Multiscale Modeling of Dense Plasmas

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Computational modeling of plasmas typically employs hydrodynamics (e.g., magnetohydrodynamics) or kinetic (e.g., Vlasov) models. In contrast, dense plasmas, such as strongly coupled plasmas, are typically modeled using Monte Carlo and/or molecular dynamics (MD) approaches; such approaches often contain higher-fidelity physics. Many important experiments, such as those involving laser heating of solids, span various regimes of dense plasma physics for which higher-fidelity physics is required, but the time and length scales of interest can be accessed only with macroscopic models. For example, it is not possible today to simulate a full Linac-Coherent-Light-Source (LCLS) experiment [1] from the solid through the warm dense matter phases, all of which include complex electronic structure, very strong ionic coupling, and radiation coupling.

All of the separate computational communities are vibrant, with new algorithms being developed on ever-newer computational architectures. The higher-fidelity approaches are gradually reaching toward macroscopic scales; over the past couple decades, we have seen MD move from simulating a few hundred particles to modeling trillions of particles. Yet, the length scales on which dense plasmas are simulated remain limited to sub-micron scales. To dramatically increase the pace of development of computational tools, it has been proposed that microscopic and macroscopic approaches be combined into a single computational approach.

Most problems in plasma physics are multiscale in some sense. For example, radiation hydrodynamics codes have as their closure an equation of state and transport coefficients that are computed from a microscopic theory (or, even better, from experiments). In this sense, the macroscale model is radiation hydrodynamics, and the microscale models are equations of state (from experimental data, theory or simulation), cross sections (opacities and nuclear), and subgrid mixing models. Other multiscale problems in plasma physics arise from very disparate scales, such as those driven by quite disparate cyclotron frequencies, electron and ion plasma frequencies, collision frequencies, wave frequencies, boundary conditions, and so forth. Here, we propose to construct multiscale plasma physics models in which there are several (usually two) distinct solvers that can be coupled in a meaningful way.

An emerging paradigm for building multiscale models of this sort is the heterogeneous multiscale model (HMM) framework [2]. HMM approaches the problem as a closure problem. If a macroscale model can be constructed from first principles, then it will not be closed because it cannot describe the microscale behavior (otherwise, it would simply be a microscale model). An example is the pressure tensor in hydrodynamics, which must be specified

approximately or computed directly in terms of higher moments that introduce more complex tensor closures. HMM introduces the notion that a microscale method can be run sequentially to provide the necessary closure information. For example, an MD code could be embedded within a hydrodynamics code and called as needed. The usual paradigm for HMM is thus to compute closure information using microscale solver, such as MD, for a limited amount of computational time and then to provide the microscale results to the macroscale solver, such as a hydrodynamics code, for use over much larger length and time scales. Ideally, one obtains a model that is almost as fast as the macroscale solver with the physics fidelity of the microscale solver.

HMM and related paradigms are currently in their infancy and, as such, have never been applied to plasma physics problems of relevance to DOE experimental facilities. Such microscale-macroscale schemes require further development from their currently nascent stage; the development of such codes could potentially lead to novel multiscale variants and be game changing and influential across many areas of plasma science. Capabilities introduced into plasma physics could include the following:

- More consistent equation-of-state information, including the correct treatment of mixtures.
- Better treatment of pre-ionized material properties.
- Deviations from true thermal equilibrium.
- Self-consistent transport coefficients.
- Inclusion of drivers (radiation, beams, etc.) and diagnostics into computational models with high-fidelity physics.

[1] P. Heimann and S. Glenzer, "Second User Workshop on High-Power Lasers at the Linac Coherent Light Source" *Synchrotron Radiation News* **28** 54 (2015) doi: 10.1080/08940886.2015.1037685

[2] *Principles of Multiscale Modeling*, Weinan E, Cambridge University Press, 2011.