Final Report: MULTISCALE ANALYSIS AND COMPUTATION FOR FLOWS IN HETEROGENEOUS MEDIA
This research is supported by DOE grant DE-FG02-06ER25727

August 4, 2016

TAMU PI: Y. Efendiev[1]
Other PI's: T.Y. Hou (PI)[2], L.J. Durlofsky [3], H. Tchelepi[4]

1 Summary

Our work in this project is aimed at making fundamental advances in multiscale methods for flow and transport in highly heterogeneous porous media. The main thrust of this research is to develop a systematic multiscale analysis and efficient coarse-scale models that can capture global effects and extend existing multiscale approaches to problems with additional physics and uncertainties. A key emphasis is on problems without an apparent scale separation.

Multiscale solution methods are currently under active investigation for the simulation of subsurface flow in heterogeneous formations. These procedures capture the effects of fine-scale permeability variations through the calculation of specialized coarse-scale basis functions. Most of the multiscale techniques presented to date employ localization approximations in the calculation of these basis functions. For some highly correlated (e.g., channelized) formations, however, global effects are important and these may need to be incorporated into the multiscale basis functions. Other challenging issues facing multiscale simulations are the extension of existing multiscale techniques to problems with additional physics, such as compressibility, capillary effects, etc.

In our project, we explore the improvement of multiscale methods through the incorporation of additional (single-phase flow) information and the development of a general multiscale framework for flows in the presence of uncertainties, compressible flow and heterogeneous transport, and geomechanics. We have considered (1) adaptive local-global multiscale methods, (2) multiscale methods for the transport equation, (3) operator-based multiscale methods and solvers, (4) multiscale methods in the presence of uncertainties and applications, (5) multiscale finite element methods for high contrast porous media and their generalizations, and (6) multiscale methods for geomechanics. Below, we present a brief overview of each of these contributions.

[1]Department of Mathematics, Texas A&M University, College Station, TX 77843-3368
[2]Applied Mathematics, Caltech, Pasadena, CA 91125
[3]Department of Energy Resources Engineering, Stanford University, Stanford, CA 94305-2220
[4]Department of Energy Resources Engineering, Stanford University, Stanford, CA 94305-2220

2 Adaptive local-global multiscale methods

The use of limited global information in multiscale methods provides a better accuracy in the simulations. In this part of our research, we have considered various ways to incorporate limited global information in two-phase flows to obtain accurate solutions and develop local-global approaches. The limited global information typically consists of single-phase flow information in two-phase flow simulations.

An earlier paper [4] on the use of limited global information is developed within the context of upscaling [4]. The procedure enables the efficient incorporation of approximate global information, determined via coarse-scale simulations, into the multiscale basis functions. The main idea of the technique in [13] (see also [17, 22, 21] for local-global and [29]) is to use the multiscale basis functions iteratively to obtain more accurate solutions. In particular, multiscale solutions over different oversampling regions are used to obtain the next iteration. These solutions can be computed efficiently since they rely on local solutions. Moreover, the basis functions can be updated using thresholding techniques similar to those developed for upscaling methods. The improvement in accuracy is due to the fact that each iteration improves the global information that is incorporated into the basis functions. The resulting procedure is formulated as a finite volume element method and is applied for a number of single and two-phase flow simulations of channelized two-dimensional systems. The level of accuracy of the resulting method is shown to be consistently higher than that of the standard finite volume element multiscale technique based on simple localized basis functions.

The global information can also be considered via the use of oversampling techniques as shown [23, 14]. Oversampling techniques are often used in porous media simulations to achieve high accuracy. The main idea of the oversampling technique is to use regions larger than the target coarse block to compute the basis functions. In particular, auxiliary solutions are computed, and then their linear combinations are used in setting up the local basis functions. In [10], we compare two type of oversampling strategies. The first oversampling approach uses generic global boundary conditions that do not reflect the actual flow boundary conditions, while the second oversampling approach replaces one of the global oversampling basis functions with the solution of the single-phase flow equation. Our numerical results show that the second approach is several times more accurate for one of the commonly used boundary conditions. We provide partial theoretical explanation for these numerical observations.

