Mathematisches Forschungsinstitut Oberwolfach

Report No. 20/2005

Mini-Workshop: Numerical Upscaling: Theory and Applications

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May 1st – May 7th, 2005

Abstract. Numerical upscaling is often the only way in which various multiscale problems can be handled. Numerics related to solving auxiliary problems appearing in asymptotic homogenization, as well as numerical treatment of multiscale problems with non-separable scales, are discussed here. Among the main topics discussed, are classification of multiscale problems and multiscale numerical algorithms; deriving coarse scale approximations via approximate truncations or based on variational principles; iterations over scales; accuracy and robustness of numerical upscaling algorithms; similarity and differences between different approaches (multigrid, multiscale FEM, heterogeneous multiscale method, etc.); convergence issues; area of applicability of the numerical upscaling, etc.

Mathematics Subject Classification (2000): 39-xx, 60-xx, 62-xx, 65-xx, 70-xx, 76-xx, 80-xx.

Introduction by the Organisers

This Mini-Workshop was attended by sixteen participants from five countries, representing different scientific schools and generations. Fifteen presentations (each accompanied with intensive discussions), two common round table discussions, and an uncountable number of discussions in couples, triples, etc. - the week flew as an instant. Mixing different generations - leading scientists working from years in the field, and ones who just finished PhD and came full with promising ideas and enthusiasm - provided a basis for versatile discussion of each question, for generating new ideas and for immediate attempts to apply these idea for solving the problems discussed. Blackboard discussions, sheets of paper, fast coding and demonstration on the laptops of results from computations - any and all ways of discussing, arguing, convincing: this is how the workshop looked.

Multiscale problems, due to their importance for many branches of science and industry, attract significant attention of the mathematical community. The main targets of this workshop were the numerical aspects of the multiscale problems: integrating numerical algorithms with asymptotic homogenization theory when the latter is applicable, and developing numerical approaches for multiscale problems with nonseparable scales. The last is especially important. Many multiscale problems are heterogeneous at each scale, and no small parameter can be introduced there. For such problems the equations at all scales are coupled, and the one way, fine-to-coarse scale procedure is not applicable. Instead, an (iterative) coupled solution at all scales is required. The mathematical studies of coupled multiscale problems are still far from the level which is achieved in the field of the asymptotic homogenization, and this has to be compensated for by intensive research. The most active mathematical research in the field of numerical upscaling is currently carried out in two directions: upscaling based on multigrid methods, and upscaling based on multiscale finite element method. Both, MG and multiscale FEM, provide a suitable framework for solving coupled multiscale problems.

Various general and particular questions were discussed during the workshop.

Among the general questions, special attention deserves the need of classification of the multiscale problems with respect to the goals seeked: For example: i) mathematical model at the fine scale is known and the solution is sought at the fine scale (coarse scale serves only to accelerate the solution procedure); ii) mathematical model at the fine scale is known, but the solution is sought at the coarse scale only (fine scale has to provide information about the model and the effective properties of the coarse scale), etc.

Another hot topic for discussions is when the scales can be separated and when not (depending on the geometry, process parameters, etc.). In particular, examples for problems with nonseparable scales, arising in Geoscience, were presented. The case when the scales can not be separated is the most difficult one, and there is no alternative to the numerical upscaling here. How to solve problems with nonseparable scales - with AMG-type approach, or with multiscale FEM, or with a combination of both; with overlapping or without overlapping for cell problems, etc., - all these questions were intensively discussed during the workshop, and they still need to be further discussed aiming at breaking the complexity of the multiscale problems considered.

Further interesting topics discussed there were:

- Different approaches for deriving coarse scale equations: based on truncated asymptotic expansions, starting from variational principles, etc.
- Different approaches for calculating effective coefficients of the coarse scale equations: matrix-dependent prolongation in multigrid; solving overlapping or non-overlapping local problems in multiscale and heterogeneous FEM, etc.
- How to put together analytical and numerical approaches for solving the auxiliary or the cell problems.

• How to benefit from the similarity between algebraic approaches (AMG agglomeration, approximate total reduction, etc.) and upscaling approaches (MsFEM, HMM, etc).

• How to combine the solution on a fine scale for a quasi–steady variable with transient computations on a coarse scale for other variables. Example from multiphase flow in porous media was presented when pressure is calculated once on the coarse scale, while contamination transport in time is simulated on a coarser scale.

• Define benchmark problems with separable and unseparable scales to test different approaches.

Some of the discussed questions are reflected in the presented abstracts, others need further research and we expect that they will appear in forthcoming papers.

Mini-Workshop: Numerical Upscaling: Theory and Applications

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Abstracts

Higher Order Gradient Continuum Description of Atomistic Models for Crystalline Solids

Marcel Arndt
(joint work with Michael Griebel)

The behavior of materials often involves quite different length scales. The effects which can be observed range from the macroscale down to the atomic length scale or even to the quantum mechanical scale. For an accurate modeling and an efficient numerical treatment, it is necessary to address the problem on the complete hierarchy of scales and to explore the relationships of different models on different length scales.

Two approaches are of special interest: upscaling and coupling techniques. Upscaling means to derive a model on one scale from a model on the next finer scale, whereas in the coupling approach, several models on different length scales are used simultaneously within one numerical simulation. Widely used coupling techniques are the quasi-continuum method [6], the bridging scales method [7] and the heterogeneous multiscale method [4].

Here we are interested in upscaling techniques from the atomic length scale to the continuum mechanical length scale for crystalline solids. The basic ingredient of an atomistic model is the potential energy $\Phi^{(\mathrm{A})}$, which is a function of the atom positions:

$$\Phi^{(\mathrm{A})}\big(\{y(x)\}_{x\in\mathcal{L}\cap\Omega}\big). \tag{0.1}$$

$\mathcal{L}$ denotes the crystal lattice, $\Omega \subset \mathbb{R}^d$ the shape of the specimen in the reference configuration and $y : \mathcal{L} \cap \Omega \to \mathbb{R}^d$ a discrete deformation function. The goal of upscaling is to assign a continuum potential energy to a continuum deformation function $y : \Omega \to \mathbb{R}^d$, making use of the atomistic potential $\Phi^{(\mathrm{A})}$. The evolution equations and other models can then be derived from the continuum potential.

A classical upscaling technique is the scaling technique, which has been analyzed e.g. in [3]. It is based on rescaling the atomistic potential energy to an arbitrary fine lattice $\varepsilon\mathcal{L}$ for $\varepsilon > 0$ and subsequently letting ε tend to zero. This coincides with the thermodynamic limit, which drives the number of particles to infinity. Under moderate assumptions, it can be shown that this procedure leads to a potential energy in the form

$$\Phi(y)^{(\mathrm{S})} = \int_\Omega \Phi^{(\mathrm{S}),x}\big(\nabla y(x)\big)\,\mathrm{d}x \tag{0.2}$$

for a continuum deformation function $y : \Omega \to \mathbb{R}^d$. It is well-known that the according evolution equation

$$\rho\frac{\partial^2 y}{\partial t^2}(x) = \operatorname{div}\Phi^{(\mathrm{S}),x'}\big(\nabla y(x)\big) \tag{0.3}$$

exhibits classical solutions only for a finite time horizon due to hyperbolic shock waves. This breakdown of solution theory stands in contrast to the discrete system, which exhibits solutions for an infinite time horizon. Moreover, the solutions lack the typical dispersive effects of the discrete system. An asymptotic analysis reveals that only partial information from the atomistic system is transferred to the continuum level, whereas other information is necessarily lost by the limit process.

As a remedy we consider the system within the so-called quasicontinuum regime, i.e. for a large, but finite number of particles. To this end, the inner expansion technique [1, 2] has been developed. It works as follows.

First, the atomistic potential $\Phi^{(\mathrm{A})}$ is localized by splitting it up into a sum

$$\Phi^{(\mathrm{A})}\big(\{y(x)\}_{x\in\mathcal{L}\cap\Omega}\big) = \sum_{\overline{x}\in\overline{\mathcal{L}}\cap\Omega} \Phi^{(\mathrm{A}),\overline{x}}\big(\{y(x)\}_{x\in\mathcal{L}\cap\Omega}\big) \tag{0.4}$$

of local potentials $\Phi^{(\mathrm{A}),\overline{x}}$, each of which describes the interaction of the atoms around the point $\overline{x}$. Nearly all physically meaningful potentials allow for such a localization.

Second, we perform a power series expansion of the continuum deformation function $y : \Omega \to \mathbb{R}^d$ around each point $\overline{x}$ up to some degree K and reformulate the potential as follows:

$$\begin{aligned}
\Phi^{(\mathrm{A})}(y) &= \sum_{\overline{x}\in\overline{\mathcal{L}}\cap\Omega} \Phi^{(\mathrm{A}),\overline{x}}\big(\{y(x)\}_{x\in\mathcal{L}\cap\Omega}\big) \\
&\approx \sum_{\overline{x}\in\overline{\mathcal{L}}\cap\Omega} \Phi^{(\mathrm{A}),\overline{x}}\left(\left\{\sum_{k=0}^{K}\frac{1}{k!}\nabla^k y(\overline{x}) : (x-\overline{x})^k\right\}_{x\in\mathcal{L}\cap\Omega}\right) \\
&=: \sum_{\overline{x}\in\overline{\mathcal{L}}\cap\Omega} \Phi^{(\mathrm{I}),\overline{x}}\left(y(\overline{x}), \nabla y(\overline{x}), \nabla^2 y(\overline{x}), \ldots, \nabla^K y(\overline{x})\right).
\end{aligned} \tag{0.5}$$

The choice of expansion points $\overline{x} \in \overline{\mathcal{L}} \cap \Omega$ strongly determines the approximation properties of the resulting continuum model. For many types of potential functions, it can be shown that the best choice for $\overline{x}$ is the barycenter of the positions of the involved atoms, since the remainder terms of the series expansion are minimized then.

The expression (0.5) still contains the finite sum over the lattice $\overline{\mathcal{L}} \cap \Omega$ of expansion points. The sum acts like a Riemann sum and is averaged in a third step

$$\begin{aligned}
\Phi^{(\mathrm{I})}(y) &= \sum_{\overline{x}\in\overline{\mathcal{L}}\cap\Omega} \Phi^{(\mathrm{I}),\overline{x}}\left(y(\overline{x}), \nabla y(\overline{x}), \nabla 2y(\overline{x}), \ldots, \nabla^K y(\overline{x})\right) \\
&\approx \overline{\alpha}^{-1}\int_{\Omega} \Phi^{(\mathrm{I}),\overline{x}}\left(y(\overline{x}), \nabla y(\overline{x}), \nabla 2y(\overline{x}), \ldots, \nabla^K y(\overline{x})\right)\,\mathrm{d}\overline{x} \\
&=: \Phi^{(\mathrm{J})}(y),
\end{aligned} \tag{0.6}$$

where $\overline{\alpha}$ denotes the volume of a unit cell of $\overline{\mathcal{L}}$. This gives us the final continuum potential $\Phi^{(\mathrm{J})}$.

The resulting continuum potential $\Phi^{(\mathrm{J})}(y)$ from (0.6) is a generalization of $\Phi^{(\mathrm{S})}(y)$ from (0.2) which involves higher order gradients. It is shown that the higher order terms allow the description of the microscopic material properties to a higher extent than commonly used continuum mechanical models like (0.2). In particular, the discreteness effects of the underlying atomistic model are captured. Moreover, convexity and boundedness properties of the atomistic system are carried over to the continuum level.

The approximation properties of the resulting continuum model are studied numerically for the model problem of a one-dimensional atomic chain. Depending on the degree K of approximation, it turns out that the dispersion is captured both qualitatively and quantitatively very well, whereas it is completely lost by the scaling technique. The inner expansion technique is then applied to the physically more relevant three-dimensional example of a silicon crystal. It is shown that the resulting continuum model is much more precise than the standard model obtained by the thermodynamic limit. Especially the three-body interactions profit from the higher order terms. Let us note that an application to shape memory alloys is given in [1].

Finally let us mention the direct expansion technique [5] as another upscaling scheme which gives an approximation of the atomistic system within the quasicontinuum regime. It is based on a power series or a Padé approximation of the evolution equation of the discrete system and is capable to preserve the microscopic properties such as the dispersion on the continuum scale as well. However, it does not preserve convexity and boundedness properties of the atomistic system in general, which often leads to ill-posed problems.

References

[1] M. Arndt, M. Griebel, *Derivation of higher order gradient continuum models from atomistic models for crystalline solids*, Multiscale Model. Simul. **4** (2005), 531–562.

[2] M. Arndt, *Upscaling from atomistic models to higher order gradient continuum models for crystalline solids*, Dissertation, Institute for Numerical Simulation, University of Bonn (2004).

[3] X. Blanc, C. Le Bris, P. L. Lions, *From molecular models to continuum mechanics*, Arch. Ration. Mech. Anal. **164** (2002), 341–381.

[4] W. E, B. Engquist, *The heterogeneous multi-scale methods*, Comm. Math. Sci. **1** (2003), 87–133.

[5] P. Rosenau, *Dynamics of nonlinear mass-spring chains near the continuum limit*, Phys. Lett. A **118** (1986), 222–227.

[6] E. B. Tadmor, M. Ortiz, R. Phillips, *Quasicontinuum analysis of defects in solids*, Philos. Mag. A **73** (1996), 1529–1563.

[7] G. J. Wagner, W. K. Liu, *Coupling of atomistic and continuum simulations using a bridging scale decomposition*, J. Comput. Phys. **190** (2003), 249–274.

Coarse Grained Mixing Parameters for Solute Transport

Sabine Attinger

Flow and transport in natural formations are dominated by the heterogeneous structure of the material. To capture observed phenomena accurately, one has to discretize numerical models by grid cells of smaller size than the scale of heterogeneity. The computational effort to solve field scale problems is very demanding and it is common to diminish the computational resolution by choosing coarser grids. Variability is lost in this case and one faces the problem how to model the impact of unresolved velocity fluctuations upon transport. Standard upscaling procedures such as homogenization and stochastic modelling compensate unresolved effects by introduction of macrodispersive fluxes. Both methods average out all heterogeneities resulting in a total loss of spatial variability in the flow and transport parameters. In general, one has to make a compromise between computational efficiency and the preciseness/correctness of the model solution. However, numerical grid cells of size much larger than the heterogeneity scale might be not desired nor might yield reliable results with respect to the required preciseness of the results. Or practical problems might be dominated by additional scales not much larger than the heterogeneity scale.

We aim at improving standard upscaling procedures by introducing a method called Coarse Graining that is capable to transfer a heterogeneous model not only on very large scales but also to intermediate scales. Standard upscaling methods are also called asymptotic methods whereas the method of Coarse Graining accounts for preasymptotic effects as well.

1. The Model

Solutes released into fluid flow are carried along with the flow but are also subject to diffusion in the presence of concentration gradients. Our focus is not on the microscopic pore scale but on the larger Darcy scale. Both, hydrodynamic dispersion and diffusion, contribute to dispersive movement of solutes and the mass conservation for solutes read

$$\theta \frac{\partial c}{\partial t} = \nabla(\theta \mathbf{D} \nabla c) - \nabla(\mathbf{u} c) + q_S c_S \tag{1.1}$$

where c denotes the solute concentration (dimensions mass/L^d). q_S is the volumetric rate of the concentration sink/source c_S and $\mathbf{u}$ is the heterogeneous Darcy velocity. $\mathbf{D}$ is the dispersion tensor. It is assumed to be diagonal and isotropic.

