An Improved Random Walk Algorithm for IMC

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Abstract
We recently implemented a modified Implicit Monte Carlo (IMC) Random Walk (RW) algorithm in the Jayenne Project software, which increases simulation efficiency for multi-group radiative transfer problems with strongly frequency-dependent opacities.

To date, the RW method has only been implemented in “fully-gray” form; that is, the multi-group IMC opacities are group-collapsed over the full frequency domain of the problem to obtain a gray diffusion problem for RW. The efficiency of this method degrades when the spatial cells are thin or the opacities are a strong function of frequency.

To address this issue, we introduce a RW frequency group cutoff in each spatial cell, which divides the frequency domain into optically thick and optically thin components. We refer to this new method as Partially-Gray Random Walk (PGRW).

Background and Motivation
The IMC method [2] has been used to model thermal radiative transfer in a large variety of physical systems, including problems in inertial confinement fusion and astrophysics. The IMC equations are numerically robust and capable of producing high-fidelity solutions (provided reasonable values are chosen for the time step and zone size). However, one of the major drawbacks of IMC is the large computational cost required to obtain a given precision for realistic problems. In particular, the IMC method is often prohibitively expensive when the problem involves very optically thick regions.

To mitigate this problem, Fleck and Canfield introduced the Random Walk acceleration scheme for IMC particles in optically thick spatial cells [1]. In the original RW method, the diffusion equation is obtained by integrating the original IMC opacities over the entire frequency domain.

This fully-gray treatment degrades the efficiency of RW acceleration, especially in problems where the opacity is a strongly-varying function of particle frequency. Because the RW problem is fully-integrated in frequency, optically thin opacity groups are lumped in with optically thick, “diffusive” opacity groups. This, in turn, limits the use of the fully-gray RW method in cells that may appear optically thick to particles in certain frequency groups, but optically thin in others.

Our PGRW method separates the cell-wise frequency domain into diffusive and transport regimes. As a result, the RW procedure can be applied to particles in diffusive frequency groups, while particles in transport frequency groups are treated with standard IMC. This increases the total number of RW steps per time-step (which consequently improves the efficiency of the simulation).

Description/Impact
The test problem presented here is a homogeneous 1-D Marshak wave. The material begins at a uniform temperature of 1 eV, and is heated by a 1 keV boundary source at $x = 0$. The opacity is temperature and frequency-dependent, and is given by

$$\sigma_a(v, T) = \frac{1000}{(hv)^3 \sqrt{kT}},$$  \hspace{1cm} (0.1)

where the quantities $(hv)$ and $(kT)$ are reported in keV.

We approximate the frequency dependence of the opacity with a 30-group multigroup structure, spanning from 0.1 eV to 100 keV. Thus, while particles in the lower frequency groups will have very short mean-free-paths, particles in the higher groups will stream long distances between collisions. We use a time-step size of $\Delta t = 0.01$ ns, and run the simulation to a total time of $t = 1$ ns.
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(100 time-steps). $10^5$ particles are simulated per time-step.

In Figure 1, we plot the material temperature profile at $t = 1.0$ ns for the left-most centimeter of the problem domain. Excellent agreement is observed between the PGRW, RW, Discrete Diffusion Monte Carlo (DDMC), and IMC solutions. Timing data is summarized in Table 1, with two variants of the PGRW method included to provide reasonable upper and lower performance bounds. This data shows that PGRW is roughly 2.7 times faster than standard IMC when the least-optimal version of PGRW is used, and $\sim 6.5$ times faster than standard IMC when PGRW is nearly optimized.

**Material temperature at $t = 1.0$ ns**

<table>
<thead>
<tr>
<th>Method</th>
<th>Wall time (s)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>PGRW (optimal)</td>
<td>619</td>
<td>6.53</td>
</tr>
<tr>
<td>PGRW (worst)</td>
<td>1496</td>
<td>2.70</td>
</tr>
<tr>
<td>RW</td>
<td>2884</td>
<td>1.40</td>
</tr>
<tr>
<td>IMC</td>
<td>4042</td>
<td>–</td>
</tr>
</tbody>
</table>

**Anticipated Impact**

When compared to standard RW, the PGRW method significantly increases the total number of RW steps performed per transport time-step; this, in turn, reduces simulation time considerably for multigroup problems with strongly frequency-dependent opacities. In general, we expect the new PGRW implementation to decrease runtimes for these problems by a factor of $\sim 2-4$ compared to standard RW, and a factor of of $\sim 3-6$ compared to standard IMC.

**Acknowledgements**


**References**
