Multiscale Computational Methods:

Research Activities

Achi Brandt
Department of Applied Mathematics & Computer Science
The Weizmann Institute of Science, Rehovot 76100, Israel

ABSTRACT

This is a brief summary of the general scope of multiscale computations, and of our recent and current research directions and results.

1. General

Multiscale (or "multilevel", or "multigrid") computation are fast methods for solving huge problems defined in a low dimensional space (e.g., the physical space or space-time), including many-variable (e.g., partial differential) equations, optimization problems and statistical field calculations. The typical multiscale algorithm uses local processing (relaxing an equation, or locally optimizing, or locally simulating a statistical rule) on each scale of the space, with inter-scale interactions: typically, the evolving solution on each scale recursively modifies the *equations* (or the Hamiltonian) on coarser scales and the *solution* on finer ones. As a result, fine scales can be employed very sparingly, and sometimes only at special and/or representative small regions. Also, the inter-scale interactions can eliminate many types of troubles, such as slow convergence (in PDE solvers), ill-posedness (e.g., of inverse problems), critical slowing down (in statistical physics), large-scale attraction basins (in global optimization), conflicts between small-scale and large-scale representations (e.g., in wave problem), numerousity of interactions (in many body problems), the need to produce many fine-level solutions (e.g., in optimal control) or very many fine-level independent samples (in statistical measurements), etc.

the first multiscale algorithm was probably Southwell's two-level relaxation for solving elliptic partial differential equations[40], first extended to more levels by Fedorenko[23]. The first multigrid solvers exhibiting the typical modern efficiency (e.g., four orders of magnitude faster than Fedorenko's estimates) were developed in the early 1970's[3,9], leading to intensive international research on the theory of such solvers and their extension to more general types of partial differential problems, with numerous scientific and engineering applications. Much of this development is reported in the books[26,35,10,38,25,32,27,22,33,31,34,28,29]. Recent developments, including in particular the development of multiscale methods outside

the field of partial differential equations, are reviewed in[5,7,11]. See also the contributions to the present conference by D. Chu, Z. Huang, J. Sun and B. Li, M. Wang, J. Xu, and G. Zhou.

Highlights from our recent and current research activities are briefly described below, summarizing mainly *conceptual* developments. *Not* included are details of collaborations in developing multigrid solvers in various application areas, such as: aerodynamics, atmospheric and oceanic research, structural mechanics, tribology, robotics, quantum mechanics, astrophysics, condensed matter, VLSI design, and tomography.

2. PDE multigrid solvers

Steady State PDEs. Traditional multigrid solves general (linear and nonlinear, scalar and non-scalar) elliptic systems in some dozens of operations per discrete unknown (see the general guide[10]), and the algorithm can naturally and fully exploit a very large number of parallel processors (see, e.g. Sec. 11 in Ref. 7). A similar efficiency has recently been obtained for general **non-elliptic systems** with one family of characteristics, such as high-Reynolds incompressible flow problems[19,20,21]. Extensions are contemplated to systems with more characteristic families, including compressible flows. (Most multigrid solvers in current use for flow problems fall orders of magnitude behind the above mentioned efficiency.)

Ways have been developed to extend the multigrid solvers, in their full above-stated efficiency, to many **new situations**, including: free boundaries[37]; thin domains[36] (much thinner than the meshsize of some of the coarser grids); singularities and discontinuities of various types; local mesh refinements[1]; severe nonlinearities[41]; topological charges (e.g., in Dirac equations)[2,11]; problems with essential but small-scale features (e.g., small holes in the problem domain) which are "invisible" on coarser grids[16]; disordered systems[11]; highly oscillating boundaries and fast changes in boundary operators[17]; etc.

Rigorous quantitative analysis of multigrid solvers for general elliptic problems has been developed[6]. Unlike other rigorous theories, the quantitative analysis provides tools, based on local Fourier expansions, for numerically predicting the exact algorithm efficiency. This can therefore be, and indeed is, used for algorithm design and program debugging. Extensions are being developed to the non-elliptic, where so far the quantitative analysis[4,19,20] is not rigorous.

Inverse problems can become well-posed when formulated in a multi-scale setting, and can be solved at a cost comparable to that of solving corresponding direct problems[42,43]. A demonstration of this is being developed for system identification and inverse gravimetric problems.

