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NUEN-618 Class Project: Actually Implicit Monte Carlo

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1 Introduction

This research describes a new method for the solution of the thermal radiative transfer (TRT) equations that is implicit in time which will be called Actually Implicit Monte Carlo (AIMC). This section aims to introduce the TRT equations, as well as the current workhorse method which is known as Implicit Monte Carlo (IMC). As the name of the method proposed here indicates, IMC is a misnomer in that it is only semi-implicit, which will be shown in this section as well.

1.1 The Thermal Radiative Transfer Equations

The TRT equations consist of a transport equation for the radiation angular intensity I, and a conservation equation for the material energy, often written in terms of the material temperature T, specific energy e, or energy density U_m. The transport equation, assuming no scattering and no external volumetric sources (which is a valid assumption in a wide variety of problems) can be written as:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mathbf{\Omega}\cdot\nabla I + \sigma I = \sigma B \ , \tag{1}$$

where c is the speed of light, $\mathbf{\Omega}$ is the direction of flight, σ is the absorption opacity, and B is Planck's function. The quantities in this equation have the following dependencies:

$$I = I\left(\mathbf{r}, \mathbf{\Omega}, \nu, t\right) \ ,$$

$$\sigma = \sigma\left(\mathbf{r}, \nu, T\left(t\right)\right) \ ,$$

$$B = B\left(\nu, T\left(t\right)\right) \ ,$$

where $\mathbf{r}$ is the position in space, ν is the photon frequency, t is time, and T is the material temperature. We will mainly be concerned here with the case where the material opacities

have no dependence on photon frequency, also known as the Gray approximation. Given this approximation, we can integrate equation 1 over all photon frequencies

$$\frac{1}{c}\frac{\partial \mathcal{I}}{\partial t} + \mathbf{\Omega} \cdot \nabla \mathcal{I} + \sigma \mathcal{I} = \frac{c\sigma a T^4}{4\pi} \,, \tag{2}$$

where

$$\mathcal{I}\left(\mathbf{r}, \mathbf{\Omega}, t\right) = \int_0^\infty I\left(\mathbf{r}, \mathbf{\Omega}, \nu, t\right) d\nu \,,$$

and

$$\int_0^\infty B\left(\nu, T\right) d\nu = \frac{caT^4}{4\pi} \,.$$

The material energy equation can be written as

$$\rho \frac{\partial e}{\partial t} = \int_0^\infty \iint_{4\pi} \sigma \left(I - B\right) d\Omega d\nu \,, \tag{3}$$

where ρ is the density and e is the specific energy related to the temperature via the equation of state (EOS). Again, assuming opacities independent of photon frequency, we can carry out the frequency integral

$$\rho \frac{\partial e}{\partial t} = \iint_{4\pi} \sigma \mathcal{I} d\Omega - c\sigma a T^4 \,. \tag{4}$$

1.2 The Implicit Monte Carlo Method

The IMC method is based upon a particular linearization and discretization in time of the TRT equations presented in the previous subsection. The resulting equations do not necessarily need to be solved via Monte Carlo, making the name of the method even more questionable. In any case, it is the linearization and discretization that is of concern here, and not the method of solution. Further details of the IMC method can be found in its original derivation by Fleck and Cummings[1], and the dissertation by Wollaber.[2] The first step is to replace the specific energy with the energy density U_m, and the T^4 terms with the radiation energy density U_r

$$\rho e = U_m \qquad ; \qquad U_r = aT^4 \,, \tag{5}$$

in order to linearize the TRT equations

$$\frac{1}{c}\frac{\partial \mathcal{I}}{\partial t} + \mathbf{\Omega} \cdot \nabla \mathcal{I} + \sigma \mathcal{I} = \frac{c\sigma U_r}{4\pi} \,, \tag{6}$$

$$\frac{\partial U_m}{\partial t} + c\sigma U_r = \iint_{4\pi} \sigma \mathcal{I} d\Omega \,. \tag{7}$$