Other research in local-global methods (see [17, 22, 21]) focused on the use of local multiscale basis functions in constructing global modes, which allow an efficient reduced-order approximation of the solution. In these methods, by constructing global modes via local multiscale basis functions, we reduce the computational complexity of the problem.

3 Multiscale methods for the transport equation

Developing multiscale methods for transport equation in two-phase systems has been a challenging task. In this part, we have developed several robust techniques for convection-dominated problems.

In [15], we propose a multiscale technique for simulation of porous media flows in a flow-based coordinate system. A flow-based coordinate system is a coordinate system that depends on single-phase flow characteristics, such as single-phase pressure and streamline functions. Flow-based coordinate systems allow us to simplify the scale interaction and derive the upscaled equations for purely hyperbolic transport equations. This is due to the fact that two-phase flow and transport properties are smooth functions in flow-based coordinate systems.

The main idea of the proposed method is to study the fine-scale model in a pressure-streamline coordinate system. We discuss the upscaling of the transport equation along streamlines as well as across streamlines. The upscaling along streamlines can be accomplished by taking harmonic averages of the velocity field. The upscaling across streamlines introduces non-local effects, which can be modeled using perturbation techniques. The upscaled transport equation is further coupled to the pressure equation which is solved using a multiscale finite volume element method on the coarse grid.

In [28], we have developed an adaptive multiscale finite-volume (MSFV) method for the transport equation of nonlinear two-phase flow in heterogeneous domains. The objective is to develop an adaptive reconstruction strategy. The method can be described using prolongation and restriction operators as in a two-level multigrid scheme. The restriction operator is defined as the volume average of the fine-scale saturations in a coarse block. Three adaptive prolongation operators are defined according to the saturation distribution, in which the physical domain is divided into three regions: (1) Region 1 where the injection fluid has not arrived, (2) Region 2, where steep saturation gradients are present, and (3) Region 3 where saturations change slowly in the wake of advancing fronts. To identify the transition between the regions, specific norm-based criteria are proposed. In Region 1, the transport equation can be completely skipped, whereas in the Regions 2 the local fine-scale transport equations are solved iteratively on a coarse grid (this is referred as Prolongation Operator I). In Regions 3, we developed two approximate prolongation operators: Prolongation Operator II that reconstructs the fine-scale velocity and is locally conservative on the fine grid, and Prolongation Operator III that interpolates saturation changes to yield a locally conservative scheme, but only on the coarse grid. The proposed adaptive multiscale method has been tested with various models, including systems with strong permeability heterogeneity. An example using the SPE 10 top layer demonstrates that the multi-scale results with adaptive transport calculations are in excellent agreement with the fine-scale reference solutions. Furthermore, the adaptive scheme for coupled flow and transport equations yields solutions that are much more computationally efficient than conventional finite difference methods.

In [3], we study a stabilization of multiscale methods for convection-dominated problems. In particular, we develop a Petrov-Galerkin stabilization method for multiscale convection-diffusion transport systems. Existing stabilization techniques add a limited number of degrees of freedom in the form of bubble functions or a modified diffusion, which may not be sufficient to stabilize multiscale systems. We seek a local reduced-order model for this kind of multiscale transport problems and develop a systematic approach for finding reduced-order approximations of the solution. We start from a Petrov-Galerkin framework using optimal weighting functions. We introduce an auxiliary variable to a mixed formulation of the problem. The auxiliary variable stands for the optimal weighting function. The problem reduces to finding a test space (a dimensionally reduced space for this auxiliary variable), which guarantees that the error in the primal variable (representing the solution) is close to the projection error of the full solution on the dimensionally reduced space that approximates the solution. We introduce snapshots and local spectral problems that appropriately define local weight and trial spaces. In particular, we use energy minimizing snapshots and local spectral decompositions in the natural norm associated with the auxiliary variable. The resulting spectral decomposition adaptively identifies and builds the optimal multiscale space to stabilize the system. We present several numerical examples, including a transport equation in highly heterogeneous porous media and show that one needs a few test functions to achieve an error similar to the projection error in the primal variable irrespective of the Peclet number.

