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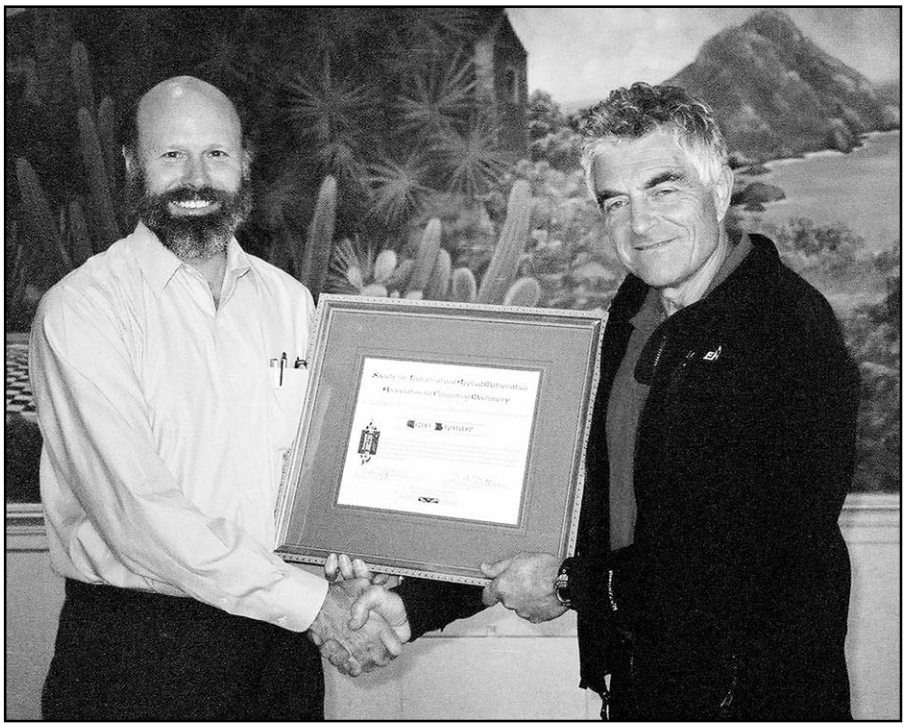
2005 CS&E Prize Honors Multilevel Methods Pioneer

For "pioneering modern multilevel methods, from multigrid solvers for partial differential equations to multiscale techniques for statistical physics," Achi Brandt of the Weizmann Institute of Science is the 2005 recipient of the SIAM/ACM Prize in Computational Science and Engineering. The prize was awarded at the third SIAM Conference on Computational Science and Engineering, held in Orlando, February 12–15. Brandt, who was also cited "for influencing almost every aspect of contemporary computational science and engineering," provided SIAM News *with the following perspective of the area in which his work has been so influential.*



SIAM past president James (Mac) Hyman presented the 2005 SIAM/ACM Prize in Computational Science and Engineering to Achi Brandt at the third SIAM Conference on Computational Science and Engineering, in Orlando, Florida.

The Scale Gap

Despite their dizzying speeds, modern supercomputers are incapable of handling many of the most vital problems in science and engineering. This is due primarily to the gap between the microscopic scale, at which physical laws are given, and the much larger scale of phenomena we wish to understand and control.

The existence of this gap implies, first of all, huge numbers of *variables* (e.g., particle locations, gridpoint values of a discretized partial differential equation, picture elements), and possibly even much larger numbers of *interactions* (e.g., among particles, each interacting with all the others). Moreover, computers simulate physical systems by moving just a few variables at a time; each such move must be extremely small, because a larger move would have to take into account all the motions to be performed simultaneously by all other variables.

Consequences of these difficulties include dynamical simulations in which only tiny time steps are allowed, iterative solvers that are very slow to converge, and critically inefficient Monte-Carlo sampling. Even more seriously, such computer schemes are incapable of moving a system across large-scale energy barriers, each of which can be crossed only by a large coherent motion of a very large number of variables. All these computational obstacles make it impossible today to calculate, say, properties of elementary particles and atomic nuclei, or to computerize chemistry, so as to enable detailed understanding and design of proteins, drugs, nano-systems, materials, chemical reactions, industrial processes. . . .

