Multiscale Computational Methods:
Research Activities

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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), numerosity 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, first extended to more levels by Fedorenko. 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 1970s, 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, Recent developments, including in particular the development of multiscale methods outside
the field of partial differential equations, are reviewed in\textsuperscript{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 \textit{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

\textbf{Steady State PDEs}. Traditional multigrid solves general (linear and non-linear, scalar and non-scalar) elliptic systems in some dozens of operations per discrete unknown (see the general guide\textsuperscript{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 \textbf{non-elliptic systems} with one family of characteristics, such as high-Reynolds incompressible flow problems\textsuperscript{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 \textbf{new situations}, including: free boundaries\textsuperscript{37}; thin domains\textsuperscript{36} (much thinner than the meshsize of some of the coarser grids); singularities and discontinuities of various types; local mesh refinements\textsuperscript{1}; severe nonlinearities\textsuperscript{41}; topological charges (e.g., in Dirac equations)\textsuperscript{2,11}; problems with essential but small-scale features (e.g., small holes in the problem domain) which are “invisible” on coarser grids\textsuperscript{16}; disordered systems\textsuperscript{11}; highly oscillating boundaries and fast changes in boundary operators\textsuperscript{17}; etc.

\textbf{Rigorous quantitative analysis} of multigrid solvers for general elliptic problems has been developed\textsuperscript{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\textsuperscript{4,19,20} is not rigorous.

\textbf{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\textsuperscript{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 \textbf{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, 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 \( \xi_j \)) 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 prob-
lem 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 implementa-
tion 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 Schröd-
ing-er 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. 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. Also,
multileveling allows parallel processing not only at each time step, but across the
total space-time domain. Extensions of such ideas to other time dependent prob-
lems, 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 itera-
tions. Moreover, in a multilevel algorithm the alignment is just a local operation,
since each level can be a union of independent, possibly overlapping patches (inter-
acting, 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.
3. Other multiscale computations

Performing general integral transforms, or solving integral and integrodifferential 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)\textsuperscript{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\textsuperscript{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\textsuperscript{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)\textsuperscript{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\textsuperscript{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\textsuperscript{5,2}.

Multilevel Monte Carlo methods for problems in statistical mechanics and lattice field theory have been initiated\textsuperscript{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\textsuperscript{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. 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

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