $\mathcal{O}(H)$ as well. Furthermore, let the family of coverings $\{\Omega_i\}$ be shape regular as $s \to \infty$. In addition let $\{\Phi_j : j = 1, \ldots, N\}$ be a set of functions in $\mathcal{V}^h$ with support of diameter $\mathcal{O}(H)$, such that $\|\Phi_j\|_\infty \lesssim 1$ and $\sum_j \Phi_j(x) = 1$ everywhere, except in a boundary layer of width $\mathcal{O}(H)$ near the boundary of Ω. These functions span a (coarse) subspace of $\mathcal{V}^h$. For simplicity let us assume here that $s = N$ and that $\Omega_i = \mathrm{supp}(\Phi_i)$. Note however that this is not necessary in general to achieve results of the kind presented below. Given $\{\Phi_i\}$ (and its associated supports $\{\Omega_i\}$) an additive two-level overlapping Schwarz preconditioner can be defined as

$$(3) \qquad M \;=\; \sum_{i=0}^{N} R_i A_i^{-1} R_i^T \,,$$

where R_i, for $i = 1, \ldots, N$, denotes the restriction matrix from freedoms in Ω to freedoms in Ω_i. The restriction to the coarse space is defined as $(R_0)_{j,k} = \Phi_j(x_k)$, where x_k, $k = 1, \ldots, n$, are the interior nodes of the fine mesh $\mathcal{T}^h$, and the matrices A_i are defined via the Galerkin product $A_i := R_i A R_i^T$.

We now state one of the main results in [14] (in the simplified case here):

Theorem.
$$\kappa(MA) \lesssim \gamma(K) \quad \text{where} \quad \gamma(K) := H^2 \max_{i=1}^{N} \|\nabla \Phi_i^T K \nabla \Phi_i\|_{L_\infty(\Omega)}$$

is an indicator for the coarse space robustness *and the hidden constant is independent of h, H and K.*

Note that, roughly speaking, $\gamma(K)$ is well-behaved if the functions Φ_i have small gradient wherever K is large. For the classical case, when $K \sim I$ and $\{\Phi_i\}$ is the standard nodal basis for the continuous piecewise linear functions on a coarse simplicial mesh $\mathcal{T}^H$, we have $\gamma(K) = \mathcal{O}(1)$ and we recover the classical theory. When K varies more rapidly, our framework leaves open the possibility of choosing the Φ_i to depend on K in such a way that $\gamma(K)$ is still well-behaved.

In [3, 4, 14, 16] we then study various possible choices for the coarse basis $\{\Phi_i\}$, such as multiscale finite elements or certain AMG coarsening strategies, such as explicit energy minimisation or smoothed aggregation, which all aim to minimise the coarse space robustness indicator and thus the energy of the coarse space. For certain model problems we are able to rigorously bound the coarse space robustness indicator, and numerical experiments confirm the sharpness of our theoretical results.

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Coarse Spaces by Constrained Energy Minimization
Panayot S. Vassilevski

We consider an unified approach of constructing operator-dependent discretization spaces (cf. [1]) on relatively coarse computationally feasible meshes. The approach utilizes natural energy functionals associated with the PDEs of interest. We construct local basis functions by minimizing the underlined functional subject to a set of constraints. The constraints are chosen so that the resulting spaces possess increasingly high order of approximation. We investigate the proposed approach from an upscaling discretization point of view which we illustrate with some preliminary numerical examples.

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A Numerical Subgrid Approach for the Brinkman Problem
Joerg Willems
(joint work with Oleg Iliev and Raytcho Lazarov)

In this talk a numerical subgrid approach for the Brinkman problem is presented. The method follows the strategy discussed by T. Arbogast in [2, 1] for the mixed formulation of Darcy's problem. The discretization used for the Brinkman problem is based on the discontinuous Galerkin discretization for the Stokes problem presented in [4]. The performance of the developed method is tested for two example geometries. The talk is concluded with an outlook aiming at improving the numerical subgrid method by introducing subsequent iterations, which allow the treatment of the approach in the framework of alternating Schwarz methods.