We then make the following definition

$$\beta\left(\mathbf{r}, T\right) = \frac{\partial U_r}{\partial U_m} \,,$$

in order to eliminate U_m from the material energy equation

$$\frac{1}{\beta}\frac{\partial U_r}{\partial t} + c\sigma U_r = \iint_{4\pi} \sigma \mathcal{I} d\Omega \; . \tag{8}$$

Thus far, no approximations have been made. The IMC discretization then assumes

$$\sigma = \sigma_n = \sigma\left(\mathbf{r}, T\left(t_n\right)\right) \qquad \text{and} \qquad \beta = \beta_n = \beta\left(\mathbf{r}, T\left(t_n\right)\right) \; .$$

where t_n is the start time of timestep n. Before going forward, it should be noted that this assumption makes it impossible for the method to be fully implicit. Furthermore, equations 7 and 8 are no longer equivalent because β has been fixed to its value at the beginning of the time step. Inserting these approximations and discretizing the remaining variables implicitly in time gives

$$\frac{1}{c}\frac{\mathcal{I}^{n+1} - \mathcal{I}^n}{\Delta t} + \mathbf{\Omega} \cdot \nabla \mathcal{I}^{n+1} + \sigma_n \mathcal{I}^{n+1} = \frac{c\sigma_n U_r^{n+1}}{4\pi} \; , \tag{9}$$

$$\frac{1}{\beta_n}\frac{U_r^{n+1} - U_r^n}{\Delta t} + c\sigma_n U_r^{n+1} = \iint_{4\pi} \sigma_n \mathcal{I}^{n+1} d\Omega \; , \tag{10}$$

$$\frac{U_m^{n+1} - U_m^n}{\Delta t} + c\sigma_n U_r^{n+1} = \iint_{4\pi} \sigma_n \mathcal{I}^{n+1} d\Omega \; . \tag{11}$$

Solving for U_r^{n+1} in equation 10 gives

$$U_r^{n+1} = \left(\frac{1}{1 + c\sigma_n\beta_n\Delta t}\right) U_r^n + \left(\frac{\beta_n \Delta t}{1 + c\sigma_n\beta_n\Delta t}\right) \iint_{4\pi} \sigma_n \mathcal{I}^{n+1} d\Omega \; . \tag{12}$$

We then define the Fleck factor

$$f_n = \frac{1}{1 + c\sigma_n\beta_n\Delta t} \; ,$$

to write this as

$$U_r^{n+1} = f_n U_r^n + \frac{1}{c\sigma_n} \iint_{4\pi} \left(1 - f_n\right) \sigma_n \mathcal{I}^{n+1} d\Omega \; . \tag{13}$$

Substituting this into equations 9 and 11 gives

$$\frac{1}{c}\frac{\mathcal{I}^{n+1} - \mathcal{I}^n}{\Delta t} + \mathbf{\Omega} \cdot \nabla \mathcal{I}^{n+1} + \sigma_n \mathcal{I}^{n+1} = \frac{c\sigma_n f_n}{4\pi} U_r^n + \frac{1}{4\pi} \iint_{4\pi} \left(1 - f_n\right) \sigma_n \mathcal{I}^{n+1} d\Omega \; , \tag{14}$$

$$\frac{U_m^{n+1} - U_m^n}{\Delta t} + c\sigma_n f_n U_r^n = \iint_{4\pi} f_n \sigma_n \mathcal{I}^{n+1} d\Omega \; . \tag{15}$$

The IMC solution then proceeds as follows:

1. Solve equation 14 for the angular intensity at the end of the time step $\mathcal{I}^{n+1}$, using standard solution methods for the linear Boltzmann transport equation, such as the Monte Carlo method or the discrete ordinates method.

2. Use $\mathcal{I}^{n+1}$ to solve equation 15 for U_m^{n+1}.
3. Use the EOS to get T^{n+1} (and hence U_r^{n+1}) given U_m^{n+1}.
4. Repeat this process for each time step.

It should be noted that we began the derivation assuming no scattering, and equation 14 appears to have a scattering source in the second term on the right hand side. The discretization presented here essentially approximates the absorption and re-emission process as a scattering event. This is useful because the re-emission time scale is likely far smaller than the time step.