Classical multigrid, and all other solution techniques, have been extremely ineffective for solving the highly indefinite system of stationary equations arising in **wave problems**, e.g., in acoustics, seismology, electromagnetic propagation and quantum mechanics. Efficient multilevel algorithms have now been developed

for such equations in their integral representation[8], and are being extended to the differential case. On each of their levels, the algorithms represent the solution as $\sum_j A_j(x) \exp(i\xi_j x)$. On increasingly coarser spatial grids (discretizing x), increasingly finer "momentum" resolutions (denser grids ξ_j) are used. The coarser the grid the more like ray formulation (geometrical optics) the equations become. This yields not only a faster solver, but also the option to treat most of the problem domain on coarse "grids", hence essentially by geometrical optics, with nested local refinements (using eventually the underlying wave equations) confined to small regions where the ray formulation breaks down. Also, the implementation of radiation boundary conditions in this representation is straightforward.

Such representations can also form the basis for a very efficient multigrid calculations of **many eigenfunctions** of a given elliptic operator; e.g., the Schrödinger operator in condensed matter applications.

For parabolic **time-dependent problems** it has been shown that multigrid techniques are extremely efficient not just in that they solve fast the system of implicit equations at each time step[14]. A large additional benefit is that only rare activation of fine scales is needed wherever the solution changes smoothly in time; e.g., wherever and whenever the forcing terms are stationary[24]. Also, multileveling allows parallel processing not only at each time step, but across the entire space-time domain. Extensions of such ideas to other time dependent problems, including high-Reynolds flows, are planned; they depend on the development described next.

Grid alignment with the characteristic lines of the problem yields much superior discretizations, both for evolution and stationary non-elliptic problems. Even when those lines are not known in advance, progressive grid alignment can naturally be integrated into the full multigrid (FMG) algorithm, needing no iterations.Moreover, in a multilevel algorithm the alignment is just a local operation, since each level can be a union of independent, possibly overlapping patches (interacting, as usual, with the coarser level, not with each other). This would provide also a tool for locally aligning grids with boundaries, which is expected to be much cheaper and more flexible than the global grid generation techniques, since the much simpler uniform cartesian grid may be used throughout the domain interior. The development of such systems is considered, but requires heavy investments in writing new basic software.

A multigrid algorithm (Sec. 7.5 of Ref. 9) provides an effective vehicle for **domain decomposition**, where many processors work in parallel to solve the problem, each processor in a different subdomain. The total solution work is only a fraction more than the work of solving just *once* in each subdomain. The communications needed between the subdomains is very small, since it is required only at coarse levels[12].

3. Other multiscale computations

Performing general **integral transforms**, or solving **integral and integro-differential equations**, discretized on n grid points, have been shown to cost, using a multigrid structure, only $O(n)$ or $O(n \log n)$ operations (even though they involve *full* $n \times n$ matrices)[15,8]. In particular this is true for performing Fourier transform on *non-uniform* grids. An extension has been devised to transforms with oscillatory kernels[8].

Calculation of the $n(n-1)$ **interactions between** n **bodies**, and even local **ground states** of such interactions, have been performed in $O(n)$ operations by embedding in a multigrid structure[8]. In case there is no good initial approximation to the ground state, however, the calculations do not converge. Methods are therefore needed similar to those discussed next.

Multilevel annealing methods have been shown as very effective for **global optimization** of systems with a multitude of local optima and with multi-scale attraction basins, in which cases the usual simulated annealing method may be extremely inefficient. This includes in particular discrete-state optimization, provided the problem is defined in a low dimensional (e.g., the physical) space (thereby allowing multiscale interactions)[18,39].

Likewise, multilevel approaches are much more effective than usual (e.g., simplex) algorithm for **linear programming** problems defined in the physical space. This has been demonstrated for the *transportation problem*[30].

In QCD calculations with interacting fermions it is required to update the value of the **determinant** of an $n \times n$ matrix (representing discretized Dirac equations) each time one of its terms (the gauge field) changes. On a model (discretized diffusion) problem, we have shown that each such update can be done in $O(1)$ to $O(\log n)$ operations, by updating a certain multigrid structure. The structure requires $O(n \log n)$ storage locations[5,2].

