Multiscale Simulation for High Energy Density Physics

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I. INTRODUCTION

To efficiently achieve major advances in multiscale simulation one *must* address three components:

1. the development of better analytic or computational models that capture the effect of under-resolved physics on the resolved physics;

2. the development of algorithms that either solve existing models faster or solve new models effectively;

3. the development of more advanced hardware.

The third will require the most money, but that money will be largely wasted without significant investment in the first two.

Historically, each of these components have contributed in similar measure to advance our simulation capabilities. For example, state-of-the-art simulations of turbulent flows can use subgrid models, spectral element methods, and distributed or parallel hardware.

Of course, in order to benefit from increased simulation capabilities, better visualization techniques and tools (including hardware) are also needed.

Here we articulate only a few points regarding the first two components, with more emphasis on the first. We will use supernova simulations as the framework for this incomplete discussion.

II. COMPRESSIBLE TURBULENCE AND MIXING

Better models are needed for compressible turbulence (including reactive and possibly stratified flows) and turbulent mixing — not just to capture their effect on fluid dynamics, but to also capture their effect on other important physics such as photon (and possibly neutrino) transport or nuclear combustion rates.

Furthermore, in many cases of interest, magnetic fields become important; and we are then faced with the additional complications of magnetohydrodynamic turbulence (for which no generally accepted subgrid model exist at present). Moreover, for some applications all this has to be done for relativistic regimes.

Of course, there is currently no fully satisfactory universal model for incompressible turbulence, much less for compressible turbulence. However, many models for incompressible turbulence have a long history and have been validated in many regimes. Ideally, every model of compressible turbulence should reduce to a well-validated incompressible model in all incompressible limits.

A key mathematical difficulty is that the problem has no scale separation, so traditional asymptotic methods fail to yield useful models.

An engineering approach is best. We should therefore consider many alternative models, holding them to high standards of validation, constantly comparing them, and using them to help quantify uncertainty in the modeling.

Modeling turbulent mixing is much harder than the already extremely difficult problem of modeling turbulence; and the effects of — for example — “chunk mixing” versus atomic mix remain to be to resolved. Because turbulent mixing between different regions of a star (or an imploding hohlraum) strongly affects the energy balance via radiation transport or nuclear combustion, and because these aspects of the physics are more readly measured, modeling these aspects of the problem gives greater validation capabilities for each mix model.

Some models of turbulence or turbulent mixing have a stochastic basis. Their dependent variables can be means, variances, correlation lengths, and other variables that capture the stochasticity of the problem. The most complicated such models might model probability density functions (PDFs) of key variables. However, complicated models are often not best, or even practical.

Other models of turbulence or turbulent mixing have the flavor of incorporating “microscopic" simulations. These can be either deterministic (say MD or lattice gas) or stochastic (say MC or Langevin). Better algorithms for such simulations must be developed. The microscopic simulations allow one to construct statistical quatities that feed the large-scale physics simulation.

In either case we must understand the sensitivity of the large-scale physics to how the small scale physics is modeled.

Our goal must be to identify the simplest models of small-scale physics that correctly captures the dominant effects on the resolved scales, even when those models do not look realistic on the unresolved scales.

For example, does getting the resolved physics correct require that the fourth moment of a PDF be correct, or just the first three moments? If not, can a microscopic simulation capture the first three moments without accurately capturing the fourth?

III. RADIATION AND NEUTRINO TRANSPORT

Because of the range of optical thicknesses encountered, the need for better photon, neutrino, and particle transport simulations will be with us for a long time.

Better transport simulations are not only important for getting the physics right inside the star, but for predicting what might emerge from the star to effect neighboring objects or to be collected by our telescopes, and for properly using the emergent radiation to infer the interior physical properties of the star.

Transport models need to be developed that build on the turbulence and turbulent mixing models. Models of transport in random media need more development. Algorithms are needed for transport through random media models that incorporate "microscopic" simulations.

Of course, the state-of-the-art for simulations in diffusion regimes is most advanced, but even here there are issues of coupling to other physics (like mixing or energy production) that need work.

For transport simulations in near-diffusion transition regimes, finite difference, finite element, finite volume, and similar methods (FXMs) do well, while particle methods can become prohibitively expensive. On the other hand, for transport simulations in near-streaming regimes, particle methods become best because FXMs degrade due to grid effects.

Many problems exhibit the gambit of regimes, from diffusion to transition to streaming. Moreover, these regimes partition phase-space, not just physical space. Hybrid diffusion-kinetic models therefore need more work.

IV. LOCAL NON-THERMODYNAMIC EQUILIBRIUM

In some situations the material is not in local thermodynamic equilibrium; this loss of LTE can occur quite inhomogeneously, adding yet another element to the multi-scale nature of the underlying problem. This can be true in the photosphere and chromosphere of a star, such as our Sun, as well as in laboratory plasmas. In such cases, the connection between the “observables” (obtained typically via remote sensing) and local physical properties becomes far more complex; and a clear understanding of the physical models used in simulations becomes essential in order to make sense of what one is observing even for the most elementary physical properties (such as plasma density).

V. QUANTIFYING UNCERTAINTY

We must learn to better quantify the uncertainty in our simulations. Models with a stochastic basis provide one handle on this issue, but will not come close to providing a complete answer.

For example, if one uses a diffusion photon transport model, how should one quantify the possible effects of deviations from the diffusion approximation?

Similarly, if one uses rate equations to model nuclear combustion, how should one quantify the possible effects of neglected reactions or of deviations from the mean field approximation?

This is a harder problem than simply quantifying the effect of uncertainties in transport coefficients or combustion rates.

Quantifying the effect of uncertainties in transport coefficients or combustion rates can be studied by sensitivity analysis using either direct, linearized, or adjoint methods. The first is quick and dirty, but is less meaningful than the latter two. The third requires the identification of object functionals, but also may be physically the most meaningful.

Uncertainties due to modeling are much greater than numerical uncertainties in most situations, but not always. Solving the same model with two very different algorithms can be very enlightening.

For example, photon transport can be simulated by Monte-Carlo or deterministic methods. The difference in two such simulations gives a useful measure of uncertainty.

VI. MICRODYNAMICS TO MACRODYNAMICS

The fundamental mathematical problem of small-scales to large-scales has to be understood better. When a “microscopic” system with chaotic dynamics is coarse-grained, the result should be a stochastic system. There is no satisfactory recipe for doing this. Coarse-grained models are therefore more commonly engineered than derived. Any breakthrough in this area will have a great impact on the way we face these problems over a wide range of applications.