More precisely, the equations under considerations are the following:

$$(1) \qquad \begin{cases} -\nabla \cdot (\widetilde{\mu} \nabla \boldsymbol{u}) + \dfrac{\mu}{K} \boldsymbol{u} + \nabla p &=& \boldsymbol{f} \quad \text{in } \Omega \subset \mathbb{R}^2 \\ \nabla \cdot \boldsymbol{u} &=& 0 \quad \text{in } \Omega \\ \boldsymbol{u} &=& \boldsymbol{0} \quad \text{on } \partial\Omega, \end{cases}$$

where $\boldsymbol{u}$ and p is the velocity and pressure, respectively, $\boldsymbol{f}$ is some forcing term, K is the permeability, and μ and $\widetilde{\mu}$ is the viscosity and effective viscosity, respectively. Typically, the permeability K may vary by several orders of magnitude over the domain Ω. Since the length-scale on which these variations occur is often much smaller than the length-scale on which one wants to obtain (a sufficiently accurate approximation of) $\boldsymbol{u}$ and p one is interested in extracting a reduced or "upscaled" problem corresponding to (1), which preserves the main features of the solution but is less costly to solve. Recently, an approach for upscaling (1) was discussed in [3]. In the procedure in [3] it is, however, assumed that the upscaled equations

of (1) are given by Darcy's problem. This seems reasonable whenever there are no large regions in Ω where K is large, i.e. regions with (almost) free flow. Otherwise, the assumption that the upscaled problem corresponding to (1) is a Darcy problem may not be justified, and a Brinkman to Brinkman upscaling seems to be more reasonable. The latter is the approach discussed in this talk.

The discretization used for the Brinkman problem follows that for the Stokes problem discussed in [4]. There the finite element space $(\mathscr{V}_H, \mathscr{W}_H)$ is chosen such that $(\mathscr{V}_H, \mathscr{W}_H) \subset \big(H_0(div; \Omega), L_0^2(\Omega)\big)$. This means that in general the space may be nonconforming in the sense that $(\mathscr{V}_H, \mathscr{W}_H) \nsubseteq \big(H_0^1(\Omega), L_0^2(\Omega)\big)$. The variational formulation of (1) thus reads

$$(2) \qquad \begin{cases} \boldsymbol{u}_H \boldsymbol{v}_H + b\,(\boldsymbol{v}_H, p_H) &=& F(\boldsymbol{v}_H) \\ b\,(\boldsymbol{u}_H, q_H) &=& 0, \end{cases}$$

with

- $b\,(\boldsymbol{v}_H, p_H) := \displaystyle\int_\Omega p_H \nabla \cdot \boldsymbol{v}_H d\boldsymbol{x}$

- $F(\boldsymbol{v}_H) := \displaystyle\int_\Omega \boldsymbol{f} \cdot \boldsymbol{v}_H d\boldsymbol{x}$

- $a\,(\boldsymbol{u}_H, \boldsymbol{v}_H) := \displaystyle\sum_{T \in \mathcal{T}_H} \int_T \widetilde{\mu} \nabla \boldsymbol{u}_H : \nabla \boldsymbol{v}_H + \frac{\mu}{K} \boldsymbol{u}_H \cdot \boldsymbol{v}_H d\boldsymbol{x} - \sum_{e \in \mathcal{E}_H} \int_e \bigg(\{\!\!\{\boldsymbol{u}_H\}\!\!\} \, [\![\boldsymbol{v}_H]\!] +$