1.3 The IMC Method as a Newton Iteration

Before moving on to the proposed method, we wish to put in writing a fact that many experts in the field know, yet is not presented clearly in the literature. This fact is that the IMC method can be viewed in the context of a single Newton iteration for the linearized, and then implicitly discretized TRT equations 9 and 10. Newton iteration to solve the system

$$\mathbf{f}\left(\mathbf{x}\right) = \mathbf{0}\,, \tag{16}$$

can be written as

$$\mathbb{J}\left(\mathbf{x}^{(l)}\right)\Delta\mathbf{x}^{(l)} = -\mathbf{f}\left(\mathbf{x}^{(l)}\right) \quad ; \quad \mathbf{x}^{(l+1)} = \mathbf{x}^{(l)} + \Delta\mathbf{x}^{(l)}\,, \tag{17}$$

where $\mathbb{J}$ is the Jacobian of $\mathbf{f}$. In the case of the linearized, and then implicitly discretized TRT equations

$$\mathbf{f} = \begin{pmatrix} m\left(U_r^{n+1}, \mathcal{I}^{n+1}\right) \\ r\left(U_r^{n+1}, \mathcal{I}^{n+1}\right) \end{pmatrix} = \begin{pmatrix} \frac{1}{\beta\Delta t}\left(U_r^{n+1} - U_r^{n}\right) + c\sigma U_r^{n+1} - \iint_{4\pi}\sigma\mathcal{I}^{n+1}d\Omega \\ \frac{1}{c\Delta t}\left(\mathcal{I}^{n+1} - \mathcal{I}^{n}\right) + \mathbf{\Omega}\cdot\nabla\mathcal{I}^{n+1} + \sigma\mathcal{I}^{n+1} - \frac{c\sigma}{4\pi}U_r^{n+1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}\,. \tag{18}$$

Note that σ and β have not been fixed at the beginning of the time step, and hence equation 18 is still non-linear. The Jacobian is given by

$$\mathbb{J} = \begin{pmatrix} J_{m,U_r} & J_{m,\mathcal{I}} \\ J_{r,U_r} & J_{r,\mathcal{I}} \end{pmatrix}\,, \tag{19}$$

where

$$J_{m,U_r} = \frac{1}{\beta\Delta t} + c\sigma\,, \tag{20}$$

$$J_{m,\mathcal{I}} = -\iint_{4\pi}\sigma\left(\cdot\right)d\Omega\,, \tag{21}$$

$$J_{r,U_r} = -\frac{c\sigma}{4\pi}\,, \tag{22}$$

$$J_{r,\mathcal{I}} = \frac{1}{c\Delta t} + \mathbf{\Omega} \cdot \nabla (\cdot) + \sigma \ . \tag{23}$$

A single newton iteration is completed by solving the following system

$$\begin{pmatrix} J^n_{m,U_r} & J^n_{m,\mathcal{I}} \\ J^n_{r,U_r} & J^n_{r,\mathcal{I}} \end{pmatrix} \begin{pmatrix} \delta U_r \\ \delta \mathcal{I} \end{pmatrix} = \begin{pmatrix} m\left(U^n_r, \mathcal{I}^n\right) \\ r\left(U^n_r, \mathcal{I}^n\right) \end{pmatrix} \ , \tag{24}$$

where we have used the values of U_r and $\mathcal{I}$ at the beginning of the time step as our initial guess. We then use a Schur complement to write

$$\left(J^n_{r,\mathcal{I}} - J^n_{r,U_r}\left(J^n_{m,U_r}\right)^{-1} J^n_{m,\mathcal{I}}\right) \delta\mathcal{I} = -r\left(U^n_r, \mathcal{I}^n\right) + J^n_{r,U_r}\left(J^n_{m,U_r}\right)^{-1} m\left(U^n_r, \mathcal{I}^n\right) \ . \tag{25}$$

With a little bit of algebra, it can easily be shown that

$$J^n_{r,U_r}\left(J^n_{m,U_r}\right)^{-1} J^n_{m,\mathcal{I}} = \frac{1}{4\pi} \iint_{4\pi} (1 - f_n)\, \sigma_n (\cdot)\, d\Omega \ , \tag{26}$$

and

$$J^n_{r,U_r}\left(J^n_{m,U_r}\right)^{-1} = -\frac{1}{4\pi}(1 - f_n) \ . \tag{27}$$

