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The objective of this study is to develop a multiscale/multiresolution method for computing wave propagation and scattering in strongly heterogeneous media. The important feature of this method is that does not require resolving the small scale details, yet it can capture their effect on the large scales. The central idea is to incorporate the small scale information into the finite element base functions, so that the effect of small scales on the large scales is correctly captured. This feature allows us to break a large scale computation into many small and independent pieces, which can be carried out in perfect parallel. As a consquence, the size of the computation is drastically reduced. This gives us the possibility to attack problems with many spatial and time scales.

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Final Report for AFOSR Grant F49620-97-1-0282

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1. Objective

The objective of this study is to develop a multiscale/multiresolution method for computing wave propagation and scattering in strongly heterogeneous media. The important feature of this method is that does *not* require resolving the small scale details, yet it can capture their effect on the large scales. The central idea is to incorporate the small scale information into the finite element base functions, so that the effect of small scales on the large scales is correctly captured. This feature allows us to break a large scale computation into many small and independent pieces, which can be carried out in perfect parallel. As a consequence, the size of the computation is drastically reduced. This gives us the possibility to attack problems with many spatial and time scales.

2. Status of effort

The idea is best illustrated by first considering the following elliptic equation.

$$-\nabla \cdot (a_\epsilon \nabla u) = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega, \tag{1}$$

where $a_\epsilon(x)$ is a positive definite matrix with a small parameter ϵ characterizing the physical small scale. Our MsFEM is based on the Galerkin finite element method. The only difference between our method and the conventional finite element methods is in the way we construct the base functions. In our MsFEM, the base function, ϕ^i, satisfies the leading order homogeneous elliptic equation within each computational element, K,

$$\nabla \cdot a(\mathbf{x}) \nabla \phi^i = 0 \qquad \text{in } K. \tag{2}$$

Let $\mathbf{x}_j \in \overline{K}$ $(j = 1, \ldots, d)$ be the nodal points of K. As usual, we require $\phi^i(\mathbf{x}_j) = \delta_{ij}$. One needs to specify the boundary condition of ϕ^i to make (2) a well-posed problem (see below). One obvious choice (but not the best one) is to use a linear boundary condition. We remark that the idea of using special base functions is not new. In the case of convection-diffusion equations with boundary layers, exponential base functions have been used to obtain uniform convergence independent of the boundary layer thickness (see, e.g., [1].

An important question is if our MsFEM can correctly capture the small scale effect on the large scales. We give a definite answer in the special case of $a_\epsilon = a(\mathbf{x}, \mathbf{x}/\epsilon)$, with $a(\mathbf{x}, \mathbf{y})$ being periodic in $\mathbf{y}$. We can prove [4] that the multiple scale FEM indeed converges to the correct homogenized solution as $\epsilon \to 0$:

$$\|u - u^h\|_{1,\Omega} \le C_1 h \|f\|_{0,\Omega} + C_2 (\epsilon/h)^{\frac{1}{2}} \qquad (\epsilon < h), \tag{3}$$

where $C_{1,2}$ are constants independent of ϵ and h.

Scale resonance and over-sampling technique

It turns out that the ratio ϵ/h in our estimate is sharp and generic. This reflects the two intrinsic scales, h, and ϵ, in the problem. Our numerical experiments have demonstrated that the method indeed fails to converge when $h \approx \epsilon$. We call this "Scale Resonance". A deeper analysis reveals that the boundary layer in the first order correction term of the base function is responsible for this resonance error. This boundary layer reflects the mismatch between the global nature of the elliptic solution operator and the local boundary condition for the base functions. By a judicious choice of boundary conditions for ϕ^i, this boundary layer can be reduced or even eliminated. This will give rise to a conservative discretization for the numerical solution. This conservative discretization leads to *cancellation of resonance errors,* and gives an improved rate of convergence $O(h^2 + \epsilon)$ to the leading order in the discrete l^2 norm. Indeed this has been observed numerically.

