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# Error Modes in Implicit Monte Carlo

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## I. Introduction

The Implicit Monte Carlo (IMC) method of Fleck and Cummings [1] has been used for years to analyze radiative transfer problems, such as those encountered in stellar atmospheres or inertial confinement fusion. Larsen and Mercier [2] have shown that the IMC method violates a maximum principle that is satisfied by the exact solution to the radiative transfer equation. Except for [2] and related papers regarding the maximum principle, there have been no other published results regarding the analysis of errors or convergence properties for the IMC method.

This work presents an exact error analysis for the IMC method by using the analytical solutions for infinite medium geometry (0-D) to determine closed form expressions for the errors. The goal is to gain insight regarding the errors inherent in the IMC method by relating the exact 0-D errors to multi-dimensional geometry. Additional work (not described herein) has shown that adding a leakage term (i.e., a "buckling" term) to the 0-D equations has relatively little effect on the IMC errors analyzed in this paper, so that the 0-D errors should provide useful guidance for the errors observed in multi-dimensional simulations.

## II. Radiative Transfer Equations

### Grey Equations for an Infinite Medium

We begin with the coupled equations (grey) of radiative transfer [3]:

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

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

where $I(\mathrm{r},\mathbf{\Omega},t)$ is the radiation intensity, $\phi(\mathrm{r},t)=\int I(\mathrm{r},\mathbf{\Omega},t)d\mathbf{\Omega}$ is the integrated intensity, $U_r(\mathrm{r},t)=a\left[T(\mathrm{r},t)\right]^4$ is the equilibrium radiation energy density, a is the radiation constant, $\sigma$ is the absorption cross section (no scattering), and $\beta(\mathrm{r},\mathrm{t}) = \frac{\partial \mathrm{U_r}(\mathrm{r},\mathrm{t})}{\partial \mathrm{U_m}(\mathrm{r},\mathrm{t})}$ relates $U_r(\mathrm{r},t)$ to the material energy density $U_m(\mathrm{r},t)$ and is a function of position, temperature, and heat capacity.

Now assume an infinite, uniform medium with constant $\beta$ (i.e., $\rho C_v \sim T^3$) and $\sigma$, and integrate Eq. (1) over angle to obtain:

$$\frac{1}{\mathrm{c}}\frac{\mathrm{d}\phi}{\mathrm{dt}} + \sigma\phi(\mathrm{t}) = \mathrm{c}\sigma U_r(\mathrm{t}) + \mathrm{Q}(\mathrm{t}) \tag{3}$$

$$\frac{1}{\beta}\frac{dU_r}{dt} = \sigma\phi(t) - c\sigma U_r(t) \tag{4}$$

Equations (3) and (4) are solved over a timestep $\Delta t = t_{n+1} - t_n$ with initial conditions $\phi(t_n) = \phi_n$ and $U_r(t_n) = U_r^n$.

The material energy (hence temperature T) is a sensitive function of the difference between energy loss due to emission and energy gain due to absorption. Thus energy conservation is key to radiative transfer. A conservation of energy principle is obtained by adding Eqs. (3) and (4):

$$\frac{1}{\mathrm{c}}\frac{\mathrm{d}\phi}{\mathrm{dt}} + \frac{1}{\beta}\frac{\mathrm{d}U_r}{\mathrm{dt}} = \mathrm{Q}(\mathrm{t}) \tag{5}$$

where we note that the second term on the left hand side is the time rate of change of the material energy density, since $\frac{\mathrm{d}U_m}{\mathrm{dt}} = \frac{1}{\beta}\frac{\mathrm{d}U_r}{\mathrm{dt}}$ by the definition of $\beta$. Thus the time rate of change of the radiation energy plus the material energy is balanced by the external source. If $\phi(\mathrm{t})$ has been found, $U_r(t)$ may be obtained by integrating (5):

$$U_r(\mathrm{t}) = U_r^n - \frac{\beta}{\mathrm{c}}\left[\phi(\mathrm{t}) - \phi_\mathrm{n}\right] + \beta\int_{\mathrm{t_n}}^{\mathrm{t}} \mathrm{Q}(\mathrm{t}')\mathrm{dt}' \tag{6}$$