Plugging these into equation 25 gives

$$\begin{aligned} \frac{1}{c}\frac{\mathcal{I}^{n+1} - \mathcal{I}^n}{\Delta t} + \mathbf{\Omega} \cdot \nabla \mathcal{I}^{n+1} - \cancel{\mathbf{\Omega} \cdot \nabla \mathcal{I}^n} + \sigma_n \mathcal{I}^{n+1} - \cancel{\sigma_n \mathcal{I}^n} - \\ \frac{1}{4\pi} \iint_{4\pi} (1 - f_n)\, \sigma_n \mathcal{I}^{n+1} d\Omega + \cancel{\frac{1}{4\pi} \iint_{4\pi} (1 - f_n)\, \sigma_n \mathcal{I}^n d\Omega} = \\ - \cancel{\mathbf{\Omega} \cdot \nabla \mathcal{I}^n} - \cancel{\sigma_n \mathcal{I}^n} + \cancel{\frac{c\sigma_n}{4\pi} U^n_r} - \cancel{\frac{c\sigma_n}{4\pi} U^n_r} + \\ \frac{c\sigma_n f_n}{4\pi} U^n_r + \cancel{\frac{1}{4\pi} \iint_{4\pi} (1 - f_n)\, \sigma_n \mathcal{I}^n d\Omega} \ . \end{aligned} \tag{28}$$

The final result is

$$\frac{1}{c}\frac{\mathcal{I}^{n+1} - \mathcal{I}^n}{\Delta t} + \mathbf{\Omega} \cdot \nabla \mathcal{I}^{n+1} + \sigma_n \mathcal{I}^{n+1} = \frac{c\sigma_n f_n}{4\pi} U^n_r + \frac{1}{4\pi} \iint_{4\pi} (1 - f_n)\, \sigma_n \mathcal{I}^{n+1} d\Omega \ , \tag{29}$$

which we recognize as equation 14. Thus, the IMC method is simply performing a single Newton iteration of the linearized TRT equations, using the temperature and radiation intensity at the beginning of the time step as the initial guess.

2 Proposed Method

Many attempts have been made to improve the accuracy and stability of the time discretization of the IMC method, and a detailed history of these attempts and other improvements is discussed in the article "Four Decades of Implicit Monte Carlo," by Wollaber.[3] As the name of that article implies, the IMC method despite its short-comings, has proven a robust tool for the solution of the TRT equations over a relatively long period of time.

Iterative techniques to fully resolve the non-linearities of the TRT equations, and hence solve them implicitly are straight-forward enough when using deterministic methods, but introduce unwanted complexity when applied to stochastic methods such as the Monte Carlo method, and the alternative presented here is not immune to such issues. Among these issues, two are unavoidable:

- In order to iterate over a time step, the state of the particles at the beginning of the time step must be kept in memory, leading to duplicate copies of all particles in census.
- Testing for convergence will be complicated by the stochastic error inherent in the Monte Carlo method, making it unlikely to reach a desired convergence tolerance without running an absurd number of particles.

Despite these complications, attempts at quite sophisticated iterative techniques and two-step methods have been made.[3][4][5] To our knowledge, no one has yet attempted the most obvious of these given the derivation above.

At the end of the previous section, we showed that the IMC method can be derived in the context of a single Newton iteration. An obvious claim might be that a simple way to make the IMC method actually implicit would be to continue the Newton iteration procedure to convergence. Perhaps such iteration would be too costly given the number of particles that would need to be simulated in order to reduce the stochastic error below the convergence tolerance; however, surely any number of iterations more than 1 would improve accuracy and stability when compared the standard IMC method.

