A Collision-Based Hybrid Method for Multiscale, Linear Transport

Cory D. Hauck†
Oak Ridge National Laboratory
hauckc@ornl.gov

Ryan G. McClarren
Texas A & M University
rgm@tamu.edu

Abstract

We present a hybrid method for simulating kinetic equations with multiscale phenomena in the context of linear transport. The method consists of (i) partitioning the kinetic equation into collisional and non-collisional components; (ii) applying a different numerical method to each component; and (iii) re-partitioning the kinetic distribution after each time step in the algorithm. Preliminary results show that for a wide range of test problems, the combination of a low-order method for the collisional component and a high-order method for the non-collisional component provides a level of accuracy that is comparable to a uniform, high-order treatment of the entire system.

Background

Problem Setup. We consider a single-group, linear transport equation of the form

$$\frac{1}{c}\frac{\partial \psi}{\partial t} + \Omega \cdot \nabla_x \psi + \sigma_t \psi = \frac{\sigma_s}{4\pi}\langle \psi \rangle + Q, \tag{1}$$

where the *angular flux* ψ depends on position $x \in \mathbb{R}^3$, direction of flight $\Omega \in \mathbb{S}^2$ (the unit sphere), and time $t > 0$ and is defined so that $c^{-1}\psi$ gives the number density of particles at time t with respect to the measure $dxd\Omega$. The particle speed c is a fixed positive scalar and $Q = Q(x, \Omega, t)$ is a source, which we assume is known. The quantities σ_a, σ_s, and $\sigma_t = \sigma_a + \sigma_s$ are the absorption, scattering, and total cross-sections. They are assumed to be functions of position only. Angle brackets are used to denote integration over $\mathbb{S}^2$ and $\phi := \langle \psi \rangle$ is the *scalar flux*.

Challenge. The use of implicit numerical schemes introduces coupling between spatial derivatives in the transport operator and the angular redistribution which occurs via particle scattering. The resulting linear systems can be difficult to solve. In regimes with low levels of scattering, a high degree of angular resolution is needed. However, because the angular components of the kinetic distribution are weakly coupled, the work required per unknown is relatively small. On the other hand, strong scattering requires a relatively small number of unknowns to resolve angular dependencies, but the unknowns are strongly coupled. The consequence of this dichotomy is that a single uniform method will have a large number of strongly coupled components.

Previous Work. The difficulty in handling this type of multiscale problem has been addressed in several ways, the main idea of each being to use low-order models as preconditioners in the solution procedure for a high-resolution angular discretization. For discrete ordinate calculations, diffusive approximations are often used to speed up the convergence of iterative solvers in strongly scattering regimes. The prototype for this approach is diffusion synthetic acceleration (DSA), but the ideas can also be reformulated as preconditioners for modern Krylov solvers [1, 8]. Another well-known approach to acceleration involves the use of nonlinear methods which combine a high-resolution discretization in angle with a low order, moment-based approximation to accelerate convergence [3, 4, 7].

Splitting

First Collision Source. Following [2], we write ψ as the sum

$$\psi = \psi_c + \psi_u\,, \tag{2}$$

where the *collided flux* ψ_c and the *uncollided flux* ψ_u satisfy

$$\frac{1}{c}\frac{\partial \psi_u}{\partial t} + \Omega \cdot \nabla_x \psi_u + \sigma_t \psi_u = Q_u, \tag{3a}$$

$$\frac{1}{c}\frac{\partial \psi_c}{\partial t} + \Omega \cdot \nabla_x \psi_c + \sigma_t \psi_c = \frac{\sigma_s}{4\pi}(\langle \psi_c \rangle + \langle \psi_u \rangle) + Q_c, \tag{3b}$$

and $Q = Q_u + Q_c$. The equation for ψ_u has no angular couping no coupling in angle and is independent of ψ_c. The angular average of ψ_u acts as a (first-collision) source for the collided equation. Integrating (3) in time with backward Euler gives

$$\frac{\psi_u^{n+1} - \psi_u^n}{c\Delta t} + \Omega \cdot \nabla_x \psi_u^{n+1} + \sigma_t \psi_u^{n+1} = Q_u^{n+1}, \tag{4a}$$

$$\frac{\psi_c^{n+1} - \psi_c^n}{c\Delta t} + \Omega \cdot \nabla_x \psi_c^{n+1} + \sigma_t \psi_c^{n+1} = \frac{\sigma_s}{4\pi}\left(\langle \psi_c^{n+1} \rangle + \langle \psi_u^{n+1} \rangle\right) + Q_c^{n+1}\,. \tag{4b}$$

The original idea of this splitting was to evaluate ψ_u using Monte-Carlo or ray tracing from localized sources and then use discrete ordinates to evaluate ψ_c. Here we propose more generally to use to any sufficient high-order angular discretization for ψ_u and any sufficient low-order angular discretization for ψ_c.

