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Improved Method for Implicit Monte Carlo

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I. Introduction

The Implicit Monte Carlo (IMC) method [1] has been used for over 30 years to analyze radiative transfer problems, such as those encountered in stellar atmospheres or inertial confinement fusion. Reference [2] provided an exact error analysis of IMC for 0-D problems and demonstrated that IMC can exhibit substantial errors when timesteps are large. These temporal errors are inherent in the method and are in addition to spatial discretization errors and approximations that address nonlinearities (due to variation of physical constants). In Reference [3], IMC and four other methods were analyzed in detail and compared on both theoretical grounds and the accuracy of numerical tests. As discussed in [3], two alternative schemes for solving the radiative transfer equations, the Carter-Forest (C-F) method [4] and the Ahrens-Larsen (A-L) method [5], do not exhibit the errors found in IMC; for 0-D, both of these methods are exact for all time, while for 3-D, A-L is exact for all time and C-F is exact within a timestep. These methods can yield substantially superior results to IMC.

This work develops a non-analog transport scheme for the C-F method, extending it beyond the original work, to permit the straightforward integration of the method into existing IMC codes. With the new sampling scheme derived below, upgrading an existing IMC code to use the more accurate C-F method should be a straightforward exercise, involving only a few dozen lines of coding. Tests of the new sampling scheme demonstrate its correctness.

II. Radiative Transfer Equations and Solution Methods

The coupled equations of grey radiative transfer [2,3] are:

$$\frac{1}{c}\frac{\partial I(\mathbf{r},\mathbf{\Omega},t)}{\partial t} + \mathbf{\Omega}\bullet\nabla I + \sigma I = \frac{c}{4\pi}\sigma U_r(\mathbf{r},t) + q(\mathbf{r},\mathbf{\Omega},t) \qquad (1)$$

$$\frac{1}{\beta(\mathbf{r},t)}\frac{\partial U_r(\mathbf{r},t)}{\partial t} = \sigma\phi(\mathbf{r},t) - c\sigma U_r(\mathbf{r},t) \qquad (2)$$

where the notation is standard [cf. 2,3]. We assume local thermodynamic equilibrium, no scattering, and that material properties (e.g., β, σ) are held constant within a timestep. Equations (1,2) are solved over a timestep $\Delta t = t_{n+1} - t_n$.

In Reference [3], five computational methods for solving Eqs. (1,2) were compared and tested using analog Monte Carlo techniques, in order to clearly illustrate fundamental differences in the methods. For analog simulation, when a photon emerges from either a collision, source, or emission event, a free-flight distance to the next collision event is randomly sampled using the total opacity σ, and then the random selection of either absorption or effective scattering is made using σ_s / σ, where σ_s is a time-dependent effective scattering cross-section. Tallies of the energy absorbed by the material are made at collision points, not during flights.

For practical application in conventional IMC codes, photon transport is modeled in a non-analog manner, as described in [1], in order to reduce statistical fluctuations and improve the computer run time. For this non-analog simulation, the free-flight distance is sampled using only the effective scattering cross-section (not the total), and then the photon energy is reduced to account for the expected absorption along the chosen flight path. The energy lost during the flight is tallied as absorption in the material. Only effective scattering is permitted at collision points. For the IMC method, the effective scattering cross-section is approximated by a constant, $\sigma_s = (1-f)\cdot\sigma$, with $f = 1/(1+\alpha c\sigma\beta\Delta t)$ during the timestep Δt, so that the free-flight distance is sampled in a simple fashion as $s \leftarrow -\ln(\xi)/\sigma_s$, where ξ is a uniform random deviate. The expected fractional loss in particle energy is $(1-e^{-f\sigma s})$. To develop a compatible non-analog scheme for the C-F method is challenging and nontrivial, since the effective scattering and absorption cross-sections are time dependent. The derivation below provides the first known scheme for doing so.

III. New Free-flight Sampling Scheme for the C-F Method

During a timestep in the C-F method, the effective scattering cross-section is given by [3]:

$$\sigma_s(t) = \sigma \cdot \left[1 - e^{-c\sigma\beta(t_{n+1}-t)}\right] \tag{3}$$

where $t_n \le t \le t_{n+1}$. Assume that the photon emerges from an event (emission, source, or collision) at time t' to begin a flight, with $t_n \le t' \le t_{n+1}$. We want to sample the free-flight distance using the effective scattering cross-section given by Eq. (3). Defining t'' as the time to the next collision, where $0 \le t'' \le t_{n+1} - t'$, and the corresponding flight distance $x = ct''$, Eq. (3) can be used to define the effective scattering cross-section as a function of the photon flight distance:

$$\sigma_s(x) = \sigma \cdot \left[1 - \gamma e^{+\sigma\beta x}\right] \tag{4}$$

for $0 \le x \le a$, where $a = c(t_{n+1} - t')$ and $\gamma = e^{-\sigma\beta a}$. Note that $\sigma_s(x)$ decreases smoothly from $\sigma(1-\gamma)$ at *x=0* to 0 at *x=a*.