What equation would be have to solve at each iteration in order to accomplish this? After all, the popularity of the IMC method stems from equation 14 so closely resembling a standard transport equation; an equation for which a wealth of information about its numerical solution is available. To derive the equation to be solved at each iteration, we denote the most recent iterate with an asterisk. In this case, each Newton iteration must solve the system

$$\begin{pmatrix} J^*_{m,U_r} & J^*_{m,I} \\ J^*_{r,U_r} & J^*_{r,I} \end{pmatrix} \begin{pmatrix} \delta U_r \\ \delta \mathcal{I} \end{pmatrix} = \begin{pmatrix} m\left(U^*_r, \mathcal{I}^*\right) \\ r\left(U^*_r, \mathcal{I}^*\right) \end{pmatrix} , \tag{30}$$

where $\delta U_r = U_r^{n+1} - U_r^*$ and $\delta \mathcal{I} = \mathcal{I}^{n+1} - \mathcal{I}^*$. We again use a Schur complement to write

$$\left(J^*_{r,\mathcal{I}} - J^*_{r,U_r}\left(J^*_{m,U_r}\right)^{-1} J^*_{m,\mathcal{I}}\right)\delta\mathcal{I} = -r\left(U_r^*, \mathcal{I}^*\right) + J^*_{r,U_r}\left(J^*_{m,U_r}\right)^{-1} m\left(U_r^*, \mathcal{I}^*\right) \ . \tag{31}$$

Again, with a little bit of algebra, it can easily be shown that

$$J^*_{r,U_r}\left(J^*_{m,U_r}\right)^{-1} J^*_{m,\mathcal{I}} = \frac{1}{4\pi}\iint_{4\pi}\left(1-f^*\right)\sigma^*\left(\cdot\right)d\Omega \ , \tag{32}$$

and

$$J^*_{r,U_r}\left(J^*_{m,U_r}\right)^{-1} = -\frac{1}{4\pi}\left(1-f^*\right) \ . \tag{33}$$

Plugging these into equation 31 gives

$$\begin{aligned}
&\frac{1}{c}\frac{\mathcal{I}^{n+1} - \cancel{\mathcal{I}^*}}{\Delta t} + \mathbf{\Omega}\cdot\nabla\mathcal{I}^{n+1} - \cancel{\mathbf{\Omega}\cdot\nabla\mathcal{I}^*} + \sigma^*\mathcal{I}^{n+1} - \cancel{\sigma^*\mathcal{I}^*} - \\
&\qquad \frac{1}{4\pi}\iint_{4\pi}\left(1-f^*\right)\sigma^*\mathcal{I}^{n+1}\,d\Omega + \cancel{\frac{1}{4\pi}\iint_{4\pi}\left(1-f^*\right)\sigma^*\mathcal{I}^*\,d\Omega} = \\
&\qquad\qquad \frac{1}{c}\frac{\mathcal{I}^n - \cancel{\mathcal{I}^*}}{\Delta t} - \cancel{\mathbf{\Omega}\cdot\nabla\mathcal{I}^*} - \cancel{\sigma^*\mathcal{I}^*} + \cancel{\frac{c\sigma^*}{4\pi}U_r^*} - \\
&\qquad\qquad \frac{1}{4\pi\beta^*\Delta t}\left(1-f^*\right)\left(U_r^* - U_r^n\right) - \frac{c\sigma^*}{4\pi}\left(\cancel{1} - f^*\right)U_r^* + \\
&\qquad\qquad\qquad \cancel{\frac{1}{4\pi}\iint_{4\pi}\left(1-f^*\right)\sigma^*\mathcal{I}^* d\Omega} \ .
\end{aligned} \tag{34}$$

The final result is

$$\begin{aligned}
&\frac{1}{c}\frac{\mathcal{I}^{n+1} - \mathcal{I}^n}{\Delta t} + \mathbf{\Omega}\cdot\nabla\mathcal{I}^{n+1} + \sigma^*\mathcal{I}^{n+1} = \\
&\qquad \left(\frac{c\sigma^* f^*}{4\pi}U_r^* - \frac{1}{4\pi\beta^*\Delta t}\left(1-f^*\right)\left(U_r^* - U_r^n\right)\right) + \frac{1}{4\pi}\iint_{4\pi}\left(1-f^*\right)\sigma^*\mathcal{I}^{n+1}d\Omega \ .
\end{aligned} \tag{35}$$

The only difference between this and equation 14 is that the collisional term, the faux scattering term, and the emission term use the opacity and Fleck factor evaluated at the most recent estimate of the temperature (σ^* and f^*), and the emission source has an extra term in it. Note that this term was present in the IMC derivation, however in that case $U_r^* = U_r^n$, and hence the second term in the emission source evaluated to zero.