Particle Relabeling. Roughly speaking, we expect that scattering events will isotropize ψ_c, making lower-order methods sufficient. It turns out that this is not exactly the case. Indeed, although scattered particles are distributed isotropically in angle, they need not remain so unless more collisions occur. To accommodate for this fact, we relabel the collided particles as uncollided after each time step. With respect to the semidiscrete scheme (4), this gives

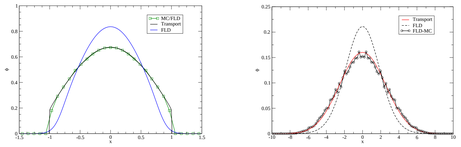
$$\Omega \cdot \nabla_x \psi_u^{n+1} + \left(\sigma_t + \frac{1}{c\Delta t}\right)\psi_u^{n+1} = \frac{1}{c\Delta t}\left(\psi_c^n + \psi_u^n\right) + Q_u^{n+1}, \tag{5a}$$

$$\Omega \cdot \nabla_x \psi_c^{n+1} + \left(\sigma_t + \frac{1}{c\Delta t}\right)\psi_c^{n+1} = \frac{\sigma_s}{4\pi}\left(\langle \psi_c^{n+1} \rangle + \langle \psi_u^{n+1} \rangle\right) + Q_c^{n+1}\,. \tag{5b}$$

The collided flux at time t^n now acts as source for the uncollided flux at time t^{n+1}. By relabeling the particles in this way, we gain high-resolution transport information from the uncollided equation. The addition cost in doing so lies in specifying the closure that must be computing when mapping from the low-order angular discretization of ψ_c^n, generated by (5b), to the high-order one which is needed in (5a). In practice, we have so far used very simple closures.

Numerical Results - 1D

The Plane Source. The plane-source problem is a torture test of whether an angular discretization method can accurately approximate solutions with strong discontinuities. Particles are emitted from an initial planar source into an infinite medium. The problem can be represented in one spatial dimension with x being the signed, normal distance to the source plane. We assume a purely scattering material with $\sigma_t = \sigma_a = 1.0$, $Q = 0$, $c = 1$, and initial conditions $\psi_u(x, \mu, 0) = 0.5\delta(x)$ and $\psi_c(x, \mu, 0) = 0$. Hybrid Monte-Carlo/diffusion solutions are given in Figure 1. Discrete ordinate hybrid solutions are given in Figure 2a.



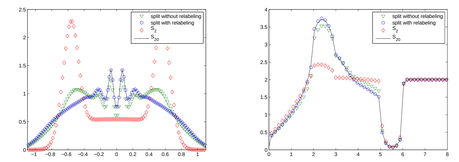
(a) $t = 1.0$ (b) $t = 10.0$

FIGURE 1: Plane source problem, comparing the Monte Carlo/Flux-limited diffusion (MC-FLD) hybrid, the (semi)-exact transport solution, and the flux-limited diffusion (FLD) solution.

Reed's Problem. Reed's problem [9] involves a slab of length $L = 8.0$ that is composed of five materials having significantly different properties. Discrete ordinate hybrid solutions are given in Figure 2a.

Region	$0 \le x < 2$	$2 \le x < 3$	$3 \le x < 5$	$5 \le x < 6$	$6 \le x < 8$
σ_s	0.9	0.1	0.0	0.0	0.0
σ_a	0.1	0.2	0.0	5.0	50.0
Q	0.0	1.0	0.0	0.0	50.0

TABLE 1: Material properties for Reed's problem.

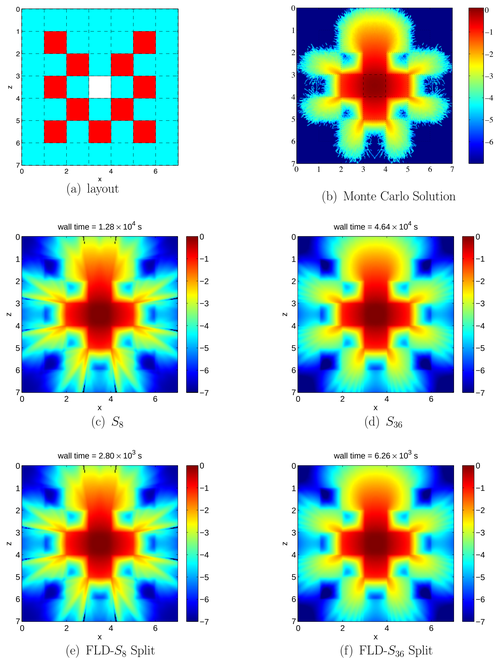


(a) Plane source (b) Reed's Problem

FIGURE 2: Discrete ordinate solutions using two (S_2) and twenty (S_{20}) Gauss-Legendre quadratures.