4 Operator-based multiscale methods and solvers

Using multiscale methods as solvers has been investigated in the works [33, 35, 34, 31, 30], where a general Algebraic Multiscale Solver (AMS) for the pressure equation was developed. We analyzed the role of the Correction Function (CF) in the context of AMS, and we showed that the CF can be seen as an independent local stage. As a local preconditioner, CF helps to capture some of the high-frequency errors, especially in the source terms, and accelerates the overall convergence rate. However, - on average - the gain in convergence rate of using CF does not compensate for the additional computational cost. Simple preconditioners, such as ILU, are found to be more efficient than CF. Note that AMS with any combination of local- and global-stage solvers al- lows for the reconstruction of a conservative velocity field, if an MSFV stage is applied as the last step. Overall, the best AMS strategy is multiscale finite element with reduced boundary conditions along with ILU. Our results indicate that the performance of AMS is comparable to advanced algebraic multigrid solvers. Our results show that AMS is quite efficient, especially if it is used as a multiscale approximate (but conservative) solver for time-dependent subsurface flow problems. We have extended the existing multiscale methods to compressible multi-phase flows.

5 Multiscale methods for stochastic porous media flow equations

In this part, we have developed multiscale methods for stochastic flow equations, where the uncertainties are due to permeability variations. The latter is important for many realistic flows.

In this paper [12], we study multiscale finite element methods for stochastic porous media flow equations as well as applications to uncertainty quantification. We assume that the permeability field is stochastic and can be described in a finite dimensional stochastic space. This is common in applications where the coefficients are expanded using chaos approximations. We discuss two types of approaches. In the first approach, the basis functions are interpolated using pre-computed basis functions computed based on some selected realizations of the permeability field. In the second approach, the stochastic solution is projected to a finite dimensional space consisting of basis functions corresponding to selected realizations. The second case does not require any interpolation in stochastic space. Basis functions can be constructed both locally and globally. The proposed multiscale method constructs multiscale basis functions corresponding to some realizations, and these basis functions are used to approximate the solution on the coarse grid for any realization. These multiscale methods are used in developing multilevel Monte Carlo methods in [27, 16], where we propose multilevel Monte Carlo (MLMC) methods. In multilevel Monte Carlo methods, more accurate (and expensive) forward simulations are run with fewer samples, while less accurate (and inexpensive) forward simulations are run with a larger number of samples. Selecting the number of expensive and inexpensive simulations based on the number of coarse degrees of freedom, one can show that MLMC methods can provide better accuracy at the same cost as Monte Carlo (MC) methods. We also apply the proposed technique to an uncertainty quantification problem where the permeability field is sampled based on oil production rates (an integrated response).

In a number of papers, we explored performing the multiscale model reduction in both physical space and stochastic space to design effective dimensional reduction method. In [7, 32], we develop a data-driven stochastic method by using multiscale model reduction for flow equations in the physical space and exploring a low-rank solution structure in the stochastic space. By upscaling in the physical space and by exploring the low rank structure in the stochastic space, we demonstrate this multiscale data-driven stochastic method gives a significant speed-up over existing stochastic methods based on generalized polynomial chaos expansion.

In [5, 6], we develop a dynamically bi-orthogonal method (DyBO) to solve compressible flow equations described by time dependent stochastic partial differential equations (SPDEs). The objective of our method is to exploit some intrinsic sparse structure in the stochastic solution by constructing the sparsest representation of the stochastic solution via a bi-orthogonal basis. The main contribution of these papers is that we derive an equivalent system that governs the evolution of the spatial and stochastic basis in the Karhunen-Loeve expansion. Unlike other reduced model methods, our method constructs the reduced basis on-the-fly without the need to form the covariance matrix or to compute its eigendecomposition. We have performed extensive numerical experiments for compressible single-phase flow in stochastic porous media to demonstrate the effectiveness of the DyBO method.

In [25], we introduce a heterogeneous stochastic FEM framework to solve single-phase flow equation described by stochastic elliptic PDEs with multiscale random coefficients. Our method explores the compactness of the inverse operator in the stochastic direction and allows for spatially heterogeneous stochastic structure. More specifically, we use the heterogeneous coupling of spatial basis with local stochastic basis to exploit the local stochastic structure of the solution space. This line of research is further explored in [26].

