An Implicit Monte Carlo Method Based on BDF-2 Time Integration for Simulating Nonlinear Radiative Transfer

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DERIVATION OF THE METHOD

Consider a gray radiative transfer problem, defined by an equation for the specific intensity of radiation, $\psi(r,\Omega,t)$,

$$\frac{1}{c}\frac{\partial\psi}{\partial t}+\Omega\cdot\nabla\psi+\sigma(T)\psi=\frac{\sigma(T)acT^4}{4\pi}+\frac{Q}{4\pi}, \tag{1}$$

and a material energy equation

$$\frac{\partial E_\mathrm{m}}{\partial t}=c\sigma(T)(E_\mathrm{r}-aT^4), \tag{2}$$

where $E_\mathrm{m}(r,t)$ is the material internal energy density which is related to the temperature by an equation of state: $\frac{\partial E_\mathrm{m}}{\partial t}=C_\mathrm{v}(T)\frac{\partial T}{\partial t}$. Also in Eq. (2), $E_\mathrm{r}(r,t)$ is the radiation energy density (a quantity proportional to the zeroth angular moment of the specific intensity): $E_\mathrm{r}(r,t)=\frac{1}{c}\int_{4\pi}\psi(r,\Omega,t)\,d\Omega$. In Eq. (1) we have neglected scattering for convenience; including scattering is straightforward and does not change our method.

We will find a means of approximating the T^4 term to develop a set of linearized equations that are suitable for solution via a Monte Carlo technique. First, we difference the time derivative in Eq. (2) using a backward difference formula of order 2 (the BDF-2 method) [1], which takes a differential equation of the form

$$\frac{du(t)}{dt}=f(u(t)),$$

and integrates over a time step Δt using the formula

$$\frac{u^{n+1}-\frac{4}{3}u^n+\frac{1}{3}u^{n-1}}{\Delta t}=\frac{2}{3}f(u^{n+1}),$$

where u^n is the value of u after the n^th time step. The BDF-2 method is second-order accurate in time, provided that any nonlinearity on the right-hand side is converged, and the method is L-stable. Our derivation assumes constant time step sizes, although this can be relaxed in a straightforward manner.

Applying the BDF-2 method to Eq. (2), and linearizing about $T^{n+1/2}$ written as

$$T^{n+1/2}=\frac{4}{3}T^n-\frac{1}{3}T^{n-1}, \tag{3}$$

leads to the expression

$$a(T^{n+1})^4=ma\left(T^{n+1/2}\right)^4+(1-m)E_\mathrm{r}, \tag{4}$$

where

$$m=\frac{1}{1+\frac{2}{3}\beta c\sigma\left(T^{n+1/2}\right)\Delta t}, \tag{5}$$

$$\beta=\frac{4a\left(T^{n+1/2}\right)^3}{C_\mathrm{v}}+\frac{\left(T^{n+1/2}\right)^4}{C_\mathrm{v}}\frac{d}{dT}\log(\sigma)\bigg|_{T=T^{n+1/2}}. \tag{6}$$

Then substituting Eq. (4) into the original radiation and material equations—Eqs. (1) and (2) respectively—we arrive at the system of equations

$$\frac{1}{c}\frac{\partial\psi}{\partial t}+\Omega\cdot\nabla\psi+\sigma\left(T^{n+1/2}\right)\psi=\frac{(1-m)c\,\sigma\left(T^{n+1/2}\right)E_\mathrm{r}}{4\pi}+\frac{m\,\sigma\left(T^{n+1/2}\right)ac\left(T^{n+1/2}\right)^4}{4\pi}+\frac{Q}{4\pi}, \tag{7a}$$

$$\frac{\partial E_\mathrm{m}}{\partial t}=mc\,\sigma\left(T^{n+1/2}\right)\left(E_\mathrm{r}-a\left(T^{n+1/2}\right)^4\right), \tag{7b}$$

