A Moment-based, Scale-bridging Algorithm for Neutral Particle Transport Problems

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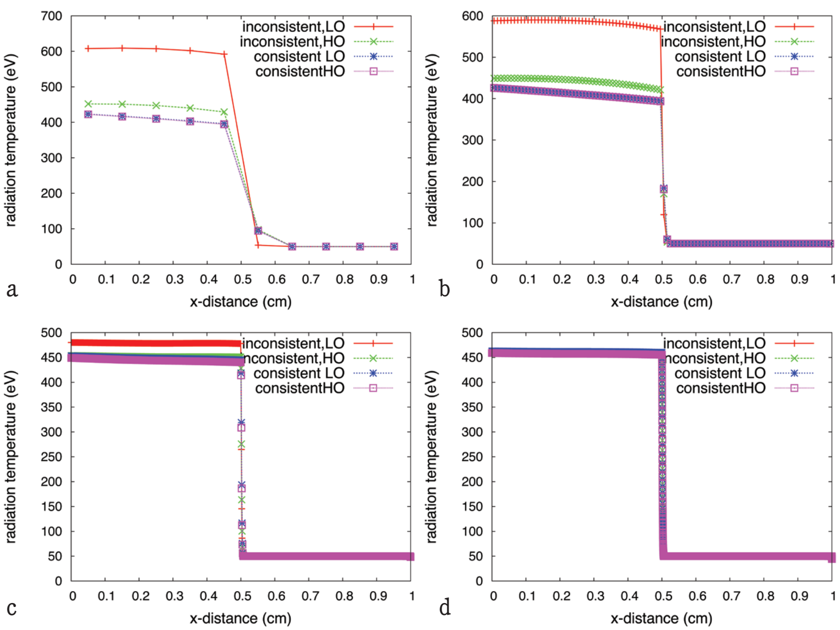
Accurate modeling of neutral particle behavior is of great importance in many science and engineering applications. Due to strong interactions between particles and surrounding media, many numerical algorithms suffer from slow convergence in optically thick regions. We are developing a moment-based, scale-bridging algorithm that can mitigate slow convergence of transport algorithms. Our algorithm utilizes the low-order (LO) continuum equations that are consistently derived from the high-order (HO) transport equation. Due to discrete consistency, the LO system can be used not only for accelerating the HO solution, but also coupling to other physics.

Fig.1. Comparison of the radiation temperature with and without the consistency term for different spatial mesh sizes: a) dx = 0.1 cm, b) dx = 0.01 cm, c) dx = 0.001 cm, d) dx = 0.0001 cm.



The Boltzmann transport equation describes the statistical behavior of particles that are interacting with surrounding media. The transport equation is used to simulate neutral particle physics in many physical systems–for example, combustion systems, nuclear power reactors, and internal confinement fusion. Unfortunately, many iterative schemes, based on an explicit scattering and re-emission source iteration, suffer from slow convergence in an optically thick region, where particles undergo a large number of scattering and/or absorption re-emission events. In such regions, a continuum description of the transport equation with an approximate closure (e.g., Fick's law of diffusion) can adequately represent the particle behaviors. On the other hand, diffusion and other approximated closure equations become invalid in an optically thin region due to the presence of significant transport effects. For computational efficiency it is natural to seek a (geometric) hybrid transport-diffusion algorithm [1,2].

As an alternative to this geometric hybrid algorithm, we are developing a new, efficient approach to solve neutral particle transport problems. In our algorithm, the transport high order (HO) and continuum low order (LO) systems lie on the same computational domain, and can be viewed as a scale-bridging algorithm. Fine-scale physics, such as particle streaming, are treated by the HO system, while large-scale, isotropic physics are treated implicitly in the LO system. Our algorithm derives a closure relationship directly from the discrete HO system and adds a *consistency* term that forces the LO truncation error to be identical to the truncation error of the HO system. Thus, the solution of the LO system is guaranteed to be consistent with the solution of the HO system upon convergence of the nonlinear system.

With increasing interest in high-fidelity, multiphysics simulations, our algorithm becomes even more attractive. Specifically, the LO system can be used to couple other physics (e.g., fluid flow, heat transfer, and chemical reactions) in a multiphysics simulation. By coupling with the LO system, we can reduce the problem dimension of the multiphysics system. Furthermore, the algorithm allows one to use not only a deterministic but also a stochastic (Monte Carlo) method for obtaining the solution of the HO system. We have applied our algorithm to many physical systems, but will focus on the following two here. The first application is time-dependent thermal radiative transfer (TRT) problems in the context of high-energy density physics [3]. The second application is neutron transport criticality [4], which is an important application in the nuclear power industry.