  $\{\!\!\{\boldsymbol{v}_H\}\!\!\} \, [\![\boldsymbol{u}_H]\!] - \dfrac{\alpha}{|e|} \, [\![\boldsymbol{u}_H]\!] \, [\![\boldsymbol{v}_H]\!] \bigg) ds,$

where

- $\{\!\!\{\boldsymbol{v}\}\!\!\}|_e := \frac{1}{2} \left(\boldsymbol{n}_e^+ \cdot \nabla(\boldsymbol{v} \cdot \boldsymbol{\tau}_e^+)|_{e^+} + \boldsymbol{n}_e^- \cdot \nabla(\boldsymbol{v} \cdot \boldsymbol{\tau}_e^-)|_{e^-} \right)$ and
- $[\![\boldsymbol{v}]\!]|_e := \boldsymbol{v}|_{e^+} \cdot \boldsymbol{\tau}_e^+ + \boldsymbol{v}|_{e^-} \cdot \boldsymbol{\tau}_e^-.$

Here, $\mathcal{T}_H$ is a triangulation and $\mathcal{E}_H$ is the set of all corresponding edges. For an edge $e \in \mathcal{E}_H$ shared by two elements T^+ and T^- $\boldsymbol{n}_e^+$ and $\boldsymbol{n}_e^-$ are the corresponding unit outer normal vectors on e. The tangential vectors forming right-hand coordinate systems with $\boldsymbol{n}_e^+$ and $\boldsymbol{n}_e^-$ are denoted by $\boldsymbol{\tau}_e^+$ and $\boldsymbol{\tau}_e^-$. α is a penalty parameter, which needs to be chosen sufficiently large to ensure the coercivity of $a\,(\cdot, \cdot)$.

To formulate the subgrid approach a fine triangulation $\mathcal{T}_h$ which is obtained by further refining $\mathcal{T}_H$ is considered. Furthermore, a finite element space $(\mathscr{V}_{H,h}, \mathscr{W}_{H,h}) = (\mathscr{V}_h \oplus \mathscr{V}_H, \mathscr{W}_h \oplus \mathscr{W}_H) \subset (L_0^2, H_0(div))$ satisfying

(1) $\nabla \cdot \mathscr{V}_h = \mathscr{W}_h$ and $\nabla \cdot \mathscr{V}_H = \mathscr{W}_H$
(2) $\boldsymbol{v}_h \cdot \boldsymbol{n} = 0$ on ∂T, $\forall \boldsymbol{v}_h \in \mathscr{V}_h$ and $\partial T \in \mathcal{T}_H$
(3) $\mathscr{W}_H \perp \mathscr{W}_h$

is considered. Note that choosing $(\mathscr{V}_H, \mathscr{W}_H)$ Brezzi-Douglas-Marini elements of order 1 (BDM1) corresponding to $\mathcal{T}_H$ and choosing $(\mathscr{V}_h, \mathscr{W}_h)$ the union of BDM1 elements with respect to $\mathcal{T}_h$ restricted to each coarse cell $T \in \mathcal{T}_H$ with homogeneous boundary conditions at ∂T satisfies 1.-3.

Considering the variational formulation (2) with respect to the space $(\mathscr{V}_{H,h}, \mathscr{W}_{H,h})$ and utilizing the unique decomposition of elements in $(\mathscr{V}_{H,h}, \mathscr{W}_{H,h})$ into elements of $(\mathscr{V}_H, \mathscr{W}_H)$ and $(\mathscr{V}_h, \mathscr{W}_h)$ one may follow the derivations in [2] to

obtain the symmetric upscaled system

$$\begin{cases} a\left(\boldsymbol{u}_H + \delta_{\boldsymbol{u}}(\boldsymbol{u}_H), \boldsymbol{v}_H + \delta_{\boldsymbol{u}}(\boldsymbol{v}_H)\right) + b\left(\boldsymbol{v}_H, p_H\right) &= F(\boldsymbol{v}_H) - a\left(\overline{\delta}_{\boldsymbol{u}}, \boldsymbol{v}_H\right), \\ b\left(\boldsymbol{u}_H, q_H\right) &= 0, \end{cases}$$