3 Results

Before presenting the results, we would like to acknowledge that they are incomplete but promising. We choose as our testing ground a typical Marshak wave problem where a semi-infinite domain ($x > 0$) is initially at $T = 0.05$, and a radiation source at $T = 1$ is placed at $x = 0$. For simplicity, $a = \sigma_{\text{sb}} = c = 1$, where σ_{sb} is the Stefan-Boltzmann constant used to convert the boundary source temperature into particles per cm^2 per second. The absorption opacity is $\sigma = 0.1T^{-3}$, the material density $\rho = 1$, and the material is an ideal gas with $c_v = 7.14$.

Figure 1 shows the solution at $t = 50$ using standard IMC with various numbers of uniform timesteps N. The way in which the numerical solution strays from the analytical or reference solution as the timesteps get larger is a known deficiency of the IMC method, sometimes referred to as overheating. In particular, this error violates the maximum principle which in this case should limit the temperature inside the domain below the source temperature of unity. Instead of the hump-shaped wave that should appear, overheating causes the temperature wave to curve upwards, and suddenly drop to zero at the wave-front.

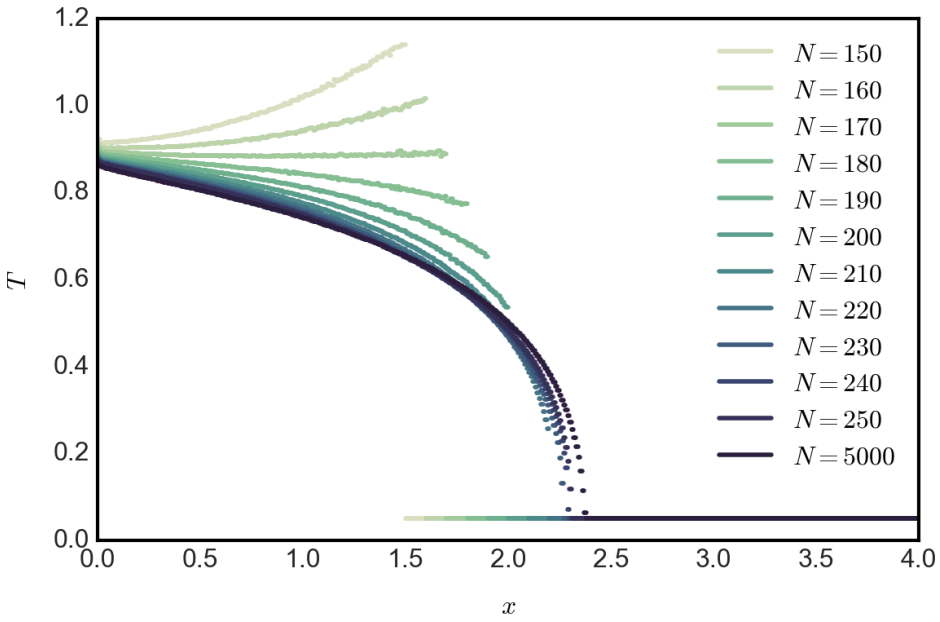

Figure 1: Solution for the test problem at $t = 50$ using standard IMC, using various uniform timestep sizes indicated here by the number of timesteps N.

