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IMPLICIT MONTE CARLO METHODS FOR COUPLED THREE-TEMPERATURE TRANSPORT

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ABSTRACT

We present three methods for extending the Implicit Monte Carlo (IMC) method to treat the time-evolution of coupled radiation, electron, and ion energies. The first method splits the ion and electron coupling and conduction from the standard IMC radiation-transport process. The second method recasts the IMC equations such that part of the coupling is treated during the Monte Carlo calculation. The third method treats all of the coupling and conduction in the Monte Carlo simulation. Using Modified Equation Analysis (MEA), we show that the third method is theoretically the most accurate. We demonstrate the effectiveness of each method on a series of nonlinear benchmark problems where the accuracy of the third method is shown to be up to ten times greater than the other coupling methods for selected calculations. Also, the third method maintains first-order accuracy in time where the other methods lose first-order accuracy in thick problems.

Key Words: thermal radiation transport, Implicit Monte Carlo, three-temperature model

1. INTRODUCTION

Nonlinear, thermal radiation transport ranks among the most difficult class of transport problems. One of the most successful and widely used methods in thermal radiation transport is Implicit Monte Carlo (IMC) [1]. This method is a two-temperature ($2T$) scheme that includes radiation and material coupling where the matter is represented by a single temperature. A more accurate description of the radiation and material coupling represents the ions and electrons by distinct, separate temperatures [2]. The resulting three-temperature ($3T$) equations for the time evolution of the radiation, electron, and ion energies include terms representing electron-ion coupling and conduction [3]. Conventionally, this system of equations is solved using radiation diffusion with operator-split conduction and coupling [4]. Fully nonlinear solutions using radiation diffusion have been shown in Ref. [2].

The objective of this paper is to extend the standard, grey IMC method to include $3T$ physics. Descriptions of matter that include separate energies for electrons and ions are important in high energy density physics applications and astrophysics [5]. The first method uses the standard IMC technique to simulate radiation transport. The conduction and coupling terms are linearized and split into separate equations that are solved independently. A second method uses a more robust splitting scheme in which half of the coupling is treated during the transport simulation. The conduction is split from the ion and electron equations and is solved subsequently. Afterward, the second half of the coupling is solved. The third method treats the conduction explicitly and includes all of the conduction and coupling in the linearization of the transport equation. This is a good approximation when the conduction timescales are much longer than the radiation-transport timescales. We expect this to be the case for most problems because the conduction timescales are related to the electron thermal velocity whereas the radiation moves at the speed of light.

The resulting system has three equations: a Monte Carlo transport equation and two decoupled energy equations for electrons and ions.

In the next part of the paper, we provide an analytical framework for determining which method performs best through Modified Equation Analysis (MEA). MEA has been shown to be a useful technique for determining the errors that result from splitting and linearization methods [6]. In MEA we formulate the continuous system of equations from the discretized system using Taylor series expansions. The resulting system of equations gives the continuous system plus the error terms that are imposed by a particular splitting or linearization strategy. This *modified* system of equations can then be solved using an unsplit, nonlinear method to evaluate the error terms imposed by the discrete method.

2. 3T IMC METHODS

We consider a $3T$ model that is split from any associated hydrodynamics effects. Thus, errors that result from splitting the radiation from the hydrodynamics are neglected. The $3T$ system consists of radiation, electron, and ion energy equations [2, 3]. The frequency-integrated (grey) form of the $3T$ equations are

$$\frac{1}{c}\frac{\partial \psi}{\partial t} + \hat{\mathbf{\Omega}} \cdot \nabla \psi + \sigma \psi = \frac{1}{4\pi} \sigma a c T_e^4 \,, \tag{1}$$

$$\frac{\partial e_e}{\partial t} = \nabla \cdot D_e \nabla T_e + \frac{C_{ve}}{\tau}(T_i - T_e) + \int \sigma \psi \, d\mathbf{\Omega} - \sigma a c T_e^4 + Q_e \,, \tag{2}$$

$$\frac{\partial e_i}{\partial t} = \nabla \cdot D_i \nabla T_i - \frac{C_{ve}}{\tau}(T_i - T_e) + Q_i \,, \tag{3}$$

where we have neglected electromagnetic effects. Here, ψ is the angular radiation intensity, T_α is the temperature for electrons or ions, e_α is the internal energy of the electrons or ions, τ is the ion-electron equilibration time, $C_{v\alpha}$ is the electron or ion specific heat, Q_α is the energy source for electrons or ions, D_α is the diffusion coefficient for electrons or ions, σ is the photon absorption opacity, a is the radiation constant, and c is the speed of light. In addition, the radiation energy density is given by

$$E(\mathbf{x}, t) = \frac{1}{c} \int \psi(\mathbf{x}, \mathbf{\Omega}, t) \, d\mathbf{\Omega} \,. \tag{4}$$

Full details regarding Eqs. (1)–(3) are available elsewhere [7].