We split the spatially fluctuating Darcy velocity into a deterministic and a random contribution,

$$\mathbf{u}(\mathbf{x}) \equiv \overline{\mathbf{u}} - \mathbf{u}'(\mathbf{x}) \quad , \tag{1.2}$$

where $\overline{\mathbf{u}}$ is the averaged Darcy velocity. The field $\mathbf{u}'(x)$ denotes the fluctuation around the mean value. The corresponding velocity auto-correlation functions are

denoted by

$$\overline{u_i'(\mathbf{x})\, u_j'(\mathbf{x}')} = \mathrm{C}_{ij}^{uu}(\mathbf{x}-\mathbf{x}') \qquad , \tag{1.3}$$

where $u_i'(\mathbf{x})$ is the i-component of the d-dimensional field $\mathbf{u}'(\mathbf{x})$, $i = 1, \ldots, d$ with isotropic correlation lengths$l$.

2. Effective Mixing Parameters

In heterogeneous media, the mixing coefficients depend implicitly on the spatial distribution of the heterogeneities, $D_{ij} = D_{ij}(c)$, via the concentration. In the stochastic approach, the large scale plume is characterized by an large scale or ensemble dispersivity which reads

$$D_{ij}^{\mathrm{ens}} \;\equiv\; D_{ij}(\overline{c}) \tag{2.1}$$

where the overbar denotes the average over the ensemble of aquifer realizations. It represents the dispersion characteristics of the whole ensemble of aquifer realizations. The 'effective' dispersivity is different from this quantity,

$$D_{ij}^{\mathrm{eff}} \;\equiv\; \overline{D_{ij}(c)} \tag{2.2}$$

The ensemble dispersion coefficient takes into account an artificial dispersion effect caused by fluctuations of the center of mass positions of the solute clouds in different realizations of the inhomogeneous medium. This effect is suppressed in the effective dispersion coefficients $D^{\mathrm{eff}}(t)$, because there the center of mass positions are superimposed before the ensemble average is performed. In general, the experimentally observable dispersion, which is a property related to one given aquifer, is represented by the effective quantity $D_{ij}^{\mathrm{eff}}(t)$.

Thus, deriving real block-scale mixing coefficients needs coarse graining of effective mixing coefficients instead of ensemble mixing coefficients if one is interested in finite time regimes. *R*ubin et al. [1999] applied coarse graining to solute transport but only stated explicit results for block-scale macrodispersivity values.

3. Results.

With this talk, we presented scale dependent or block-scale effective mixing coefficients as a completation of the work of *E*fendiev et al. and *R*ubin et al..

The ensemble dispersion approaches its long time value on time scales larger than $t \gg \tau_{\mathrm{u}}$. For infinite Peclet numbers, we get

$$\delta D_{11}^{\mathrm{ens}}(\lambda) \;=\; \sqrt{\pi/2}\sigma_f^2\, \overline{u} l \left(1 - \frac{1}{(1+\lambda^2/4l^2)^{(d-1)/2}}\right) \tag{3.1}$$

where λ denotes the scale which is still resolved by the model or the width of the Coarse Graining filter. The ensemble dispersion coefficient displays artificial mixing effects due to the spatial filter. Even without any physical small scale mixing mechanism $D = 0$, the ensemble dispersion reaches finite long time values. This scale or resolution dependent ensemble dispersion coefficient is comparable to the block-effective macrodispersion coefficient introduced by *R*ubin [1999].

The effective dispersion coefficient approaches its constant long time value for very large times only. The long time value is identical to that of the ensemble quantity. Increasing the width of the filter, the time scales split. Similar to the time behavior of the effective mixing coefficients in Stochastic Modelling, the difference between ensemble and effective mixing vanishes only after the plume has sampled dispersively a sufficiently large region in space. We find

$$\delta D_{11}^{\mathrm{eff}}(t,\lambda) = \delta D_{11}^{\mathrm{ens}}(t,\lambda) - \sqrt{\frac{\pi}{2}}\,\gamma^{-2}\,\sigma_f^2\,\overline{u}\,l \left(\left(1+4\,\frac{t}{\tau_{\mathrm{D}}}\right)^{-(d-1)/2} - \left(1+\frac{\lambda^2}{4l^2}+4\,\frac{t}{\tau_{\mathrm{D}}}\right)^{-(d-1)/2} \right) \tag{3.2}$$

The sufficiently large region, mentioned above, is not determined by the heterogeneity scale l but by the width of the spatial filter λ. If the plume has spread over the width of the filter, the filtering procedure displays no artificial mixing any more and consequently ensemble and effective mixing coefficients become identical.

4. Conclusions.

We demonstrated that the ensemble dispersion coefficient displays artificial mixing effects overestimating the real scale dependent mixing. The artificial filtering effects could be suppressed making use of the concept of effective mixing parameters. Closed results are stated for weakly heterogeneous media, avoiding empirical functions as needed in *E*fendiev et al [2000]. For further information, the reader is referred to *A*ttinger [2005].

References

[1] Attinger S., *Coarse Grained Ensemble and Effective Mixing Parameters for solute Transport*, submitted for publication to Water Resour. Res., (2005)

[2] Y. Efendiev, L.J. Durlofsky and S.H. Lee, *Modeling of subgrid effects in coarse-scale simulations of transport in heterogeneous porous media*, Water Res. Res., **36(8)**, (2000), 2031–2041

[3] Rubin, Y., A. Sun, R. Maxwell and A. Bellin, *The concept of block-effective macrodispersivity and a unified approach for grid-scale and plume-scale dependent transport*, Journal of FluidMech., **395**, (1999), 161-180.

Multiscale finite element methods for nonlinear problems

Yaslchin Efendiev

Many processes involve a wide range of scales. Because of the scale disparity in multiscale problems, it is often impossible to resolve the effects of small scales directly. For this reason some type of coarsening or upscaling is performed. The main idea of upscaling techniques is to form coarse-scale equations with a prescribed analytical form that may differ from the underlying fine-scale equations. In multiscale methods, by contrast, the fine-scale information may be carried throughout the simulation, and the coarse-scale equations are generally not expressed analytically, but rather formed and solved numerically.

Recently a number of multiscale numerical methods, such as residual free bubbles, variational multiscale method, multiscale finite element method (MsFEM), two-scale finite element methods, two-scale conservative subgrid approaches, and heterogeneous multiscale method (HMM) have been proposed. We remark that special base functions in finite element methods have been used earlier in [1], where using special base function, the generalized finite element method is introduced. We have generalized MsFEM to nonlinear problems. Originally, MsFEM is proposed for linear equations and its main idea is to use oscillatory base functions to capture the local-scale information. The pre-computed multiscale base functions allow us to interpolate a coarse-scale function, defined at the nodal values of the coarse grid, to the underlying fine grid. This idea can be naturally generalized to nonlinear problems if one considers, instead of the base functions, a multiscale map from the coarse grid space to the underlying fine grid space. This multiscale map is constructed using the solutions of the local problems and provides us with the interpolation of the coarse-scale function, defined at the nodal values of the coarse grid, to the underlying fine grid. For linear problems, our multiscale map is linear and, thus, the image of the coarse dimensional space is a linear space with the same dimension. A basis for the multiscale space can be obtained by mapping a basis of the coarse dimensional space. The latter gives us the multiscale finite element basis functions introduced in [4]. Once the multiscale mapping is defined, we can formulate the global finite element formulation of the problem. Our multiscale finite element methods use a Petrov-Galerkin formulation in which we use multiscale finite element bases as basis functions and standard linear finite elements as test functions. We would like to stress that the formulation of MsFEM does not require any assumptions on the nature of heterogeneities, such as periodicity, almost periodicity, or etc.

We considered the analysis of MsFEM for general nonlinear elliptic equations, $u_\epsilon \in W_0^{1,p}(\Omega)$

$$-\mathrm{div}(a_\epsilon(x, u_\epsilon, D_x u_\epsilon)) + a_{0,\epsilon}(x, u_\epsilon, D_x u_\epsilon) = f, \tag{0.1}$$

where $a_\epsilon(x, \eta, \xi)$ and $a_{0,\epsilon}(x, \eta, \xi)$, $\eta \in \mathbb{R}$, $\xi \in \mathbb{R}^d$ satisfy some assumptions, which guarantee the well-posedness of the nonlinear elliptic problem (0.1). Here $\Omega \subset \mathbb{R}^d$ is a Lipschitz domain and ϵ denotes the small scale of the problem. The homogenization of nonlinear partial differential equations has been studied previously (see, e.g., [5]). It can be shown that a solution u_ϵ converges (up to a sub-sequence) to u in an appropriate norm, where $u \in W_0^{1,p}(\Omega)$ is a solution of a homogenized equation

$$-\mathrm{div}(a^*(x, u, Du)) + a_0^*(x, u, Du) = f. \tag{0.2}$$

The homogenized coefficients can be computed if we make an additional assumption on the heterogeneities, such as periodicity, almost periodicity, or when the fluxes are strictly stationary fields with respect to spatial variables. In these cases, an auxiliary problem is formulated and used in the calculations of the homogenized fluxes, a^* and a_0^*. Our motivation in considering this type of equation stems from porous media applications, where nonlinear fluxes arise. In particular, we

are interested in porous media flows in unsaturated media and the transport of two-phase flows in heterogeneous porous media. In these examples, nonlinearities arise due to the interaction between the phases and components.

We have studied the convergence of the generalized MsFEM for periodic as well as random heterogeneities. To analyze the method for periodic case, we first approximate the solutions of the local problems by introducing appropriate correctors, which are periodic with respect to the fast variables. These approximations of the local solutions allow us to extract the homogenized behavior of MsFEM solutions and compare it with the homogenized solutions of the continuous equations. Sharp estimates for the corrector approximations are obtained. The analysis allows us to understand the resonance error and propose an oversampling technique as in [4]. Numerical examples are presented to show the accuracy of the oversampling method. We use both periodic and random fields with long-range correlation structures (with and without discontinuities) in our numerical experiments. We present numerical examples for both multiscale finite element and multiscale finite volume element methods. Multiscale finite volume element methods are very closely related to multiscale finite element method, where the formulation of the method follows the standard finite volume element methods. All the examples clearly demonstrate the advantages of the oversampling method. In particular, the oversampling approach provides small errors for relatively large coarsening. Finally, we would like to note that the resonance errors are a common feature of multiscale methods unless periodic problems are considered and the solutions of the local problems in an exact period are used. In this case, one can solve the local problems in one period to approximate the multiscale map.

The results can be extended to parabolic equations. These results and applications of the method are presented in [2, 3].

References

[1] I. Babuška and E. Osborn, *Generalized finite element methods: Their performance and their relation to mixed methods*, SIAM J. Numer. Anal., 20 (1983), pp. 510–536.

[2] ———, *Numerical homogenization of nonlinear random parabolic operators*, SIAM Multiscale Modeling and Simulation, 2(2) (2004), pp. 237–268.

[3] Y. Efendiev, T. Hou, and V. Ginting, *Multiscale finite element methods for nonlinear problems and their applications*, Comm. Math. Sci., 2 (2004), pp. 553–589.

[4] T. Y. Hou and X. H. Wu, *A multiscale finite element method for elliptic problems in composite materials and porous media*, Journal of Computational Physics, 134 (1997), pp. 169–189.

[5] A. Pankov, *G-convergence and homogenization of nonlinear partial differential operators*, Kluwer Academic Publishers, Dordrecht, 1997.

Upscaled models for porous media flows

Richard Ewing

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 base elements. In this work we develop a similar approach using finite volume framework. Because of their conservative features, finite volume 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. In particular, we employ perturbation analysis to derive the macrodiffusion that represents the effects of subgrid heterogeneities. The macrodiffusion, in particular, can be written as a covariance between the velocity fluctuations and fine-scale quantity that represents the length of the fine-scale trajectories. For the computation of the fine-scale

quantities we use detailed information that is contained in the multiscale base functions.

We note that the resulting macrodispersion depends on the concentration of the components due to the functional dependence of the velocities on it. Thus, a mere use of this macrodispersion model would require saving the velocities for each time. We implemented a procedure to overcome the aforementioned impracticality by proposing a recursive relation relating the length of the fine-scale trajectories to the velocities. The recursive relation is based on the invariance of the trajectory viewed at two different time levels, as long as these two time levels are reasonably close to each other. In previous approaches [4] the authors use simplified models for macrodispersion, where only pre-asymptotic behavior of the macrodispersion is modeled. These simplifications limit the applications of macrodispersion models to general flow scenarios. A procedure for the computation of two-point correlations of spatial velocity fields is proposed. The latter allows the use of our approach for more general flow scenarios. These results are presented in [6, 7].

In this talk, we also 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].

References

[1] J. W. Barker and S. Thibeau. A critical review of the use of pseudo-relative permeabilities for upscaling. *SPE Res. Eng.*, 12:138–143, 1997.

[2] L. J. Durlofsky. Numerical calculation of equivalent grid block permeability tensors for heterogeneous porous media. *Water Resour. Res.*, 27:699–708, 1991.

[3] L. J. Durlofsky. Coarse scale models of two phase flow in heterogeneous reservoirs: Volume averaged equations and their relationship to the existing upscaling techniques. *Computational Geosciences*, 2:73–92, 1998.

[4] Y. R. Efendiev and L. J. Durlofsky. Numerical modeling of subgrid heterogeneity in two phase flow simulations. *Water Resour. Res.*, 38(8), 2002.

[5] Y. R. Efendiev, V. Ginting, T. Hou and R. Ewing. Accurate multiscale finite element methods for two-phase flow simulations *submitted to J. Computational Physics.*

[6] V. Ginting, R. Ewing, Y. Efendiev and R. Lazarov. Upscaled modeling for multiphase flow *to appear in Journal of Computational and Applied Mathematics.*

[7] V. Ginting, R. Ewing, Y. Efendiev and H. Wang. Upscaled Modeling for multicomponent miscible flows *submitted toComputational Geoscience.*

[8] T. Y. Hou and X. H. Wu. A multiscale finite element method for elliptic problems in composite materials and porous media. *Journal of Computational Physics*, 134:169–189, 1997.

Upscaling: A review of some numerical methods

Chris Farmer

Upscaling refers to the process of approximating one system of, usually differential, equations by a system of equations that is easier to solve but with the same average or large scale behaviour. This is a classical activity referred to as homogenisation in the mathematical literature and effective medium theory in the theoretical physics literature.

In this talk a classification of some numerical approaches was given. The problem of single phase, incompressible fluid flow through porous media was taken as a model problem. This has practical importance in the modelling of oil recovery, groundwater management and pollution modelling.

Incompressibility leads to the condition that the flux is divergence-free, $divu = 0$. Darcy's law provides the condition that the flux is proportional to a potential gradient, $u = -k\nabla p$ where a unit viscosity is assumed. The permeability coefficient, k, is in general a positive definite symmetric tensor. Various combinations of boundary conditions are applied to this model problem. The full problem involves multiple phases and leads to a system of parabolic equations, some of which are nearly elliptic and some nearly hyperbolic. The upscaling problem is to find a smoother, or at least simpler, permeability coefficient, k, so that the average behaviour is preserved. A detailed review of upscaling can be found in Farmer (2002). For general background see Farmer (2005).

If a physical experiment is performed on a heterogeneous material the permeability is calculated by taking the ratio of the gradient of the average flux to the average gradient. Numerical approaches to upscaling involve simulating such physical experiments. As most numerical experiments involve a grid, and as the detailed model will require a large, fine grid, we refer to the detailed model as the fine grid model. The equivalent simpler model is called the coarse grid model. Thus there is a fine grid experimental stage and a coarse grid *calibration* stage. Calibration involves inferring coarse grid coefficients by solving inverse problems with the fine grid results as input data. To make the calibration calculation easy, the numerical experiment is designed so that the flow is, on average, one dimensional and with a spatially constant pressure at one end of the system and a constant, lower, pressure at the other end.

There are two types of fine grid numerical experiment. One type involves experiments on small subregions which, in many cases, become the grid cells in the coarse grid model. We refer to such small scale experiments as *local*. The other type of experiment involves solving the fine grid model on a large part of the original problem domain. The fine grid experiment might, exceptionally, solve the original problem. When the fine grid problem involves a substantial portion of the domain we refer to the experiment as *global*.