Numerical Results - 2D

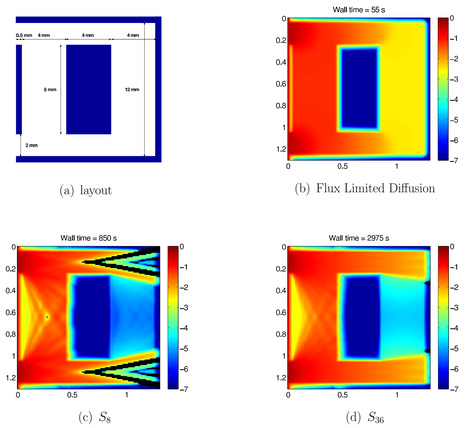
The Lattice Problem. We consider a checkerboard of highly absorbing material embedded in a scattering material. This problem, originally due to Brunner [5,6], has become a common test problem of angular discretizations of the transport equation. The problem domain (see Figure 3a) is 7 cm × 7 cm with vacuum boundaries. The red squares are pure absorbers with $\sigma_t = \sigma_a = 10$ cm^{-1}; the light blue and white regions are pure scatterers with $\sigma_t = \sigma_s = 1$ cm^{-1}; the white region also has an isotropic source $Q = 1$ cm^{-3} s^{-1}. Initially, there are no particles in the domain.



(a) layout (b) Monte Carlo Solution (c) S_8 (d) S_{36} (e) FLD-S_8 Split (f) FLD-S_{36} Split

FIGURE 3: The layout and solution for the lattice problem using several angular discretization techniques. The color scale on the figures shows $\log_{10}\phi$ at $t = 3.2$ s. Wall times denoted in the figures are the computational time to get a solution for each problem. The Monte Carlo solution is taken from [5] for reference.

The Hohlraum Problem. We consider a variation of a simplified hohlraum configuration that has been considered previously in [5] and is applicable to the study of inertial confinement fusion. (The original problem is coupled nonlinearly to the material via blackbody radiation. Here we use scattering to represent the emission of particles from the material.) The layout and dimensions of the problem are shown in Figure (a). The spatial domain is made up of two materials: a dense material with $\sigma_t = 100$ and $\sigma_a = 99$ that makes up the walls and central target and a dilute, purely scattering, material with $\sigma_t = \sigma_s = 0.1$ that sits between the walls and central target. The dense material is representative of the solid density materials in an experiment and the dilute material is representative of the material ablated from the walls. The problem has vacuum boundary conditions on the top, bottom, and right sides and an isotropic incoming boundary condition is imposed on the left boundary.



(a) layout (b) Flux Limited Diffusion (c) S_8 (d) S_{36} (e) FLD-S_8 Split (f) FLD-S_{36} Split

FIGURE 4: Layout and solutions to the hohlraum problem at $t = 1.3$ s. In these figures the color scale shows $\log_{10}\phi$ and negative values of ϕ are shown in black. The wall times denoted in the figure are the computational time to get a solution for each problem.

References

[1] M. L. Adams and E. W. Larsen, *Fast iterative methods for discrete-ordinates particle transport calculations*, Progress in Nuclear Energy, 40 (2002), pp. 3 – 159.

[2] R. Alcouffe, R. O'Dell, and F. W. Brinkley, Jr., *A first collision source method that satisfies discrete S_N transport balance*, Tech. Rep. LA-UR-89-304, 1989.

[3] D. Y. Anistratov and V. Y. Gol'Din, *Nonlinear methods for solving particle transport problems*, Transport Theory and Statistical Physics, 22 (1993), pp. 125–163.

[4] D. Y. Anistratov and E. W. Larsen, *Nonlinear and linear [alpha]-weighted methods for particle transport problems*, Journal of Computational Physics, 173 (2001), pp. 664 – 684.

[5] T. A. Brunner, *Forms of approximate radiation transport*, Tech. Rep. SAND2002-1778, Sandia National Laboratories, 2002.

[6] T. A. Brunner and J. P. Holloway, *Two-dimensional time dependent Riemann solvers for neutron transport*, J. Comput. Phys., 210 (2005), pp. 386–399.

[7] V. I. Goldin, *The mathematical modeling of problems of continuous media with nonequilibrium transfer*, in Current Problems of Mathematical Physics and Computational Mathematics, 1982, pp. 113–127.

[8] E. W. Larsen and J. E. Morel, *Advances in discrete-ordinates methodology*, in Nuclear Computational Science, Springer Netherlands, 2010, pp. 1–84.

[9] W. Reed, *New difference schemes for the neutron transport equation.*, Nucl. Sci. Eng., 46 (1971), pp. 31–39.

†The research of this author is sponsored by the Office of Advanced Scientific Computing Research, U.S. Department of Energy. The work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. De-AC05-00OR22725.