We propose three schemes for solving Eqs. (1)–(3). Extensive details on the derivation of these methods can be found in Ref. [7]. The principal difficulty when adding electron and ion effects to IMC is treating the conduction operator in Eqs. (2) and (3). One approach is to assume that conduction will operate at slow timescales relative to the radiation flow so that the conduction operators can be treated explicitly. This approximation will, in general, be valid because the radiation moves at the speed of light whereas the conduction is a function of the electron thermal velocity. Also, the magnitude of conduction effects is sometimes small compared to the coupling in high energy density physics problems. Using these

approximations we derive the explicit-conduction IMC (ECIMC) equations,

$$\frac{1}{c}\frac{\partial \psi}{\partial t} + \hat{\mathbf{\Omega}} \cdot \nabla \psi + \sigma^n \psi = \frac{1}{4\pi}\Big[\bar{f}\sigma^n c\phi^n + (1-\bar{f})\int \sigma^n \psi \, d\mathbf{\Omega} + (1-\bar{f})S^n\Big] , \tag{5}$$

$$\frac{e_e^{n+1} - e_e^n}{\Delta t} = \frac{C_{ve}^n}{C_{ve}^n - \alpha\Delta t}\Big[\bar{f}\int \sigma^n \psi \, d\mathbf{\Omega} - \bar{f}\sigma^n c\phi^n + \bar{f}S^n\Big] , \tag{6}$$

$$\begin{aligned}\frac{e_i^{n+1} - e_i^n}{\Delta t} &= Q_i^n + Q_e^n + \nabla \cdot D_e^n \nabla T_e^n + \nabla \cdot D_i^n \nabla T_i^n - S^n \\ &\quad - \frac{\alpha\Delta t}{C_{ve}^n - \alpha\Delta t}\Big[\bar{f}\int \sigma^n \psi \, d\mathbf{\Omega} - \bar{f}\sigma^n c\phi^n + \bar{f}S^n\Big] .\end{aligned} \tag{7}$$

Here, the modified form of the standard IMC Fleck factor, $\bar{f}$, is defined

$$\bar{f} = \frac{C_{ve}^n - \alpha\Delta t}{(1+\beta^n\sigma^n c\Delta t)C_{ve}^n - \alpha\Delta t} , \tag{8}$$

and

$$S^n = \nabla \cdot D_e^n \nabla T_e^n + \alpha T_e^n + S_i^n + Q_e^n , \tag{9}$$

$$S_i^n = \frac{C_{ve}^n}{\tau^n\gamma}\Big(\frac{C_{vi}^n}{\Delta t}T_i^n + Q_i^n + \nabla \cdot D_i^n \nabla T_i^n\Big) , \tag{10}$$

$$\alpha = \frac{C_{ve}^n}{\tau^n}\Big(\frac{C_{ve}^n}{\tau^n\gamma} - 1\Big) , \tag{11}$$

$$\gamma = \frac{C_{vi}^n}{\Delta t} + \frac{C_{ve}^n}{\tau^n} . \tag{12}$$

Also, here and in all that follows,

$$\phi = aT_e^4 , \tag{13}$$

$$\beta = \frac{4aT^3}{C_{ve}} , \tag{14}$$

and the n denotes a quantity evaluated at time t^n.

The description of propagation of radiation based on the speed of light is not always accurate. In highly diffusive media the wave-speed that defines the radiation flow can be subsonic. In these cases we may not be able to treat the conduction explicitly. Therefore, the system of equations is split such that the resulting conduction equations can be treated implicitly. To preserve the physical coupling between conduction and the electron-ion coupling, half of the electron-ion coupling is solved before the conduction equations. The second-half of the electron-ion coupling is solved afterward. This technique is the split-conduction IMC