Once the fine grid result is obtained a coarse grid model is calibrated that reproduces some aspects of the large scale behaviour. When this is done using just a small part of the coarse model, we refer to a local calibration, and when the whole coarse model is calibrated (probably involving a large scale optimisation problem) we refer to a *global calibration*. We thus arrive at four types of upscaling local-local, local-global, global-local and global-global. The first word of the pair refers to the fine grid experiment and the second word to the method of calibration. The local-global method as defined here is not used. However, speculation as to what might be involved in such a local-global method is a fruitful activity in analysing the way in which mathematical upscaling techniques are applied by engineers (see Farmer 2005 for further discussion).

Generally upscaling methods work if the length scales of the problem are well-separated. This means that the methods are subject to the same limitations as homogenisation approaches. However, numerical upscaling methods, although heuristic, are applicable in practice to a wide range of problems. Upscaling methods can be applied recursively, over several levels in cases where the fine grid model is only defined implicitly as for example by a probability density function. This is very similar to the real space renormalisation group method used in statistical physics. When the length scales are not well separated then the global-local and global-global upscaling methods will be best, as long as the boundary conditions are not too different from those used in the fine grid experiments.

More recently new approaches to upscaling problems have been devised. Of particular note are the multiscale basis function methods of Hou (1997) and of Jenny at al (2003). For simple problems, although better founded in theory, multiscale methods are practically the same as upscaling approaches. For more complicated problems the methods are of wider applicability. Nevertheless, these methods are only useful in cases where the fine grid model is available as a well defined numerical modelling. The work of Durlofsky (2003) involves an iterative approach, whereby a coarse grid calculation is used to obtain a possibly more accurate boundary condition for a repetition of the fine grid experiments.

References

[1] Y.Chen, L.J.Durlofsky, M.Gerritsen and X.H.Wen. A coupled local-global upscaling approach for simulating flow in highly heterogeneous formations. Advances in Water Resources, 26, 2003, 10411060.

[2] C.L. Farmer. Upscaling: A Review. Numerical Methods in Fluids, 40, 63-78, 2002.

[3] C.L. Farmer. Geological Modelling and Reservoir Simulation. In: Mathematical Methods and Modelling in Hydrocarbon Exploration and Production, Edited Armin Iske and Trygve Randen, Springer, 2005. pp 119-212.

[4] T.Hou and X.H. Wu. A multiscale finite element method for elliptic problems in composite materials and porous media. J. Comput. Phys., 134:169-189, 1997.

[5] P.Jenny, S.H. Lee, and H.A. Tchelepi. Multi-scale finite-volume method for elliptic problems in subsurface flow simulation. J. Comput.. Phys., 187:47-67, 2003.

Upscaling of two-phase flow processes in highly heterogeneous porous media including interfaces on different scales

Rainer Helmig

Environmental remediation and protection has provided an especially important motivation for multiphase research in the course of the last 15 years [4, 15]. The release of non-aqueous phase liquids, both lighter and denser than water (LNAPLs and DNAPLs), into the environment is a problem of particular importance to researchers and practitioners alike [14]. Of late, such work has focused on the construction of mathematical models which can be used to test and advance our understanding of complex multiphase systems, evaluate risks to human and ecological health, and aid in the design of control and remediation methods.

One of the foremost problems facing the reliable modeling of multiphase porous medium systems is the problem of scale. Roughly speaking, a model is assembled from a set of conservation equations and constitutive, or closure, relations. One must identify constitutive relations and system-specific parameters that are appropriate for the spatial and temporal scales of interest. Often, however, a disparity exists between the measurement scale in the field or laboratory and the scale of the model application in the field. Furthermore, neither the measurement nor the field application scales are commensurate with the scale of theoretical or empirical process descriptions. Both closure relation forms and parameters are subject to change when the system of concern is heterogeneous in some relevant respect.

Figure 1 graphically depicts the range of spatial scales of concern in a typical porous medium system. It illustrates two important aspects of these natural systems: several orders of magnitude in potentially relevant length scales exist, and heterogeneity occurs across the entire range of relevant scales. A similar range of temporal scales exists as well, from the pico-seconds over which a chemical reaction can occur on a molecular length scale to the decades of concern in restoring sites contaminated with DNAPLs.

A careful definition of relevant length scales can clarify any investigation of scale considerations, although such definitions are a matter of choice and modeling approach [6]. We define the following length scales of concern: the molecular length scale, which is of the order of the size of a molecule; the microscale, or the minimum continuum length scale on which individual molecular interactions can be neglected in favor of an ensemble average of molecular collisions; the local scale, which is the minimum continuum length scale at which the microscale description of fluid movement through individual pores can be neglected in favor of averaging the fluid movement over a representative elementary volume (REV) – therefore this scale is also called the REV-scale; the mesoscale, which is a scale on which local scale properties vary distinctly and markedly; and the megascale or field-scale. Measurements or observations can yield representative information across this entire range of scales, depending on the aspect of the system observed and the nature of the instrument used to make the observation. For this reason, we do not specifically define a measurement scale.

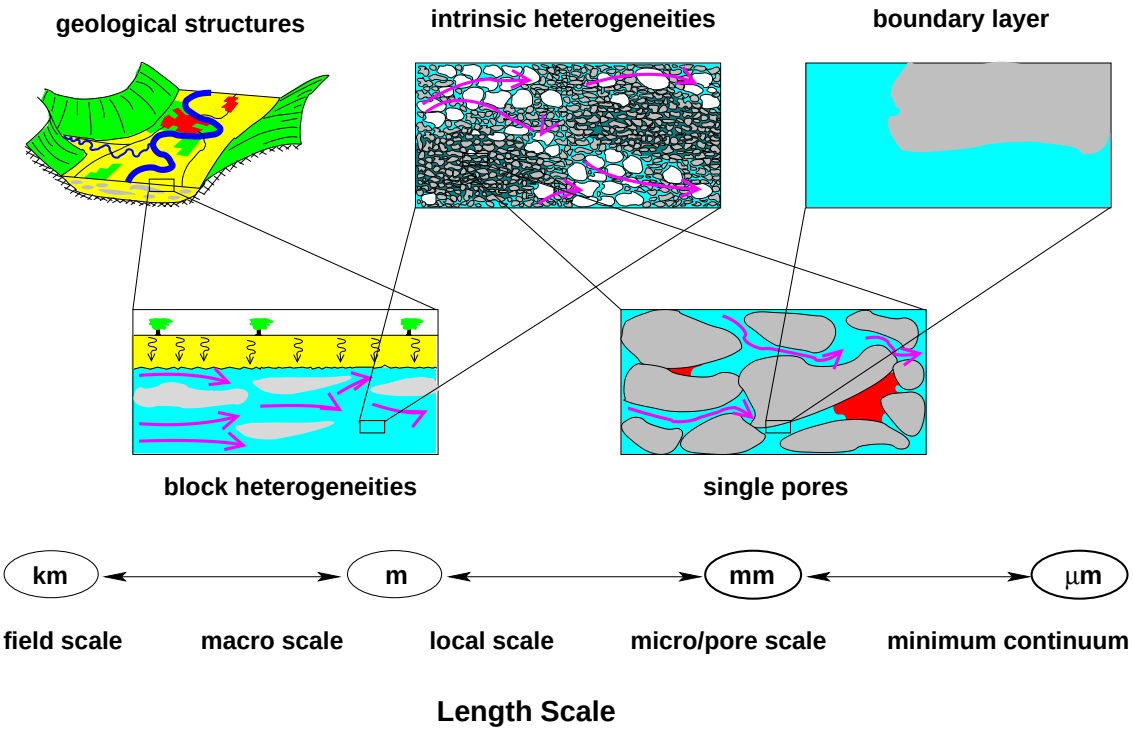

FIGURE 1. Different scales for flow in porous media

For the minimum continuum length scale, we take the boundaries of the different grains directly into account. For the microscale, we look at a variety of pore throats and pore volumes. Note that, for both scales, we average over the properties of the fluids only (achieving for example density, viscosity).

When looking at the REV-scale, we average over both fluid–phase properties and solid–phase properties. In Figure 2, we show schematically the averaged properties (e.g. the porosity). While averaging over a representative elementary volume (REV), we assume that the averaged property P does not oscillate significantly. In Figure 2 this is the case in the range of V_0 to V_1 with $V_0 < V_1$, so any volume V with $V_0 \leq V \leq V_1$ can be chosen as REV. Accordingly, we do not assume any heterogeneities on the REV-scale. For our model, we assume that the effects of the sub–REV–scale heterogeneities are taken into account by effective parameters. The super–REV–scale heterogeneities have to be taken into account by applying different parameters to the domain of interest. Both steady transitions as well as jumps have to be considered for the parameters. We denominate those heterogeneities with jumps within the spatial parameters as block heterogeneities. Within the context of this work, we assume that block heterogeneities can be described by subdomains with well–defined interfaces. In this paper, we do not consider heterogeneities on the field scale.

Because the scale of interest in this paper is ultimately the meso–scale, one can usually ignore molecular-scale phenomena, although these effects are embodied in continuum–conservation equations and associated closure relations. However,

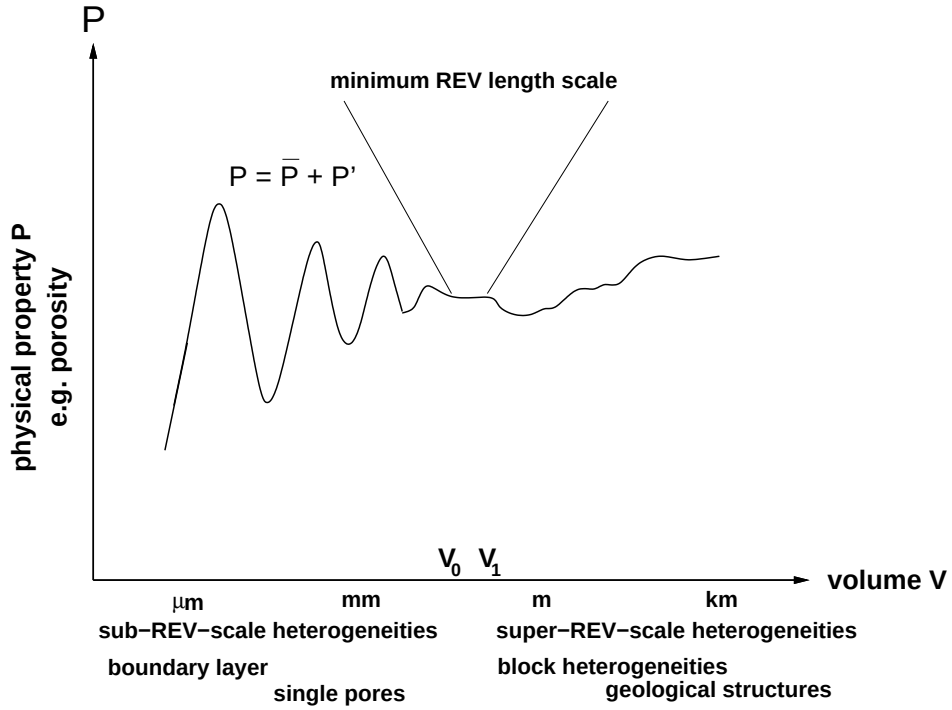

FIGURE 2. Different scales for flow in porous media (schematically for Figure 1)

we must consider all other important and relevant scales in the current study of multiphase porous–medium systems.

Conceptually, one wishes to describe phenomena at a given scale using the minimum amount of information from smaller scales. This process gives rise to quantities at each scale that may not be meaningful at smaller scales. For example, fluid pressures are not relevant to individual collisions at the molecular scale, and point-wise fluid saturations or volume fractions do not necessarily reflect the microscale fluid composition at that point. A conceptually satisfying theoretical approach – one that could fundamentally increase the field's maturity – must provide a method for incorporating models on a given scale sparingly into models on the next larger scale using rigorous mathematics and sound physical reasoning.

For example, microscale models can be developed to describe fluid flow in individual pores by solving the Navier-Stokes equations [1] or Boltzmann equation [2] over an appropriate domain. These methods can in turn be used to model systems consisting of many pores, even of a size equivalent to an REV for a REV-scale porous–medium system. Such approaches have been used to develop REV-scale closure relations based upon microscale processes [5].

As yet, this kind of connection does not exist across relevant length scales for all the phenomena considered in multiphase porous–medium systems. Valid questions remain about the importance of heterogeneities for specific processes, the appropriate form and parameterization of closure relations for heterogeneous

multiphase porous–medium systems, and effective ways of simulating such systems economically.

In spite of the problems of scale, we need reliable efficient multiphase flow and transport simulators that represent the dominant flow and transport mechanisms in heterogeneous multiphase porous–medium systems. The REV-scale modeling problem has been operationally separated from the more general problem of cascading scales, although the two problems are formally entwined. The two have been split apart because of the urgent need to respond practically to such problems, even before we understand them fully. The operational separation of local scale modeling from a more comprehensive theoretical modeling methodology has resulted in many practical models and experimental studies of complex multiphase phenomena [16, 10, 7, 11, 8, 9]. Engineering has played an important role in implementing this practical response.

¿From the mesoscopic perspective, two basic classes of multiphase applications have received attention in the literature and deserve further consideration: the imbibition of DNAPL into a heterogeneous porous–medium system [8, 9, 3] and the removal of a DNAPL originally in a state of residual saturation [12, 13]. The former class determines the morphology of the DNAPL distribution at residual saturation, which, therefore, determines the initial condition of the latter problem. While the public is greatly concerned with remediating DNAPL–contaminated soils, many questions concerning DNAPL imbibition and removal still hinder our remediation efforts.

The overall goal of this work is to advance our understanding of models for heterogeneous multiphase porous–medium systems across a range of scales. Our specific objectives are (1) to evaluate the role of the spatial scale in determining the dominant process for multiphase flow; (2) to investigate the influence of pore-scale heterogeneity on microscale and REV-scale flow processes; (3) to summarize conventional continuum-scale mathematical models; (4) to evaluate the accuracy and efficiency of a set of spatial and temporal discretization approaches for solving multiphase flow and transport; (5) to compare numerical simulations with experimental observations for heterogeneous mesoscopic systems; and (6) to point the way toward important future areas of research in the field.

References

[1] P. M. Adler. *Porous Media: Geometry and Transports*. Butterworth-Heinemann, Boston, 1992.

[2] S. Chen and G. D. Doolen. Lattice Boltzmann method for fluid flows. *Annual Review of Fluid Mechanics*, 30:329–364, 1998.

[3] R. Helmig and R. Huber. Comparison of Galerkin-type discretization techniques for two-phase flow in heterogeneous porous media. *Advances in Water Resources*, 21(8):697–711, 1998.

[4] Rainer Helmig. *Multiphase flow and transport processes in the subsurface - a contribution to the modeling of hydrosystems*. Springer Verlag, 1997.

[5] M. Hilpert, J. F. McBride, and C. T. Miller. Investigation of the residual-funicular nonwetting-phase-saturation relation. *Advances in Water Resources*, 24(2):157–177, 2001.