Proceeding similar to [6], define

$$\tau(x) = \int_0^x \sigma_s(x')dx' = \sigma x - \gamma\left(e^{\sigma\beta x} - 1\right)/\beta \tag{5}$$

so that the probability of <u>not</u> colliding in the interval [*0,a*] is

$$P_{NC} = e^{-\tau(a)} = \exp\left[-\sigma a + \gamma\left(e^{\sigma\beta a} - 1\right)/\beta\right] = \exp\left[-\sigma a + (1-\gamma)/\beta\right] \tag{6}$$

With probability $P_C = 1 - P_{NC}$, a collision occurs within the interval [*0,a*], and the flight distance must be sampled from the probability density function (pdf)

$$f(s)=\frac{1}{G}\sigma_s(s)\cdot\exp\left[-\int_0^s\sigma_s(x)dx\right]=\frac{1}{G}\sigma\cdot\left[1-\gamma e^{+\sigma\beta s}\right]\exp\left[-\sigma s+\gamma(e^{\sigma\beta s}-1)/\beta\right] \quad (7)$$

where G is a normalization factor given by

$$G=\int_0^{\tau(a)}e^{-\tau}d\tau=1-e^{-\tau(a)}=1-\exp\left[-\sigma a+(1-\gamma)/\beta\right] \quad (8)$$

We have devised efficient rejection methods for sampling Eq. (7) for the case of $\beta>1$, but have not been successful for $\beta\ll 1$. Since β can vary arbitrarily as material properties change and extreme changes are expected, rejection methods will not be used. Instead, a direct sampling method will be derived. Using Eq. (5), Eq. (7) may be rewritten as

$$f(\tau)=f(s)\cdot\frac{ds}{d\tau}=\frac{1}{G}e^{-\tau} \quad (9)$$

for $0\le\tau\le\tau_{\max}$, where $\tau_{\max}=\sigma a-(1-\gamma)/\beta$. Given that a collision occurs in the interval $[0,a]$, the free-flight distance is found from Eq. (9) by solving the following equation for $\hat{\tau}$, and then solving Eq. (5) for the corresponding free-flight distance:

$$\xi=\int_0^{\hat{\tau}}f(\tau)d\tau, \qquad 0\le\hat{\tau}\le\tau_{\max} \quad (10)$$

Eqs. (8-10) are immediately recognized as sampling $\hat{\tau}$ from a truncated exponential pdf, which has the solution

$$\hat{\tau}=-\ln(1-G\cdot\xi) \quad (11)$$

Substituting $\hat{\tau}$ for τ, and $\hat{s}$ for x in Eq. (11) gives:

$$\hat{\tau}=\sigma\hat{s}-\gamma(e^{\sigma\beta\hat{s}}-1)/\beta \quad (12)$$

Equation (12) is a transcendental equation for $\hat{s}$ which is readily solved numerically using a simple Newton iteration with an initial guess of $\hat{s}_0=\hat{\tau}/\sigma$:

$$\hat{s}_{n+1}=\hat{s}_n-g(\hat{s}_n)/g'(\hat{s}_n), \quad \text{where } g(s)=\hat{\tau}-\tau(s), \quad g'(s)=-\sigma_s(s) \quad (13)$$

This will always converge for an initial guess in the interval $(0,a)$ because $g'(s)<0$, hence $g(s)$ is monotone. We have found that only 1-3 iterations are needed to converge $\hat{s}$ within 10^{-6}, even for extreme values of σ, β, and a, so that this approach is actually faster than rejection schemes. Figure (1) compares the results of this direct sampling method to the exact PDF given by Eq. (7) for several values of t' for collisions near the beginning, middle, and end of the timestep.

III. Modifications to the C-F Method

To summarize, the modifications necessary to the C-F method are:

1. Sample the flight distance to effective scattering, $\hat{s}$:
   If $\xi_1\le P_{NC}$, set $\hat{s}=a$. Otherwise, set $\hat{\tau}=-\ln(1-G\cdot\xi_2)$, then use Eq. (13) to solve for $\hat{s}$.
2. Transport the photon a distance $\hat{s}$.
3. Reduce the photon energy to $E'=E\exp\left[-\int_0^{\hat{s}}[\sigma-\sigma_s(x)]dx\right]=E\exp\left[-\gamma(e^{\sigma\beta\hat{s}}-1)/\beta\right]$.
4. Tally the absorbed energy for the flight given by $(E-E')$.

5. For collision analysis, consider only effective scattering (i.e., absorption-reemission), disallowing absorption events.

Numerical tests of the modified C-F method were carried out for the Su-Olsen transport benchmark problem [7] and compared with the conventional IMC method, the exact analog method of Ahrens and Larsen [5], and the exact analytic solution. Figure(2) shows the results for t=10 and $t = 30$, using a coarse timestep of $\Delta t = 10$. It can be seen that the modified C-F method gives essentially exact results, while IMC shows substantial errors. Computer running times were 60 seconds for the C-F method and 50 seconds for IMC using a 1 GHz Pentium-III processor and the Metroworks C++ compiler.