In upscaling a stochastic PDE describing flow equations, how to define an appropriate local boundary condition is crucial for accuracy of the upscaled problem. In [24], we propose a local oversampling method to construct basis functions that have optimal local approximation property. Our methodology is based on the compactness of the solution operator when restricted to local regions of the spatial domain, and does not depend on any scale-separation or periodicity assumption of the coefficient. We construct a special type of basis functions that are harmonic on each element and have optimal approximation property. Rigorous error estimates can be obtained through thresholding in constructing the basis functions. Numerical results for single-phase flow with multiple spatial scales and high contrast inclusions are presented to demonstrate the compactness of the local solution space and the capacity of our method in identifying and exploiting this compact structure to achieve computational savings.

6 Multiscale methods for high contrast porous media and their generalizations

To take into account the high contrast in the media properties, we have developed a general multiscale framework, Generalized Multiscale Finite Element Method, which extends multiscale finite element method. In [20, 18, 19], we have presented a general framework for solving multiscale problems with a high contrast. The main idea of the GMsFEM is to introduce snapshots on a coarse grid and identify dominant modes in the snapshot space. The snapshot space represents a set of functions that can be used to calculate the local solution space accurately. The snapshots typically consist of local solutions with randomized boundary conditions, which represent point sources distributed on the boundaries. The snapshot vectors are similar to the snapshots used in global model reduction, however, they are constructed without solving expensive global problems and similar to cell problems in homogenization. The snapshot vectors are computed by using random boundary conditions. To avoid the effects of randomization and improve the accuracy, we use oversampling techniques and compute snapshots in domains slightly larger than the target coarse block. The local spectral decomposition is performed in the space of snapshots by identifying local spectral decomposition based on the analysis. The analysis consists of decomposing the error into local regions and bounding these error components. We have demonstrated applications of the method to two-phase flow systems in [21].

The multiscale methods in the presence of the high contrast has also been rigorously investigated in [8, 9] for some special permeability fields. The authors have introduced a new variant of the multiscale finite element method which is able to accurately capture solutions of high contrast elliptic interface problems using uniform coarse meshes which are not required to resolve the interfaces [8, 9]. A typical application would be the modeling of a number of highly permeable inclusions in a low-permeability matrix. Under moderate assumptions, we prove that our methods have convergence of $O(H)$ in the energy norm and $O(H^2)$ in the L_2 norm, independent of the contrast, where H is the (coarse) mesh diameter. Our methods are conforming and employ multiscale finite element approximation with novel interior boundary conditions on element edges which intersect the interface. The method reduces to standard linear approximation on elements which do not intersect the interface. The new boundary conditions depend not only on the contrast but also on the local angles of intersection of the interface with the element edges. Our numerical experiments have confirmed our theoretical results. This is the first convergence result for the multiscale interface problem in which one can obtain an optimal convergence result independent of the contrast of the coefficients without requiring the media being periodic in order to use homogenization theory.

7 Multiscale methods for geomechanics

One of the proposed areas included geomechanics, where the flow and mechanics equations are coupled. We have investigated the application of multiscale methods to geomechanics in [1, 2].

In [1], the numerical solution of poroelasticity problems is studied. The system is of Biot type, for which a general algorithm for solving coupled systems is developed. The challenges associated with mechanics and flow problems in heterogeneous media are discussed. The two primary issues being the multiscale nature of the media and the solutions of the fluid and mechanics variables traditionally developed with separate grids and methods. For the numerical solution we develop and implement a Generalized Multiscale Finite Element Method (GMsFEM) that solves problem on a coarse grid by constructing local multiscale basis functions. The procedure begins with construction of multiscale bases for both displacement and pressure in each coarse block. Using a snapshot space and local spectral problems, we construct a basis of reduced dimension. Finally, after multiplying by a multiscale partitions of unity, the multiscale basis is constructed in the offline phase and the coarse grid problem then can be solved for arbitrary forcing and boundary conditions. The algorithm is implemented on two heterogeneous media and the errors are computed between the multiscale solution with the fine-scale solutions.