[6] D. T. Hristopulos and G. Christakos. An analysis of hydraulic conductivity upscaling. *Nonlinear Analysis*, 30(8):4979–4984, 1997.
[7] B. H. Kueper, W. Abbott, and G. Farquhar. Experimental observations of multiphase flow in heterogeneous porous media. *Journal of Contaminant Hydrology*, 5:83–95, 1989.
[8] B. H. Kueper and E. O. Frind. Two-phase flow in heterogeneous porous media, 1. Model development. *Water Resources Research*, 27(6):1049–1057, 1991.
[9] B. H. Kueper and E. O. Frind. Two-phase flow in heterogeneous porous media, 2. Model application. *Water Resources Research*, 27(6):1059–1070, 1991.
[10] R. J. Lenhard and J. C. Parker. Measurement and prediction of saturation-pressure relationships in three-phase porous media systems. *Journal of Contaminant Hydrology*, 1:407–424, 1987.
[11] R. J. Lenhard, J. C. Parker, and J. J. Kaluarachchi. A model for hysteretic constitutive relations governing multiphase flow 3. Refinements and numerical simulations. *Water Resources Research*, 25(7):1727–1736, 1989.
[12] A. S. Mayer and C. T. Miller. An experimental investigation of pore-scale distributions of nonaqueous phase liquids at residual saturation. *Transport in Porous Media*, 10(1):57–80, 1993.
[13] A. S. Mayer and C. T. Miller. The influence of mass transfer characteristics and porous media heterogeneity on nonaqueous phase dissolution. *Water Resources Research*, 32(6):1551–1567, 1996.
[14] National Research Council. Groundwater contamination: Overview and recommendations. In National Research Council, editor, *Groundwater Contamination*, pages 3–20. National Academy Press, Washington, DC, 1984.
[15] National Research Council. *Natural Attenuation for Groundwater Remediation*. National Academy Press, Washington, DC, 2000.
[16] J. C. Parker and R. J. Lenhard. A model for hysteretic constitutive relations governing multiphase flow 1. Saturation-pressure relations. *Water Resources Research*, 23(12):2187–2196, 1987.

On averaging of the non-periodic conductivity coefficient using two-scale extension

Vsevolod Laptev
(joint work with S. Belouettar)

It is usually difficult to predict a global behavior of some process in heterogeneous media (for example composite/porous materials) although the physics of the process might be well understood locally. The reason lying in the complexity of the microstructure gives rise to different upscaling methods.

Heterogeneities having periodic microstructure play a central role in the development of upscaled models. From one side they represent an important particular case of general heterogeneous media and on the other there are well developed mathematical techniques (e.g. the two-scale asymptotic expansion method), which help to derive formally and often rigorously the upscaled model. As a result many physical processes in heterogeneous media having periodic microstructures are well investigated both from theoretical and from practical points of view and the periodicity assumption is usually a starting point for the upscaling procedures [2],[5],[6].

Although this assumption is valid in only limited number of cases, mostly in artificially created materials. Therefore for practical purposes one should be able to deal with non- periodic structures.

The deterministic homogenization procedure starts from a sequence of problems $\{\mathcal{P}^\varepsilon\}$. In the periodic case the heterogeneity in $\mathcal{P}^\varepsilon$ is usually described by an ε-periodic function $a^\varepsilon(x) = a(x/\varepsilon)$ (where $a(y)$ is a given 1-periodic function). Quite often the purely periodic coefficient can be generalized without difficulties to the locally periodic coefficient $a^\varepsilon(x) = a(x, x/\varepsilon)$ (where $a(x, y)$ is a given 1-periodic function in y). In the following steps one has to investigate the convergence of the sequence (in a wide sense) and to find a limit problem $\mathcal{P}^0$. The solution of the limit problem can be used in order to approximate the solutions of the problems $\mathcal{P}^\varepsilon$ for small enough ε.

The coefficients $a(y)$ or $a(x, y)$ are considered in mathematical literature as given functions belonging to some functional spaces, without paying much attention where they come from.

In this presentation we start from a rapidly oscillated (non-periodic) coefficient $a_M(x)$ given in Ω and define a two-scale extension for $a_M(x)$ – any 1-periodic in y function $a(x, y)$ satisfying for some $\bar{\varepsilon} > 0$ the equality $a(x, x/\bar{\varepsilon}) = a_M(x)$ in Ω.

If $a_M(x)$ is a coefficient in a problem $\mathcal{P}$ then the resulting sequence $\{\mathcal{P}^\varepsilon\}$ (constructed from the two-scale extension $a(x, y)$) passes through the problem $\mathcal{P}$ when $\varepsilon = \bar{\varepsilon}$. And if the sequence $\{\mathcal{P}^\varepsilon\}$ has a limit problem $\mathcal{P}^0$ then the solution of $\mathcal{P}^0$ can be used in order to approximate the solution of $\mathcal{P}$. Roughly speaking, $\mathcal{P}^0$ is an upscaled problem for $\mathcal{P}$.

The two-scale extension is not unique and different two-scale extensions lead to different upscaled problems. The trivial extension is given by $a(x, y) = a_M(x)$. More useful extensions can be constructed in the following way (assuming that $a_M(x)$ is known in a larger domain $\widetilde{\Omega} \supset \Omega$ to avoid uncertainties close to $\partial\Omega$):

- we choose $\bar{\varepsilon} > 0$ (small in comparison to the typical size of Ω);
- for each $x \in \Omega$ we choose an $\bar{\varepsilon}$-cube W_x containing x and $W_x \subset \widetilde{\Omega}$ (W_x is a cubic Representative Elementary Volume around x);
  It is reasonable to distinguish two main choices for W_x:
  - W_x is an $\bar{\varepsilon}$-cube with the center x.
  - Having a partition $\overline{\Omega} = \cup_j \overline{\Omega_j}$ ($\Omega_i \cap \Omega_j = \emptyset$, $i \neq j$) that each Ω_j has an $\bar{\varepsilon}$-cube W_j ($\Omega_j \subseteq W_j$) then for each $x \in \Omega_j$ we can define $W_x := W_j$.

Now we fix $x \in \Omega$ and construct $a(x, \cdot)$:

(1) $\tilde{a}(x, y) = a_M(y)$, $y \in W_x$;
(2) $\tilde{a}(x, y)$ is extended $\bar{\varepsilon}$-periodically in y to the whole space.
(3) $a(x, y) = \tilde{a}(x, \bar{\varepsilon}y)$ is the two-scale extension.

The discontinuity of such two-scale extensions can be partially compensated by "admissibility" in the sense of the two-scale convergence method [1].

Applying this approach to the second order elliptic equation with homogeneous Dirichlet boundary conditions, the initial problem is

$$\mathcal{P}: \qquad -\nabla \cdot (a_M(x)\nabla u) = f \qquad \text{in } \Omega, \qquad u|_{\partial\Omega} = 0,$$

the imaginary sequence of problems with the two-scale extension $a(x, y)$ is

$$\mathcal{P}^\varepsilon : \qquad -\nabla \cdot (a(x, x/\varepsilon)\nabla u_\varepsilon) = f \qquad \text{in } \Omega, \qquad u_\varepsilon|_{\partial\Omega} = 0,$$

and the averaged (upscaled) problem with $A(\cdot)$ calculated using the standard homogenization algorithm [2],[5],[6] is

$$\mathcal{P}^0: \qquad -\nabla \cdot (A(x)\nabla U) = f \qquad \text{in } \Omega, \qquad U|_{\partial\Omega} = 0,$$

where the solution of a cell problem depending on $a_M(\cdot)$ in W_x is used to determine the averaged tensor coefficient $A(x)$.

For several 1D and 2D test problems we have compared numerically u with U and $\widehat{U}$, where $\widehat{U}$ is a so-called H^1 correction of U, calculated a posteriori from U and the cell problem solutions. The dependency of the approximation error and the averaged coefficient on $\bar{\varepsilon}$ was shown and discussed.

There are many algorithms currently known for practical calculation of $A(\cdot)$ [3],[4]. Some of them (having the same local problem with periodic boundary conditions) can be recovered by a special choice of the two-scale extension. This gives them a justification by an asymptotical argument as well as some freedom for improvement and generalization. The two-scale extensions might be also useful for better understanding fundamental questions related to upscaling.

References

[1] G. Allaire, *Homogenization and two-scale convergence*, SIAM J. Math. Anal. **23**, No. 6 (1992), 1482-1518.

[2] A. Bensoussan, J.L. Lions and G. Papanicolaou, *Asymptotic Analysis for Periodic Structure*, North Holland, Amsterdam, 1978.

[3] Y. Chen, L.J. Durlofsky, M. Gerritsen, X.H. Wen, *A coupled local-global upscaling approach for simulating flow in highly heterogeneous formations*, Advances in Water Resources, **26** (2003), 1041-1060.

[4] C.L. Farmer, *Upscaling: A Review*, Numerical Methods in Fluids, **40** (2002), 63-78.

[5] E. Sanchez-Palencia, *Non-Homogeneous Media and Vibration Theory*, Springer-Verlag, Berlin, 1980.

[6] V.V. Zhikov, S.M. Kozlov, O.A. Oleinik, *Homogenization of Differential Operators and Integral Functionals*, Springer-Verlag, Berlin, 1994.

On averaging of the non-periodic conductivity coefficient using two-scale extension

Vsevolod Laptev

(joint work with S. Belouettar)

It is usually difficult to predict a global behavior of some process in heterogeneous media (for example composite/porous materials) although the physics of the process might be well understood locally. The reason lying in the complexity of the microstructure gives rise to different upscaling (averaging, homogenization) methods.

Heterogeneities having periodical structure play a central role in the development of upscaled models. From one side they represent an important particular

case of general heterogeneous media and on the other there are well developed mathematical techniques (e.g. two-scale asymptotic expansion method), which help to derive formally and often rigorously the upscaled model. As a result many physical processes in heterogeneous media having periodical microstructures are well investigated both from theoretical and from practical points of view and the periodicity assumption is usually a starting point for the upscaling procedures. Although this assumption is valid in only limited number of cases, mostly in artificially created materials. Therefore for practical purposes one should be able to deal with non- periodical structures.

In this presentation we define a notion of two-scale extension for a given non-periodic coefficient and present several ways to construct it. The main purpose is to adapt the upscaling results known for problems with (locally) periodic coefficients to problems with non-periodic coefficients. The locally periodic coefficient is a natural generalization of a purely periodic coefficient. It is often used in homogenization as a given two-scale function. Its form determines the sequence of problems depending on a small parameter as well as the final form of the upscaled model. Instead of treating the locally periodic coefficient as a given function we try to construct it (two-scale extension) in such a way that the resulting sequence of problems passes through the given problem with non-periodic coefficient. This is a key idea of using two-scale extensions. Different two-scale extensions lead to different upscaled problems.

The classical averaging algorithm for the second order elliptic equation with the locally periodic coefficient is used to calculate an effective coefficient for the particular non-periodic problem by solving finite (or infinite) number of cell problems, covering the whole domain.

The discontinuity of the proposed two-scale extensions can be partially compensated by "admissibility" in the sense of the two-scale convergence method.

The averaging approach was tested on several problems in 1D and 2D with randomly generated conductivity.

Multiscale preconditioning

Nicolas Neuss

1. Introduction

In this contribution, we consider the numerical solution of discrete equations arising from the discretisation of a multiscale problem. We show that the multiscale nature can be used to construct an efficient preconditioner. In contrast to [8], we do not require conditions of cell symmetry here, but require a sufficient resolution of the fine scale problem which allows to transfer the continuous approximation result of homogenisation theory to the discrete situation.

2. Microscopic problem

For $k \geq 1$, let $A \in C^{0,1}_{\text{per}}(\mathbb{R}^d, \mathbb{R}^{d\times d})$ be a Lipschitz-continuous, 1-periodic, matrix-valued function which satisfies $A_{ij}(x) = A_{ji}(x)$ for all $x \in \mathbb{R}^d$ together with the ellipticity and continuity condition that there exist constants $0 < \lambda_1 \leq \lambda_2 < \infty$ such that

$$\lambda_1|\xi|^2 \leq (\xi, A(x)\xi) \leq \lambda_2|\xi|^2\,, \quad x \in \mathbb{R}^d\,. \tag{2.1}$$

Now, let $\varepsilon = 1/N$ for some $N \in \mathbb{N}$ and $\Omega = (0,1)^d$. Given $f \in L2(\Omega)$, we search for $u^\varepsilon \in H1_0(\Omega)$ satisfying

$$a^\varepsilon(u^\varepsilon, v) := \int_\Omega \nabla v(x) A(\frac{x}{\varepsilon})\nabla u^\varepsilon(x)dx = \int_\Omega f(x)v(x)dx \tag{2.2}$$

for all test functions $v \in H1_0(\Omega)$. The Lemma of Lax-Milgram then guarantees unique solvability of this problem.

3. Homogenised problem

Homogenisation theory (c.f. [7]) proves that, for small ε, a good approximation of the solution u^ε of problem (2.2) can be constructed by solving the following *homogenised* problem: find $u0 \in H1_0(\Omega)$ satisfying

$$a0(u0, v) := \int_\Omega \nabla v : A0\,\nabla u0 dx = \int_\Omega v\, f dx, \quad v \in H1_0(\Omega), \tag{3.1}$$

where the constant coefficient matrix $A0$ is defined as an average

$$A0_{ij} = \int_Y \left(A_{ij}(y) + \sum_{l=1}^{d} A_{il}(y)\frac{\partial N_j}{\partial y_l}(y) \right) dy, \tag{3.2}$$

over $Y = (0,1)^d$ with functions $N_k \in \dot{H}^1(Y), k = 1, \ldots, n$ satisfying

$$a(N_k, V) := \int_Y \nabla V(y) : A(y)\nabla N_k(y)dy = -\int_Y \nabla\varphi(y) : A(y)e_k dy \tag{3.3}$$

for all $V \in \dot{H}^1(Y)$, where $e_k \in \mathbb{R}^d$ is the vector with components $(\delta_{jk})_{j=1,\ldots,n}$.

Theorem 1. *Let u^ε be the solution of (2.2), N_k be the solutions of (3.3), and $u0$ be the solution of (3.1). Consider the first-order corrector*

$$u^{1,\varepsilon}(x) := u0(x) + \varepsilon \sum_{k=1}^{d} N_k(\frac{x}{\varepsilon})\frac{\partial u0}{\partial x_k}(x) \tag{3.4}$$

and the boundary correction $\theta^\varepsilon = \theta^\varepsilon(\nabla u0)$ defined by $\theta^\varepsilon = u^{1,\varepsilon}$ on $\partial\Omega$ and

$$\int_{\Omega^\varepsilon} \nabla v^\varepsilon(x) \cdot A^\varepsilon(x)\nabla\theta^\varepsilon(x)dx = 0, \quad v^\varepsilon \in V_0^\varepsilon\,. \tag{3.5}$$

Then we have the error estimate

$$\|\nabla(u^\varepsilon - u^{1,\varepsilon} + \theta^\varepsilon)\|_{L2(\Omega^\varepsilon)} \leq C\varepsilon\|f\|_{L2(\Omega)}. \tag{3.6}$$

Proof. See, e.g., [7], [8], [9]. □

4. Discretisation

Let $T_{\hat{h}}$ denote a quasi-uniform mesh of the unit cell Y which fits across the identified boundary ∂Y. Thus, $T_{\hat{h}}$ can be scaled by ε and repeated periodically, such that we obtain a ε-periodic mesh T_h on Ω of meshsize $h = \varepsilon\hat{h}$. Both T_h and $T_{\hat{h}}$ may contain simplices or tensor products of simplices (i.e. triangles and/or quadrangles for $n = 2$). With T_H we denote the cube mesh of meshsize $H = \varepsilon$.

On T_h, we discretise problem (2.2) with standard conforming finite elements of order 1 and denote the ansatz space with Dirichlet boundary conditions by $S1_{h,0}$. In the same way, we discretise problem (3.3) on $T_{\hat{h}}$, and denote the ansatz space consisting of periodic functions with zero mean value by $S1_{\hat{h}}$. Solving the arising finite-dimensional problem gives us approximations $\mathbf{N}_{\hat{h}} \in S_{\hat{h}}$ of N, and using $\mathbf{N}_{\hat{h}}$ instead of $\mathbf{N}_{\hat{h}}$ in (3.2) gives us an approximation $\mathbf{A}^0_{\hat{h}}$ to $\mathbf{A}^0$. Finally, we can use $\mathbf{A}^0_{\hat{h}}$ for discretizing (3.1) using an ansatz space $S1_{H,0}$ consisting of conforming multilinear finite elements on T_H.