(SCIMC) method and is represented by

$$\frac{1}{c}\frac{\partial\psi}{\partial t} + \hat{\mathbf{\Omega}}\cdot\nabla\psi + \sigma^n\psi = \frac{1}{4\pi}\Big[\hat{f}\sigma^n c\phi^n + (1-\hat{f})\int \sigma^n\psi\, d\mathbf{\Omega} + (1-\hat{f})\hat{S}^n\Big]\,, \tag{15}$$

$$\frac{e'_e - e^n_e}{\Delta t} = \frac{C^n_{ve}}{C^n_{ve} - \hat{\alpha}\Delta t}\Big[\hat{f}\int \sigma^n\psi\, d\mathbf{\Omega} - \hat{f}\sigma^n c\phi^n + \hat{f}\hat{S}^n\Big]\,, \tag{16}$$

$$\frac{e'_i - e^n_i}{\Delta t} = Q^n_i + Q^n_e - \hat{S}^n - \frac{\hat{\alpha}\Delta t}{C^n_{ve} - \hat{\alpha}\Delta t}\Big[\hat{f}\int \sigma^n\psi\, d\mathbf{\Omega} - \hat{f}\sigma^n c\phi^n + \hat{f}\hat{S}^n\Big]\,, \tag{17}$$

$$\frac{e''_e - e'_e}{\Delta t} = \nabla\cdot D_e\nabla T''_e\,, \tag{18}$$

$$\frac{e''_i - e'_i}{\Delta t} = \nabla\cdot D_i\nabla T''_i\,, \tag{19}$$

$$\frac{e^{n+1}_e - e''_e}{\Delta t} = \frac{C_{ve}}{2\tau}(T^{n+1}_i - T^{n+1}_e)\,, \tag{20}$$

$$\frac{e^{n+1}_i - e''_i}{\Delta t} = -\frac{C_{ve}}{2\tau}(T^{n+1}_i - T^{n+1}_e)\,. \tag{21}$$

The modified Fleck factor and source for this method are

$$\hat{f} = \frac{C^n_{ve} - \hat{\alpha}\Delta t}{(1+\beta^n\sigma^n c\Delta t)C^n_{ve} - \hat{\alpha}\Delta t}\,, \tag{22}$$

$$\hat{S}^n = \hat{\alpha}T^n_e + \hat{S}^n_i + Q^n_e\,, \tag{23}$$

$$\hat{\alpha} = \frac{C^n_{ve}}{2\tau^n}\Big(\frac{C^n_{ve}}{2\tau^n\hat{\gamma}} - 1\Big)\,, \tag{24}$$

$$\hat{S}^n_i = \frac{C^n_{ve}}{2\tau^n\hat{\gamma}}\Big(\frac{C^n_{vi}}{\Delta t}T^n_i + Q^n_i\Big)\,, \tag{25}$$

$$\hat{\gamma} = \frac{C^n_{vi}}{\Delta t} + \frac{C^n_{ve}}{2\tau^n}\,. \tag{26}$$

The final $3T$ Monte Carlo method we will consider is a fully-split scheme. Here, we use standard IMC [1] to solve for the radiation intensity and electron energy at t^*. The rest of the coupling terms are split and can be solved after the Monte Carlo transport simulation. Effectively, the fully-split IMC (FSIMC) method is

similar to the SCIMC scheme except we add an additional split,

$$\frac{1}{c}\frac{\partial \psi}{\partial t} + \hat{\mathbf{\Omega}} \cdot \nabla \psi + \sigma^n \psi = \frac{1}{4\pi}\Big[f\sigma^n c\phi^n + (1-f)\int \sigma^n \psi \, d\mathbf{\Omega} + (1-f)Q_e^n \Big] , \tag{27}$$

$$\frac{e_e^* - e_e^n}{\Delta t} = f\int \sigma^n \psi \, d\mathbf{\Omega} - f\sigma^n c\phi^n + fQ_e^n , \tag{28}$$

$$\frac{e_e' - e_e^*}{\Delta t} = \frac{C_{ve}^n}{2\tau^n}(T_i' - T_e') , \tag{29}$$

$$\frac{e_i' - e_i^n}{\Delta t} = -\frac{C_{ve}^n}{2\tau^n}(T_i' - T_e') + Q_i^n , \tag{30}$$

$$\frac{e_e'' - e_e'}{\Delta t} = \nabla \cdot D_e \nabla T_e'' , \tag{31}$$

$$\frac{e_i'' - e_i'}{\Delta t} = \nabla \cdot D_i \nabla T_i'' , \tag{32}$$

$$\frac{e_e^{n+1} - e_e''}{\Delta t} = \frac{C_{ve}}{2\tau}(T_i^{n+1} - T_e^{n+1}) , \tag{33}$$

$$\frac{e_i^{n+1} - e_i''}{\Delta t} = -\frac{C_{ve}}{2\tau}(T_i^{n+1} - T_e^{n+1}) . \tag{34}$$

Equations (27) and (28) are identical to the standard, $2T$ IMC equations. The Fleck factor f is defined

$$f = \frac{1}{1 + \beta^n \sigma^n c \Delta t} . \tag{35}$$

The principal advantage of this method is that it can be easily integrated with an existing IMC implementation.