Multilevel Monte Carlo methods for problems in statistical mechanics and lattice field theory have been initiated[18], and are being further developed. Usual Monte Carlo methods, which update one site at a time, require $O(L^{d+z})$ operations to produce each new (nearly independent) statistical sample, where d is the problem dimension, L is the linear size of the lattice and typically $z \approx 2$. For some model problems it has been shown that, due to multigrid acceleration on one hand and sampling on coarse levels on the other hand, a new sample may on the average be produced in only $O(1)$ operations[13,11].

Multilevel Monte-Carlo (MC) methods are also being developed for **many particle** (e.g. atom) simulations. Usual MC methods, moving one particle at a time, are extremely slow, since one particle can move very little when all others are fixed. Moreover, since its neighbors in their turn move very little too, the particle is likely to reverse much of its movement in subsequent MC sweeps. Initial multilevel experiments have shown to alleviate this slowness very much, since they perform

collective displacements of the particles. Much further development is planned.

Multilevel techniques to accelerate **protein folding** and similar calculations are expected to emerge from our multilevel Monte Carlo and global optimization methods (see above). A preliminary exploration has started.

We have shown in several examples that the multilevel processing can yield **macroscopic equations** for the computed system. These equations can be much simpler than those derived by group renormalization methods, since they can retain a certain (properly bounded) amount of iterative interaction with finer levels[13]. Much more can and will be done in this direction. The birth of macroscopic particles, or rays, from microscopic PDEs (like the above mentioned wave equations), and the birth of macroscopic PDEs (e.g. continuum mechanics) from atomic motions, are just examples.

Development of multilevel techniques in **image processing** has been started. One of the first objectives, for example, is to demonstrate, for a noised picture with N pixels, that all statistically significant smooth lines and edges can be discovered in $O(N \log N)$ operations.

4. References

1. D. Bai and A. Brandt, *SIAM J. Sci. Stat. Comp.* **8** (1987) 109.

2. R. Ben-Av, A. Brandt, M. Harmatz, E. Katznelson, P.G. Lauwers, S. Solomon and K. Wolowesky, *Phys. Lett. B.* **253** (1991) 185.

3. A. Brandt, in *Proc. 3rd Int. Conf. Numerical Methods in Fluid Mechanics*, ed. H. Cabannes and R. Temam, (Springer-Verlag, 1973) 82.

4. A. Brandt, *Multi-grid solvers for non-elliptic and singular-perturbation steady-state problems*, (Weizmann Institute of Science, 1981).

5. A. Brandt, in *Multigrid Methods: Theory, Applications and Supercomputing*, ed. S.F. McCormick, (Marcel-Dekker, 1988) 35.

6. A. Brandt, in *Prel. Proc. 4th Copper Mountain Conf. on Multigrid Methods*, (1989). An extended and corrected version is a report entitled: "Rigorous Quantitative Analysis of Multigrid", April, 1991.

7. A. Brandt, in *Proc. 4th Copper Mountain conf. on Multigrid Methods*, ed. J. Mandel et al., (SIAM, 1989) 13.

8. A. Brandt, *Computer Phys. Communications* **65** (1991) 24.

9. A. Brandt, *Math. Comp.* **31** (1977) 333.

10. A. Brandt, Multigrid Techniques: 1984 Guide, with Applications to Fluid Dynamics. (Monograph, 1984). Available as GMD-Studien Nr. 85 from GMD-F1T, Postfach 1240, D-5205, St. Augustin 1, Germany. Also available from Secretary, Math. Dept., Univ. of Colorado at Denver, Denver, CO 80217-3364.

11. A. Brandt, in *Proc. Lattice 91*, eds. M. Fukugita et al, to appear in *Nuc. Phys. B* (Proc. Suppl.), 1992.

12. A. Brandt, In Proc. 6th Domain Decomposition Conf., Como, Italy, June 1992.

13. A. Brandt, M. Galun and D. Ron, Optimal multigrid algorithms for calculating thermodynamic limits, *J. Stat. Phys.*, submitted.

14. A. Brandt and J. Greenwald, in: *Multigrid Methods III*, eds. W. Hackbusch and U. Trottenberg, (Birkhäuser-Verlag, 1991) 143.