where the local responses $\delta_{\boldsymbol{u}}(\cdot)$ and $\overline{\delta}_{\boldsymbol{u}}$ are defined by

$$\begin{cases} \begin{cases} a\left(\boldsymbol{u}_H + \delta_{\boldsymbol{u}}(\boldsymbol{u}_H), \boldsymbol{v}_h\right) + b\left(\boldsymbol{v}_h, \delta_p(\boldsymbol{u}_H)\right) &= 0 \quad \forall \boldsymbol{v}_h \in \mathscr{V}_h \\ b\left(\delta_{\boldsymbol{u}}(\boldsymbol{u}_H), q_h\right) &= 0 \quad \forall q_h \in \mathscr{W}_h \end{cases} \\ \begin{cases} a\left(\overline{\delta}_{\boldsymbol{u}}, \boldsymbol{v}_h\right) + b\left(\boldsymbol{v}_h, \overline{\delta}_p\right) &= F(\boldsymbol{v}_h) \quad \forall \boldsymbol{v}_h \in \mathscr{V}_h \\ b\left(\overline{\delta}_{\boldsymbol{u}}, q_h\right) &= 0 \quad\quad \forall q_h \in \mathscr{W}_h. \end{cases} \end{cases}$$

The subgrid algorithm can then be formulated as follows:

- Solve for the fine responses $(\overline{\delta}_{\boldsymbol{u}}, \overline{\delta}_p)$ and $(\delta_{\boldsymbol{u}}(\boldsymbol{\varphi}_H), \delta_p(\boldsymbol{\varphi}_H))$ for coarse basis functions $\boldsymbol{\varphi}_H$ and each coarse cell.
- Solve upscaled equation for $(\boldsymbol{u}_H, p_H)$.
- Piece together the solution $(\boldsymbol{u}_{H,h}, p_{H,h}) = (\boldsymbol{u}_H, p_H) + (\delta_{\boldsymbol{u}}(\boldsymbol{u}_H), \delta_p(\boldsymbol{u}_H)) + (\overline{\delta}_{\boldsymbol{u}}, \overline{\delta}_p)$.

The error of the presented algorithm compared to a full fine solve comes from the fact that information across coarse cell boundaries can only be communicated by functions in $(\mathscr{V}_H, \mathscr{W}_H)$. This can also be seen in the presented numerical results, which exemplify that the error is caused by an insufficient resolution of solution features across coarse cell boundaries.

The talk is concluded with a proposal for extending the algorithm aimed at mitigating the deficiency just described. It is proposed to solve local problems in "tube" regions around coarse edges with right hand side F and boundary conditions from the previously computed solution. Thus, fine scale solutions are obtained for all edges, which can then be used as boundary data for the recomputation of $(\overline{\delta}_{\boldsymbol{u}}, \overline{\delta}_p)$. This procedure may now be iterated until fine scale features across coarse cell boundaries are resolved sufficiently well. Note, that the responses of the basis functions $(\delta_{\boldsymbol{u}}(\boldsymbol{\varphi}_H), \delta_p(\boldsymbol{\varphi}_H))$ do not have to be recomputed. It is also important to note that this iterative process is actually an alternating Schwarz method. Unfortunately, at the time of the talk there were no numerical results available for this extended algorithm, which is a topic of further research.

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Reservoir Modeling Using Adaptive Gridding with Global Scale-up

Xiao-Hui Wu

An accurate and efficient reservoir modeling process is essential for developing and producing hydrocarbon reserves, especially from unconventional resources. In this talk, we address some of the main challenges associated with modeling complex reservoir geometry and heterogeneous reservoir properties. We present recently developed techniques for generating adaptive, constrained, 2.5D Voronoi grid and for generic global flow-based scale-up. We demonstrate that the combination of the two techniques is effective in constructing accurate coarse reservoir models.