Remark 4.1. *Because of Theorem 1, the most interesting case is $h \leq \varepsilon 2$, because otherwise the solution to the homogenised problem (3.1) together with a boundary layer approximation according to (3.5) would yield an equally good or even better approximation at lower computational cost.*

5. Multiscale preconditioning

If h is small (e.g. of size $\varepsilon 2$ as indicated in Remark 4.1), the efficient solution of problem (2.2) on $S1_{h,0}$ becomes large, and efficient solution techniques are called for. Here, we propose to use a domain decomposition with respect to the subdomains

$$\Omega^{\varepsilon}_{\vec{k}} = \Omega \cap \varepsilon(\vec{k} + (-1,1)^d)\,, \quad 1 \leq \max_{i=1,\ldots,d} |k_i| \leq \frac{1}{\varepsilon} - 1 \tag{5.1}$$

together with a coarse space defined by solving the discrete homogenised problem. More precisely, let $V_h = S1_{h,0}$, and for $1 \leq i \leq m = \frac{1}{(1/\varepsilon - 1)^d}$, let $i \mapsto \vec{k}^{(i)}$ be a numbering of the set $\{\vec{k} \in \mathbb{Z}^d : 0 \leq k_j \leq \frac{1}{\varepsilon} - 1\}$.

Theorem 2. *Let*

$$V_i = \{v \in V_h : \mathrm{Supp}(v) \subset \Omega_{\vec{k}^{(i)}}\}\,, \quad i = 1, \ldots, n\,, \tag{5.2}$$

and set $V_0 = \mathrm{Range}(p^h_H)$, where $p^h_H : V_H \to V_h$ is defined as

$$u_H \mapsto I_h \circ (u_H + \varepsilon \sum_{k=1}^{d} N_k \frac{\partial u_H}{\partial x_k}) \tag{5.3}$$

with $I_h : C0(\Omega) \to S_h$ denoting the projection operator defined by nodal evaluation. For $i = 1, \ldots, n$ let $A_i : V_i \to V_i'$ be defined by restricting the bilinear form a^{ε} from (2.2) to V_i. For $i = 0$, choose A_0 to be a discretisation of the homogenised problem.

ε	1/2	1/4	1/8	1/16
ρ	0.0004	0.36	0.45	0.5

TABLE 1. Convergence rates for solving the diffusion problem.

If $\hat{h} \lesssim \varepsilon$, and $H \sim \varepsilon$, then every $v \in V_h$ has a decomposition $v = \sum_{i=0}^{n} v_i$ with $v_i \in V_i$ such that for some $K_1 > 0$ independent of ε and h, we have

$$\Big(\sum_{i=0}^{n} \|v_i\|_{A_i}^2 \Big)^{\frac{1}{2}} \leq K_1 \|v\|_A \,. \tag{5.4}$$

and there exists $K_2 > 0$ such that for arbitrary $u_i \in V_i$,

$$\sum_{k=0}^{n} \sum_{i=0}^{n} a(v_k, u_i) \leq K_2 \|v\|_A \Big(\sum_{i=1}^{n} \|u_i\|_{A_i}^2 \Big)^{\frac{1}{2}} \,. \tag{5.5}$$

Proof. For $v_h \in V_h$, let v_H denote the solution of

$$a_H(v_H, w_H) = a^{\varepsilon}(v_h, p_H^h w_H) \,, \quad w_H \in V_H \,,$$

and set $v_0 = p_H^h v_H$. Then it is a straightforward combination of standard finite element error estimates and Theorem 1 to show that the remainder $w = v_h - v_0$ satisfies $\|w\|_{L2(\Omega)} \lesssim \varepsilon$. This is sufficient to show that (5.4) is satisfied for the decomposition $w = \sum_{i=1}^{n} v_i$, if v_i is defined as $I_h \circ (w\psi_i)$ for $\{\psi_i\}_{i=1,\ldots,m}$ denoting the set of standard nodal basis functions in S_H with $\psi_i(\vec{k}^{(j)}) = \delta_{ij}$. (5.5) follows, because no more than $2^d + 1$ of the subspaces have nonempty intersection. □

Corollary 3. *A parallel subspace correction using the subspaces $V_0, \ldots, V_n$ defined above yields an optimal preconditioner for problem (2.2) discretised on $V_h = S1_{h,0}$.*

6. Numerical results

We look at a special case of problem (2.2), with a scalar diffusion coefficient

$$\mathbf{A}_{ij}(y) = \frac{\delta_{ij}}{(2 + 1.8\sin(2\pi y_1))(2 + 1.8\sin(2\pi y_2))} \,.$$

We discretize and solve this problem according to Sections 4 and 5. As solver for the local subproblems we used a simple CG iteration with Jacobi preconditioning. The implementation was done using the program FEMLISP, see [5]. We vary $\hat{h} = \varepsilon$, $H = \varepsilon$, $h = \varepsilon 2$ simultaneously with ε and obtain the convergence rates shown in Table 1. Of course, a more practical version of this algorithm would not use an exact solver on each subspace, but an approximate hierarchical solver. The numerical results do not change significantly in this case and also Theorem 2 can be adapted easily.

Finally, we want to remark that the technique described here can also be applied to higher order discretisations, systems of equations like linear elasticity, and even to situations where the micro- and macroproblem are of rather different character. For example, consider the problem of solving Stokes equation in a domain Ω^{ε} with

ε	1/2	1/4	1/8	1/16
ρ	0.65	0.69	0.69	0.7

TABLE 2. Convergence rates for solving the Stokes problem.

periodically distributed holes of size ε, with no-slip boundary conditions posed on $\partial\Omega^\varepsilon$. Here the homogenised equation is a diffusion equation (Darcy's law) with a certain permeability which can be computed by solving flow problems on a representative cell. Preliminary results for $\hat{h} = \text{const}$ (which corresponds to the setting of [8]) and a very cheap choice of overlapping subspaces centered at vertices of T_h show a robust convergence independent of ε, see Table 2. However, the theoretical analysis of this method as well as the analogous method with $\hat{h} \sim \varepsilon$ is still open.

References

[1] N. Bakhvalov and G. Panasenko. *Homogenisation: Averaging Processes in Periodic Media*. Kluwer, Dordrecht, 1989.

[2] F. Brezzi and L. D. Marini. *Augmented spaces, two-level methods, and stabilizing subgrids*. Internat. J. Numer. Meth. Fluid, 40:31–46, 2002.

[3] W. E and B. Engquist. The heterogeneous multi-scale method. *Comm. Math. Sci.*, 1:87–133, 2003.

[4] C. L. Farmer Upscaling: A review. in *Proc. ICFD Conference on Num. Meth. Fluid Dyn., Oxford, UK*, 2001.

[5] Femlisp. Homepage. `http://www.femlisp.org`.

[6] T. Y. Hou, X. H. Wu, and Z. Cai. Convergence of a multiscale finite element method for elliptic problems with rapidly oscillating coefficients. *Math. Comp.*, 68:913–943, 1999.

[7] V. V. Jikov, S. M. Kozlov, and O. A. Oleinik. *Homogenisation of Differential Operators and Integral Functionals*. Springer–Verlag, Berlin, 1994.

[8] N. Neuss, W. Jäger, and G. Wittum. Homogenization and multigrid. *Computing*, 66:1–26, 2001.

[9] M. Neuss-Radu. The boundary behavior of a composite material. *M2AN*, 35:407–435, 2001.

Numerical analysis of coarse-grained stochastic lattice dynamics

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(joint work with Markos A. Katsoulakis, Alexandros Sopasakis)

Introduction. In [13, 16] the authors started developing systematic mathematical strategies for the coarse-graining of microscopic models, focusing on the paradigm of stochastic lattice dynamics and the corresponding MC simulators. In these papers a hierarchy of coarse-grained stochastic models–referred to as coarse-grained MC (CGMC) – was derived from the microscopic rules through a stochastic closure argument. The resulting *stochastic coarse-grained processes* involve Markovian birth-death and generalized exclusion processes and their combinations.

The CGMC algorithms discussed here are related to a number of methods involving coarse-graining at various levels. For example, corrections to the CGMC

dynamics from the renormalization group flow given by RGMC and multigrid MC methods [2, 6, 8] will improve approximation properties of CGMC. Various coarse-graining approaches may yield explicitly derived stochastic coarse models such as CGMC or [9, 11, 18], or can be statistics-based [19] or may rely on on-fly simulations, e.g., equation-free [17], heterogeneous multi-scale [7] or multi-scale FEM methods [10]. A systematic approach to upscaling of stochastic systems has been developed in [1, 4, 3, 5].

Microscopic lattice models. The presented analysis applies to the class of Ising-type lattice systems. For the sake of simplicity we assume that the computational domain is defined as the discrete periodic lattice $\Lambda_N = \frac{1}{n}\mathbb{Z}^d \cap \mathbb{T}$ which represents discretization of the d-dimensional torus $\mathbb{T} = [0,1)^d$. The microscopic degrees of freedom or the microscopic order parameter is given by the spin-like variable $\sigma(x)$ defined at each site $x \in \Lambda_N$. In this paper we discuss only the case of discrete spin variables, i.e., $\sigma(x) \in \Sigma$ with $\Sigma = \{-1, 1\}$, $\Sigma = \{0, 1\}$ (Ising model) or $\Sigma = \{0, 1, \dots s\}$ (Potts models). We denote $\sigma = \{\sigma(x) \,|\, x \in \Lambda_N\}$ a configuration of spins on the lattice, i.e., an element of the configuration space $\mathcal{S}_N = \Sigma^{\Lambda_N}$. The interactions between spins at a given configuration σ are defined by the microscopic Hamiltonian

$$H(\sigma) = -\frac{1}{2} \sum_{x \in \Lambda_N} \sum_{y \neq x} J(x-y)\sigma(x)\sigma(y) + \sum_{x \in \Lambda_N} h(x)\sigma(x)\,, \tag{0.1}$$

where $h(x)$ denotes the external field at the site x. The two-body inter-particle potential J accounts for interactions between individual spins. We consider the class of potentials with the given interaction range L, $J(x-y) = \frac{1}{L^d} V\left(\frac{n}{L}|x-y|\right)$, $x, y \in \Lambda_N$, where $V(r) = V(-r)$, $V(r) = 0$ if $|r| \geq 1$. The canonical equilibrium state is given in terms of the Gibbs measure.

The microscopic dynamics is defined as a continuous-time jump Markov process that defines a change of the spin $\sigma(x)$ with the probability $c(x, \sigma; \xi)\Delta t$ over the time interval $[t, t + \Delta t]$. The probability that over the time interval $[t, t + \Delta t]$ the spin at the site $x \in \Lambda_N$ spontaneously changes from $\sigma_t(x)$ to a new value in the state space $\xi \in \Sigma$ is $c(x, \sigma; \xi)\Delta t + O(\Delta t^2)$. We denote the resulting configuration $\sigma^{x,\xi}$. In the case of the Ising-type state space and spin-flip dynamics we omit ξ in this notation. The generator $\mathcal{L} : L^\infty(\mathcal{S}_N) \to L^\infty(\mathcal{S}_N)$ of the Markov process acting on a bounded test function $\phi \in L^\infty(\mathcal{S}_N)$ defined on the space of configurations is given by

$$(\mathcal{L}f)(\sigma) = \sum_{x \in \Lambda_N} \int_\Sigma c(x, \sigma; \xi) \left(\phi(\sigma^{x,\xi}) - \phi(\sigma)\right) \, d\xi\,. \tag{0.2}$$

We require that the dynamics is of the relaxation type such that the invariant measure of this Markov process is the Gibbs measure.

Approximation of the coarse-grained process The coarse-graining is defined in a geometric way introducing the coarse-grained observables as block-spin variables. We define the coarse-graining operator $\mathbf{T} : \mathcal{S}_N \to \mathcal{S}^c_{M,q}$, where the coarse configuration space $\mathcal{S}^c_{M,q}$ is defined on the coarse lattice Λ^c_M, and with the new

state space Σ^c. The coarse configuration $\eta = \mathbf{T}\sigma \in \mathcal{S}^c_{M,q}$ is defined on a smaller lattice with M lattice sites and with the coarse state space Σ^c for the new lattice spins $\eta(k)$. The parameter q defines the coarse-graining ratio. The operator $\mathbf{T}$ induces an operator $\mathbf{T}_*$ on the space of probability measures $\mathbf{T}_* : \mu(\sigma) \mapsto \mu^c(\eta) := \mu\{\sigma \in \mathcal{S}_N \,|\, \mathbf{T}\sigma = \eta\}$. For example, the projection operator defines the block spin at the coarse site k as $(\mathbf{T}\sigma)(k) := \sum_{x\in C_k} \sigma(x)$. Given the Markov process $(\{\sigma_t\}_{t\geq 0}, \mathcal{L})$ with the generator $\mathcal{L}$ we obtain a coarse-grained process $\{\mathbf{T}\sigma_t\}_{t\geq 0}$ which is *not*, in general, a Markov process. From the computational point of view this may cause significant difficulties should sampling of such a process be implemented on the computer. Therefore we derive an *approximating* Markov process $(\{\eta_t\}_{t\geq 0}, \bar{\mathcal{L}}^c)$ which can be easily implemented once its generator is given explicitly.

We define the configuration δ_k defined on the coarse state space is equal to zero at all sites except the site $k \in \Lambda^c_M$ where it is equal 1. The exact generator for the coarse process can be written in the form

$$\mathcal{L}^c\psi(\eta) = \sum_{k\in\Lambda^c_M} c_a(k)\left[\psi(\eta+\delta_k) - \psi(\eta)\right] + \sum_{k\in\Lambda^c_M} c_d(k)\left[\psi(\eta-\delta_k) - \psi(\eta)\right], \tag{0.3}$$

where the new rates are $c_a(k) = \sum_{x\in C_k} c(x,\sigma)(1-\sigma(x))$, $c_d(k) = \sum_{x\in C_k} c(x,\sigma)\sigma(x)$ correspond to the adsorption and desorption processes. Now it is reasonable to propose an approximating Markov process, which for the case of desorption/adsorption is a *birth-death* process $\{\eta_t\}_{t\geq 0}$ defined on the state space $\Sigma^c = \{0, 1, \dots q\}$. This process is defined by the generator $\bar{\mathcal{L}}^c$ of the form (0.3) where the rates c_a and c_d are replaced by approximate rates $\bar{c}_a(k,\eta) = d_0(q-\eta(k))$, and $\bar{c}_d(k,\eta) = d_0\eta(k)e^{-\beta\bar{U}(\eta)}$. The new interaction potential $\bar{U}(\eta)$ represents the approximation of the original interaction $U(\sigma)$,

$$\bar{U}(l,\eta) = \sum_{\substack{k\in\Lambda^c_M \\ l\neq k}} \bar{J}(l,k)\eta(k) + \bar{J}(0,0)(\eta(l)-1) - \bar{h}(l)\,. \tag{0.4}$$

In the talk we present detailed derivation of the approximating process $(\{\eta_t\}_{t\geq 0}, \bar{\mathcal{L}}^c)$. Furthermore, we analyse the approximation properties of this process from the two different points of view deriving *information theory estimates* and *weak convergence estimates*. As an example of the former we discuss theorems of the following type

Theorem 1 ([15])**.** *Suppose the process $\{\eta_t\}_{t\in[0,T]}$, defined by the coarse generator $\bar{\mathcal{L}}^c$ is the coarse approximation of the microscopic process $\{\sigma_t\}_{t\in[0,T]}$ then for any $q < L$ and N, $Mq = N$ the information loss as $q/L \to 0$ is*

$$\frac{1}{N}\mathcal{R}\left(\mathbf{T}_* Q_{\mathbf{T}_*\sigma_0,[0,T]} \,|\, Q^c_{\eta_0,[0,T]}\right) = T\,O\left(\frac{q}{L}\right) \tag{0.5}$$

This gives an estimate on *relative entropy* $\mathcal{R}$ of the coarse-grained process in terms of the ratio between the coarse-graining level q and the interaction range L.