**IMC Approximation**

It is a straightforward exercise [3,4] to apply the IMC method to Eqs. (3) and (4), which results in the following approximate transport equation:

$$\frac{1}{\mathrm{c}}\frac{\mathrm{d}\varphi}{\mathrm{dt}} + \sigma f \varphi(\mathrm{t}) = \sigma f V_r^n + \mathrm{Q}_0 \tag{7}$$

where $\varphi(t)$ and $V_r(t)$ are the IMC approximations to the actual solutions $\phi(t)$ and $U_r(t)$, $f = \frac{1}{1+\alpha c\beta\sigma\Delta t}$ is the "Fleck" factor, and $\alpha$ is the time weighting factor defined by the IMC approximation which expresses the instantaneous equilibrium radiation energy density in terms of its beginning and end of timestep values:

$$V_r(t) \simeq \alpha V_r^{n+1} + (1-\alpha)V_r^n .$$

Reference [1] notes that to avoid oscillations in the numerical solution, one should impose $(1-\alpha)\beta c\sigma\Delta t \le 1$ which for many applications results in the condition $\alpha = 1$.

## III. Analytical Solutions

**Solutions to Exact Equations**

Equations (3) and (4) can be rearranged into a single second order equation:

$$\frac{1}{c}\frac{d}{dt}\left(\frac{d\phi}{dt}\right) + \sigma(1+\beta)\frac{d\phi}{dt} = c\sigma\beta Q_0 \tag{8}$$

where the initial conditions are $\phi(t_n) = \phi_n$ and $\left.\frac{d\phi}{dt}\right|_{t=t_n} = \sigma c^2 U_r^n - \sigma c\phi_n + cQ_0$. The solution to Eq. (8) is easily found:

$$\begin{aligned}\phi(t) = \phi_n + \left(\frac{\sigma}{c\gamma}\right)\left(cU_r^n - \phi_n\right)\left(1-e^{-\gamma(t-t_n)}\right) + \frac{cQ_0}{\gamma}\left(1-e^{-\gamma(t-t_n)}\right) \\ + \frac{\sigma c^2\beta Q_0}{\gamma}t - \frac{\sigma c^2\beta Q_0}{\gamma}\left(1-e^{-\gamma(t-t_n)}\right)\end{aligned} \tag{9}$$

where $\gamma = \sigma c(1+\beta)$ .

Now substitute (9) into (6) to find $U_r(t)$ for the case of a fixed source $Q_0$ within the timestep:

$$U_r(t) = U_r^n + \beta Q_0(t - t_n) - \frac{\beta}{c}\left(\phi(t) - \phi_n\right) \tag{10}$$

**Solutions to IMC Equations**

The IMC equation (7) may be solved for $\varphi(t)$:

$$\varphi(t) = \varphi_n e^{-c\sigma f(t-t_n)} + \left(cV_r^n + \frac{Q_0}{c\sigma f}\right)\left(1-e^{-c\sigma f(t-t_n)}\right) \tag{11}$$

which is then substituted into (6) to find the equilibrium radiation energy density:

$$V_r(\mathrm{t}) = V_r^n + \beta \mathrm{Q}_0(\mathrm{t}-\mathrm{t_n}) - \frac{\beta}{\mathrm{c}}\left(\varphi(\mathrm{t}) - \varphi_\mathrm{n}\right) \qquad (12)$$

The IMC solution is only relevant at the end of the timestep since the factor *f* depends on the timestep $\Delta\mathrm{t}$ and a conventional IMC calculation will only yield the end of timestep solution. However, one can obtain the within-timestep variation of the IMC solution is desired (this is plotted in the results to be discussed in the next section). Therefore, the analytical IMC solutions at $\mathrm{t} = \mathrm{t_{n+1}}$ are given by:

$$\varphi_\mathrm{n+1} = \varphi_\mathrm{n} \mathrm{e}^{-\mathrm{c}\sigma f \Delta\mathrm{t}} + \left( cV_r^n + \frac{\mathrm{Q}_0}{\mathrm{c}\sigma f} \right)\left(1 - \mathrm{e}^{-\mathrm{c}\sigma f \Delta\mathrm{t}}\right) \qquad (13)$$

$$V_r^{n+1} = V_r^n + \beta \mathrm{Q}_0 \Delta\mathrm{t} - \frac{\beta}{\mathrm{c}}\left(\varphi_\mathrm{n+1} - \varphi_\mathrm{n}\right) \qquad (14)$$