V. Summary and Conclusions

We have extended the C-F method for solving the grey radiative transfer equations to the case of non-analog transport. A new method for sampling the flight distance using the C-F effective scattering cross-section was developed and verified. Testing of the modified C-F method has demonstrated that it can give nearly exact results for radiative transfer problems even when very large timesteps are used, eliminating the significant temporal errors inherent in the conventional IMC method at a modest 20% increase in computer time.

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Figure 1. Verification of Sampling Scheme for Modified Carter-Forest Method, for scattering at beginning, middle, and end of timestep

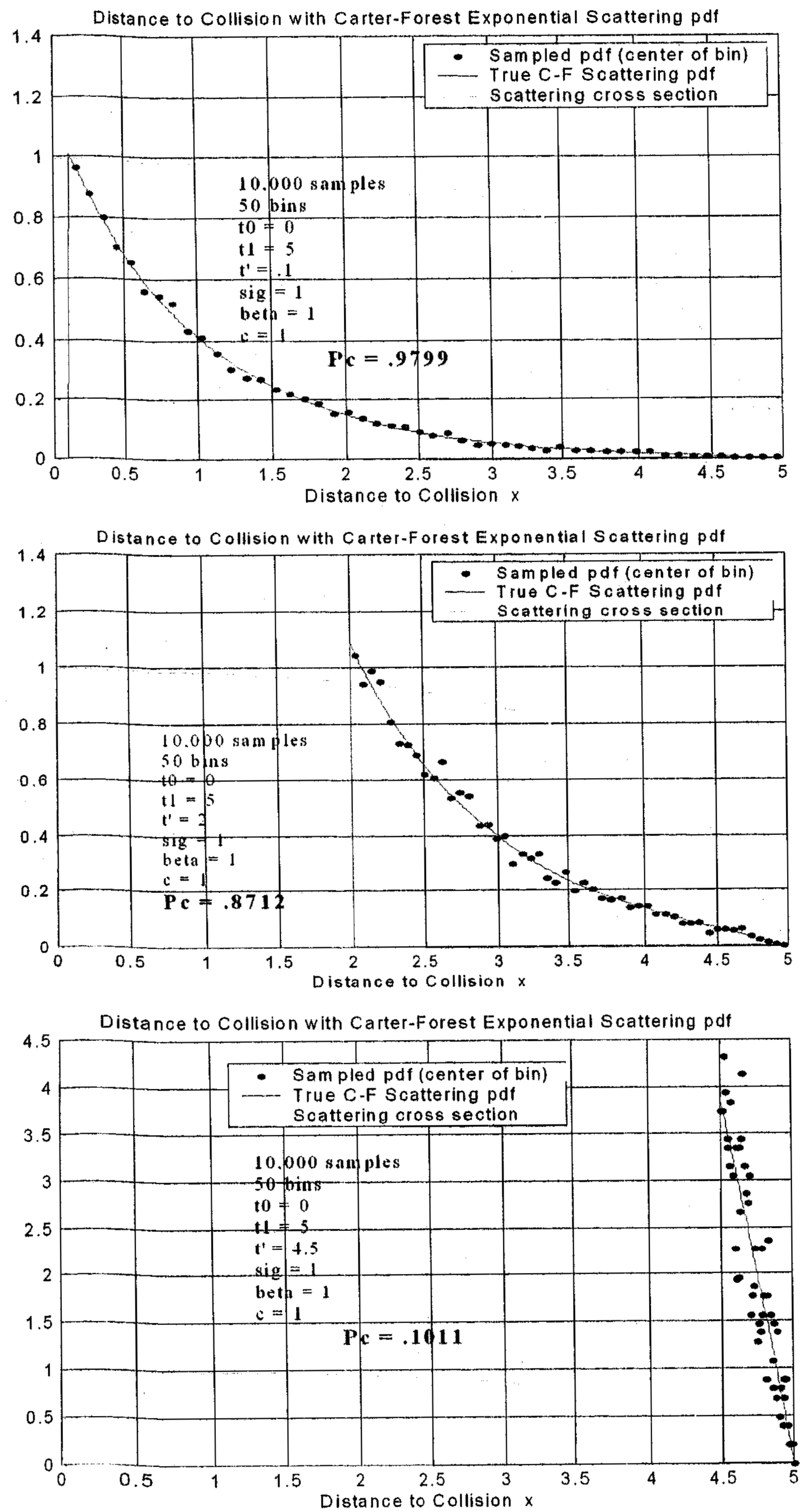

Figure 2. Integrated Radiation Intensity for Su-Olsen Benchmark Problem, 200,000 particles, 200 mesh cells, $\Delta t = 10$, $\sigma = \beta = c = 1$, no scattering