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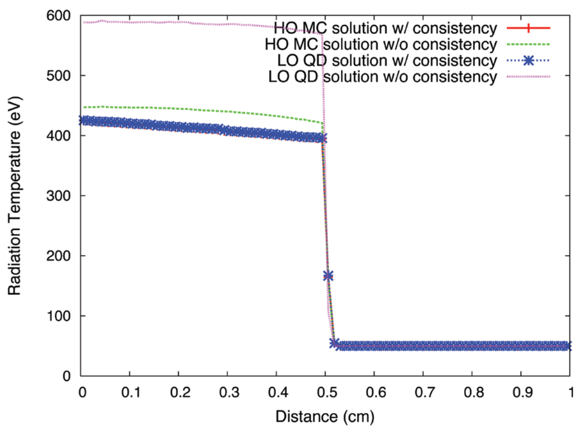

Fig. 2. Comparison of radiation temperature profile using Monte Carlo HO solver.

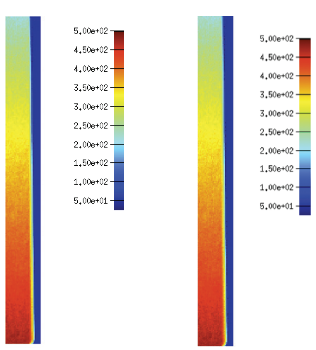

Fig. 3. Comparison of the radiation temperature in IMC HO solver: a) LO radiation temperature, b) HO radiation temperature.

Figure 1 shows the radiation temperature profiles for a 1D multimaterial TRT problem, solved with and without the consistent LO formulation. Without consistency, the LO radiation temperature exhibits an unphysical solution. This error is due to poor resolution of the solution gradient near the material interface. Because insufficient energy is transferred into the thick material, excessive energy is deposited in the thin material. By using the consistent LO formulation, the radiation flux at the material interface is properly evaluated, eliminating the unphysical solution. Although the LO and HO radiation temperatures approach each other without the consistency term under mesh refinement, mesh resolution on the order of a mean-free-path (not reasonable) is required to obtain a reasonable solution. Figure 2 shows the comparison as similar to Fig. 1, but the HO system is solved with a Monte Carlo method. With the Monte Carlo HO solver, the LO and HO solution are consistent. With the help of the LO problem, the particle tracking in the Monte Carlo simulation becomes simpler and faster, enabling a larger number of histories with the same CPU time. Figure 3 shows the radiation temperature profiles of a 2D multimaterial problem. The simulation was performed using a LANL large-scale multiphysics simulation code interfaced with an Implicit Monte Carlo (IMC) code. Both are production-level codes used regularly by a practitioner for realistic simulations. With the new algorithm, we observed CPU speed-ups of a factor of 8 to 20, compared to the standalone IMC code.

These same algorithms can be applied to neutron transport in nuclear power reactors. Figure 4 shows an eigenvalue convergence comparison between standard power iteration (PI) and our algorithm (NDA-NCA) in a 2D nuclear reactor criticality problem. The outer iteration corresponds to the number of HO solves, which is the major contributor to the CPU time. The NDA-NCA algorithm [4] reduces the outer iteration by a factor of 600 and reduces the CPU time by a factor of 400. Note that our algorithm not only accelerates scattering source via the scale-bridging algorithm, but also utilizes an accelerated eigenvalue computation in the LO system, which is possible due to the consistent formulation between the HO and LO systems. The next step is multiphysics coupling with this scale-bridging algorithm [5].

Finally, this scale-bridging algorithm may map well to emerging parallel computing architectures. Specifically, the computationally expensive HO solution algorithm is suited for GPU computation, while we can capitalize on the state-of-art parallel computing software for solving the LO system across nodes. Moreover, a relatively small communication requirement between the HO and LO systems may ease the communication bottleneck of the heterogeneous parallel architecture.

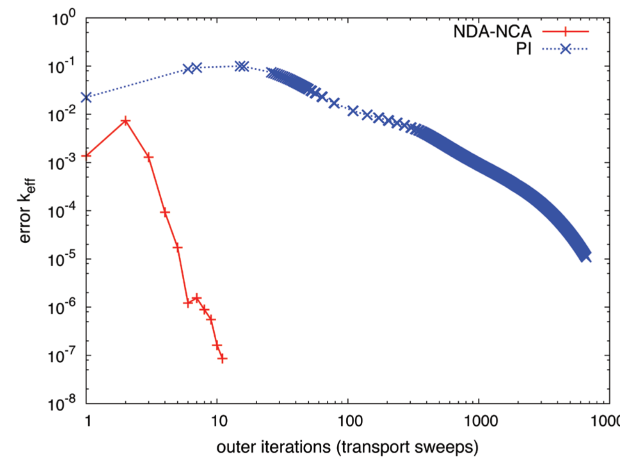

Fig. 4. Convergence comparison between NDA-NCA and PI for the LRA-BWR problem.

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