## IV. Numerical Results

The above error analysis was applied to a number of test problems to investigate the IMC errors. Illustrative results are given in Figure 1 for a thermal relaxation problem with $\phi_0 = 1000$, $U_r^0 = 1$, and $\mathrm{Q}_0 = 0$, and parameters $\sigma = 1$, $\beta = 1$, $\alpha = 1$, c = 1, and $\Delta$t = 5. Physically, this problem simulates a cold medium that is irradiated by a relatively hot photon flux. The problem data corresponds to a relatively long timestep where photons may undergo several absorptions and re-emissions, since the mean thermal relaxation time (time to re-emit following absorption) is $\beta^{-1} = 1$ and the mean absorption time is $(\sigma\mathrm{c})^{-1} = 1$, compared to the timestep $\Delta$t=5. It is convenient to show the radiation energy density $E(\mathrm{t}) = \frac{1}{\mathrm{c}}\phi(\mathrm{t})$, since $E(\mathrm{t}) \to U_r(\mathrm{t})$ as t increases.

Figure 1 includes three plots of the exact solutions for $E(\mathrm{t})$ and $U_r(\mathrm{t})$ compared with the IMC solutions for different choices of the time weighting factor $\alpha$. Figure 1a shows the $\alpha$=1 ("implicit") case, which is the conventional choice for IMC. This plot shows that the errors in the IMC solutions are substantial initially, then decrease rapidly as the solution equilibrates. Figure 1b gives the $\alpha$=.5 (time-centered) case, showing severe oscillations in the solution which diminish with increasing t. (The Ref. [1] criterion results in $\alpha \geq .8$ although oscillations are observed for $\alpha = 1$ that are strongly damped.) Figure 1c depicts the $\alpha$=0 ("fully explicit") case and the oscillations are persistent and undamped, indicating clearly the unstable behavior of explicit timestepping. Therefore, the typical choice to use $\alpha$=1 with IMC is supported by these 0-D results. (For some other types of problems, such as a cold medium that has a photon source turned on at t=0, the best results may be obtained by choosing $\alpha$<1, typically in the range .5-1.)

To examine the variation of the error with timestep and beta, only the error in the first timestep was tabulated as a function of these two parameters. Figure 2a depicts the dependence of the first timestep error as a function of $\Delta$t for $\beta$=1 while Figure 2b shows the dependence of the first timestep error as a function of $\beta$ for $\Delta t = 5$. It can be seen that relatively large errors (20-80%) occur for a large range of $\Delta t$ and $\beta$.

When the above analysis is modified to include leakage, via a "buckling" term, it is found that the solution to the exact system contains two exponential terms while the exact IMC solution has only one exponential term to approximate the true solution. A number of cases were analyzed with various amounts of leakage, including equilibration and source problems. Interestingly, the errors for the cases with leakage were not substantially different from the zero leakage cases, even with relatively large leakage terms, e.g., with a leakage rate comparable to the absorption rate. This indicates that for the 0-D equations, leakage does not seem to make the IMC errors any worse.

## V. Summary and Conclusions

We have derived an analytical solution to the infinite medium grey radiative transfer equations and have performed an exact error analysis for the IMC method. For large timesteps and/or small values of $\beta$, it was shown that substantial errors arise in the IMC solutions. 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).

As discussed in [3], two alternative schemes for solving the radiative transfer equations, the Carter-Forest (C-F) method [5] and the Ahrens-Larsen (A-L) method [4], do not exhibit the errors described herein; 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 yield substantially superior results to IMC for the chosen test problems, as expected.

