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# An Adaptive $\alpha$ for the Implicit Monte Carlo Equations (U)

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During the derivation of Fleck and Cumming's Implicit Monte Carlo (IMC) equations, a global user parameter $\alpha$ is introduced that may be adjusted in the range $0.5 \leq \alpha \leq 1.0$ in order to control the degree of "implicitness" of the IMC approximation of the thermal radiative transfer equations. For linear (and certain nonlinear) problems, it can be shown that the IMC equations are second-order accurate in the time step size $\Delta_t$ if $\alpha = 0.5$, and they are first-order accurate otherwise. However, users almost universally choose $\alpha = 1$ in an attempt to avoid unphysical temperature oscillations that can occur for problem regions in which the optical time step is large. In this paper, we provide a mathematically motivated, adaptive value of $\alpha$ that dynamically changes according to the space- and time-dependent problem data. We show that our $\alpha \rightarrow 0.5$ in the limit of small $\Delta_t$, which automatically produces second-order accuracy. In the limit of large time steps, $\alpha \rightarrow 1$; this retains the "fully implicit" time behavior that is usually employed throughout the entire problem. An adaptive $\alpha$ also has the advantages of being trivial to implement in current IMC implementations and allowing the elimination of a user input parameter that is a potential source of confusion. Test problems are presented to demonstrate the accuracy of the new approach.

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## Introduction

In the derivation of the Implicit Monte Carlo (IMC) equations, one of the most dubious approximations is to write the "equilibrium" radiative energy density $U_r(t)$ as a combination of its beginning- and end-of-time-step values through the introduction of the user parameter $\alpha$ [1]. The resulting expression for $U_r(t)$ is only correct in a time-average sense, and even then, only if the "right" value of $\alpha$ is chosen. If $\alpha = 0.5$ is chosen, then, for linear and certain nonlinear problems, it can be shown that the IMC equations are second-order accurate in the limit of small time steps $\Delta_t$ [2, 3]. However, choosing $\alpha = 0.5$ can lead to unphysical temperature oscillations, and this value of $\alpha$ is the lowest possible setting for which the IMC equations are unconditionally stable [4, 5]. Therefore, in practice, most users choose $\alpha = 1$, although temporal oscillations can occur even for this value [5].

Recently, we presented an alternative approach that uses a different, more accurate approximation that preserves the character of the IMC equations at the expense of adding a new, *time-dependent* Fleck factor [6, 7]. We referred to this as the IMC-TDF approach (Implicit Monte Carlo with a Time-Dependent Fleck factor). This approach also avoids the introduction of the user-defined parameter $\alpha$. As a first step towards implementing the IMC-TDF approach, we suggested that the *average* of the time-dependent Fleck factor be used in lieu of the original Fleck factor, and that this can be accomplished by equating the two Fleck factors and solving for $\alpha$. This produces a value of $\alpha$ that varies with $\Delta_t$ and other problem data such that $0.5 \leq \alpha \leq 1.0$.

In this paper we demonstrate how this choice of $\alpha(\Delta_t)$ leads to $O(\Delta_t^2)$ accuracy for certain classes of linear and nonlinear problems, and how in the limit of large time steps, $\alpha \to 1$, thereby reproducing the behavior of the usual form of the IMC equations. It is also trivial to implement this approach in most existing IMC codes, and it allows for the elimination of a rarely used and potentially confusing user input parameter. We present numerical test problems that demonstrate accuracy from the adaptive $\alpha$ approach and comparable solution efficiencies to IMC.

## An Adaptive $\alpha$

During the derivation of the IMC equations, the "equilibrium" radiative energy density is approximated as [1]:

$$\frac{1}{\Delta_t}\int_{t_n}^{t_{n+1}} U_r(t)\,dt \approx (1-\alpha)U_{r,n} + \alpha U_{r,n+1}\,, \approx U_r(t),$$

where $\Delta_t$ is the time step size, $U_{r,n} = U_r(t_n)$, and $\alpha$ is a a *user parameter* such that $0.5 \leq \alpha \leq 1$. Because users typically choose $\alpha = 1$ due to stability concerns, the first relationship is not exact. The second approximation (replacing the $U_r(t)$ by its mean) is made in order to get the thermal radiative transfer equations into a lower triangular form. In this paper, we focus on sharpening the first approximation.