where $T^{n+1/2}$ is defined in terms of T^n and T^{n-1} by Eq. (3). The system given in (7) contains the equations we seek to solve with a particle-based Monte Carlo method. This procedure closely follows that of standard IMC as presented by Fleck and Cummings [2]. Equation (7a) is a time-dependent, linear transport equation with a known source: this equation can be solved using standard Monte Carlo procedures on a prescribed spatial grid [2, 3]. In this equation, $m\sigma$ is an effective absorption cross-section for thermal radiation and $(1-m)\sigma$ is the effective scattering for thermal radiation. The Monte Carlo solution transports the thermally emitted particles and tallies net energy deposition to the material.

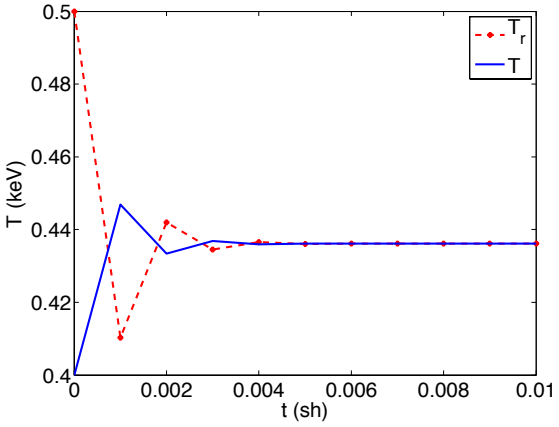
We can generalize the form of m found in Eq. (5) to

$$m=\frac{1}{1+\theta\beta c\sigma\left(T^{n+1/2}\right)\Delta t}, \tag{8}$$

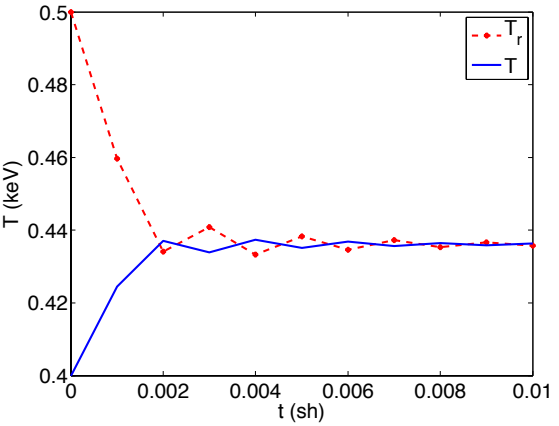
where θ is a parameter between $\frac{2}{3}$ and 1. The value of $\frac{2}{3}$ gives the BDF-2 scheme as derived. Using a different value for θ adds a first-order in Δt error to the temperature update, though, as numerical experiments have bourne out, using a value of 1 gives more robust solutions. We call this approach "time lumping" because it resembles lumping in finite element methods where an error term is added to enhance stability.

PROPERTIES OF THE METHOD

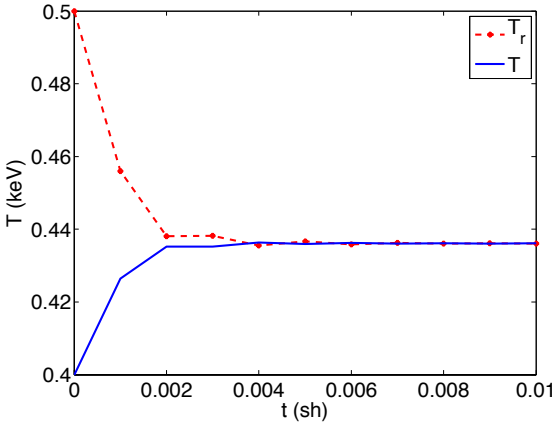
The above method has many similarities to the Implicit Monte Carlo (IMC) method originally promulgated by Fleck and Cummings [2] and later advanced by many authors (see, for instance, Refs. [4, 5, 6, 7, 8, 9, 10]). In IMC the absorption/emission process during a time step is partially modeled



