Systematic Multiscaling in Materials Science Computations

A. Brandt

Department of Mathematics
University of California, Los Angeles, CA 90095
email: abrandt@math.ucla.edu

ABSTRACT

The multiscale computational methodology is a systematic approach to achieve efficient calculations of systems that inclue very many degrees of freedom (particle locations, discrete-function values, etc.). It includes fast multigrid solvers for discretized partial-differential equations (PDEs) and for other large systems of local equations; fast summation of long-range (e.g. electrostatic) interactions and fast solvers of integral and inverse PDE problems; collective computation of many eigenfunctions; slowdown-free Monte Carlo simulators; multilevel methods of global optimization; and general systematic upscaling procedures, which start at a microscopic scale where first-principle laws are known and lead scale-by-scale to processing rules of collective variables at increasingly larger scales.

1. The Scale Gap

Most difficulties in computing materials are primarily due to *the scale gap*, which exists between the microscopic scale at which physical laws are given and the much larger scale of phenomena we wish to understand.

This gap implies, first of all, a huge number of *variables* (e.g., atoms or grid-points), and possibly even a much larger number of *interactions* (e.g., one force between every pair of atoms). Moreover, computers simulate physical systems by moving *one variable at a time*; as a result, each such move must be extremely small, since a larger move would have to take into account all the motions that should in parallel be performed by all other variables. Such a computer simulation is particularly incapable of moving the system across large-scale *energy barriers*, which can each be crossed only by a large, and unknown, *coherent* motion of very many variables.

A general current approach to overcome the scale gap is by *multiscale modeling* (MSM; also called "multiscale simulation"). It studies a physical system by employing several different ad-hoc models, each describing a very different scale of the system. They are usually linked by *fine-to-coarse parameter passing*, in which data obtained from simulating a finer scale model, often coupled with experimental observations, are used to determine certain parameters of a larger scale model, regarding the latter as a coarse graining of the former.

Successful as MSM is in various special cases, its applicability and accuracy are generally severely limited, especially when the different simulated scales are not well separated, or when they interact with (possibly many) intermediate scales that introduce their own characteristics. Also, the calculation of the large-scale parameters usually still requires the full simulation of very large systems with painfully small steps.

2. Multiscale Algorithms

Past studies have demonstrated that the slowness associated with the necessarily small steps of moving one variable at a time can be overcome by multiscale algorithms. Such algorithms have first been developed in the form of fast **multigrid solvers** for discretized PDEs [1]. These solvers are based on two processes: (1) classical *relaxation* schemes, which are generally slow to converge but fast to *smooth* the error function; (2) approximating the smooth error on a *coarser grid* (typically having twice the meshsize), by solving there equations which are derived from the PDE and from the fine-grid residuals; the solution of these coarse-grid equations is obtained by using recursively the same two processes. As a result, large scale changes are effectively calculated on correspondingly coarse grids, based on residual information gathered from finer grids. In many years of research, the range of applicability of these methods has steadily grown, to cover most major types of linear and nonlinear large systems of equations appearing in sciences and engineering. This has been accomplished by diversifying the types of coarse representations, to include for instance grid-free solvers, called *algebraic multigrid* [2], non-deterministic problems ([3], [4]) and multiple coarse-level representations for wave equations [5].

Structural mechanics PDEs, discretized on well-structured grids, can be solved by multigrid in just several dozen operations per discrete unknown. For *unstructured* discretizations (e.g., by finite-element or finite-volume or mesh-free methods) algebraic multigrid solvers come close to achieving similar efficiency.

Nonlinear problems are solved as fast, with no need for global linearization, by a multigrid version called FAS. In this version, the relaxed solution at each fine level supplies corrections to the *equations* of the next coarser level. These *fine-to-coarse defect corrections* (DCs) can be calculated *locally*, just on a small patch of the fine level at a time, and they rarely need updating upon re-solving the problem. Thus, solving a problem many times (as part of some **evolution in time**, or in **optimizing design or control**) can usually be made mostly on very coarse grids with fixed DCs, rarely updating the DCs by visits to finer levels. Moreover, the finer the level the smaller the subdomain on which its DCs will usually need updating (e.g., a smaller neighborhood of the changes being introduced for optimizing the design).

In case of a **singularity (e.g., a material defect)**, increasingly finer patches introduced over progressively smaller neighborhoods of the singularity restore the *regular efficiency* (i.e., the same order of accuracy per unit work obtained in the absence of singularities). Such local-refinement patches can use their own *coordinates* (providing grids fitted to local boundaries, local solution characteristics, etc.) and their own *PDEs* (e.g., adding singular-perturbation terms at boundary layers). In particular, while the global description is in terms of continuum-mechanics PDEs, the local patches description can be *atomistic*. (This **quasi-continuum** method, as it is called today, was already described in §1.1 of [4].)

3. Upscaling

Such methods, that employ finer resolutions very sparingly, depend of course on having coarser-level (larger-scale) models. In some cases such models are readily available (e.g., a coarser discretization of the same PDE, or a continuum-mechanics description corresponding to the given fine-level atomistic model), but generally they need to be *derived*, one coarsening level at a time, starting from the known fine-level model. Since there is no reason to assume that accurate coarse-level descriptions will have nice analytic form (like simple PDEs), a general approach should derive them in the form of numerical tables.

Systematic Upscaling (SU) is a recent methodology for doing just that. It offers systematic procedures to iterate back and forth between all the scales of the physical problem, with a general criterion for choosing appropriate variables that operate at increasingly coarser levels (larger scales), and general techniques to derive their operational rules. Indefinitely large systems can in this way be simulated, with computation at each level being needed only within certain windows containing only a limited number (typically several thousands) of variables. Each level derives its operational rules (e.g., a Hamiltonian-like functional implying transition probabilities) from the next finer level, while the windows where it operates, and their boundary conditions, are provided by the next coarser level.

Unlike conventional ad-hoc multiscale modelling, SU is in principle generally applicable, free of slowdowns and bears fully-controlled accuracy.

First examples of SU, for simple polymers and fluids in equilibrium are described in the general review paper [6] and references therein. Other examples are currently under development, including solids and non-equilibrium examples. Variables at increasingly coarser levels have been identified, suitable for a variety of situations, indirectly describing features such as local crystal dimensions and directions, defects, dislocation, grains, etc.

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