If instead we were to start with a small timestep, and slowly ramp up to the timesteps taken in Figure 1, we would get Figure 2. In this figure, the initial time step taken is $\Delta t = 0.01$, and it is increased by 10% each timestep until the desired timestep size is reached, at which point the timestep is kept uniform throughout the duration of the simulation. It is

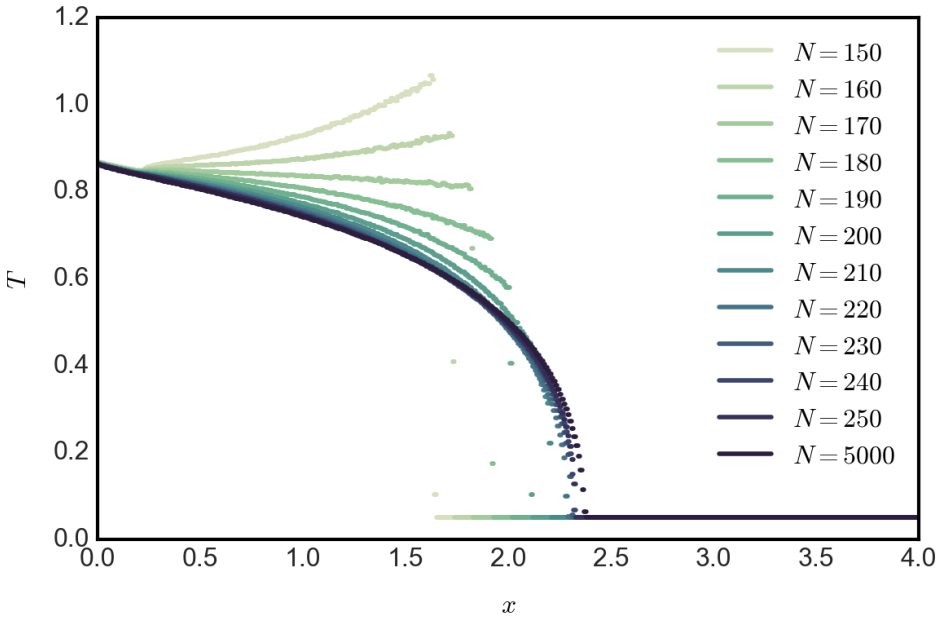

Figure 2: Solution for the test problem at $t = 50$ using standard IMC, using eventually uniform timestep sizes of the same size as in Figure 1, starting with $\Delta t = 0.01$, and increasing by 10% each step until the size limit is reached.

recognized that the legend in this case is misleading, since N no longer indicates the number of steps taken, but the number of steps that would have been taken if the timestep size were uniform from the start. The legend is only kept the same for comparison to Figure 1. It appears that the only improvement gained from slowly ramping the timestep to its desired value is the offset in time at which the overheating begins.

Now that we have our test case, we perform the same exact problem using just two Newton iterations (i.e. one more iteration than standard IMC) per timestep. The results are shown in Figures 3 and 4. It appears that even without ramping up the timestep, the solution for the same time step sizes are drastically more accurate, and the only noticeable error occurs in the first few zones of the domain. If we ramp the timestep using just two iterations, even this small error is avoided, and the solution for all timestep sizes are visibly indistinguishable from the reference solution.