(a) IMC



(b) BDF-2, $\theta = \frac{2}{3}$



(c) BDF-2, $\theta = 1$

Fig. 1. Infinite medium solutions to a problem with $C_v = 0.01$ GJ/cm^3-keV, $\sigma(T) = 100$ cm^{-1}, and an initial radiation temperature, $T_r = (E_r/a)^{1/4} = 0.5$ keV and an initial material temperature of $T = 0.4$ keV. The time step size is $\Delta t = 0.001$ sh.

by an effective scattering process. The IMC procedure defines the Fleck factor, as

$$f = \frac{1}{1 + \alpha\sigma\,(T^n)\hat{\beta}c\Delta t}, \tag{9}$$

with α an implicitness parameter between 0 and 1. Typically, $\hat{\beta} = 4a\,(T^n)^3/C_v$, although Gentile [8] explored the inclusion of the derivative of the opacity in a slightly different form than Eq. (6) and found that including this information could lead to a more accurate method. Nevertheless, the $\hat{\beta}$ described above is the most common formulation.

The BDF-2 is not self-starting, that is, it cannot be used for the very first time step of a calculation because two previous solutions are needed, and in the first time step only the initial condition is available. One approach is to use the IMC method to get a mid-step value of the temperature for the first time step, and then use this mid-step temperature and the initial condition to do a full BDF-2 update. This is the method we use to start the calculations in this summary.

INFINITE MEDIUM TESTS

In an infinite medium our method can be simplified into a system of ODEs

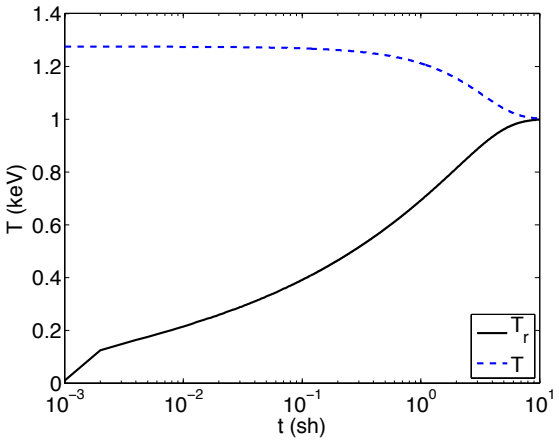
$$\frac{dE_r}{dt} = -mc\sigma\left(T^{n+1/2}\right)\left(E_r - a\left(T^{n+1/2}\right)^4\right) + Q. \tag{10a}$$

$$\frac{dE_m}{dt} = mc\sigma\left(T^{n+1/2}\right)\left(E_r - a\left(T^{n+1/2}\right)^4\right). \tag{10b}$$

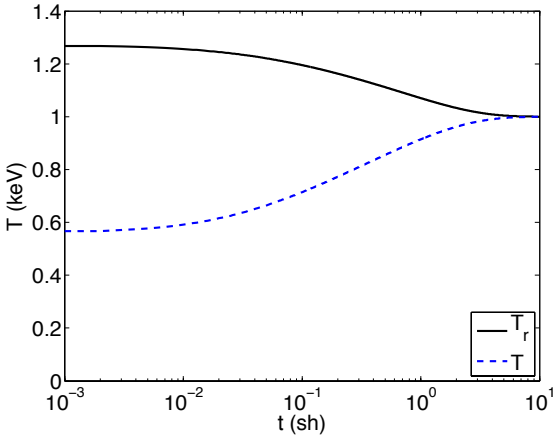
The solution of these equations represents the solution the Monte Carlo procedure would obtain in the limit of an infinite number of particles.