In [2], The numerical solution of some *nonlinear* poroelasticity problems is considered. This Biot type system is solved by a novel general algorithm. The difficulties associated with flow and mechanics in heterogeneous media with nonlinear coupling are discussed. The central issue being how to handle the nonlinearities and the multiscale scale nature of the media. To compute an efficient numerical solution we develop and implement a Generalized Multiscale Finite Element Method (GMsFEM) that solves nonlinear problems on a coarse grid by constructing local multiscale basis functions and treating part of the nonlinearity locally as a parametric value. After linearization with a Picard Iteration, the procedure begins with construction of multiscale bases for both displacement and pressure in each coarse block by treating the staggered nonlinearity as a parametric value. Using a snapshot space and local spectral problems, we construct an offline basis of reduced dimension. From here an online, parametric dependent, space is constructed. Finally, after multiplying by a multiscale partitions of unity, the multiscale basis is constructed and the coarse grid problem then can be solved for arbitrary forcing and boundary conditions. The algorithm is implemented on a geometry with a linear and nonlinear pressure dependent permeability field. The errors are computed between the multiscale solution with the fine-scale solutions.

References

[1] D. L Brown and M. Vasilyeva. A generalized multiscale finite element method for poroelasticity problems i: linear problems. *Journal of Computational and Applied Mathematics*, 294:372–388, 2016.

[2] D. L Brown and M. Vasilyeva. A generalized multiscale finite element method for poroelasticity problems ii: nonlinear coupling. *Journal of Computational and Applied Mathematics*, 297:132–146, 2016.

[3] V. M Calo, E.T Chung, Y. Efendiev, and Wing Tat Leung. Multiscale stabilization for convection-dominated diffusion in heterogeneous media. *arXiv preprint arXiv:1509.06833*, 2015. CMAME, Volume 304, 1 June 2016, Pages 359-377.

[4] Y. Chen and L.J. Durlofsky. Adaptive local-global upscaling for general flow scenarios in heterogeneous formations. *Transport in Porous Media*, 62:157–185, 2006.

[5] M. Cheng, T. Y. Hou, and Z. Zhang, A Dynamically Bi-Orthogonal Method for Time-Dependent Stochastic Partial Differential Equations I: Derivation and Algorithms. *J. Comput. Phys.*, 242:843-868, 2013.

[6] M. Cheng, T. Y. Hou, and Z. Zhang, A Dynamically Bi-Orthogonal Method for Time-Dependent Stochastic Partial Differential Equations II: Adaptivity and Generalizations. *J. Comput. Phys.*, 242:753-776, 2013.

[7] M. Cheng, T. Y. Hou, M. Yan, and Z. Zhang, A Data-driven Stochastic Method for Elliptic PDEs with Random Coefficients. *SIAM/ASA J. for Uncertainty Quantification*, 1:452-493, 2013.

[8] C.C. Chu, Ivan Graham, and T-Y Hou. A new multiscale finite element method for high-contrast elliptic interface problems. *Mathematics of Computation*, 79(272):1915–1955, 2010.

[9] C.C. Chu. *Multiscale methods for elliptic partial differential equations and related applications.* PhD thesis, California Institute of Technology, 2010.

[10] C. C. Chu, Y. Efendiev, V. Ginting, and T. Y. Hou. Flow based oversampling technique for multiscale finite element methods. *Advances in Water Resources*, 31(4):599–608, 2008.

[11] M. Ci, T. Y. Hou, and Z. Shi, A Multiscale Model Reduction Method for Partial Differential Equations. *Mathematical Modeling and Numerical Analysis (M2AN)*, 48(2):449-474, 2014.

[12] P. Dostert, Y. Efendiev, and T. Y Hou. Multiscale finite element methods for stochastic porous media flow equations and application to uncertainty quantification. *Computer Methods in Applied Mechanics and Engineering*, 197(43):3445–3455, 2008.

[13] L.J. Durlofsky, Y. Efendiev, and V. Ginting. An adaptive local-global multiscale finite volume element method for two-phase flow simulations. *Advances in Water Resources*, 30:576–588, 2007.

[14] Y. Efendiev and T. Hou. *Multiscale Finite Element Methods: Theory and Applications*, volume 4 of *Surveys and Tutorials in the Applied Mathematical Sciences*. Springer, New York, 2009.

