Development of a Moment-based, Two-way, Scale-bridging Algorithm for the DOE Exascale Initiative

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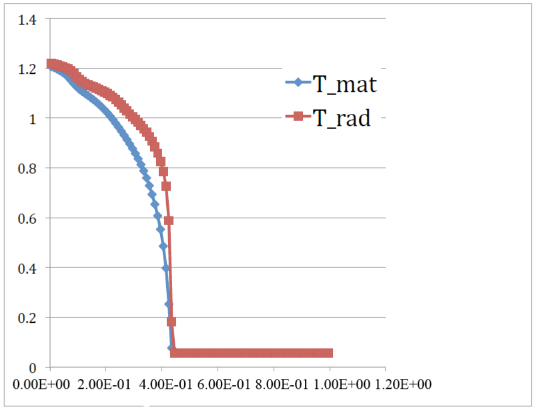
Multi-time-scale and multi-space-scale phenomena are ubiquitous, and define a large fraction of the problems of interest at LANL. In today's landscape, we find numerous studies that resort to an approximation (such as approximate closure) of the equations governing the small-scale, computationally demanding processes. Such approximations can be useful, but do not solve the equations at the finest of scales. We also find brute force simulation of the fine-scale equation, but over a reduced spatial domain and on shorter-than-desired time scales.

We are developing a moment-based, two-way, scale-bridging algorithm that can accelerate the solution of the fine-scale equations to the point where coarse time and length scales are achievable. Our prototype fine-scale problem has time, configuration space, and phase space as independent variables. This fine-scale model is often referred to as the "kinetic" problem, and the discretized version of this problem will be referred to as the high order (HO) problem. We accelerate the solution to this fine problem using a low order (LO) problem as a nonlinear "coarse space" correction. The LO problem is derived from a small number of phase space moments of the HO problem, and can also be solved on a coarser configuration space mesh. We self-consistently determine the higher-order moments required by the LO problem with the phase-space solution of the HO problem. This moment-based algorithm has a clear connection to multigrid ideas from numerical linear algebra. The LO problem is an efficient way to relax the "long wave length" components of the desired fine scale solution, and the HO problem is only used to relax the "short wavelength" components of the solution.

Fig. 1. Material and radiation temperature at a specific point in time.



No general scale-bridging algorithm of the type we propose currently exists, although one can find publication of foundational ideas that support this more general algorithmic direction [1-3]. The potential impact for the algorithmic advancement is best summarized by a selected list of applications. These could include neutron transport, photon transport plasma kinetic simulation, rarefied gas dynamics, transport in condensed matter (e.g., semiconductors), simulating the evolution of matter in the universe, and molecular dynamics material science and biology. All of these problems (and more) have an underlying fine-scale description that has significant impact over long time scales and large space scales.

It is very important to realize that the two-level nature of the algorithm may allow it to map well to modern heterogeneous parallel computing architectures (an early example of the computational co-design philosophy). The communication between levels is fairly limited–it is just the moments of the fine-scale distribution function going from HO to LO, and a few specific configuration space fields going from LO to HO. As a result of this simple fact, and the broad range of potential applications, we expect this fundamental algorithmic idea to have a significant impact on the evolving philosophy of computational co-design and the rapidly developing Department of Energy (DOE) Exascale computing initiative.

In a related form, this moment-based algorithm is already being used and making a positive impact on neutron transport for industrial fission reactor physics calculations [3]. A reduced moment system (diffusion-like) LO problem is constructed from the underlying HO transport problem by taking the zero and first angular moments of the HO problem. The LO problem is solved for the scalar flux on a coarse mesh. This scalar flux is used to define the scattering and fission source in the transport equation (HO problem), which is solved on a more refined mesh for the angular flux. Moments of the angular flux are required to define the coefficients required in the diffusion-like (LO) problem. We

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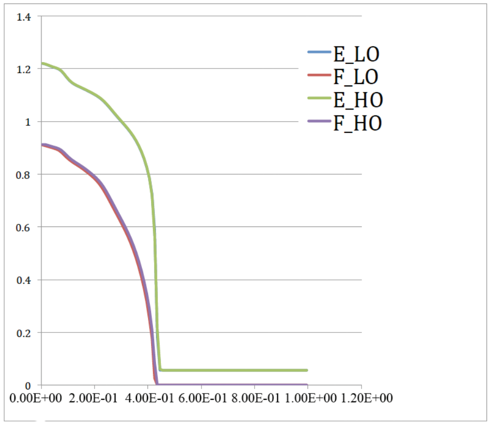

Fig. 2. The solution coming from the LO problem is consistent with moments of the solution from the HO problem.

have extended this algorithmic concept by providing a tighter Newton-based coupling in the HO/LO iteration [4], and by bringing the k-eigenvalue computation inside the Newton-based nonlinear iteration [5]. The combination of these extensions is providing a new level of efficiency in transport-based nuclear reactor k-eigenvalue calculations [5].

There is a strong need for an efficient scale-bridging algorithm in magnetic fusion energy research, space weather, and inertial confinement fusion. A simple model for addressing algorithm development here is the Vlasov-Poisson equation system. To implement the moment-based approach we require the first two velocity space moments of the ion and electron Vlasov equations. These equations, along with the appropriate Maxwell equations, are the LO problem. The HO problem (The Vlasov equations) will get the electric potential from the LO problem, and the HO problem solution will provide consistent closure for the ion and electron pressure tensors, which are required for the advance of the LO problem [6].

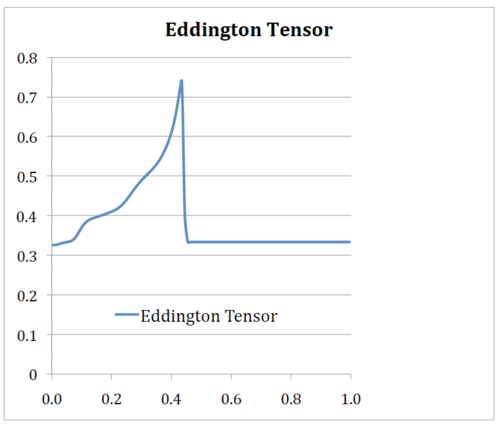

Fig. 3. Plot of the Eddington tensor (factor in this case) required for the solution of the LO problem, the second angular moment of the HO solution. If diffusion theory is valid, the Eddington factor would be 1/3 everywhere.

We are currently extending this algorithm for the solution of thermal radiation transport. The moment-based algorithm is intended to replace the historically successful implicit Monte Carlo (IMC) algorithm. In a grey model problem example of the moment-based approach, the LO problem is a nonlinear system which includes the material energy balance along with the zero and first angular moments of the photon transport equation. This LO problem provides a consistent emission source to the HO (transport) problem. The HO problem provides the numerically exact closure of the Eddington tensor (factor in 1D) required for the solution of the LO problem. Figures 1-3 show an example result from a 1D nonequilibrium thermal wave.

As can be seen, this moment-based, scale-bridging algorithm has significant potential for application, although significant algorithmic research is required to bring most of this to fruition. Furthermore, this work is a young example of potential algorithm co-design in action, as the mapping of the algorithm to evolving hybrid parallel computing architectures appears to have a clear route. We have started to explore alterations of these algorithmic ideas for the application to scale-bridging in computational materials science. We expect this exciting area of algorithmic research to blossom at LANL with the evolving DOE initiative in Exascale computing.

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