In many practical MC simulations the main goal is to estimate averages (expected values) of specific observables. Therefore it is natural to analyse the weak error, defined as the quantity $e_w := |\mathbb{E}_S[\mathbf{T}\sigma_t] - \mathbb{E}_S[\eta_t]|$, where the expectation

$\mathbb{E}_S[\mathbf{T}\sigma_t]$ is defined for the path conditioned on the initial configuration $\mathbf{T}\sigma_0 = S$ and $\mathbb{E}_S[\eta_t]$ on $\eta_0 = S$. We discuss results of the following type:

Theorem 2 ([14], *Weak error*)**.** *Let $\phi \in L^\infty(\mathcal{S}_N)$ be a test function (observable) on the microscopic space. Given the initial configuration Let $(\{\sigma_t\}_{t\geq 0}, \mathcal{L})$ be a microscopic process with $\mathbf{T}\sigma_0 = S$ and $(\{\gamma_t\}_{t\geq 0}, \mathcal{L}^\gamma)$ be the corresponding synthetic process, then the weak error satisfies for $0 < T < \infty$*

$$|\mathbb{E}_S[\phi(\sigma_T)] - \mathbb{E}_S[\phi(\gamma_T)]| \leq C_T \left(\frac{q}{L}\right)^2, \tag{0.6}$$

where the constant C_T is independent of q and L but depends on T.

We propose a technical tool (the synthetic process $\{\gamma_t\}_{t\geq 0}$) that allows us to compare the projected process $\{\mathbf{T}\sigma_t\}_{t\geq 0}$ with the approximating process $\{\eta_t\}_{t\geq 0}$. We refer to [14] for more details and proofs as well as numerical simulations that confirm the error analysis and demonstrate also good approximation of quantities that depend on the path. We also discuss computational speed-up and efficiency.

References

[1] D. Ron A. Brandt and D. J. Amit. Multi-level approaches to discrete-state and stochastic problems. In W. Hackbusch and U. Trottenberg, editors, *Multigrid Methods, II*, pages 66–99. Springer-Verlag, 1986.

[2] M. Galun A. Brandt and D. Ron. Optimal multigrid algorithms for calculating thermodynamic limits. *J. Stat. Phys.*, 74:313–348, 1994.

[3] D. Bai and A. Brandt. Multiscale computation of polymer models. In J. Bernholc A. Brandt and K. Binder, editors, *Multiscale Computational Methods in Chemistry and Physics*, volume 177 of *NATO Science Series: Computer and System Sciences*, pages 250–266. IOS Press, 2001.

[4] A. Brandt. Multigrid methods in lattice field computations. *Nucl. Phys. B*, 26:137–180, 1992.

[5] A. Brandt and V. Ilyin. Multilevel monte carlo methods for studying large-scale phenomena in fluids. *J. of Molecular Liquids*, 105:253–256, 2003.

[6] A. Brandt and D. Ron. Renormalization multigrid: Statistically optimal renormalization group flow and coarse-to-fine Monte Carlo acceleration. *J. Stat. Phys.*, 102:231–257, 2001.

[7] Weinan E and Bjorn Engquist. Multiscale modeling and computation. *Notices Amer. Math. Soc.*, 50(9):1062–1070, 2003.

[8] J. Goodman and A. D. Sokal. Multigrid monte carlo methods for lattice field theories. *Phys. Rev. Lett.*, 56:1015–1018, 1986.

[9] Q. Hou, N. Goldenfeld, and A. McKane. Renormalization group and perfect operators for stochastic differential equations. *Phys. Rev. E*, 6303:6125, 2001.

[10] Thomas Y. Hou and Xiao-Hui Wu. A multiscale finite element method for PDEs with oscillatory coefficients. In *Numerical treatment of multi-scale problems (Kiel, 1997)*, volume 70 of *Notes Numer. Fluid Mech.*, pages 58–69. Vieweg, Braunschweig, 1999.

[11] A. E. Ismail, G. C. Rutledge, , and G. Stephanopoulos. Multiresolution analysis in statistical mechanics. I, II. *J. Chem. Phys.*, 118:4414, 2003.

[12] M. A. Katsoulakis, A. J. Majda, and D. G. Vlachos. Coarse-grained stochastic processes and Monte Carlo simulations in lattice systems. *J. Comput. Phys.*, 186(1):250–278, 2003.

[13] M. A. Katsoulakis, A. J. Majda, and D. G. Vlachos. Coarse-grained stochastic processes for microscopic lattice systems. *Proc. Natl. Acad. Sci. USA*, 100(3):782–787 (electronic), 2003.

[14] M. A. Katsoulakis, P. Plecháč, and A. Sopasakis. Error control and analysis in coarse-graining of stochastic lattice dynamics. 2005. submitted to SIAM J. Sci. Comp.

[15] M. A. Katsoulakis and J. Trashorras. Information loss in coarse-graining of stochastic particle dynamics. Technical report, University of Massachussets, 2004. submitted to J. Stat. Phys.
[16] M. A. Katsoulakis and D. G. Vlachos. Hierarchical kinetic Monte Carlo simulations for diffusion of interacting molecules. *J. Chem. Phys*, 112(18), 2003.
[17] I. G. Kevrekidis, C. W. Gear, and G. Hummer. Equation-free: the computer aided analysis of complex multiscale systems. *AIChE Journal*, 50(7):1346–1355, 2004.
[18] A. J. Majda, I. Timofeyev, and E. Vanden Eijnden. A mathematical framework for stochastic climate models. *Comm. Pure Appl. Math.*, 54:891, 2001.
[19] F. Muller-Plathe. Coarse-graining in polymer simulation: from the atomistic to the mesoscale and back. *Chem. Phys. Chem.*, 3:754, 2002.

Toward upscaling of flow in deformable porous media

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(joint work with Oleg Iliev and Andro Mikelic)

Many important engineering applications such as ground water flow, reservoir engineering, various filtering devices used in chemical processing, to name a few, involve flow in deformable porous media [3]. The upscaling of deformable porous media involves two coupled physical processes. At the microscopic (pore) level one has a deformable skeleton surrounded by a fluid. The solid is usually described by the Lamé equations of linear elasticity and the fluid by the Stokes equations.

In general the upscaling problem for poroelasticity medium is not separable even when the microscopic heterogeneity (the pores) is well separated. This is due to the fact that the skeleton can deform arbitrarily large due to different parameters such as macroscopic displacements, pressure and velocity. However, for certain classes of poroelastic problems it is possible to derive macroscopic equations.

The problem has been first studied experimentally by Biot [5, 3] who formulated the macroscopic equations for the effective medium. The application of the asymptotic homogenization method [4, 8, 2, 9] has lead to theoretical justification of Biot's equation [1, 8, 6] along with appropriate cell problems from which the macroscopic parameters can be computed numerically. The macroscopic equations are derived under the assumption that the solid-fluid interface displacements are small compared to the pore size. This allows to apply interface conditions at the initial position of the fluid solid interface and important properties such as periodicity of the unit cell are preserved. A wide range of applications, for example, in soil acoustics fall within these limits. However, many other important engineering problems cannot be considered under such severe restrictions.

Under more relaxed assumptions Lee and Mei [7] have derived a nonlinear macroscopic governing equations by assuming periodic media and allowing the interface displacements to be of the same order as the pore size. It is also assumed that the total deformation of a the unit-cell can be decomposed into a rigid-body motion of each unit cell after which the interface displacement become infinitely small in the new reference frame. Under certain symmetry assumptions of the

unit cell prior to the deformation it is shown that macroscopic equations reduce to Biot's law.

The focus of this work is the case when, due to problem parameters such as macroscopic pressure and displacement, the fluid-solid interface deforms considerably at the pore level. When the interface cannot be approximated by a rigid body motion of its initial position it is necessary to consider the Fluid-Structure Interaction (FSI) problem at pore level as a problem with an unknown interface.

Therefore, this work first formulates the stationary FSI problem in terms of incompressible Newtonian fluid and a linearized elastic solid. The flow is assumed to be characterized by very low Reynolds number and is described by the Stokes equations. The strains in the solid are small allowing for the solid to be described by the Lame equations. However, no restrictions are applied to the magnitude of the displacements with respect to the pore size, thus leading to strongly coupled, nonlinear fluid-structure problem. Then, under certain assumptions, an asymptotic solution to the FSI problem is developed for a long channel geometry. A nonlinear Darcy-type upscaled equation is obtained:

$$\frac{\partial}{\partial x}\left(\gamma^3(x)\frac{\partial p^0}{\partial x}\right) = 0, \tag{0.1}$$

where the channel runs along the x axis, $p^0(x)$ is the y-averaged pressure, and $\gamma(x)$ is the half-width of the fluid part of the channel. This width is found to depend on the channel geometry, solid material parameters and the y-averaged pressure:

$$\gamma(x) \approx 1 + \delta\frac{1}{\lambda_s + 2\mu_s}p^0(x), \tag{0.2}$$

Here λ_s and μ_s are the Lame constants for the solid, and δ is the thickness of the solid part of the channel.

Further, a numerical method for the FSI problem is developed and used to verify the analytical result. The microscale FSI problem is treated numerically by an iterative procedure which solves sequentially fluid and solid subproblems. Each of the two subproblems is discretized by finite elements and the fluid-structure coupling is reduced to an interface boundary condition. Numerical and asymptotic solutions are found to converge to each other, thus validating both the numerical solver and the analytical derivation (0.1), (0.2). Numerical computations are also used to perform permeability computations for different geometries.

In conclusion, while upscaling the FSI problem under such general conditions for arbitrary pore geometry is unlikely, the results in this work can be used to select parameters for numerical upscaling. Based on the indication from the long channel that the most important upscaling parameter is the averaged pore pressure various numerical upscaling schemes can be devised for more general geometries.

A more detailed description of the results is available in Technical report No.65, 2004 of Fraunhofer ITWM (www.itwm.fhg.de).

References

[1] J.-L. Auriault and E. Sanchez-Palencia, *Étude du comportement macroscopique d'un milieu poreux saturé déformable*, Journal de Mécanique, **16**, (1977), 575-603.

[2] N. Bakhvalov and G. Panasenko, *Homogenization: Averaging Processes in Periodic Media*, Kluwer Academic Publishers, Dordrecht, 1990.

[3] J. Bear, *Dynamics of Fluids in Porous Media*, Dover, New York, 1972.

[4] A. Bensoussan, J.L. Lions and G. Papanicolaou, *Assymptotic Analysis for Periodic Structures*, North-Holland, Amsterdam, 1978.

[5] M.A. Biot, *General theory of three dimensional consolidation*, J. Appl. Phys. **12** (1941), 155-164.

[6] C.C. Mei and J.-L. Auriault, *Mechanics of Heterogeneous Porous Media with Several Spatial Scales*, Proc. Roy. Soc. Lond. A, **426**, (1989), 391-423.

[7] C.K. Lee and C.C. Mei, *Re-examination of the equations of poroelasticity*, Int. J. Eng. Sci., **35**, (1997), 329-352.

[8] E. Sanchez-Palencia, *Non-Homogeneous Media and Vibration Theory*, Springer-Verlag, Berlin, 1980.

[9] V.V. Zhikov, S.M. Kozlov and O.A. Oleinik, *Homogenization of Differential Operators and Integral Functionals*, Springer-Verlag, Berlin, 1994.

On numerical upscaling of flow in anisotropic porous media

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(joint work with Oleg Iliev)

Introduction. Multiscale problems can be conditionally subdivided to two large groups. In the first, solution at the fine scale is sought, while solution at the corse scale is a target for the second group. Typical examples from the second group are flow in porous media, heat conductivity of heterogeneous materials, etc. Here we are interested in such a class of problems, for which the mathematical model (including the coefficients) is given at the fine scale, while the model (equation and/or coefficients) and the solution are sought at the coarse scale. That is, given fine scale model L_f, b_f: $L_f u_f = b_f$, find L_c, b_c, u_c such that $L_c u_c = b_c$ and $\| < u_f >_B - u_c \|_A$ is small. Here B, A are some proper operators defining averaging and a norm, respectively.

Essential success was achieved during the last decades in the studies of problems with clearly separated fine and coarse scales (e.g., periodic microstructure, or statistically homogeneous porous media). When the fine and the coarse scales can be decoupled, solving a multiscale problem reduces to one way two-stage procedure: i) solve fine scale 'cell-problem" and use its solution to upscale the effective properties of the multiscale media; ii) solve coarse scale equations with the calculated effective coefficients. That is, a cell problem with a given L_f is solved, its solution is used to find L_c, and finally $L_c u_c = b_c$ is solved for any specified b_c.

The separation of scales, however, is not always possible, and developing numerical upscaling techniques for such problems is the subject of this presentation. An iterative local-global upscaling approach is proposed in [1] for simulating flow in highly heterogeneous formations with diagonal permeability tensor. Recall, that

we are interested only in the solution at the coarse scale, therefore we do not mention here the many multigrid and multilevel methods, which are used to solve multiscale problems when solution at the fine scale is the final target. Currently, we are working on further developments of the approach from [1] and here we present our first results.

Fine scale problem. In rectangular domain Ω we consider 2-D pressure equation obtained by combining the continuity equation ($\nabla \cdot u = f$) and Darcy's law ($u = -K \cdot \nabla p$) for steady state incompressible single phase flow in porous media

$$-\nabla \cdot (K \cdot \nabla p) = f, \quad \text{in } \Omega,$$

with full symmetric permeability tensor K. The tensor coefficients can be discontinuous, the following interface conditions are satisfied in such a case: $[p] = 0, \quad \left[K \frac{\partial p}{\partial \mathbf{n}}\right] = 0.$

The above equation is discretized with finite volume method. In the domain $\bar{\Omega}$, we consider $N_1 \times N_2$ control volumes. The pressure p is calculated at the centers of the control volumes. Each cell is split into four subcells by the lines joining adjacent cell centers. To discretize, we derive piecewise linear interpolating polynomials (linear in each subcell), such that the pressure gradient is constant in each subcell, the fluxes are continuous across the cell faces, and the pressure is continuous only in the centers of the cell's faces. Such approach was also used in [2, 4]. In the case when the solution is smooth, second order convergence for the pressure is observed even when the tensor coefficient is discontinuous.

Multiscale algorithm. The local-global iterative method from [1] could be considered as overlapping domain decomposition with a coarse grid correction, if the fine scale solution would be the target of the computations. On the other case, for a periodic or statistically homogeneous medium this approach is equivalent to applying homogenization for calculating the coarse scale coefficients, followed by solving the coarse scale problem. The algorithm is based on decomposing the computational domain into overlapping subdomains, solving local problems in each subdomain to calculate (homogenize) effective coefficients for this subdomain, and a solution of the coarse scale problem with the just calculated coefficients. Iterations over scales are carried out until convergence of the coarse scale coefficients. A critical part of the algorithm is how to choose the boundary conditions for each local problem, after the current coarse scale iterate is calculated. Certain summation along faces is suggested in [1]. However, this summation does not guarantee even monotonicity for the boundary condition, what contradicts to the essence of the considered elliptic problem. Instead, we suggest solving local one dimensional problems between each two coarse scale nodes as a part of the procedure for recovering the local boundary conditions for pressure for the local fine scale problem. Such a procedure preserves a piecewise constant solution. The effective permeability in each coarse block is calculated from the local solution in the way described in [3]. It guarantees the symmetry and positive definiteness of the coarse scale problem. The type and interpolation of fine scale (local) pressure boundary conditions from coarse scale ones is subject of further research.