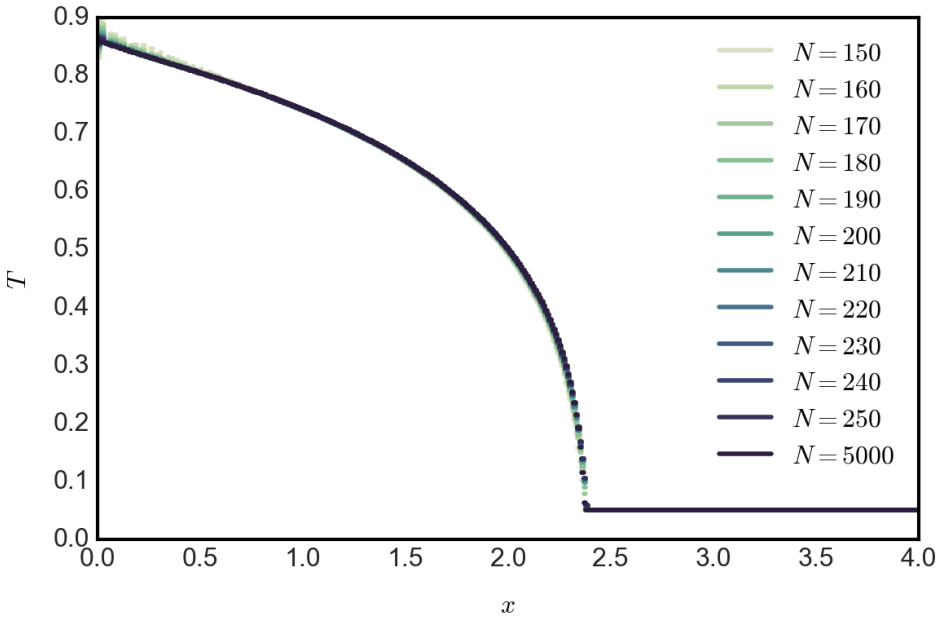

Figure 3: Solution for the test problem at $t = 50$, using two iterations per timestep, using various uniform timestep sizes indicated here by the number of timesteps N.

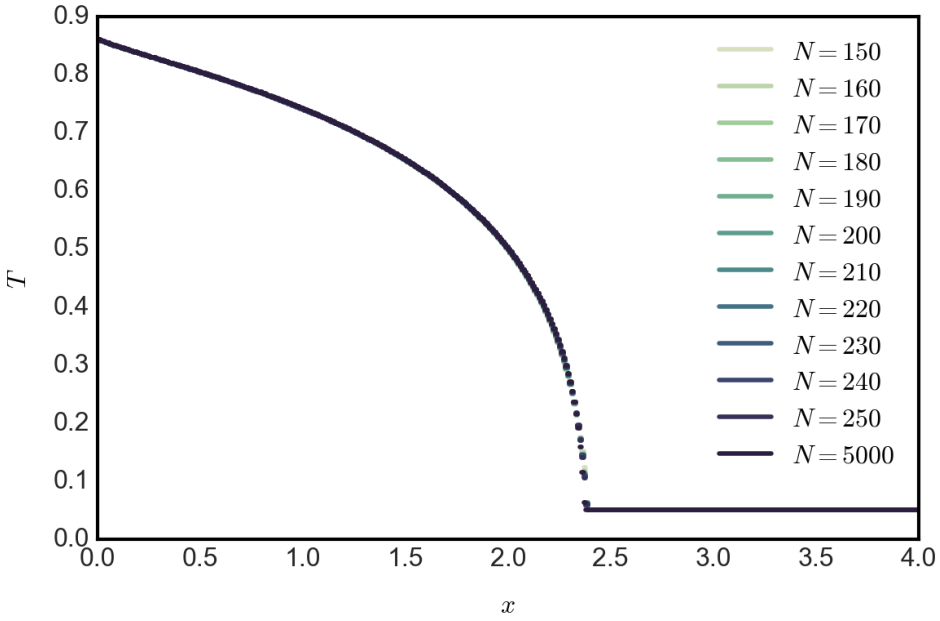

Figure 4: Solution for the test problem at $t = 50$, using two iterations per timestep, using eventually uniform timestep sizes of the same size as in Figure 3, starting with $\Delta t = 0.01$, and increasing by 10% each step until the size limit is reached..

References

[1] J. A. Fleck and J. D. Cummings, "An Implicit Monte Carlo Scheme for Calculating Time and Frequency Dependent Nonlinear Radiation Transport," *Journal of Computational Physics*, vol. 8, no. 3, pp. 313 – 342, 1971.

[2] A. B. Wollaber, *Advanced Monte Carlo Methods for Thermal Radiation Transport*. PhD thesis, University of Michigan, 2008.

[3] A. B. Wollaber, "Four Decades of Implicit Monte Carlo," *Journal of Computational and Theoretical Transport*, vol. 45, no. 1-2, pp. 1–70, 2016.

[4] R. B. Lowrie, "A Comparison of Implicit Time Integration Methods for Nonlinear Relaxation and Diffusion," *Journal of Computational Physics*, vol. 196, no. 2, pp. 566 – 590, 2004.

[5] N. A. Gentile and B. C. Yee, "Iterative Implicit Monte Carlo," *Journal of Computational and Theoretical Transport*, vol. 45, no. 1-2, pp. 71–98, 2016.