The first test we will perform has $C_v = 0.01$ GJ/cm^3-keV, $\sigma(T) = 100$ cm^{-1}, and an initial radiation temperature, $T_r = (E_r/a)^{1/4} = 0.5$ keV and an initial material temperature of $T = 0.4$ keV. We use units where $c = 299.9$ cm/sh (1 sh $= 10^{-8}$ s) and a $= 0.01372$ GJ/cm$^3\cdot$ keV^4. This problem was first solved by Densmore and Larsen to examine the behavior of different Monte Carlo methods in the diffusion limit [6]. This test problem will isolate the effect of the BDF-2 approach on the emission term because the opacity is not temperature dependent.

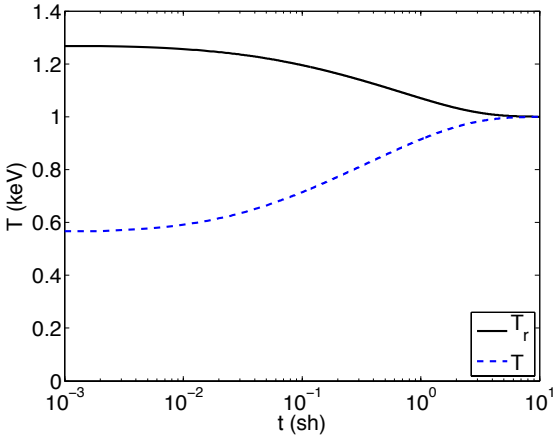
The results for this problem using standard IMC and BDF-2 with two values of θ are shown in Figure 1. From these plots we see a stark contrast between the IMC and BDF-2 schemes. The IMC scheme has the material temperature overshooting the radiation temperature in the first time step. This is a non-physical result as the solution should have the radiation and material temperatures approach the equilibrium temperature monotonically. The BDF-2 results do not have the material temperature overshoot the radiation temperature in the initial time step. We do note, however, both the IMC and BDF-2 solutions have slight oscillations around the equilibrium temperature. This oscillation is more pronounced in the BDF-2



(a) IMC



(b) BDF-2, $\theta = 1$, with derivative of $\sigma(T)$ term in β



(c) BDF-2, $\theta = 1$, without derivative of $\sigma(T)$ term in β

Fig. 2. $C_v = 0.05$ GJ/cm^3-keV, $\sigma(T) = 0.001T^{-5}$ cm^{-1} with T in keV, and an initial radiation temperature, $T_r = (E_r/a)^{1/4} = 1.465122$ keV and an initial material temperature of $T = 0.01$ keV. The time step size is $\Delta t = 0.001$ sh. Note in (a), the radiation temperature is below the material temperature.

solution when $\theta = \frac{2}{3}$ compared to the solution with $\theta = 1$. We have seen similar phenomenon in a variety of test problems, which suggest that $\theta = 1$ is more stable.

We next turn to a problem with a temperature dependent opacity. As first posed by Gentile [8], the problem we will solve has $C_v = 0.05$ GJ/cm^3-keV, $\sigma(T) = 0.001T^{-5}$ cm^{-1} with T in keV, and an initial radiation temperature, $T_r = (E_r/a)^{1/4} = 1.465122$ keV and an initial material temperature of $T = 0.01$ keV; our solutions to this problem appear in Figure 2. This problem has an equilibrium temperature of 1 keV, though the equilibrium temperature is approached very slowly because the opacity decreases rapidly with increasing temperature—an interesting aspect of this problem is that the material emits *less* radiation as it heats up. In the IMC results (Figure 2(a)) we see a vexing phenomenon, first identified by Gentile, whereby the radiation and material temperatures "flip" in the first time step and never recover. The material temperature remains above the radiation temperature until equilibrium is reached. This phenomenon motivated Gentile to include the derivative of the opacity in the IMC linearization. In our BDF-2 results we see that the BDF-2 solution does not have this flip of the temperatures, regardless of whether or not the derivative of the opacity is included in the simulation. Also, the behavior of the BDF-2 solutions is consistent with the analytic solution provided by Gentile in his work; the IMC solution takes much longer to reach equilibrium than the analytic solution. Therefore, we conjecture that the use of the derivative of the opacity is not necessary to capture the correct behavior when using the BDF-2 method.

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