A key challenge in reservoir modeling is accurate representation of the reservoir geometry of both the structural framework (i.e., horizons/major depositional surfaces that are nearly horizontal and fault surfaces that can have arbitrary spatial size and orientation) and the detailed stratigraphic layering. For typical reservoir geometries with a high aspect ratio of horizontal to vertical dimensions, 2.5D (prismatic) Voronoi grids, constructed by projection or extrusion of a 2D Voronoi grid in vertical or nearly vertical direction, are a natural choice for reservoir simulations. Our main contribution is in generating the 2D constrained Voronoi grid using a new constrained Delaunay triangulation algorithm and a rigorous procedure of constructing a Voronoi grid that conforms to piecewise linear constraints. More specifically, we construct protection areas around the linear constraints i.e., intersecting polylines, using intersecting circles along the polylines and concentric circles around the intersections. The protection areas are then defined by linking the intersections between the circles and additional points distributed on the circles into polygons. Inside the protection areas, unique Voronoi tessellations match the linear constraints and their intersections exactly; outside the protection areas, the constrained Voronoi gridding problem is converted into a constrained Delaunay triangulation problem, which is solved by using our new algorithm that enables adaptivity of the Voronoi grid to specified density functions. Therefore, we can generate adaptive Voronoi grids that honor both the faulted structural frameworks and important reservoir heterogeneities.

In addition to advanced grid generation, we also need an accurate scale-up of reservoir properties (such as permeability) to the coarse grid. To address this challenge, we developed a global scale-up method based on generic flow solutions (i.e., flows calculated from generic boundary conditions) [1]. Numerical examples are provided to demonstrate the advantages, both in efficiency and accuracy, of combining adaptive gridding with the global scale-up method in building accurate coarse reservoir models.

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Energy Minimizing Bases for Efficient Multiscale Modeling and Linear Solvers

LUDMIL TOMOV ZIKATANOV

(joint work with James J. Brannick, Jinchao Xu, Olivier Dubois, Ilya D. Mishev)

This work is on some of the techniques used in algebraic multigrid methods (AMG) to construct coarse scale models. We will focus on the choice of coarse spaces and their approximation properties, as well as relation to compatible relaxation technique and construction of piece-wise harmonic bases via energy minimization. Such idea was probably first introduced in [1, 2]. Proof that energy minimizing basis is piece-wise a-harmonic as well as optimal algorithms how to construct this basis is in [3, 4]. Most of the work that we present here is done in collaboration with Rob Falgout and Panayot S. Vassilevski (LLNL) and also Rob Scheichl, I. Graham (University of Bath).

The works on AMG methods date from about 30 years ago. Probably the first paper on AMG is by Brandt, McCormick, and Ruge [5]. An important early work is also by Ruge and Stüben [6]. Since then much progress has been made both in algorithmic development and in two-grid theoretical analysis. For recent results and comprehensive review of many AMG methods, we refer to Vassilevski [7]. In general the techniques that we use here in both two level [8, 9, 10] and multilevel analysis are via the method of subspace corrections [11, 12]. Related to the considerations here, and more sophisticated are the adaptive approaches for constructing coarse spaces via or adaptive smoothed aggregation and AMG [13, 14, 15], and Bootstrap AMG (A. Brandt, 2000).

Model problem and approximation from coarser space. Consider for example a positive definite problem in a weak form on a Lipschitz domain Ω in 2 or 3 spatial dimensions: Find $u \in V$ ($V = H_0^1(\Omega)$ or $V = H^1(\Omega)$) such that

$$a(u,v) := \int_\Omega a\nabla u\nabla v = \int_\Omega fv =: f(v), \quad \text{for all} \quad v \in V.$$

