

Title:

**Multigrid Homogenization of Heterogeneous  
Porous Media**

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Submitted to:

DOE Office of Scientific and Technical Information (OSTI)

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NATIONAL LABORATORY

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## Multigrid Homogenization of Heterogeneous Porous Media

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### Abstract

This is the final report of a three-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL); this report, however, reports on only two years' research, since this project was terminated at the end of two years in response to the reduction in funding for the LDRD Program at LANL. The numerical simulation of flow through heterogeneous porous media has become a vital tool in forecasting reservoir performance, analyzing groundwater supply and predicting the subsurface flow of contaminants. Consequently, the computational efficiency and accuracy of these simulations is paramount. However, the parameters of the underlying mathematical models (e.g., permeability, conductivity) typically exhibit severe variations over a range of significantly different length scales. Thus the numerical treatment of these problems relies on a homogenization or upscaling procedure to define an approximate coarse-scale problem that adequately captures the influence of the fine-scale structure, with a resultant compromise between the competing objectives of computational efficiency and numerical accuracy. For homogenization in models of flow through heterogeneous porous media, We have developed new, efficient, numerical, multilevel methods, that offer a significant improvement in the compromise between accuracy and efficiency. We recently combined this approach with the work of Dvůrák [6] to compute bounded estimates of the homogenized permeability for such flows and demonstrated the effectiveness of this new algorithm with numerical examples.

### Background and Research Objectives

The flow of oil, water, chemicals, or heat in a porous underground formation can be modeled as a coupled system of nonlinear partial differential equations (PDEs) describing the flow, mass conservation and chemical or biological reactions of individual species. In many petroleum reservoir and aquifer computer models, a 2D fine mesh simulation has a resolution of 10 - 20 meters. This scale is much larger than the natural length scale of the permeability in the reservoir. In homogenizing or upscaling heterogeneous media, the macroscopic equations are averaged over the microscopic length scales and treated as locally homogeneous with variations on the much larger macroscopic length scale.

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For some material properties, this upscaling is trivial. For example, the average porosity or saturation of a volume can be accurately approximated by the arithmetic average of all the porosities or saturations within that volume. However, this simplistic approach fails for other medium characteristics, such as the effective permeability. Models that use simplistic averages or sampling of the heterogeneity have historically underestimated the travel times or extent of subsurface contaminant plumes. Even when fine-scale variations in the permeability are small relative to the scale of the homogenized cell volume, the geostatistical arithmetic, geometric or harmonic averages of the fine-scale permeability can differ by orders of magnitude from the true effective permeability. Hence, the inherent complexity of the upscaling or homogenization process stems from the competing numerical objectives of accuracy and efficiency.

In addition, the increasing use of geostatistical techniques to infer physically meaningful fine-scale realizations of heterogeneous geological formations from sparse and inherently multi-scale measurement data demands more accurate and efficient homogenization procedures. Major analytical and algorithmic advances are needed before we can adequately model general multiphase flows on the coarse grids required by three space dimensional simulations. The upscaling approaches we have developed have demonstrated a significant increase in accuracy when compared to these methods.

### **Importance to LANL's Science and Technology Base and National R&D Needs**

The multigrid homogenization algorithm provides the first opportunity to accurately and efficiently homogenize a fine-scale problem with a full three-dimensional permeability tensor for simulating three-dimensional flow through porous media. In particular, the three key advantages of this approach are its computational efficiency, the ability to capture a dense coarse-scale permeability tensor and the absence of artificial internal boundary conditions. Moreover, the theoretical analysis provides a means to predict the error that is inherent in the coarse-scale model.

This research will lead to significant improvements in upscaling, homogenization, and mesoscale modeling of single and multiphase flows and will provide techniques for more accurate and realistic simulations of underground aquifers and reservoirs. Researchers at Sandia, Spectra, Chevron, and Los Alamos that model large scale subsurface flows (including WIPP, Yucca Mountain and oil reservoirs) have expressed a keen interest in employing our MGH algorithm.

The broad applicability of this approach will also impact other fields such as neutron transport in heterogeneous media and heat conduction in composite materials. The insight obtained from this approach will, ironically, also improve the efficiency of multigrid solution techniques.

### **Scientific Approach and Accomplishments**

The objective of this project was to develop new, numerical, multilevel upscaling techniques based on a solid mathematical foundation that would facilitate the efficient and accurate coarse-scale numerical treatment of flow through heterogeneous porous media.

