Time Step Control for Iterative Multifrequency Corrected Implicit Monte Carlo[1]

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ABSTRACT

In this work we outline a new time step controller that has been designed for Iterative Multifrequency Corrected Implicit Monte Carlo (IMC^2). This time step controller is directly derived from the analysis performed by Cleveland and Wollaber for the original Locally Corrected Implicit Monte Carlo (LCIMC). IMC^2 is an iterative extension of LCIMC that guaranties adhearance to the maximum principle for frequency dependent thermal radiative transfer (TRT) problems. In this work we compare solutions to an analytic Marshak wave problem with and without our new time step controller.

INTRODUCTION

Iterative Multifrequency Corrected Implicit Monte Carlo (IMC^2 or IMC-squared) [1] is a non-negative, nonlinear, iterative, TRT solver that is guaranteed, upon convergence, to preserve the maximum principle. This solver is an iterative extension of Locally Corrected Implicit Monte Carlo (LCIMC) recently developed by Cleveland and Wollaber [2]. The maximum principle states that, in the absence of external source, all internal temperatures must be equal to or less than the boundary temperatures of the problem [3]. IMC^2 does not suffer from the same efficiency and robustness issue associated with the current implementations of Iterative Implicit Monte Carlo [4, 5], which was also developed to mitigate maximum principle violations. IMC^2 was designed for Monte Carlo solvers, though it should be noted that it is not limited to this, in that it is non-negative and rapidly converging for reasonable time step sizes. In the follow section we will provide a full description of the equations that are being solved. However, much of the details of the derivation will be left out for brevity.

IMC^2

This derivation begins by defining a linearization around the current iteration, which is constrained by setting it equal to the fully implicit emission temperature for the current iteration.

$$T_{i+1}^4\Delta t \equiv \int_{t_n}^{t_{i+1}} \left(T_n^4 + 4T_{c,i+1}^3 \frac{dT}{dt}\Delta t \right) dt. \tag{1}$$

where T_{i+1} is the implicit temperature for the current iteration i. Given this integration we obtain the definition of $T_{c,i}$ defined by Cleveland and Wollaber [2],

$$T_{c,i+1}^3 \equiv \left(\frac{1}{4} \frac{(T_{i+1}^4 - T_n^4)}{(T_{i+1} - T_n)} \right). \tag{2}$$

The expansion (Eqs. 1 and 2) of the implicit emission term can be substituted back into the original TRT equations, as was done by Fleck and Cummings [6], to yield a new "IMC like" set of TRT equations. If we define a correction $\epsilon_{i+1} = f_{c,i+1} - f_{c,i}$, as was done by Cleveland and Wollaber [2], we can operator split the implicit ϵ_i term to form a set of non-linear TRT equations for a single iteration i,

$$\frac{1}{c}(I_i - I_n) + \overline{\Omega \cdot \nabla I_i} + \overline{\sigma(\nu, T_n) I_i} = f_{c,i} \frac{\sigma(\nu, T_n) b(\nu, T_i)}{4\pi} acT_n^4 \Delta t + \frac{\sigma(\nu, T_n) b(\nu, T_i)}{4\pi \sigma_{p,i}} \int \int \overline{(1 - f_{c,i}) \sigma(\nu, T_n) I_i} d\nu d\Omega, \tag{3}$$

$$\rho c_v (T_{i+1} - T_n) = \frac{f_{c,i+1}}{f_{c,i}} S_{c,i}, \tag{4}$$

and

$$\frac{1}{c}(I_{n+1} - I_i) \quad = \quad -\frac{\sigma(\nu, T_n) b(\nu, T_i,)}{4\pi \sigma_{p,i}} \frac{\epsilon_{i+1}}{f_{c,i}} S_{c,i}, \tag{5}$$

where T_i is the current iterate's guess for the implicit material temperature (or the T_{i+1} from the previous iteration),

$$S_{c,i} = \left(\int \int \overline{f_{c,i} \sigma(\nu, T_n) I_i} d\nu d\Omega - f_{c,i} ac \sigma_{p,i} T_n^4 \Delta t \right), \tag{6}$$

$$f_{c,i+1} = \frac{1}{1 + \frac{\sigma_{p,i} 4acT_{c,i+1}^3 \Delta t}{\rho c_v}}, \tag{7}$$

$$f_{c,i} = \frac{1}{1 + \frac{\sigma_{p,i} 4acT_{c,i}^3 \Delta t}{\rho c_v}}, \tag{8}$$

and,

$$T_{c,i}^3 \equiv \left(\frac{1}{4} \frac{(T_i^4 - T_n^4)}{(T_i - T_n)} \right). \tag{9}$$

Note that this form is slightly different than what was previously presented by Cleveland and Wollaeger where the iteration scheme was not properly carried through the linearization[1]. As our initial guess in the iteration scheme we use $T_{i+1} = T_i = T_n$, where T_n is the initial material temperature for the current time step. Then we evaluate Eq. 3 using Monte Carlo. Given the energy deposition information for the current iteration (i) we perform a Newton solve on Eq 4, making use of Eqs. 2, 7, 8 and 9, until we converge on a new T_{i+1}. Then we check if the intensity correction (Eq. 5) will adhere to the maximum principle. We can define an inequality for correction source (ϵS_c) that will guarantee that the maximum principle ($I_{n+1} \leq B(\nu, T_u)$) is satisfied [3] (T_u denotes the maximum temperature in the problem including any sources). We already know from the analysis performed by Cleveland and Wollaber that the LCIMC equations guarantee that $T_{i+1} \leq T_u$ [2] for any given iteration. The following