15. A. Brandt and A.A. Lubrecht, *J. Comp. Phys.* **90** (1990) 348.

16. A. Brandt and V. Mikulinsky, Recombining iterants in multigrid algorithms and problems with small islands. Report, (1991).

17. A. Brandt and V. Mikulinsky, Multigrid treatment of problems with highly oscillating boundary and boundary conditions. Report, (1991).

18. A. Brandt, D. Ron and D.J. Amit, in *Multigrid Methods II*, eds. W. Hackbusch and U. Trottenberg, (Springer Verlag, 1986) 66.

19. A. Brandt and I. Yavneh, On multigrid solution of high-Reynolds incompressible entering flows, *J. Comp. Phys.*, in print.

20. A. Brandt and I. Yavneh, Accelerated multigrid convergence for high-Reynolds recirculating flows, *J. Comp. Phys.*, submitted.

21. A. Brandt and I. Yavneh, in: *Prel. Proc. 5th Copper Mountain Conf. on Multigrid Methods*, (1991).

22. W. Briggs, Multigrid Tutorial. (*SIAM*, Philadelphia, 1987).

23. R.P. Fedorenko, *Ž. Vyčisl. Mat. i Mat. Fiz.* **4** (1964) 559.

24. J. Greenwald, Ph.D. Thesis, Weizmann Institute of Science, Rehovot, Israel, 1992.

25. W. Hackbusch, *Multigrid Methods and Applications*, Springer-Verlag, (1985).

26. W. Hackbusch and U. Trottenberg, (eds.), *Multigrid Methods*, Lecture Notes in Math. **960** (Springer-Verlag, 1981).

27. W. Hackbusch and U. Trottenberg, (eds.), *Multigrid Methods II*, Lecture Notes in Math. **1228** (Springer-Verlag, 1985).

28. W. Hackbusch and U. Trottenberg (eds.), *Multigrid Methods III.* (ISNM 98, Birkhäuser Verlag, 1991).

29. W. Hackbusch and U. Trottenberg (eds.), *Multigrid Methods: Special Topics and Application II.* (GMD-Studien Nr. 189, ISBN 3-88457-189-3, 1991).

30. R. Kaminsky, *Multilevel solution of the long transportation problem*, M.Sc. Thesis, The Weizmann Institute of Science, Rehovot, Israel, 1989.

31. J. Mandel et al (eds.), *Proc. 4th Copper Mountain Conf. on Multigrid Methods*, (SIAM, 1989).

32. S. McCormick (ed.), *Appl. Math. Comp.* **19** (1986) 1–372 (special issue).

33. S. McCormick (ed.), *Multigrid Methods: Theory, Applications and Supercomputing* (Marcel Dekker, 1988).

34. S.F. McCormick, *Multilevel Adaptive Methods for PDEs*, (Frontiers in Applied Science **6**, *SIAM*, Philadelphia, 1989).

35. S. McCormick and U. Trottenberg, (eds.), *Appl. Math. Comp.* **13** (1983) 213–474 (special issue).

36. V. Mikulinsky: Multigrid treatment of "thin" domains. Report, 1991, Dept. of Appl. Math., Weizmann Institute of Science, Rehovot, Israel.

37. V. Mikulinsky and A. Brandt, in: *Multigrid Methods: Special Topics and Applications II*, eds. W. Hackbusch and U. Trottenberg, (GMD-Studien Nr. 189, GMD, Sankt Augustin, Germany, 1991) 215.

38. D.J. Paddon and H. Holstein, (eds.) *Multigrid Methods for Integral and Differential Equations*, (Clarendon Press, 1985).

39. D. Ron, *Development of fast numerical solvers for problems of optimization and statistical mechanics*, Ph.D. Thesis, The Weizmann Institute of Science, Rehovot, Israel, 1989.

40. R.V. Southwell, *Proc. Roy. Soc. London, Ser A* **151** (1935) 56.

41. S. Ta'asan, *SIAM J. Sci. Stat. Comp.* **11** (1990) 51.

42. S. Ta'asan and P.K. Dutt, *Quarterly of Applied Mathematics* **XLVIII** (1990) 387.

43. S. Ta'asan, M.D. Salas and G. Kuruvila, in *Proc. AIAA 30th Aerospace Sciences Meeting and Exhibit*, Reno, NV (1992).