The development of the multigrid homogenization (MGH) algorithm was motivated by the observation that equivalent multiscale issues arise in the development of multi-level iterative methods. In particular, the efficiency of a multigrid method is tightly coupled to both the coarse-grid operator's approximation of the fine-grid operator's coarse-scale influence and to the ability of the inter-grid transfer operators to approximate the interaction of the various scales. Early work in multigrid methods considered utilizing simple averages such as the arithmetic and harmonic average to define the coarse-grid operators, in conjunction with standard inter-grid transfer operators (i.e., full weight restriction, bilinear interpolation). Not surprisingly this approach was fragile, yielding convergence rates that were strongly dependent on the fine-scale structure and variability of the permeability [1]. Considerable research in this area eventually led to robust and efficient multigrid methods [3,4], strongly suggesting that the corresponding coarse-grid operators provide an excellent approximation of the equivalent homogenized operators.

Based on this premise we derived a local, explicit expression that defines the two by two cell-based permeability tensor in terms of a given coarse-grid operator. We have shown that this permeability tensor is symmetric positive definite, and moreover, that --- when fine-scale structure dictates --- a dense coarse-scale tensor will result, even from a fine-scale isotropic permeability.

We have demonstrated the effectiveness of this approach on two standard, classic problems. The first has a square-shaped internal inhomogeneity with diffusion coefficient  $d$  inside this square and  $1.0$  outside, for which theory shows the tensor must be a diagonal multiple of the identity. We originally obtained excellent agreement of the black box homogenized permeability coefficient over eight orders of magnitude in  $d$ .

As  $d$  approaches 0, the harmonic mean overestimates the answer by 10%, and as  $d$  approaches infinity the arithmetic mean underestimates the answer by 10%, whereas the relative error of the MGH results compared with the rigorous results of Bourgat [2] is less than 2% over the entire range of  $d$ . The second problem has an L-shaped inhomogeneity, for which we originally obtained, remarkably, the exact axes of diffusion and relative errors in the magnitudes of the eigenvalues of 5% and 0.4%.

Recently, Dvorák [6] noticed that use of the Ritz finite element discretization and its dual could be used to compute upper and lower bounds of homogenized permeability. By exploiting this observation we were able to bound the error from above and below. By employing the arithmetic average of these two bounds, we demonstrated that the relative error in the first problem was reduced to 1% and that the relative errors in the second case were changed to 1.1% and 2.9%.

For the first case, the best of the Hashin-Shtrikman bounds [7], which is not known *a priori*, is nearly as good as the MGH results, but since these bounds are based on volume fractions, they do not change when the square-shaped region of inhomogeneity changes to a circle-shaped or lozenge-shaped region. The MGH bounds do change and continue to yield estimates within 1% relative error compared with the rigorous results of Bourgat [2].

Our preliminary investigation was restricted to single-phase saturated flow in two-dimensional periodic media. But Dendy's multigrid algorithm has demonstrated its efficiency and robustness for general boundary conditions in two- and three-dimensional problems [3,4]. We recall that the fundamental component of this algorithm, and hence our MGH algorithm, is the operator-induced variational coarsening. Thus, we began by using the variational formulation of this coarsening procedure to extend our local expression for the homogenized permeability to accommodate general boundary conditions. The resulting MGH algorithm has two distinct advantages over computationally competitive methods: the global domain is coarsened without the use of artificial internal boundary conditions, and a dense coarse-scale permeability tensor results. We anticipate that these important features of our method will play an even more important role in three dimensions.

The upper and lower bounds obtained with the variational formulation are a critical step in establishing a strong mathematical foundation for the MGH algorithm and for multilevel upscaling in general; however, such a mathematical foundation is far from complete.

We believe that the variational formulation provides an excellent starting point to build a mathematical foundation for this algorithm. This approach may be augmented by the equivalent algebraic view, that this coarsening procedure recursively utilizes approximations of the Schur complement. A succeeding direction of this theoretical investigation could be tight error bounds. This investigation may also suggest improvements that can be made to the coarsening procedure, and hence, may lead to improvements in the multigrid solution algorithms themselves.

In the increasingly common situation that geostatistical techniques are used to generate many fine grid realizations of porous media, there are two applications of the MGH algorithm that still need to be investigated. The first, direct, approach is to utilize the MGH algorithm to compute a corresponding set of coarse-grid realizations, followed by the multigrid solution of the corresponding flow problems.

Another potential area to pursue are extensions to multiphase saturated and unsaturated flow. The direct application of single-phase techniques has already shown promising performance [5].

### **Publications**

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