### References

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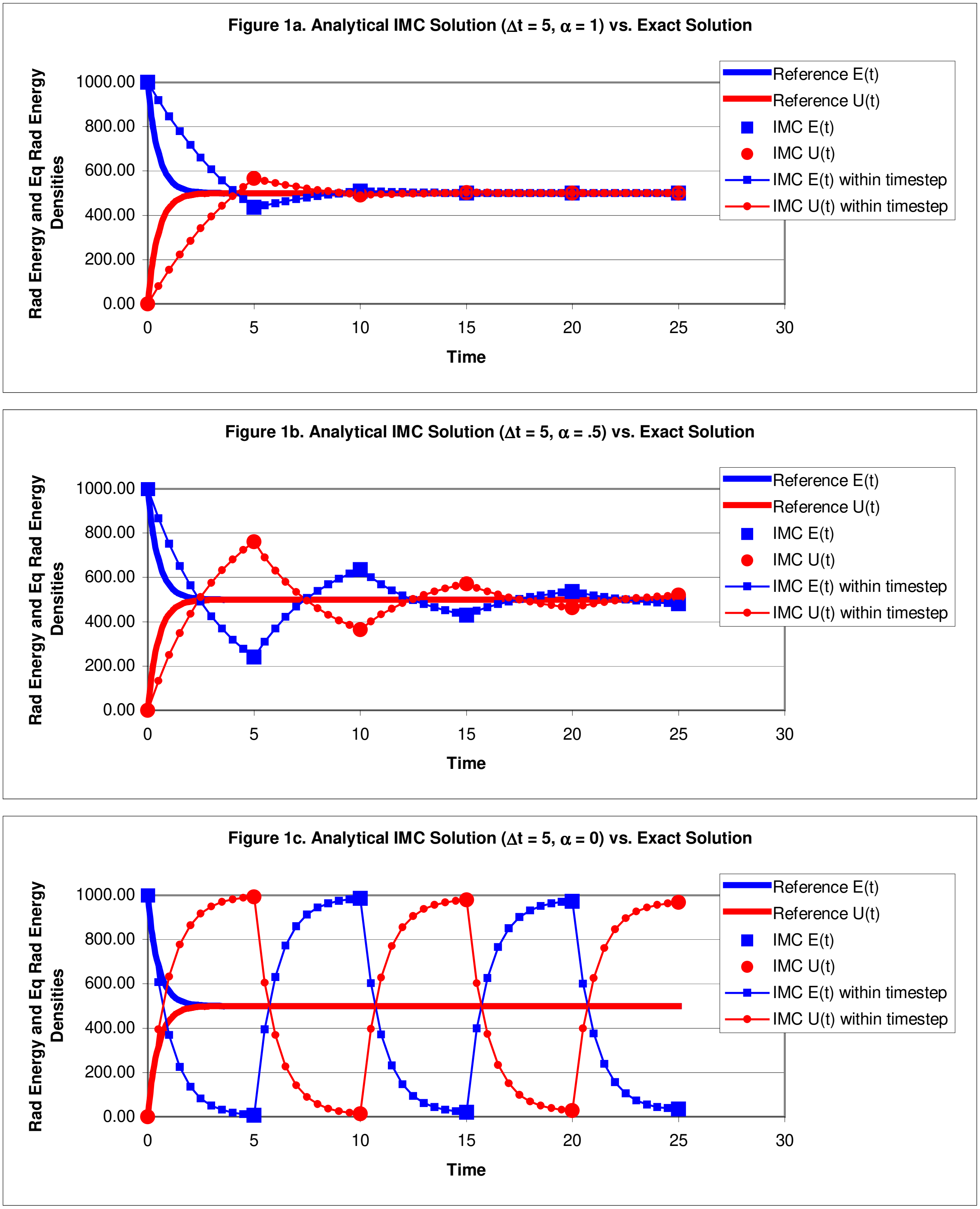
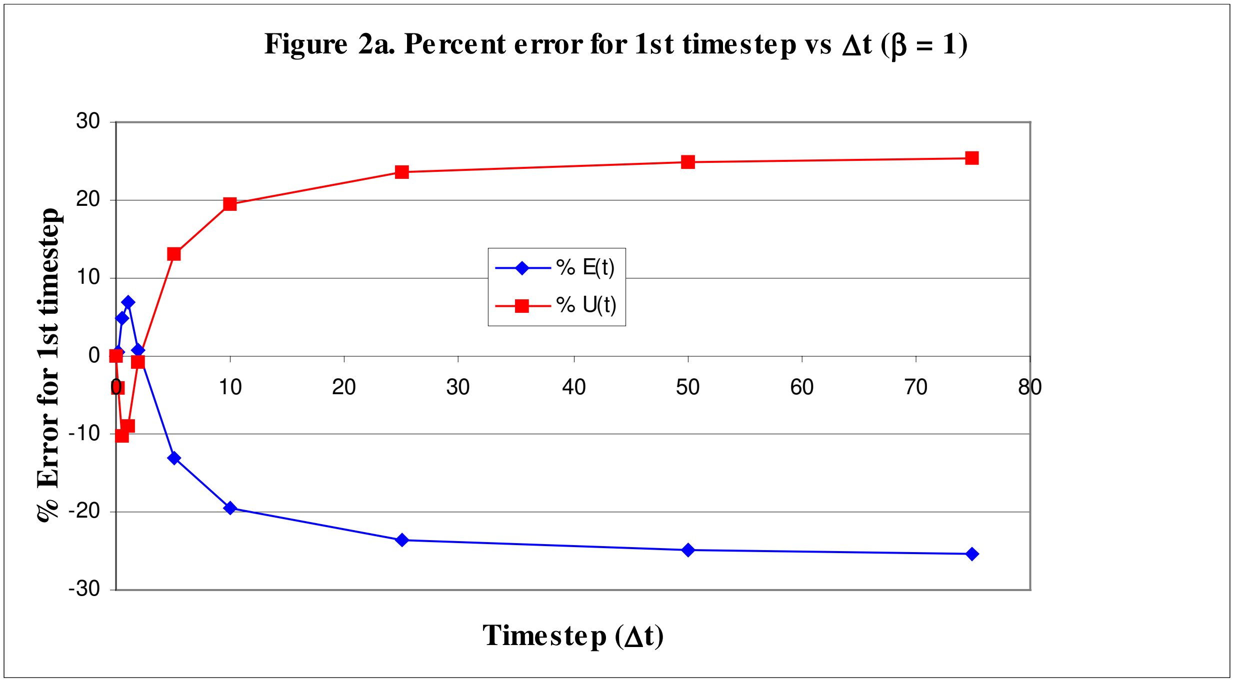