Multiscale Computation

In methodical work on several different model problems, it has been shown that all types of scale-related bottlenecks can be removed by a variety of multiscale algorithms. Such algorithms were first developed in the form of fast *multigrid solvers* for discretized PDEs. These solvers iteratively employ local processing (relaxation) on the given grid and then on increasingly coarse grids, with each grid level providing corrections to the equations governing the next-coarser level and to the solution forming at the next-finer level.

It has been shown that these (and more elaborate) interscale interactions can indeed eliminate many scale-associated difficulties, such as slow convergence (e.g., in optimization processes or in PDE solvers); critical slowing down (in statistical mechanics); ill-posedness (e.g., of inverse problems); conflicts between small- and large-scale representations (e.g., in wave phenomena, bridging the gap between wave equations and geometric optics); extremely large numbers of long-range interactions (in many-body systems or integral equations); and the need to rapidly update very large determinants (in quantum chromodynamics) or to produce many fine-level solutions (e.g., in time-dependent problems or optimal control) or very many fine-level independent samples (in statistical physics). Multigrid-like methods called *algebraic multigrid* (AMG) can rapidly solve highly disordered systems, such as Dirac equations on critical gauge fields and linear and nonlinear systems of PDEs discretized on unstructured grids. The AMG methods are also being modified to make them useful in the efficient solution of many types of graph, data mining, and vision problems.

Systematic Upscaling

Physical systems with huge numbers of variables are always highly *repetitive*: A small set of underlying laws (in the form of equations or statistical rules) governs throughout the problem domain. This has opened the way to a new computational paradigm, called systematic upscaling (SU), in which, at each coarser level, a set of governing equations that are valid everywhere is constructed once and for all, derived from the next-finer level by calculations that are *conducted only in some small representative "windows."* This removes the need for fine-scale resolution of the entire system.

Figure 1. *Selection of coarse-level variables for a polymer. Each pseudoparticle at the next-coarser level (large dots) is placed at the geometric center of three fine-level atoms (small dots).*

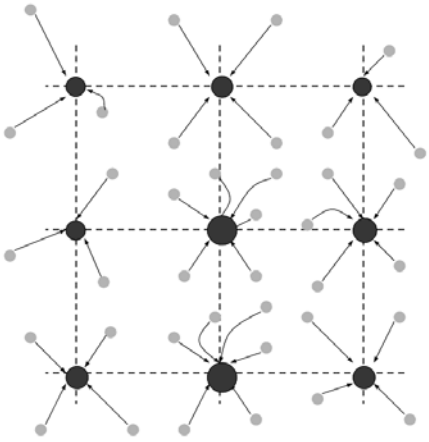


Figure 2. *Coarse-level variables for an atomistic fluid are defined at the points of a lattice; each variable describes an average property of the surrounding atoms (small dots).*

Based on coarsening procedures encountered in renormalization group methods and on multigrid-like interscale feedback, SU includes, first of all, a rigorous approach for selection, at each level, of the set of *variables* that can adequately represent the next-coarser level. Figures 1 and 2 illustrate examples of coarse-level variables (developed in collaborations with Dov Bai and Valery Ilyin). For a polymer (chain of small dots, Figure 1), the variables at the (first) coarse level are the locations of pseudo-particles (large dots); each such particle is placed at the geometric center of three fine-level atoms. For an atomistic fluid (Figure 2), the coarse level consists of variables defined at the points of a lattice; each variable describes an average property of the surrounding atoms (small gray dots): density, average charge or dipole moment, and so forth. Coarse variables of other types would enter at lower temperatures, as the fluid approached solidification.

Furthermore, SU includes procedures by which calculations at each level dictate the operational rules (e.g., equations) that should govern the next-coarser level and the windows at which the next-finer-level calculations should be conducted. Iterating back and forth between all the levels leads quickly to multilevel self-consistency. Such interlevel interactions allow very efficient computation. For example, while atom-by-atom simulation of polymers, including proteins, is extremely slow, because of energy barriers at all scales, even the first level of coarsening depicted here is free of all the more local barriers. Consequently, it allows simulations that are two orders of magnitude faster. Likewise, the multiscale computation of fluids, recursively employing progressively coarser lattices of the type shown here, allows the study of phase transitions inaccessible to one-level simulations.

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