In the case of periodic oscillatory coefficients, one can find a perfect boundary condition for ϕ^i which does not contain spurious numerical boundary layers in the corrector. Unfortunately, this perfect boundary condition involves solving a cell problem, which is not available for general non-periodic oscillatory coefficients. To overcome this difficulty, we propose to use an over-sampling technique in [4]. The idea is quite simple and easy to implement. Since the boundary layer in the corrector is thin, $O(\epsilon)$, we can sample in a domain with size larger than $h + \epsilon$. Use only the interior sampled information to construct the base. By doing this, the boundary layer in the larger domain has no influence on the base functions. We have showed through numerical experiments that this simple technique is very effective for a wide range of applications, including problems with continuous scales (see [3]).

Another advantage of our method is its ability to scale down the size of a large scale problem. This offers a big saving in computer memory. For example, let N to be the number of elements in each spatial direction, and M be the number of subcell elements in each direction for solving the base functions. Then there are total $(MN)^n$ (n is dimension) elements at the fine grid level. For a traditional FEM, the computer memory needed for solving the problem on the fine grid is $O(M^n N^n)$. In contrast, MsFEM requires only $O(M^n + N^n)$ amount of memory. If $M = 32$ in a 2-D problem, then traditional FEM needs about 1000 times more memory than MsFEM.

From the homogenization theory [2], we expect that the idea of MsFEM can be successfully applied to the scalar wave equation and the Maxwell equations with strongly heterogeneous media. In the time domain, we use implicit time discretization. An implicit discretization is preferred because larger time steps can be used. This is important for computing long distance propagation of waves. For the spatial discretization, the MsFEM formulation for the elliptic problem can be used directly. One of the results of homogenization for wave equations is that the possible oscillation in time induced by spatial oscillation disappear upon spatial averaging [2]. Thus, it is possible to use large time steps for the large scale solution. There are several other advantages using our method. First of all, the multiscale base functions are only computed initially. Once they are obtained, we can use them for computations at later time steps. And the computations at later times are all on coarse grid with large time steps. This gives a tremendous saving in computation times and memory, and allows us to attack practical problems with many scales.

3. Accomplishments/New Findings

We have applied our method to study wave propagation through multiscale random media with singular geometric boundary. We found that when the wave number is not very large, our method gives an accurate approximation even on a relatively coarse grid. For problems with large wave numbers, our MsFEM does not capture very well the interaction between the high frequency component introduced by the large wave numbers and the small scale spatial heterogeneous media. Our main effort in the past year or so is to improve our current MsFEM so that we can also capture effectively the high frequency information induced by the large wave numbers. We achieve this by incorporating the phase function (consequently the oscillatory wave form $\exp(ik\psi(x))$) into our finite element base functions. To this end, we need to approximate the leading order phase function in the wave equation (or the Helmholtz equation in the frequency domain). We expect that this correction would enable us to capture effectively the high frequency solution induced by both the small scale spatial heterogeneous media and the high frequency wave number.

Our another effort is to develop a new effective model equation in two and three space dimensions via the integral equation approach to capture the small scale information for wave scattering in rough surfaces with large wave numbers. The advantage of this model is that it reduces the problem by one dimension, and yet it can be evaluated via FFT with $N\log(N)$ operation count, where N is the number of grid points in the scatter surface. This gives rise to a very fast and robust method to study wave scattering in rough surfaces. Another important feature of this model equation is that it can capture very accurately the small scale feature of the scattering solution, such as corners, cusps, and jump discontinuities introduced by rough surfaces. Our preliminary numerical experiments have demonstrated that our model equation is indeed very effective and robust even for surfaces with order one roughness and very large wave numbers. The potential applications of this approach seem to be very promising.