Results. The discretization was first validated on problems with known solution, and second order convergence for the pressure was observed for discontinuous full tensor coefficient in the case of smooth solutions. Further, the following multiscale problem from [5] was considered.

$$K = \begin{pmatrix} a^\varepsilon(x,y) & 0 \\ 0 & a^\varepsilon(x,y) \end{pmatrix},$$

$$a^\varepsilon(x,y) = \frac{1}{6}\left(\frac{1.1+\sin(2\pi x/\varepsilon_1)}{1.1+\sin(2\pi y/\varepsilon_1)} + \frac{1.1+\sin(2\pi y/\varepsilon_2)}{1.1+\cos(2\pi x/\varepsilon_2)} + \frac{1.1+\cos(2\pi x/\varepsilon_3)}{1.1+\sin(2\pi y/\varepsilon_3)} + \right.$$
$$\left. \frac{1.1+\sin(2\pi y/\varepsilon_4)}{1.1+\cos(2\pi x/\varepsilon_4)} + \frac{1.1+\cos(2\pi x/\varepsilon_5)}{1.1+\sin(2\pi y/\varepsilon_5)} + \sin\left(4x^2y^2\right) + 1 \right),$$

where $\varepsilon_1 = 1/5$, $\varepsilon_2 = 1/13$, $\varepsilon_3 = 1/17$, $\varepsilon_4 = 1/31$, $\varepsilon_5 = 1/65$.

Numerical results (comparison with a reference solution on a fine grid) demonstrating the convergence of the pressure with O(H) are summarized below. We do not observe here the so called resonanse effect, this should be studied further.

$N_x \times N_y$	$m_x \times m_y$	$\left\|\left\langle p^f \right\rangle - p^c\right\|_C$
5×5	4×4	0.105836
10×10	4×4	0.049314
20×20	4×4	0.025197
50×50	4×4	0.011173
100×100	4×4	0.005172

The following notations are used here: $N_x \times N_y$ – number of coarse blocks; $m_x \times m_y$ – number of fine blocks; $\left\langle p^f \right\rangle$ – volume average of fine grid solution; p^c – coarse grid solution. In [5] authors reported that they did not succeed to solve this problem with both, HMM (Heterogeneous multiscale method) and MsFEM (Multiscale finite element method). Our algorithm solves the problem, probably a reason is the accurate discretuization for the fluxes used in our case.

Finally, a problem with anisotropic heterogeneous coefficients and unseparable scales was solved by the presented local-global iterative approach, results will be reported in a forthcoming paper.

Future work. As a long term perspective we plan:

1. to study the convergence of the global-local iterative algorithm in the case of tensor coefficients;
2. to analyse different boundary conditions for the auxiliary cell problems at the fine scale;
3. to analyse the influence of the order of approximation of the fluxes in solving the auxiliary cell problems on the convergence of the local-global iterative process;
4. to reformulate the local-global method as a kind of multigrid method with nonlinear coarse scale operator;
5. to develop approach with a limited usage of the fine scale information (in the

case when some a priori information for the variation of the coefficients is known. The last means that we would like to solve the coarse scale problem at a coarse scale price (i.e., cheap). Currently, we 'touch' each fine scale point, and in this sense the algorithm is still expensive in its memory requirements. The difference between, e.g., classical MG or AMG approaches which solve the fine scale problem, and the current algorithm, is in aiming at a convergence for the coarse scale solution here, and in using nonlinear coarse scale operator in solving a linear fine scale problem.

References

[1] Chen Y., Durlofsky L.J., Gerritsen M., Wen X.H., A coupled local-global upscaling approach for simulating flow in highly heterogeneous formations, Advances in Water Resources, 26(2003), pp. 1041–1060.

[2] Lee S.H., Durlofsky L.J., Lough M.F., Chen W.H., Finite difference simulation of geologically complex reservoirs with tensor permeabilities, SPE Reservoir Evaluat. Eng., 1(1998), pp. 567–574.

[3] Wu X.H., Efendiev Y., Hou T.Y., Analysis of upscaling absolute permeability, Discrete and continuous dynamical systems - series B, 2(2002), No.2, pp. 185–204.

[4] Ware A.F., Parrott A.K., Rogers C., A finite volume discretisation for porous media flows governed by non-diagonal permeability tensors, Proceedings of CFD95, Third Annual Conference of the CFD Society of Canada, Banff, Alberta, Canada, 25–27 June, 1995, ??(????), pp. ??–???.

[5] Ming P., Yue X., Numerical methods for multiscale elliptic problems, www.math.princeton.edu/multiscale/

Multiscale analytical solutions and homogenization of n-dimensional generalized elliptic equations

Rosangela F. Sviercoski

(joint work with A. W. Warrick, C. L. Winter)

1. Analytical solutions

Let $\Omega = [0,1]^n$, and $K : \Omega \to R$ such that $K(x) \in L^p(\Omega)$ with $1 < p < \infty$ and is one of the forms:

$$K(x) = \frac{c_1}{\sum_{i=1}^{n} k_i(x_i)} \quad (0.1) \qquad K(x) = \frac{c_2}{\prod_{i=1}^{n} k_i(x_i) + d_2} \quad (0.2)$$

The constants c_1, c_2, d_2 are nonzero so that $K(x) > 0$ for all $x \in \Omega$. For the form (0.2) we assume that for each $i = 1, .., n$, $k_i(x_i)$ is a positive function.

Theorem 1. *The weak solution $w_i(x) \in L^p(\Omega)$ for the BVP:*

$$(1.1) \qquad \begin{cases} \nabla \cdot (K(x) \nabla w_i(x)) = -\nabla \cdot (K(x) e_i) & x \in \Omega \\ w_i(x) = 0 & \text{along the } i^{th} \text{ boundary} \\ (K(x) \nabla w_i(x)) \cdot e_j = 0 & j \neq i \end{cases}$$

is given, up to a constant, by

$$w_i(x) = \frac{\int_0^{x_i} \frac{d\tau}{K(x_1,..,\tau,..,x_n)}}{\int_0^1 \frac{d\tau}{K(x_1,..,\tau,...,x_n)}} - x_i \tag{1.2}$$

Proof. The solution is obtained in 2-D, without loss of generality, by assuming that $w_i(x)$ is a separable function but not $K(x)$. See [7]. □

Corollary 2. *Under the assumptions of theorem 1,* $w(x) = \sum_{i=1}^n w_i(x) \in L^p(\Omega)$ *is the weak solution of:*

$$\begin{cases} \nabla \cdot (K(x) \nabla w(x)) = -\nabla \cdot (K(x)\mathbf{1}) & x \in \Omega \\ w(x) = \sum_{j \neq i} w_j(x) & \text{on each } i^{th} \text{ boundary} \end{cases} \tag{1.3}$$

with $\mathbf{1} = (1, ..1)$.

Corollary 3. *Under the assumptions of theorem 1,* $u(x) = \sum_{i=1}^n u_i(x) = \sum_{i=1}^n w_i(x) + x_i \in L^p(\Omega)$ *is the weak solution for the BVP*

$$\begin{cases} \nabla \cdot (K(x) \nabla u(x)) = 0 & x \in \Omega \\ u(x) = \sum_{j \neq i} u_j(x) + x_i + d & \text{on each } i^{th} \text{ boundary} \end{cases} \tag{1.4}$$

where d corresponds to any source (or sink) at the corner of the boundary.

Corollary 4. ***(Periodic case)*** *If* $K(x)$ *is a periodic function then the solutions to (1.1) and (1.3) are periodic and (1.2) satisfies:* **(i)** $\int_\Omega w_i(x)\,dx = 0$*;* **(ii)** $\int_\Omega \nabla w_i(x)\,dx = 0$*;* **(iii)** $\int_\Omega K(x) \frac{\partial w_i}{\partial x_j} dx = 0$ *for* $j \neq i$.

2. Homogenization of Linear Elliptic Equation

Consider the family of linear BVP's, with $K^\varepsilon \in L^p(\Omega)$ for all $\varepsilon > 0$:

$$\begin{cases} \nabla \cdot (K^\varepsilon(x) \nabla u^\varepsilon(x)) + f(x) = 0 & x \in \Omega \\ u(x) = u_D(x) & x \in \partial\Omega \end{cases} \tag{2.1}$$

Assume that the coefficient $K^\varepsilon(x) = K\left(\frac{x}{\varepsilon}\right) = K(y)$ for all $x \in \Omega$, meaning that K is $Y-$ periodic in R^n with ε a scale parameter. To obtain a homogenized approximation to (2.1), as in [2], [4] and [7], we consider the two-scale asymptotic expansion $u^\varepsilon(x) = u^0(x,y) + \varepsilon u^1(x,y)$, make this substitution into (2.1) and perform the two-scale differentiation. By using the periodicity assumption, we obtain that the solution $u^0(x) \in L^p(\Omega)$ satisfying the equation

$$\sum_{i,j=1}^n K^0_{i,j} \partial_{ij} u^0(x) + f(x) = 0 \tag{2.2}$$

approximates weakly in $L^p(\Omega)$, the solution of (2.1) as $\varepsilon \to 0$.

By setting $R_i(y) = \frac{1}{\int_0^1 \frac{d\tau}{K(y_1,y_2,\ldots,\tau,\ldots,y_n)}}$, the effective coefficient K^0 is defined by:

(2.3)
$$K_{ij}^0 = \int_Y K(y)\left(\delta_{i,j} + \partial_{y_i} w_i(y)\right) dy = \begin{bmatrix} \int_Y R_1 dY & 0 & \ldots & 0 \\ 0 & \int_Y R_2 dY & \ldots & 0 \\ : & : & : & : \\ 0 & 0 & \ldots & \int_Y R_n dY \end{bmatrix}$$

In [7] we had shown that this effective coefficient satisfies the Voigt-Reiss inequality and the known results in the literature are particular cases. We also had performed error analyses to obtain convergence properties for given $K(x)$ functions as well as numerical experiments demonstrating the applicability of this result to different types of BVP.

3. Homogenization of Nonlinear Elliptic Equation

Under the same assumptions on the coefficient function, as in the linear case, we obtain the weak approximation in $L^p(\Omega)$ of the solution $u^\varepsilon(x)$ of the nonlinear BVP:

(3.1)
$$\begin{cases} \nabla \cdot \left(K^\varepsilon\left(x, u^\varepsilon(x)\right) \nabla\left(u^\varepsilon(x)\right)\right) + f(x) = 0 & x \in \Omega \\ u^\varepsilon(x) = u_D(x) & x \in \partial\Omega \end{cases}$$

by $u^0(x)$, the solution of the BVP

(3.2)
$$\sum_{i,j=1}^{n} K_{ij}^0(u^0(x)) \partial_{ij} u^0(x) + f(x) = 0$$

Considering $P_i\left(y_1, .., y_n, u(x)\right) = \frac{1}{\int_0^1 \frac{d\tau}{K(y_1,.\tau,.,y_n,u(x))}}$, we have that the effective nonlinear coefficient is given as

(3.3)
$$K_{i,j}^0(u^0(x)) = \int_Y \begin{bmatrix} P_1 & 0 & \ldots & 0 \\ 0 & P_2 & .. & 0 \\ 0 & .. & P_i & 0 \\ 0 & .. & .. & P_n \end{bmatrix} dY$$

We also have shown the application of this result for different types of nonlinear BVP's, including an example with a body force.

4. Comparison with numerical results

By considering $K(x)$ in either (0.1) or (0.2), we have the following: (**a**) The elements in the diagonal are given as the arithmetic average of the harmonic average in each direction. (**b**) The effective coefficient is a diagonal matrix given that the original $K(x)$ is periodic. (**c**) K^0 is isotropic given that $K(x)$ is symmetric about the axis $x_1 = x_2$. Our hypothesis is that these facts hold for more general forms of coefficient functions. Indeed, in [7] we have compared the analytical form with the numerical results obtained by [1], where the rectangular inclusion type have been considered and we obtain a difference less than 10% on average. We also compared our analytical coefficient K^0 with the numerical approximations K^{num}

[3] and K^{bb} [6], where inclusions of different shapes have been considered. The table show that the differences, between K^{num} and K^0, again are less than 10% on average.

Shape	K^{num}	K^{bb}	K^0	Relative Difference (RD)
square	1.548	1.598	**1.409**	9 %
disk	1.516	1.563	**1.403**	8 %
lozenge	1.573	1.608	**1.417**	11 %

References

[1] Amaziane, B., Bourgeat, A., Koebbe, J. *Numerical Simulation and Homogenization of Two-Phase Flow in Heterogeneous Porous Media*, Transport in Porous Media 6:519-547, (1991).

[2] Bensoussan, A., Lions, J.L., Papanicolau, G. *Asymptotic Analysis for Periodic Structures*, Noth-Holland (1978).

[3] Bourgat, J.F. *Numerical Experiments of the Homogenization Method for Operators with Periodic Coefficient.*in Computing Methods in Applied Science and Engineering, I, Versailles, December 5-9, 1977, edited by R. Glowinski and J.L.Lions p. 330, Springer-Verlag (1978).

[4] Cioranescu, D., Donato P. *An Introduction to Homogenization*, Oxford Lecture Series in Mathematics and its Application, Vol. 17 (1999).

[5] Jikov, V.V., Kozlov, S.M., Oleinik, O.A. *Homogenization of Differential Operators and Integral Functionals*. Springer Verlag (1994).

[6] Moulton, J.D., Dendy, J.E., Hyman, J.M. *The Black Box Multigrid Numerical Homogenization Algorithm*. Journal of Computational Physics, 142:80-108 (1998).

[7] Sviercoski, R.F. *Multiscale Analytical Solutions and Homogenization of n-Dimensional Generalized Elliptic Equations*, Ph.D. Dissertation, University of Arizona, (2005).

From fine to coarse and/or from coarse to fine - an attempt to clarify multiscale terminology

Ulrich Trottenberg

In this talk, we have tried to clarify terminology. There is a large variety of approaches in numerical simulation addressing different scales and the terminology used in this context is rather confusing. From this list, we would like to mention here: *multiscale modelling; upscaling, averaging, coarsening, homogenization; downscaling, refinement; filtering, smoothing; multiscale/multilevel/multigrid computing; cyclic/total reduction, AMG, renormalization group;* related approaches are addressed by *grid partitioning, domain decomposition, multidisciplinary coupling* and the like.

In the following, we will not explain each of these terms, but for the purpose of clarification and *simplification* introduce the following fundamental distinctions:

a. *multiscale modelling* versus *multiscale computing*

b. *going one way* (from fine to coarse or from coarse to fine) versus *going both ways* (from fine to coarse and from coarse to fine)

c. *reduction type* versus *multigrid type* methods.

a. **Multiscale modelling** versus **multiscale computing**

Multiscale modelling: In trying to understand, describe and control natural and technical phenomena and processes, it often turns out that different scales play an important role: Very small (atomistic, nano-, microscopic) scales may influence and determine phenomena on much larger (meso-, macro-) scales, or more generally different scales interact with each other significantly. When modelling such multiscale phenomena, an approach is needed which takes all relevant scales into account. For such situations and for corresponding approaches, we use the term multiscale modelling. In multiscale modelling, one may have or not have a target scale in mind, on which the simulation result ('the solution') is finally wanted.

Multiscale computing is an algorithmic approach. Assuming that we want to calculate the solution on a target scale, additional scales are used auxiliarily in order to make the calculation more efficient.

The classical and most elaborate approach in this context is multigrid [2]. Looking at multigrid as an iterative solver one goes from fine to coarse and back from coarse to fine in an iterative manner. Classical multigrid is a combination of smoothing (filtering) and approximation (coarse grid correction) procedures. In classical (geometric) multigrid a hierarchy of grids (finer and coarser ones) is predefined based on geometric (grid) information. More sophisticated multigrid approaches like Algebraic Multigrid (AMG) make use (only) of the algebraic information that is provided by the matrix representing the discretized problem. In AMG the coarse grid structures are constructed automatically.