We begin from the nonlinear, frequency-dependent thermal radiative transfer (TRT) equations with no scattering and succinctly rederive the pertinent part of the IMC-TDF equations [6, 7]. The radiation transport equation is

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mathbf{\Omega}\cdot\nabla I + \sigma I = \frac{1}{4\pi}\sigma bcU_r\,, \tag{1a}$$

with the energy balance equation

$$\frac{1}{\beta}\frac{\partial U_r}{\partial t} + \sigma_p c U_r = \iint \sigma I\; d\Omega' d\nu'\,, \tag{1b}$$

(or, equivalently):

$$\frac{\partial U_m}{\partial t} + \sigma_p c U_r = \iint \sigma I\; d\Omega' d\nu'\,. \tag{1c}$$

In these equations, the unknowns are the specific intensity $I = I(\mathbf{x}, \mathbf{\Omega}, \nu, t)$, the material energy

density $U_m = U_m(\mathbf{x}, t)$, and the "equilibrium" radiative energy density $U_r = U_r(\mathbf{x}, t) = aT^4$. The material temperature $T$ is related to the material energy density $U_m$ by the specific heat $c_v$:

$$c_v = \frac{dU_m(T)}{dT}, \tag{2}$$

$\beta$ is given by

$$\beta(x,t) = \frac{\partial U_r}{\partial U_m} = \frac{dU_r}{dT}\frac{dT}{dU_m}, \tag{3}$$

the normalized Planck spectrum $b$ is

$$b = b(\nu, T) = \frac{15\nu^3}{\pi^4 T^4}\left(e^{\nu/T} - 1\right)^{-1}, \tag{4}$$

and the Plank opacity $\sigma_p$ is the result of frequency-weighting the absorption opacity $\sigma(\nu)$ against the Planck spectrum $b(\nu, T)$.

The first approximation is to "freeze" the opacities and $\beta$ at the initial time $t_n$, which destroys the equivalency of Eqs. (1b) and (1c). Next, we "solve" Eq. (1b) for $U_r(t)$:

$$\begin{aligned} &U_r(t)e^{\beta_n\sigma_{p,n}c(t-t_n)} - U_{r,n} \\ &= \int_{t_n}^{t} e^{\beta_n\sigma_{p,n}c(t'-t_n)}\beta_n \iint \sigma_n I(t')\, d\Omega'\, d\nu'\, dt'. \end{aligned} \tag{5}$$

This expression contains no additional approximations.[1] Here we approximate the time integral by treating $I(t)$ "implicitly":

$$\begin{aligned} &U_r(t)e^{\beta_n\sigma_{p,n}c(t-t_n)} \approx U_{r,n} \\ &+\frac{1}{\sigma_{p,n}c}\left(e^{\beta_n\sigma_{p,n}c(t'-t_n)} - 1\right)\iint \sigma_n I(t)\, d\Omega'\, d\nu'. \end{aligned}$$

Solving for $U_r(t)$, we obtain:

$$\begin{aligned} U_r(t) &= U_{r,n}f_n(t) \\ &+ \frac{1 - f_n(t)}{\sigma_{p,n}c}\iint \sigma_n I(t)\, d\Omega'\, d\nu'. \end{aligned} \tag{6}$$

[1] This is actually the final form employed in the Carter-Forest method [8].

where we have defined a *time-dependent Fleck factor* $f_n(t)$ as:

$$f_n(t) \equiv e^{-\beta_n\sigma_{p,n}c(t-t_n)}. \tag{7}$$

Eq. (6) has exactly the same character as its counterpart in the original IMC equations, and we have previously discussed the necessary modifications to convert an IMC implementation into an IMC-TDF implementation [6, 7]. However, we note that the time-average value of $f_n(t)$ (denoted by $\overline{f_n(t)}$) will generally differ from $f_n$ (the "original" Fleck factor) unless $\alpha$ is chosen to satisfy the relationship:

$$\frac{1}{\Delta_t}\int_{t_n}^{t_{n+1}} f_n(t)\, dt = f_n = \frac{1}{1 + \alpha\beta_n\sigma_{p,n}c\Delta_t}, \tag{8}$$

which produces

$$\alpha(\Delta_t) = \frac{1}{1 - e^{-\beta_n\sigma_{p,n}c\Delta_t}} - \frac{1}{\beta_n\sigma_{p,n}c\Delta_t}. \tag{9}$$

Using this $\alpha(\Delta_t)$ on a cell-wise basis should be more accurate, and it eliminates user-dependence. This is the central result of our paper.

## Analysis

We next demonstrate that the adaptive $\alpha(\Delta_t)$ contains desirable limits for both short and long time steps. Defining a "scaled" time step:

$$4(\tau - \tau_n) = \beta_n\sigma_{p,n}c(t - t_n), \tag{10}$$

where $\tau = 1$ can be interpreted as the mean free time between absorption and reeemission [5], the scaled version of the "traditional" Fleck factor is

$$f = \frac{1}{1 + 4\alpha\Delta_\tau}, \tag{11}$$

and the Fleck factor with an adaptive $\alpha$ is

$$\overline{f_n(\tau)} = \frac{1}{4\Delta_\tau}\left(1 - e^{-4\Delta_\tau}\right). \tag{12}$$