Figure 1. Comparison of Analytical IMC Solution vs. Exact Solution for Different α (Equilibration Test Problem)



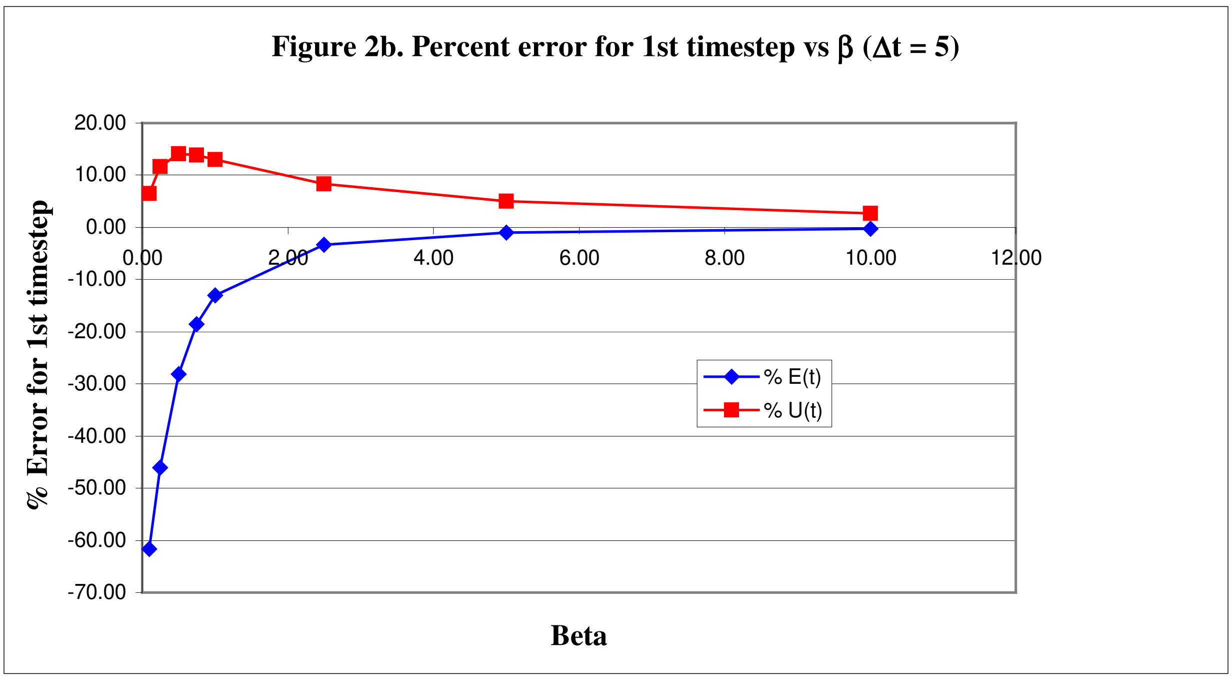




Figure 2. Percent Error in IMC Solution for 1st Timestep vs. Δt and β
(Equilibration Test Problem)