Set $\|u\|_a^2 := a(u,u)$. An interesting problem then is (in upscaling, as well as discretizations of PDE): Given an integer number n_H, find "coarse space" $V_H \subset V$ and such that: $\sup_{u \in V} \frac{1}{\|u\|_a^2} \inf_{v \in V_H} \|u - v\|_{L_2}^2$ is at minimum (with respect to the space V_H). Oftentimes, the solution to such problem is the space of the eigenfunctions corresponding to the lowest n_H eigenvalues (whenever the inverse of our differential operator is compact). Hence we should approximate this space (lowest eigenmodes). Of course, it could be computationally rather expensive to find basis in and the space exactly, because such basis will in general be globally supported. One can also observe that the basis in the "best" V_H solves also the minimization problem:

$$(1) \qquad \sum_{i=1}^{n_H} \|\phi_i\|_a^2, \quad \to \min, \quad \sum_{i=1}^{n_H} \phi_i = \boldsymbol{e}.$$

Here, if $V = H^1$ one may take $e = 1$. In all cases e should be a smooth function (say the eigenmode corresponding to the minimal eigenvalue of $a(.,.)$). Thus, the goal is to construct minimize the same functional, by imposing constraint on the supports of the basis.

Discretizations. Suppose that $V = \text{span}\{\phi_i\}_{i=1}^n$ is a finite element (FE) space. The bilinear form then defines a bounded linear operator on V, by: $(Au, v) := a(u, v)$ for all u and all v in V. Here we assume that V corresponding to the finest scale, the scale on which a continuous linear FE discretization resolves all the oscillations in $a(x)$. Then the we seek V_H by constructing a basis in it, whose elements are linear combinations of $\{\phi_i\}_{i=1}^n$. The coefficients in this linear combinations give a matrix (a.k.a. prolongation/interpolation matrix P). Thus, constructing coarse space and an upscaled (or equivalently a coarse scale) problem then involves two "generic" steps: (1) Selection of coarse "grid" degrees of freedom (a set of coarse variables C); (2) **Sparse** interpolation operator $P : \mathbb{R}^{n_H} \mapsto V$. The first step, in the simplest case considered here corresponds to picking a set of coarse variables (C-variables), e.g., indices $C = \{i_1, \ldots, i_{n_H}\}$. The remaining indices are called F-variables. Define $V_H = \text{span}\{\psi_k\}_{k=1}^{n_H}$, such that each ψ_k is supported in Ω_k (for a vector: $\Omega_k \subset \{1, \ldots, n\}$) and each ψ_k has the form: $\psi_k = 1 \cdot \phi_{i_k} + \text{tail}$, where *tail* is also supported in Ω_k. The coefficients in the above representation form the columns of $P : \mathbb{R}^{n_H} \mapsto V$ and P looks like $P = \begin{bmatrix} W \\ I \end{bmatrix}$, if we first order the so-called F-variables and then the C-variables.

Two level methods and their convergence. A two level subspace correction method is as follows: Given initial approximation to u (say u_0): (i) Find $u_H \in V_H$ such that: $a(e_H, w) = f(w) - a(u_0, w), \quad \forall w \in V_H$; (ii) Set $v_0 = u_0 + e_H$; (iii) Fine grid smoothing: Find $e_h \in V$ (V is the "fine" scale), $a_2(e_h, w) = f(w) - a(v_0, w), \quad \forall w \in V$; (iv) Set then $u_1 = v_0 + e_h$. This is one iteration of a two level method. One may continue such iterations until convergence. The bilinear form $a_2(.,.)$ is an approximation to $a(.,.)$, and do not need to be good at that. In all cases $a_2(.,.)$ defines an operator M which is called smoother. The convergence rate of such two level method then is $\|\mathcal{E}_{TG}\|_A^2 = 1 - 1/K$, where $K = \sup_v \frac{\|(I - \pi_{\bar{M}})v\|_{\bar{M}}^2}{\|(I - \pi_A)v\|_A^2}$. Suppose that we would like now to pick a coarse space $V_H \subset V$ of a fixed dimension n_H that minimizes K, or an upper bound of it. For example an explicit formula for the solution of minimizer of $\mu(P) = \sup_v \frac{\|(I - \Pi)v\|_{\bar{M}}^2}{\|(I - \pi_A)v\|_A^2}$ which is such an upper bound is known. The quantity $\mu(P)$ is known as *measure of the quality of the coarse space*. The solution (optimal P) is the so called "ideal" interpolation $P_\star$, that minimizes the trace of the operator A (same solution as given by the lowest eigenmodes earlier), when restricted to V_H. If we split A in 2×2 blocks corresponding to splitting the variables in C-coarse and F-fine, then the upper block in the definition of $P_\star$ is $W_\star = -A_{FF}^{-1} A_{FC}$. It can be shown that such choice of P results in an optimal two level algorithm, for which the so called "weak approximation property holds". That is fine, but this is not practical as well, because A_{FF}^{-1} is usually a dense matrix. We aim to approximate $P_\star$ with a sparse P, and as it turns out,