In the limit of optically small time steps, or as $\Delta_\tau \to 0$,

$$\overline{f_n(\tau)} = \frac{1}{4\Delta_\tau}\left[1 - (1 - 4\Delta_\tau + 8\Delta_\tau^2 + O(\Delta_\tau^3))\right] ,$$
$$= \frac{1}{4\Delta_\tau}\left[4\Delta_\tau - 8\Delta_\tau^2 + O(\Delta_\tau^2)\right] ,$$
$$\overline{f_n(\tau)} = 1 - 2\Delta_\tau + O(\Delta_\tau^2) . \quad (13a)$$

For the traditionally-defined, constant Fleck factor, this limit is:

$$f_n = \frac{1}{1 + 4\alpha\Delta_\tau} = 1 - 4\alpha\Delta_\tau + O(\Delta_\tau^2) , \quad (13b)$$

so, to leading order, the adaptive $\alpha(\Delta_t)$ limits to the traditional Fleck factor with $\alpha = 0.5$ when short time steps are used, "automatically" obtaining $O(\Delta_t^2)$ accuracy for linear and certain nonlinear problems.

In the limit of optically large time steps, or as $\Delta_\tau \to \infty$:

$$\overline{f_n(\tau)} = \frac{1}{4\Delta_\tau} + O\left(e^{-4\Delta_\tau}\right) , \quad (14a)$$

and

$$f_n = \frac{1}{1 + 4\alpha\Delta_\tau} = \frac{1}{4\alpha\Delta_\tau} + O\left(\frac{1}{\Delta_\tau^2}\right) , \quad (14b)$$

so, to leading order, the adaptive $\alpha$ limits to the traditional Fleck factor with $\alpha = 1.0$.

Fig. 1 illustrates the asymptotic behaviors of $\alpha(\Delta_\tau)$ over a range of $\Delta_\tau$ from 0 to 100, and confirms the above analysis – for $\Delta_\tau = 0$, $\alpha = 0.5$, but it quickly rises to a value near 1 as $\Delta_\tau$ is increased and then asymptotically approaches 1.0 thereafter.

## Results

To numerically assess the temporal order of accuracy, we consider a dimensionless, linear, gray, 0-D sample problem with $\sigma = a = c = 1$ and

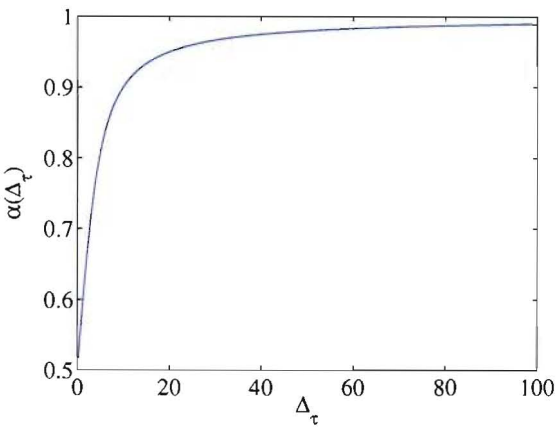


**Figure 1: Example behavior of $\alpha(\Delta_\tau)$**

$c_v = 7.14T^3$. The temperature is set to an initial condition of 0.1, and the initial intensity $\phi$ is $\approx 2.79$ (it is chosen to ensure that the equilibrium temperature is 1). The problem is solved using a variable number of time steps with an ending time fixed at $t = 10$, at which point the fine-mesh temperature solution is 1.0. We calculated exact numerical solutions of the IMC equations applied to this linear, 0-D problem; no Monte Carlo calculation was performed. We define the root mean square error of the time-dependent temperature solutions by

$$\text{RMS error} = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(T_n - T_{\text{exact},n})^2} , \quad (15)$$

where $T_n$ is provided by an IMC method, and $T_{\text{exact},n}$ is the exact solution. The results are provided in Fig. 2, which indicate that the adaptive $\alpha$ method correctly produces $O(\Delta_t^2)$ accuracy for this linear problem, as we asserted earlier. For this problem, it also happens to be the most accurate of the four IMC-based approaches.

As a more realistic test, the 1-D Su-Olson benchmark [9] was simulated using the IMC