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inequality ensures that the photon intensity will adhere to the maximum principle in each cell

$$\left(1 + \frac{\left(\frac{1}{c}\int\int I_i d\nu d\Omega + \epsilon_i S_{c,i} - aT_u^4\right)}{aT_u^4}\right)^{-1} \geq 1 \qquad (10)$$

Note that it is possible to satisfy this inequality after a single iteration if the energy exchange is well approximated by the original Fleck and Cummings expansion. If this inequality is not satisfied for all cells we update $T_{c,i}^3$ and f_i based on the new T_{i+1}, then set $T_i = T_{i+1}$, and continue to iterate. After Eq. 10 is satisfied in all cells we update the final photon intensity (I_{n+1}) using Eq. 5 and set the final material temperature $T_{n+1} = T_{i+1}$. Note that IMC^2 can produce negative corrections to the intensity for Eq. 5. Rather than reducing the current census energy we simply set the correction $\epsilon S_c = 0$. The negativity is an indication that the linearization in the current iteration will not overheat or excessively cool the cell, therefore we can accept it without fear of violating the maximum principle. This is equivalent to taking a semi-implicit IMC step, that will not violate the maximum principle, without a correction.

TIME STEP CONTROLLER

Although IMC^2 will adhear to the maximum principle, upon iteration convergence, a time step controller can still be valuable to both ensure accuracy and computational efficiency. If the coupling in a problem is sufficiently stiff it could take many transporter iterations per time step to converge. Additionally, because we are currently lagging the opacity, wave stagnation can occur for large time steps. Therefore we wish to define a time step control that attempts to maximise the correction for a single iteration. This can be achieved making Eq. 10 an equality and multiplying both sides by Δt such that

$$\Delta t_c = \Delta t_n \left(1 + \frac{\left(\frac{1}{c}\int\int I_i d\nu d\Omega + \epsilon_i S_{c,i} - aT_u^4\right)}{aT_u^4}\right)^{-1} \qquad (11)$$

This represents an assumed first order relationship between the overheating and the time step size. To prevent us from taking too large of a time step we set a max increase in the time step as $\Delta t_{max} = 1.5\Delta t_n$. Using this max change in time step size the final time step controller can be defined as

$$\Delta t_{n+1} = \min(\Delta t_c, \Delta t_{max}) \qquad (12)$$

where Δt_c is the most restrictive time step for all cells.

PRELIMINARY RESULTS AND CONCLUSIONS

We compare IMC^2 with and without our time step controller to standard IMC for an analytic Marshak Wave. This problem is composed of an initially cold ($T(t = 0) = 0.1$ [keV]) slab of material that is heated by a $T(x = 0) = 1$ [keV] surface source. The material has a constant specific heat $c_v = 0.1$ [Jerks/g/keV] and density $\rho = 1.0$ [g/cc]. All simulations used a fixed $\Delta x = 0.005$ [cm] cell spacing in the domain $0 \leq x \leq 1$ [cm]. We used 10^4 particles/iteration to evolve the radiation intensity.

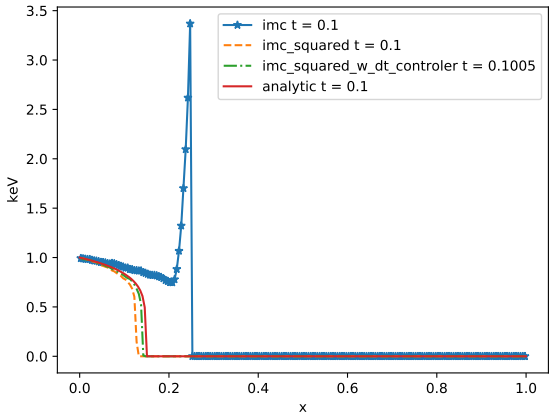

Fig. 1: IMC and IMC^2 results for the analytic Marshak wave problem.

Fig. 1 compares IMC and IMC^2 with a fixed time step size of 0.002 [ns] to IMC^2 with our new time step controller. In comparing these results we see that IMC^2 ensures that we do not violate the maximum principle even for large time steps ($\Delta t = 0.002$ [ns]) that cause IMC to violate. We see that IMC^2 with the time step controller (where the first time step size is chosen as $\Delta t_n = 0.002$) also adheres to the maximum principle and produces an improved agreement with the analytic result. The time step controller additionally improves the computational performance of the calculation. To understand this we can look at the total number of Monte Carlo iterations (the number of times Eq. 3 is evolved using Monte Carlo) and the number of time steps required to evolve the solution with and without the time step controller. The time step controller forced the simulation to take 230 time steps as opposed to the 50 required for the fixed $\Delta t = 0.002$ [ns]. The number of Monte Carlo iterations that IMC^2 with and without the time step controller, 439 and 420 respectively, are similar. However, many of the iterations taken when using the time step controller were at a smaller time step sizes than the fixed time step size. Given that for a fixed number of particles per iteration, Monte Carlo work scales proportionately to the size of the time step, we expect a reduced amount of computation time to iterate during smaller time steps. This explains the slight improvement in runtime 1187 [sec] for IMC^2 with the time step controller as compared to 1227 [sec] for IMC^2 without the time step controller.

These preliminary results shows some of the major benefits of IMC^2 using our proposed time step controller. Future publications will include more results comparing IMC and IMC^2 on multi-material, multi-frequency, and multi-dimensional problems. We will also present updated proofs, similar to those presented by Cleveland and Wollaber for LCIMC [2], of positivity and adherence to the maximum principle.

ACKNOWLEDGEMENTS

This research was performed by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396.

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