the P whose columns minimize the energy (the trace of the coarse grid operator) is the best approximation to P_* in a suitable norm. It is well known that the i-th column of the solution to the minimization problem given at the beginning (with restrictions on the sparsity) is: $[P]_i = I_i A_i^{-1} I_i^t M_a \boldsymbol{e}$, where $M_a^{-1} = \sum_{i=1}^{n_H} I_i A_i^{-1} I_i^t$. Here $I_i \in \mathbb{R}^{n \times n_i}$ and $(I_i)_{kl} = \delta_{kl}$ if both k and l are in Ω_i and zero otherwise, and $A_i = I_i^t A I_i$. We have the following theorem:

Theorem. Let P be the unique solution of the minimization problem (1). Then $\|P_\star - P\|_A = \min_Q \|P_\star - Q\|_A$, where the minimum is taken over all matrices Q that have the same prescribed sparsity as P, and $\|X\| := \mathrm{trace}(X^T A X)$.

The choice of sparsity pattern of P and is done via examining the *strength-of-connections* in A (connectivity in the weighted graph defined by A). We construct the supports Ω_i in the following way: we fix the cardinality of each Ω_i to be n_i (i.e. the number of non-zeros per column of P). Then, starting with initial guess $W_0 = 0 \in \mathbb{R}^{n_s \times n_H}$, we iterate towards the solution of $A_{FF} W = A_{FC}$ by computing the polynomial of degree $\leq \ell$, which is the best approximation to $1/x$ on an interval defined by estimates on the extreme eigenvalues of A_{FF}. Such polynomial $p_\ell(A_{FF})$ is easy to construct if bounds on the spectrum of A_{FF} are known and is obtained via:

$$
\begin{aligned}
p_0(A) &= \frac{\eta(1+\delta)}{(1-\delta)^2} I, \quad p_1(A) = -\left(\frac{\eta}{1-\delta}\right)^2 A + \frac{2\eta}{(1-\delta)^2} I, \\
p_{k+1}(A) &= [(1+\delta)I - \eta A] p_k(A) - \delta p_{k-1}(A) + \eta I.
\end{aligned}
$$

It approximates A_{FF}^{-1} quite well, if A_{FF} is *well-conditioned*. The parameters δ and η depend on the estimates of the extreme eigenvalues of A_{FF}. We note here that this we only use to define the sparsity of P and not the actual entries, which are defined via energy minimization procedure. This also tells us that we need to choose the coarse grid variables in a way that A_{FF} is well-conditioned. This in turn can be done via compatible relaxation [16, 17]. The following rationale can be applied then when constructing algorithms for upscaling or AMG methods: (1) Pick C-variables via compatible relaxation so that A_{FF} is well conditioned; (2) Construct the supports of coarse grid basis functions using approximate strength of connections by polynomial approximation to A_{FF}^{-1}; and (3) Define the basis and coarse scale model via energy (trace) minimization.

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