3. Personnel Supported: This grant provides one-month salary support for Thomas Y. Hou (PI), a full salary support a postdoc, Yu Zhang, who is responsible for most of the code development and implementation of the multiscale finite element method for wave propagation scattering in heterogeneous media.

Publications

1. Y. Efendiev, T. Y. Hou, and X. H. Wu, *Convergence of a Nonconforming Multiscale Finite Element Method*, to appear in SIAM J. Numer. Anal.
2. T. Y. Hou and X. H. Wu, *A Multiscale Finite Element Method for Elliptic Problems in Composite Materials and Porous Media,* J. Comput. Phys., **134**, pp. 169-189, 1997.
3. T. Y. Hou, X. H. Wu, and Z. Cai, *Convergence of a Multiscale Finite Element Method for Elliptic Problems With Rapidly Oscillating Coefficients,* to appear in Math. Comput..
4. X. H. Wu, Y. Efendiev, and T. Y. Hou, *Analysis of Upscaling the Absolute Permeability*, submitted to Computational Geosciences.

Interactions/Transitions:

The work on multiscale finite element methods has been presented by Hou in the Fourth SIAM Meeting on Mathematical and Computational Issues on Geosciences in Alberquerque in June of 97. Hou is also invited to give a key note lecture on this topic in the European Congress on "Applied Mathematics for Industrial Flows" to be held in Spain from Oct. 1 to 3, 1998.

We are in the process of transferring our knowledgement on the multiscale finite element method to a practical oil reservoir scale-up code. This is currently carried out by my graduate student, Efendiev, who spent his summer working at the research center of Chevron Petroleum Technology Company at La Habra, CA. Our main contacts are Dr. Louis Durlofsky, and Dr. Wen Chen. The telephone number for Durlofsky is 310/694-9103, and his email address is jljdu@chevron.com. Our purpose here is to combine the moment correction method developed at Chevron with our multiscale finite element method to develop a process independent up-scaling method.

Another technology transition activity is with Dr. Don Zhang in the Earth and Geoscience Division in Los Alamos. The telephone number for Dr. Zhang is (505)667-3541, and his email address is dzhang@vega.lanl.gov. The purpose is to develop a robust upscaling method for two-phase flows by combining the stochastic modeling based on the stream-tube method with our multiscale finite element method. The experts in the EES5 division of LANL are very enthusiastic about our results and would like to have a long term interaction with us on various applications of our method.

New Discoveries, Inventions or Patent Disclosures: None.

Honors and Awards:

Hou is invited to give a 45-Minute Lecture at the International Congress of Mathematicians in Berlin, 1998. This is considered a very high honor for mathematicians. He was the co-recipient (with Lowengrub and Shelley) of the 1998 Francois N. Frenkiel Award from the American Physical Society for the best paper in Phys. Fluids. He also received the Feng Kang Prize in Scientific Computing in August of 1997. In addition, he was invited to give a plenary lecture in the European congress on "Applied Mathematics for Industrial Flows" to be held in Spain in October of 1998 and the First International Congress of Chinese Mathematicians to be held in Beijing in December of 1998.

References

[1] I. Babuška and W. G. Szymczak, *An Error Analysis for the Finite Element Method Applied to Convection-Diffusion Problems,* Comput. Methods Appl. Math. Engrg., **31**, pp. 19-42, 1982.

[2] A. Bensoussan, J. L. Lions, and G. Papanicolaou, *Asymptotic Analysis for Periodic Structures,* volume 5 of Studies in Mathematics and its Applications. North-Holland Publ., 1978.

[3] T. Y. Hou and X. H. Wu, *A Multiscale Finite Element Method for Elliptic Problems in Composite Materials and Porous Media,* J. Comput. Phys., **134**, pp. 169-189, 1997.

[4] T. Y. Hou, X. H. Wu, and Z. Cai, *Convergence of a Multiscale Finite Element Method for Elliptic Problems With Rapidly Oscillating Coefficients,* to appear in Math. Comput..