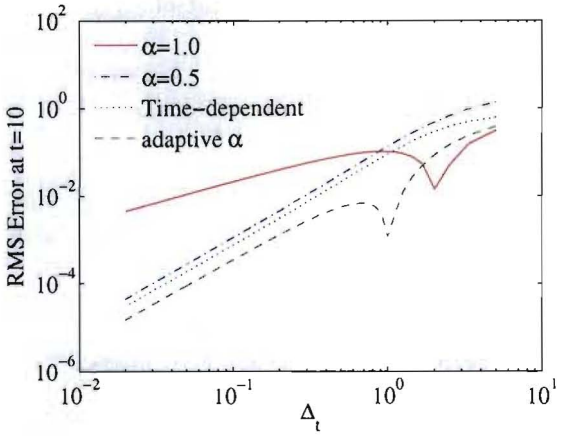


**Figure 2: The numerically-calculated order of temporal error for a linear problem for traditional IMC with $\alpha = 1$ and $\alpha = 0.5$, for IMC with the time-dependent Fleck factor $f_n(t)$, and for the adaptive $\alpha$ method.**

method with $\alpha = 1$ and the adaptive $\alpha(\Delta_t)$ approach. Because this benchmark test is linear, there are no temporal truncation errors, which implies that differences in solution accuracies should solely be due to the differences with which $\alpha$ is employed. In addition to the tabular reference solutions provided in [9] and shown in Fig. 3 in symbolic form, we have also simulated a more spatially-refined version of the Ahrens-Larsen "Semi-analog Monte Carlo" equations [5, 10], which are exact for any $\Delta_\tau$ in this linear problem (up to statistical errors). Fig. 4 depicts the relative differences in the $T^4$ solutions resulting from using $\alpha = 1$ and the adaptive $\alpha(\Delta_t)$ for times $\tau = 1.0$, 3.16228, 10.0 and 31.6228. The time discretization for this problem was to use (roughly) $\Delta_\tau = 0.1$ up to $\tau = 1.0$, $\Delta_\tau = 0.21623$ up to $\tau = 0.31623$, $\Delta_\tau = 0.341885$ up to $\tau = 1.0$, $\Delta_\tau = 0.72076$ up to $\tau = 3.16628$, $\Delta_\tau = 1.70943$ up to $\tau = 10.0$, and $\Delta_\tau = 4.32456$ up to $\tau = 31.6228$ (these seemingly strange values were chosen to match the benchmark times). Because the time steps increase as the simulation progresses, the overall trend is for the adaptive $\alpha(\Delta_\tau)$ to be more accurate than the

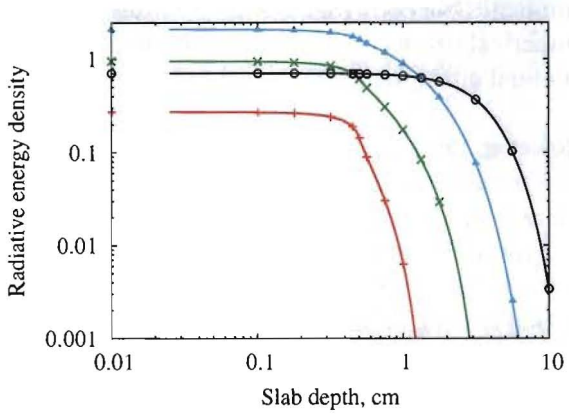


**Figure 3: $T^4$ Reference Solution (Su-Olson + Semi-Analog Monte Carlo) for times $\tau = 1.0$, 3.16228, 10.0 and 31.6228.**

$\alpha = 1$ solutions, but for the magnitude of the accuracy gain to reduce as time progresses.

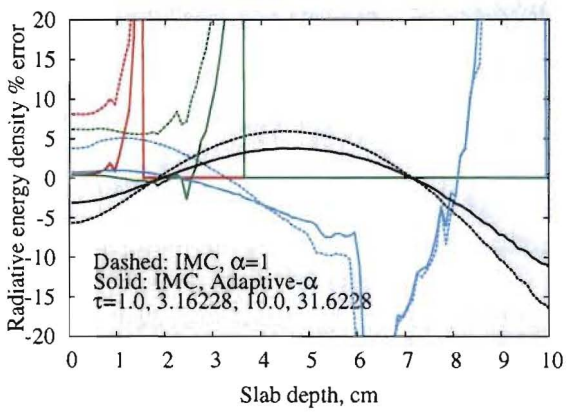


**Figure 4: Error comparison of $T^4$ for IMC with $\alpha = 1$ and adaptive $\alpha$**

## Conclusions and Future Work

We have presented a new, adaptive $\alpha(\Delta_t)$ for use in the IMC equations that (1) automatically retains $O(\Delta_t^2)$ accuracy in the limit of small time steps for linear and certain nonlinear problems, that (2) retains the more stable $\alpha = 1$ behavior for optically large time steps, and (3) completely

eliminates the need for the IMC code user to set a numerical parameter in an IMC simulation at minimal effort to the IMC code developer.

However, this technique, although more accurate than the IMC equations with $\alpha = 1$, does not address what we consider to be the largest source of error in the approximate IMC equations: the linearization error arising from freezing $\sigma$, $\beta$, and $b(\nu)$ at the beginning of the time step. As future work, we intend to test this approach against nonlinear, frequency-dependent problems in order to discern the overall magnitude of the accuracy enhancement.

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