[15] Y. Efendiev, T.Y. Hou, and T. Strinopoulos. Multiscale simulations of porous media flows in flow-based coordinate system. *Comp. Geosciences*, 12(3):257–272, 2008.

[16] Y Efendiev, O Iliev, and C Kronsbein. Multilevel monte carlo methods using ensemble level mixed msfem for two-phase flow and transport simulations. *Computational Geosciences*, 17(5):833–850, 2013.

[17] Y. Efendiev, J. Galvis, and E. Gildin. Local–global multiscale model reduction for flows in high-contrast heterogeneous media. *Journal of Computational Physics*, 231(24):8100–8113, 2012.

[18] Y. Efendiev, J. Galvis, and T. Y Hou. Generalized multiscale finite element methods (gmsfem). *Journal of Computational Physics*, 251:116–135, 2013.

[19] Y. Efendiev, J. Galvis, G. Li, and M. Presho. Generalized multiscale finite element methods: Oversampling strategies. *International Journal for Multiscale Computational Engineering*, 12(6), 2014.

[20] Y. Efendiev, J. Galvis, and X.-H. Wu. Multiscale finite element methods for high-contrast problems using local spectral basis functions. *Journal of Computational Physics*, 230(4):937–955, 2011.

[21] Y. Efendiev and M. Presho. Multiscale model reduction with generalized multiscale finite element methods in geomathematics. *Handbook of Geomathematics*, pages 679–701, 2015.

[22] M. Ghommem, M. Presho, V. M Calo, and Y. Efendiev. Mode decomposition methods for flows in high-contrast porous media. global–local approach. *Journal of computational physics*, 253:226–238, 2013.

[23] 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.

[24] T. Y. Hou and P. Liu, Optimal Local Multi-scale Basis Functions for Linear Elliptic Equations with Rough Coefficient. *Discrete and Continuous Dynamical Systems*, accepted, 2015, arXiv: 1508.00346v1 [math.NA], August 3, 2015.

[25] T. Y. Hou and P. Liu, A Heterogeneous Stochastic FEM Framework for Elliptic PDEs. *J. Comput. Phys.*, 281:942-969, 2015.

[26] T. Y. Hou, P. Liu, and Z. Zhang, A Model Reduction Method for Elliptic PDEs with Random Input Using the Heterogeneous FEM Framework. *Bulletin of the Institute of Mathematics, Academia Sinica (New Series)*, 11(1):179-216, 2016.

[27] C. Kronsbein. *On selected efficient numerical methods for multiscale problems with stochastic coefficients*. PhD thesis, Technische Universität Kaiserslautern, 2012.

[28] S. H Lee, H Zhou, and H. A Tchelepi. Adaptive multiscale finite-volume method for non-linear multiphase transport in heterogeneous formations. *Journal of Computational Physics*, 228(24):9036–9058, 2009.

[29] R. Millward. *A new adaptive multiscale finite element method with applications to high contrast interface problems*. PhD thesis, University of Bath, 2011.

[30] Y. Wang, H Hajibeygi, and H Tchelepi. Algebraic multiscale linear solver for heterogeneous elliptic problems. In *ECMOR XIII-13th European Conference on the Mathematics of Oil Recovery*, 2012.

[31] Y. Wang, H. Hajibeygi, and H. A Tchelepi. Algebraic multiscale solver for flow in heterogeneous porous media. *Journal of Computational Physics*, 259:284–303, 2014.

[32] Z. Zhang, M. Ci and T. Y. Hou, A multiscale data-driven stochastic method for elliptic PDEs with random coefficients. *SIAM Multiscale Modeling and Simulation*, 13(1):173-204, 2015.

[33] H. Zhou and H. Tchelepi. perator based multiscale method for compressible flow. SPE 106254,theProceeding of the 2007 SPE Reservoir Simulation Symposium, Houston, Texas, 26-28 February 2007.

[34] H. Zhou. *Operator based multiscale method for compressible flow*. PhD thesis, STANFORD UNIVERSITY, 2006.

[35] H. Zhou and H. A Tchelepi. Two-stage algebraic multiscale linear solver for highly heterogeneous reservoir models. *SPE Journal*, 17(02):523–539, 2012.