Novel MC TRT method: vectorizable variance reduction for energy spectra

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INTRODUCTION

Several production-scale multigroup Thermal Radiation Transport (TRT) codes use the Monte Carlo method as their primary solution technique. One such example is *Jayenne* from Los Alamos National Lab, which samples a single energy group for a particle then transports it [1]. In this work we created a novel TRT variance-reduction method to better resolve the energy spectra with large group structures and fewer particles, with a goal to decrease computational time at a given fidelity of solution in the energy spectra.

TRT EQUATIONS

The explicit TRT equations discretized in frequency, using a multi-group assumption, and in zero-dimensional space, are [2]

$$\frac{1}{c}\frac{\partial I_g(t)}{\partial t} + \sigma_{a,g}(T)I_g(t) = x_g(T)B_g(T) \tag{1}$$

$$c_v\frac{dT}{dt} = \sum_0^G \sigma_g(T)I_g(t) - x_g(T)B_g(T) \tag{2}$$

for $t > 0$ and $G \geq 1$, where $I_g(T)$ is the specific intensity in a given group g, c is the speed of light, $\sigma_{a,g}(T)$ is the absorption opacity in a given group g, $B_g(T)$ is Planck's function for a given group g, c_v is the specific heat of the material (which is assumed constant), and $x_g(T)$ is the Planck weighted opacity for given group g.

Note that we discretize the material equation in time using a forward Euler scheme [3]:

$$T_{n+1} = T_n + \Delta t c_v \frac{dT_n}{dt}\ , \tag{3}$$

where n is the time index. This means error is proportional to $O(\Delta t)$.

FLOCKING PARTICLES

We propose a method in which a single pseudo-particle carries an energy probability distribution function (PDF) representing particles across all energy groups in a given simulation. This could be thought of as a "flock" of particles all moving together through space, angle, and time. When an event occurs, instead of sampling for a new energy group, as is traditionally done, the energy weight is reallocated in the pseudo-particle's PDF.

We also required this method to be transient by using a particle census to move particles between time steps with weight-based combing for population control [4]. Traditionally combing only requires the conservation of energy across particles and does not explicitly consider spectral shape; however, with this new method, we also had to ensure that we conserve energy across all groups to preserve the shape of the PDF.

Potential computational performance hindrances come when a minimum distance to an event is found. The energy weights in **all** groups must be attenuated, requiring the computation of an exponential, and the manipulation of energy weights in **all** groups.

Consider a 200 group problem employing our novel technique: instead of computing a single exponential attenuation as in the single-group MC scheme, we must repeat this exponential calculation 200 times (once for each frequency group in the problem). Thus for *one* pseudo-particle's history, in *one* time step, the number of exponentials required is now proportional to the number of groups, hindering effective performance gains.

However, there is still hope: The attenuation calculation involves the conducting of the same operation on multiple discrete pieces of data; said another way: single instruction/multiple data (SIMD). SIMD hardware (a type of vector processor unit) is widely deployed, and can be found in production x86 CPUs with AVX instructions as well as machines purpose built to operate on vectors. It is also relatively easy to enable through the use of compiler flags on modern C++ compilers [5]. As a result, this method will be able to use accelerators that already exist and commonly remain idle, to speed up our novel method and dampen the hit to performance.

RESULTS AND DISCUSSION

We developed a test code in C++ to examine this method's performance, first as a time-dependent zero spatial dimension problem, then as a time-dependent single spatial dimension problem. Both ran gray and multi-group test cases and compared results to analytical solutions (if available) as well as current production codes.

Zero-dimensional problem

The 0D test is a simple time-dependent equilibration problem. We compared a gray case to both the analytical Mosher [6] solution as well as production codes. Then, we performed simulations with up to 200 energy groups in the *Jayenne* Implicit Monte Carlo code from Los Alamos National Lab, examining both time to equilibration and the spectrum of the results. We found that to get roughly the same fidelity of solution our novel method required the simulation of only 1×10^4 particles, while the production code required 1×10^6 particles. With these results we felt confident to move our novel method into

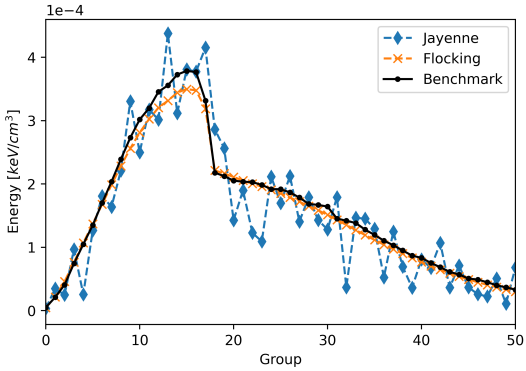

Fig. 1. High-variance solution produced from production code, a low-variance solution produced by our novel method, and a benchmark solution produced in the same cell, cycle, and with the same number of particles (1×10^4).

one dimension.

One-dimensional problem

To compare the results of our testbed with those from production codes, we employ a Marshak wave test, again starting from the gray case, then moving to multigroup with up to 200 groups.

After confirming that the temperature profiles over time matched we moved to examine their spectra in specific mesh cells at specific time steps. Figure 1 shows the spectrum produced by either code at ten-thousand particles compared to a benchmark solution of the production code ran with 5 million particles. The variance for the production code solution is very high (lots of jagged peaks) while the spectrum produced by our novel method is smooth and accurate at this low particle count. This demonstrates that the variance reduction works.

While a slight deviation of the spectral shape near the peak is observed, we believe this stems from the use of spatial tilt for source position sampling in Jayenne that has not yet been implemented in our test-bed code. When implemented we expect this discrepancy to disappear and we will be able to use a traditional Figure of Merit comparison to fully demonstrate the novel method's variance reduction abilities.

We must also consider run times. Table I confirms that this method is vectorizable, and will be able to take advantage of the specialized vector processing components of modern CPUs. It also shows that this has a huge impact on run time for this method; cutting a fully optimized solution (using the Intel icpc compiler flag `-Ofast`) in half when they are turned on (using a SIMD reduction flag above the attenuation loop).

To confirm that this method will result in an overall performance increase when considering the energy spectra, we raced the production code against the novel method at various particle counts and examined their spectra. Table II shows that the novel method does take slightly longer. However, if a well resolved spectrum is the goal of the computation than we have effectively reduced the computational time as fewer particles are required to get a well defined solution.

Optimized?	Vectorized?	Runtime [s]
no	no	1855.2
yes	no	353.2
yes	yes	184.7

TABLE I. Run-times of the 1D novel method test bed under various compiler flag conditions. Ran on Intel Skylake Gold (AVX-512).

Method	N particles	Runtime [s]
single-group	1×10^4	70.97
single-group	1×10^6	3005.50
flocking	1×10^4	92.0
flocking	1×10^6	3775.12

TABLE II. Comparing the run-times of the 1D test case between Jayenne and novel method test bed. Ran on Intel Haswell.

CONCLUSIONS

We have successfully produced a novel variance reduction technique for the energy spectra for Monte Carlo Thermal Radiation Transport. Continued work is required before the method is stable enough to implement on production codes. Specifically we need to implement physical scattering, source tilting [4], and post-collisions group splitting (to prevent highly unlikely interactions across various energy regimes in optically thin material) in the testbed.

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