Views on State of the Art

at the Conference on Computational Methods in Multiscale Analysis and Applications
Gainesville, Florida, February 29–March 2, 2004

Numerical methods that allow for the bridging of different scales in simulations have found applications in various areas ranging from atomistic simulations to continuum scale problems. Even for problems without multiple scales, multilevel algorithmic structures have been used to capture the solution efficiently. Advances in multiscale and multilevel techniques have now made possible engineering analysis of large-scale problems that were previously not within the reach of computational resources.

1. **Multiscale techniques.** Approaches to handle multiscale problems are as varied as the applications in which the problems arise. The approaches presented at the conference could be divided into four broad categories: asymptotic expansions for solutions of partial differential equations, analysis of discrete network models, numerical methods for PDEs which are designed to handle a multiscale structure, and techniques which are application specific. The asymptotic methods for differential equations which were discussed include homogenization theory, high frequency asymptotics, small spatial scale asymptotics, and boundary layer analysis. All these closely tie in with modern numerical methods designed to handle multiple scales including special finite element basis functions derived from homogenization theory so as to capture fine spatial properties, and high order quadrature and discretization schemes which can capture a wide range of frequency scales. The discrete network models are useful for bridging atomistic and continuum scales and at the same time are related to discretization and numerical schemes. Application specific approaches include models for large eddy simulation, turbulent flows, modeling in biotechnology and nanotechnology, and continuum models for granular flows.

Several important future directions for research have been identified by conference participants. From the point of view of asymptotic and numerical analysis, these include extending multiscale asymptotic and computational frameworks to discrete problems, using adaptive error control for multiscale problems, understanding the behavior of boundary/interior layers which arise from multiple scales, the development of methods to efficiently compute these boundary layers, and combining analytic and statistical techniques to accurately model microscale data. In electromagnetics, problems in which the structures span a large number of wavelengths will be important in the near future for a variety of applications. Another set of interesting problems are those with disparate time scales, without any assumptions of temporal periodicity. From the applications point of view, important research areas in which these mathematical techniques play a significant role include biomedical engineering, circuit design, photonics, nanotechnology, and composite materials.

2. **Multigrid techniques.** In this area, advances have been made both in theory and algorithm design. While a theory for geometric multigrid methods has matured over the last few decades, new developments have taken place, such as nontrivial applications of the theory to problems in electromagnetics, and a new additive multigrid theory improving previous estimates. Simultaneously, there is a resurgence of interest in algebraic multigrid methods (AMG), wherein recent advances include AMGe, spectral AMG, Matching AMG, AMG using energy minimization, adaptive smoothed aggregation, and sharp convergence theory for two level methods.

The future of multigrid is likely to involve applications to more demanding physical problems, e.g., electromagnetics, fluid flows, elasticity, and non-convex minimization problems. Multigrid techniques are likely to play a fundamental role in the fast solution of higher order problems (like strain-gradient systems in elasticity and Cahn-Hilliard type equations in nanoscience). While new applications engender new discretizations (DG, mortar, etc) which will in turn require new multigrid solvers, one can also expect multigrid techniques to be used to develop new discretizations (e.g., least squares). A better understanding of how to use multigrid together with homogenization of multiscale problems will benefit many applications. While an efficient AMG algorithm to solve arbitrary linear systems is probably out of reach, development of reliable and robust AMG algorithms for systems of partial differential equations (elasticity, electromagnetics, multiple physical couplings, etc.) seems to be within reach. The present convergence theory for AMG (beyond two level theory) leaves much room for further research.

The development of efficient, adaptive, and robust multigrid methods will certainly have a great impact in many fields. By providing efficient and reliable tools for solving linear systems, multigrid algorithms will allow us to model physical phenomena with billions and even trillions of degrees of freedom, putting many previously untouched scientific phenomena within the reach of computational modeling.

3. **Inverse problems.** Multiscale asymptotic, numerical and modeling techniques have recently been and will continue to be useful for developing methods to solve inverse problems. Although an inversion problem without any *a* priori knowledge is frequently computationally unstable, a multiscale model of the problem could yield stable and less computationally intensive techniques. We have seen these ideas used in the recovery of small-scale inhomogeneities (small, for example, relative to the electromagnetic wavelength), and separately in the recovery of large-scale properties of subsurface flows. In this general direction an important problem will be to apply multiscale models towards the recovery of the media on several scales at once. Again, due to uncertainties which may be present, the combination of analytic and statistical methods may be needed here. Numerical methods which are designed for inverse problems and multiple scales are needed for validation and optimization of inverted data. Application areas include geophysics and biomedical imaging.

4. **Application areas.**

Computational fluid mechanics: Many outstanding research problems here involve multiple scales. The examples, as reflected by the presentations, include turbulence (wide range and continuous distribution of wave numbers), multiphase flows (different material properties, sizes, and interactions), non-Newtonian fluids (memory and shear-induced property variations), fluid-structure interactions (multiple materials, high degree of stiffness, moving boundaries), cavitation (disparate time scales and Mach numbers), biodynamics (functions, properties, length and time scales). In short, development of multiscale techniques have direct consequences in engineering, physical and biomedical sciences. Groundbreaking works will be based on marriage between large scale computing, insightful modeling, and sound numerical and analytical tools.

Developing subareas seem to be delineated by the two fundamentally different ways in which multiple scales can arise in fluids: (i) boundary or interior layers, which we see in singular perturbation type of problems, and (ii) immersed multiple scales, such as turbulence, where all scales co-exist in the same space rather than being separated. New ideas are needed to address both types of problems.

Computational solid mechanics: This area was represented in the conference by talks on materials with microscale, fracture mechanics, composite materials, and granular flows. It is a challenge to account for the effects of microstructure distributions on the singularity of the elasticity solution such as in the case of cracks or re-entrant corners. An important application would be to micro and nanocomposites. Progress on development of continuum models and constitutive relations for granular flows was reported.

The effects of microscale phenomena such as microcracks, debonding, corrosion embrittlement, dislocation transport, microscale thermal and viscous effects, can have a dramatic impact on the macroscopic behavior of engineering systems. Current methods which rely on classical homogenization techniques (which smear the effects) and considerable experimentation, are not often capable of providing reliable information needed to support the design of future products. New paradigms that can resolve multiscale effects as well as intelligently incorporate them into engineering design are needed.

Computational electromagnetics: Quite effective numerical techniques to solve low frequency problems in computational electromagnetics (CEM) have been developed in the last few decades (e.g., finite elements, multipole methods, multigrid). A central challenge that remains involves high-frequency applications, i.e., applications where the structures span a large number of wavelengths, e.g., in communications (optical fibers), in high-frequency radar (military and civilian), in geophysics (prospection), etc. Current methods rely on approximations such as the eikonal model of geometrical optics.

Recent advances in CEM include the development of multigrid solvers, multipole techniques and other "accelerated method" (e.g., those based on arrays of "equivalent sources") for scattering applications, the use of Eulerian geometrical-optics solvers, the introduction of effective high-order quadrature schemes for the integral equations modeling wave-propagation, and the design of efficient error-controllable hybrid algorithms for high-frequency applications. Industrial applications that will require further algorithmic advances include applications in medicine and health (e.g., tomography, power-line safety, etc), in circuit or magnetic storage design, and in photonics.