All of the splits proposed in this paper are designed to preserve the physical connection between the electron-ion conduction and coupling. We have not considered schemes which totally separate conduction from coupling. However, if the conduction is not highly dependent on the coupling, one could consider schemes in which the conduction equations are solved either before or after the solution of the combined radiation-coupling equations. These schemes will be the topic a future study.

3. ERROR ANALYSIS AND COMPUTATIONAL RESULTS

Modified Equation Analysis (MEA) is a useful technique for analyzing time-integration errors that result from operator splits and linearization. In short, MEA uses Taylor series expansions to bring all variables and state vectors to the advanced time level for a system of equations. The procedure employed here follows closely the analysis shown in Ref. [6].

We will apply MEA to the three IMC schemes that have been proposed to solve Eqs. (1)-(3). For simplicity, we will only consider infinite medium solutions. Additionally, we will make the assumption that C_{ve}, C_{vi} and τ are constant. Using these assumptions, if we ignore the spatial terms in Eqs. (1)-(3) and integrate the transport equation over angle, we have

$$\frac{\partial E}{\partial t} + \sigma c E = \sigma c \phi , \tag{36a}$$

$$C_{ve}\frac{\partial T_e}{\partial t} = \frac{C_{ve}}{\tau}(T_i - T_e) + \sigma c E - \sigma c \phi , \tag{36b}$$

$$C_{vi}\frac{\partial T_i}{\partial t} = -\frac{C_{ve}}{\tau}(T_i - T_e) + Q_i . \tag{36c}$$

Note that $Q_e = 0$ in this analysis. Equations (36) are not written in strong conservation form, and the principal unknowns are E, T_e, and T_i.

By ignoring space dependence in Eqs. (36b–c) we do not account for conduction effects on the splitting and linearization errors. When conduction can be neglected in a particular problem, the ECIMC method is the preferred option. The ECIMC method absent conduction is derived by removing the $\nabla \cdot D\nabla T$ terms from Eqs. (10), (9), and (7). This method has no splits in the radiation solution, and it will be more accurate than simulating the standard IMC equations followed by an electron-ion coupling solve. In the analysis that follows we will consider the SCIMC and FSIMC methods with the splits that bound the conduction solve, even though the conduction splits are not present in the simplified equations. The analysis will show the errors that result from splitting the electron-ion coupling if conduction were present.

A full derivation of the modified equations for each of the IMC methods is given in Ref. [7]. We can use the modified equations to estimate the errors that result from the various linearization and splitting schemes that we employ in our IMC methods. The error terms are estimated by solving the modified equations with fully resolved nonlinearities. In this study, Newton's method is used to generate nonlinear solutions to the modified equations.

To begin, we write the system of modified equations with first-order differencing,

$$\frac{E - E^n}{\Delta t} + \sigma c(E - \phi) = \xi_1 \,, \tag{37a}$$

$$C_{ve}\frac{T_e - T_e^n}{\Delta t} - \frac{C_{ve}}{\tau}(T_i - T_e) + \sigma c(\phi - E) = \xi_2 \,, \tag{37b}$$

$$C_{vi}\frac{T_i - T_i^n}{\Delta t} + \frac{C_{ve}}{\tau}(T_i - T_e) - Q_i = \xi_3 \,, \tag{37c}$$

with ϕ given by

$$\phi = \frac{\xi_4 + \phi^n + \beta\Delta t\frac{C_{ve}}{\tau}(T_i - T_e) + \beta\sigma c\Delta t E}{1 + \beta\sigma c\Delta t} \,. \tag{38}$$

The error terms, $\{\xi_1, \xi_2, \xi_3, \xi_4\}$, are unique to the IMC method for which the modified equations are defined:

ECIMC:

$$\xi_1 = c\frac{\partial\sigma}{\partial T_e}(T_e - T_e^n)(E - \phi) \,; \tag{39a}$$

$$\xi_2 = c\frac{\partial\sigma}{\partial T_e}(T_e - T_e^n)(\phi - E) \,; \tag{39b}$$

$$\xi_3 = -\Delta t\dot{Q}_i \,; \tag{39c}$$

$$\begin{aligned}\xi_4 = {} & c\frac{\partial\sigma}{\partial T_e}(T_e - T_e^n)(\phi - E) - \frac{1}{\beta}\frac{C_{ve}}{\tau}\frac{\partial\beta}{\partial T_e}(T_e - T_e^n)(T_i - T_e) \\ & + \frac{1}{\beta}\frac{\partial\beta}{\partial T_e}\sigma c(T_e - T_e^n)(\phi - E) \,;\end{aligned} \tag{39d}$$