In addition, there are further sophisticated multigrid approaches like FMG, where iterative geometric multigrid is combined with a global refinement strategy. In FAC and MLAT (multilevel adaptive technique) local grid structure refinements and coarsenings are dynamically constructed during the calculation, based on error estimator criteria.

b. **Going one way** versus **going both ways**

From fine to coarse: In the context of (multiscale) modelling, the concept of upscaling [1] refers to the transition of a fine scale model to a coarse(r) scale model. The idea of this transition is reduction of complexity, i.e. reducing the degrees of freedom in a given model substantially, but maintaining its essential features under consideration.

Typical ways of carrying out such transitions from fine to coarse are averaging and homogenisation. Others (in context of discretisation and matrix representation) are aggregation and reduction type approaches as well as the renormalization group method (in computational physics), see below.

The concept of upscaling also includes the option of making use of a hierarchy of scales, repeating the transition (coarsening) process several times.

From coarse to fine: In discretizing and iteratively solving (nonlinear) partial differential equations there is a long tradition in using coarse grid (or coarse level) approximations as first guesses on finer grids.

Going both ways, from fine to coarse and from coarse to fine: The approaches, from fine to coarse and from coarse to fine, sketched so far are not necessarily one-directional, but in many cases can be and are used in a bi-directional manner. For example, if upscaling is used to replace a primary fine scale model by a coarser one, the coarse scale 'solution' (simulation result) may well be interpreted and be used for a more detailed look on the finer scale. Similarly, a primary coarse scale model may be considered (locally or globally) on a finer scale in order to study important local phenomena or to better understand fine scale influences.

Going from fine to coarse usually is intended to gain efficiency and going from coarse to fine to gain accuracy (and insight).

However, multigrid and multigrid related algorithmic approaches are not optionally, but fundamentally bi-directional. Multigrid and AMG type methods, make essential use of finer and coarser scales and transition processes between the scales: Indeed, these methods draw their efficiency out of the interplay between smoothing processes on finer levels and coarse scale corrections on coarser levels. Although there are multigrid algorithms the overall structure of which is from coarse to fine, viz. FMG [2] the individual steps of FMG are bi-directional!

Other related approaches like 'cascadic multigrid' which are essentially one-directional, are not regarded as multigrid methods in a strict sense.

c. Reduction type versus multigrid type methods

In going from fine to coarse, there are essentially two different objectives that can be pursued. One is to construct a coarse scale model/problem that is mathematically equivalent to the fine scale model for those unknowns/degrees of freedom which the two scales have in common (reduction type). The other (more general) objective is to define a coarse scale model/problem that is an adequate approximation representing the essential information of the original model on the coarse scale (multigrid type).

Reduction type methods: Cyclic reduction (for 1D-problems) and total reduction methods (for 2D and 3D partial differential equations) transform fine grid problems equivalently to coarser grids, in a simple and typically numerical stable way. In that respect, these methods can be regarded as specific, particularly efficient elimination processes (for discrete partial differential equations).

Similarly, renormalization group methods in theoretical physics intend to transform a fine scale problem equivalently to a coarser scale.

Algebraic multigrid (AMG) can be interpreted both as a generalization of (total) reduction, and - from the multigrid point of view - as an extension of classical geometric multigrid to matrix represented linear algebra problems.

Multigrid type (filtering) processes. In classical multigrid, relaxation type procedures are used for smoothing which means that the high frequency components of the errors which are visible only on the fine scale (grid) are filtered out. After applying such error smoothing procedures, the remaining low frequency components can without essential loss of information, but with considerably reduced computational effort be treated further on the coarser scales (grids).

Finally, we would like to mention (confess) that the distinctions we made for clarification may be regarded as somewhat artificial: In practice the different approaches addressed in this talk are often combined ...

References

[1] Brandt, A.: Multiscale solvers and systematic upscaling in computational physics. Proc. Conf. on Computational Physics 2004, September 2004, Genova. Italy. COMPHY 2927, Computer Physics Communication, Elsevier.

[2] Trottenberg, U.; Oosterlee, C.; Schüller, A.: Multigrid, Academic Press, 2001

Selecting coarse grid operators within a multigrid algorithm by local Fourier analysis

Roman Wienands

We consider a two-dimensional discrete boundary value problem

$$L_h u_h(\boldsymbol{x}) = f_h(\boldsymbol{x}) \quad (\boldsymbol{x} \in \Omega_h), \qquad B_h u_h(\boldsymbol{x}) = g_h(\boldsymbol{x}) \quad (\boldsymbol{x} \in \partial\Omega_h)$$

with discrete differential operator L_h, discrete boundary operator B_h defining the boundary conditions, discrete domain Ω_h, meshsize h and given functions f_h, g_h.

Suppose that L_h can be locally represented by a stencil $\left[\ell^h_{\boldsymbol{\kappa}}(\boldsymbol{x})\right]_h$, i.e.,

$$L_h u_h(\boldsymbol{x}) = \sum_{\boldsymbol{\kappa} \in J_h} \ell^h_{\boldsymbol{\kappa}}(\boldsymbol{x})\, u_h(\boldsymbol{x} + \boldsymbol{\kappa} h) \quad \text{with} \quad \boldsymbol{x} \in \Omega_h,$$

stencil entries $\ell^h_{\boldsymbol{\kappa}}(\boldsymbol{x}) \in \mathbb{R}$ and a certain index set $J_h \in \mathbb{Z}^2$ containing $(0,0)$. For ease of presentation we consider only consistent discretizations, i.e.,

$$\sum_{\boldsymbol{\kappa} \in J_h} \ell^h_{\boldsymbol{\kappa}}(\boldsymbol{x}) = 0.$$

Solving the discrete boundary value problem with the help of an appropriate multigrid method [1, 2] necessitates the construction of a sequence of discrete domains with coarser resolutions and corresponding coarse grid approximations for L_h. A

standard choice for the determination of coarser grids is to repeatedly double the mesh size in each spatial direction yielding Ω_{2h}, L_{2h}, Ω_{4h}, L_{4h}, etc.

In this talk, we proposed a strategy to automatically select coarse grid discretizations within a multigrid solution method with the help of local Fourier analysis [1, 2, 3]. For the application of local Fourier analysis it is necessary to consider locally frozen operators with constant coefficients ($L_h \stackrel{\wedge}{=} \left[\ell^h_{\boldsymbol{\kappa}}\right]_h$) which are extended to an infinite grid G_h. The corresponding eigenfunctions (or Fourier components) and the related eigenvalues (or Fourier symbols) read

$$\phi_h(\boldsymbol{x},\boldsymbol{\theta}) := e^{i\,\boldsymbol{\theta}\boldsymbol{x}/h} \quad (\boldsymbol{\theta}\in[-\pi,\pi]^2), \qquad \widetilde{L}_h(\boldsymbol{\theta}) := \sum_{\boldsymbol{\kappa}\in J_h} \ell^h_{\boldsymbol{\kappa}} e^{i\,\boldsymbol{\theta}\boldsymbol{\kappa}}.$$

The Fourier symbols for $L_{2h} \stackrel{\wedge}{=} \left[\ell^{2h}_{\boldsymbol{\kappa}}\right]_{2h}$ are obviously given by

$$\widetilde{L}_{2h}(\boldsymbol{\theta}) := \sum_{\boldsymbol{\kappa}\in J_{2h}} \ell^{2h}_{\boldsymbol{\kappa}} e^{i\,\boldsymbol{\theta}2\boldsymbol{\kappa}}.$$

Hence, Fourier components $\phi_h(\boldsymbol{x},\boldsymbol{\theta})$ with $\boldsymbol{\theta}\notin\Theta_{\text{low}} := [-\pi/2,\pi/2]^2$ can not be represented on G_{2h} as they coincide with certain Fourier components $\phi_h(\boldsymbol{x},\boldsymbol{\theta}^*)$ with $\boldsymbol{\theta}^*\in\Theta_{\text{low}}$ due to the periodicity of the exponential function. This observation is known as aliasing and frequencies $\boldsymbol{\theta}\in\Theta_{\text{low}}$ are called low frequencies. Due to the aliasing of Fourier components, the coarse grid discretizations should be good approximations of L_h especially w.r.t. the (very) low frequencies. In order to satisfy this requirement, the coarse grid approximations are constructed by the minimization of a certain low-frequency L^2-norm. More precisely, the coarse grid discretization is derived in such a way that its Fourier symbol is a best approximation (w.r.t. low frequencies) of the Fourier symbol of the fine grid operator. To formulate this approximation problem we consider the function space

$$L^2_{\text{low}} := \left\{ v \,:\, \Theta_{\text{low}}\to\mathbb{C} \quad \text{with} \quad \left(\int_{\Theta_{\text{low}}} |v(\boldsymbol{\theta})|^2\, d\boldsymbol{\theta}\right)^{1/2} < \infty \right\}$$

with corresponding inner product and norm, respectively:

$$\langle v,w\rangle_{\text{low}} := \int_{\Theta_{\text{low}}} v(\boldsymbol{\theta})\overline{w(\boldsymbol{\theta})}\, d\boldsymbol{\theta}, \qquad \|v\|_{\text{low}} := \sqrt{\langle v,v\rangle_{\text{low}}} \qquad \left(v,w\in L^2_{\text{low}}\right).$$

L^2_{low} equipped with $\langle\,,\,\rangle_{\text{low}}$ yields a Hilbert space. For the derivation of L_{2h} we are looking for the optimal (w.r.t. $\|\,.\,\|_{\text{low}}$) approximation of $\widetilde{L}_h\in L^2_{\text{low}}$ in the following subspace

$$F_{2h} := \text{span}\left\{ e^{i\,2\boldsymbol{\theta}\boldsymbol{\nu}} - 1 \,:\, \nu\in J_{2h}\setminus\{(0,0)\}\right\} \subset L^2_{\text{low}}.$$

This is a classical approximation problem which can be easily solved. The occurrence of "-1" within each basis function ensures a consistent coarse grid discretization (i.e., $\sum_{\boldsymbol{\kappa}\in J_{2h}} \ell^{2h}_{\boldsymbol{\kappa}} = 0$).

To illustrate the presented procedure we consider the construction of a coarse grid discretization given by a compact 5-point stencil:

$$L_{2h} \triangleq \begin{bmatrix} & \ell^{2h}_{(0,1)} & \\ \ell^{2h}_{(-1,0)} & -\sum_{\kappa\neq(0,0)} \ell^{2h}_{\boldsymbol{\kappa}} & \ell^{2h}_{(1,0)} \\ & \ell^{2h}_{(0,-1)} & \end{bmatrix}_{2h}, \quad F_{2h} := \operatorname{span}\{\phi_1,\, \phi_2,\, \phi_3,\, \phi_4\}$$

$$\text{with} \quad \phi_1(\boldsymbol{\theta}) := e^{i\,2\boldsymbol{\theta}(-1,0)} - 1, \quad \phi_2(\boldsymbol{\theta}) := e^{i\,2\boldsymbol{\theta}(1,0)} - 1,$$
$$\phi_3(\boldsymbol{\theta}) := e^{i\,2\boldsymbol{\theta}(0,-1)} - 1, \quad \phi_4(\boldsymbol{\theta}) := e^{i\,2\boldsymbol{\theta}(0,1)} - 1 \qquad (\boldsymbol{\theta} \in \Theta_{\text{low}}).$$

The optimal coarse grid stencil is then given by the following linear system

$$(\langle \phi_i, \phi_j \rangle_{\text{low}})_{i,j=1,\ldots,4} \begin{pmatrix} \ell^{2h}_{(-1,0)} \\ \ell^{2h}_{(1,0)} \\ \ell^{2h}_{(0,-1)} \\ \ell^{2h}_{(0,1)} \end{pmatrix} = \left(\langle \widetilde{L}_h, \phi_i \rangle_{\text{low}} \right)_{i=1,\ldots,4}.$$

We would like to emphasize that each inner product occurring in the above linear system is a linear combination of certain integrals which can be explicitly calculated

$$\int_{\Theta_{\text{low}}} e^{i\,(\theta_1\kappa_1+\theta_2\kappa_2)}\, d\boldsymbol{\theta} = \begin{cases} 4\pi^2/n^2 & \text{for } \kappa_1 = \kappa_2 = 0 \\ 4\pi \sin(\pi\kappa_2/n)/(\kappa_2 n) & \text{for } \kappa_1 = 0, \kappa_2 \neq 0 \\ 4\pi \sin(\pi\kappa_1/n)/(\kappa_1 n) & \text{for } \kappa_1 \neq 0, \kappa_2 = 0 \\ -2[\cos(\pi(\kappa_1+\kappa_2)/n) & \text{for } \kappa_1, \kappa_2 \neq 0 \\ -\cos(\pi(\kappa_1-\kappa_2)/n)]/(\kappa_1\kappa_2) & \end{cases}$$

with $\Theta_{\text{low}} := [-\pi/n, \pi/n]^2$. This means that the matrix $(\langle \phi_i, \phi_j \rangle_{\text{low}})_{i,j=1,\ldots,m}$ can be precomputed for a given coarse grid pattern J_{2h}. Hence, general formulas for the stencil entries $\ell^{2h}_{\boldsymbol{\kappa}}$ can be calculated in terms of $\ell^{h}_{\boldsymbol{\kappa}}$. The complete sequence of coarse grid operators $(L_{2h},\, L_{4h},\, L_{6h},\, \ldots)$ can be obtained by a repeated application of the above strategy yielding a black-box method for the construction of coarse grid operators! Analyzing this approach we made the following important observation: Choosing $\Theta_{\text{low}} = [-\pi/2, \pi/2]^2$ yields bad coarse grid approximations whereas considering only very low frequencies (i.e., $\Theta_{\text{low}} = [-\pi/n, \pi/n]$ with $n \to \infty$) yields excellent coarse grid approximations. Moreover, the analytical formulas for the coarse grid stencil entries converge to fixed expressions for $n \to \infty$. For example, one obtains the following formulas for a 5-point coarse grid operator assuming a 5-point fine grid stencil:

$$\ell^{2h}_{(-1,0)} = \frac{3}{8}\,\ell^{h}_{(-1,0)} - \frac{1}{8}\,\ell^{h}_{(1,0)}, \quad \ell^{2h}_{(1,0)} = -\frac{1}{8}\,\ell^{h}_{(-1,0)} + \frac{3}{8}\,\ell^{h}_{(1,0)},$$
$$\ell^{2h}_{(0,-1)} = \frac{3}{8}\,\ell^{h}_{(0,-1)} - \frac{1}{8}\,\ell^{h}_{(0,1)}, \quad \ell^{2h}_{(0,1)} = -\frac{1}{8}\,\ell^{h}_{(0,-1)} + \frac{3}{8}\,\ell^{h}_{(0,1)}.$$

Similar analytical expressions can be obtained for other fine and coarse grid stencil patterns. In this way it was possible to recover well-established coarse grid operators in simple situations and (even more important) to obtain improvements for

more difficult situations. The method has been successfully applied to Poisson-type equations, problems with jumping coefficients, convection diffusion equations, etc.

Finally, we would like to mention that the presented approach can be easily modified for other regular coarsening strategies like semi or red-black coarsening and for discrete operators with $\sum_{\boldsymbol{\kappa}\in J} \ell_{\boldsymbol{\kappa}} \neq 0$. The underlying analysis can even be used to judge between coarsening strategies and different patterns of coarse grid stencils.

References

[1] A. Brandt, *Multi-level adaptive solutions to boundary-value broblems*, Math. Comp. **31** (1977), 333–390.
[2] U. Trottenberg, A. Schüller, and C.W. Oosterlee, *Multigrid*, Academic Press, London, 2001.
[3] R. Wienands and W. Joppich, *Practical Fourier analysis for multigrid methods*, CRC Press, Boca Raton, 2004.

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