SCIMC:

$$\xi_1 = c\frac{\partial\sigma}{\partial T_e}(T_e - T_e^n)(E-\phi) - \Delta t\sigma c\beta\frac{C_{ve}}{2\tau}(T_i - T_e)\,; \tag{40a}$$

$$\begin{aligned}\xi_2 = {} & c\frac{\partial\sigma}{\partial T_e}(T_e - T_e^n)(\phi - E) + \Delta t\frac{C_{ve}}{4\tau^2}\Big(\frac{C_{ve}}{C_{vi}} + 1\Big)(T_i - T_e) \\ & + \Delta t\sigma c\beta\frac{C_{ve}}{2\tau}(T_i - T_e)\,;\end{aligned} \tag{40b}$$

$$\xi_3 = -\Delta t\dot{Q}_i - \Delta t\frac{C_{ve}}{4\tau^2}\Big(\frac{C_{ve}}{C_{vi}} + 1\Big)(T_i - T_e)\,; \tag{40c}$$

$$\begin{aligned}\xi_4 = {} & c\frac{\partial\sigma}{\partial T_e}(T_e - T_e^n)(\phi - E) + \Delta t\frac{C_{ve}}{4\tau^2}\Big(\frac{C_{ve}}{C_{vi}} + 1\Big)(T_i - T_e) \\ & + \Delta t\sigma c\beta\frac{C_{ve}}{2\tau}(T_i - T_e) - \frac{1}{\beta}\frac{C_{ve}}{\tau}\frac{\partial\beta}{\partial T_e}(T_e - T_e^n)(T_i - T_e) \\ & + \frac{1}{\beta}\frac{\partial\beta}{\partial T_e}\sigma c(T_e - T_e^n)(\phi - E)\,;\end{aligned} \tag{40d}$$

FSIMC:

$$\xi_1 = c\frac{\partial\sigma}{\partial T_e}(T_e - T_e^n)(E-\phi) - \Delta t\sigma c\beta\frac{C_{ve}}{\tau}(T_i - T_e)\,; \tag{41a}$$

$$\begin{aligned}\xi_2 = {} & c\frac{\partial\sigma}{\partial T_e}(T_e - T_e^n)(\phi - E) + \Delta t\frac{C_{ve}}{4\tau^2}\Big(\frac{C_{ve}}{C_{vi}} + 1\Big)(T_i - T_e) \\ & + \Delta t\sigma c\beta\frac{C_{ve}}{\tau}(T_i - T_e)\,;\end{aligned} \tag{41b}$$

$$\xi_3 = -\Delta t\dot{Q}_i - \Delta t\frac{C_{ve}}{4\tau^2}\Big(\frac{C_{ve}}{C_{vi}} + 1\Big)(T_i - T_e)\,; \tag{41c}$$

$$\begin{aligned}\xi_4 = {} & c\frac{\partial\sigma}{\partial T_e}(T_e - T_e^n)(\phi - E) + \Delta t\frac{C_{ve}}{4\tau^2}\Big(\frac{C_{ve}}{C_{vi}} + 1\Big)(T_i - T_e) \\ & + \Delta t\sigma c\beta\frac{C_{ve}}{\tau}(T_i - T_e) - \frac{1}{\beta}\frac{C_{ve}}{\tau}\frac{\partial\beta}{\partial T_e}(T_e - T_e^n)(T_i - T_e) \\ & + \frac{1}{\beta}\frac{\partial\beta}{\partial T_e}\sigma c(T_e - T_e^n)(\phi - E)\,.\end{aligned} \tag{41d}$$

These equations constitute the discrete forms of the modified equations for each IMC method defined for the simplified system in Eqs. (36a–c). The reader should note that the $\partial\sigma/\partial T_e$ and $\partial\beta/\partial T_e$ terms result from first-order evaluations of $\partial\sigma/\partial t$ and $\partial\beta/\partial t$ such that

$$\frac{\partial\sigma}{\partial t} \approx \frac{\partial\sigma}{\partial T_e}\frac{T_e - T_e^n}{\Delta t}\,, \tag{42}$$

and that these evaluations account for the missing Δt on some of the error terms. All of the error terms are $O(\Delta t)$.

We define a model problem with a Gaussian ion source centered at 10 ns and a peak source rate of 30 GJ/cm^3/ns. Second-order benchmark solutions for this problem are calculated using Crank-Nicolson differencing with nonlinear Newton iteration and timesteps of 10^{-5} ns. A comparison of results from each IMC method with the benchmark solution to this problem is shown in Fig. 1. The ECIMC method is the

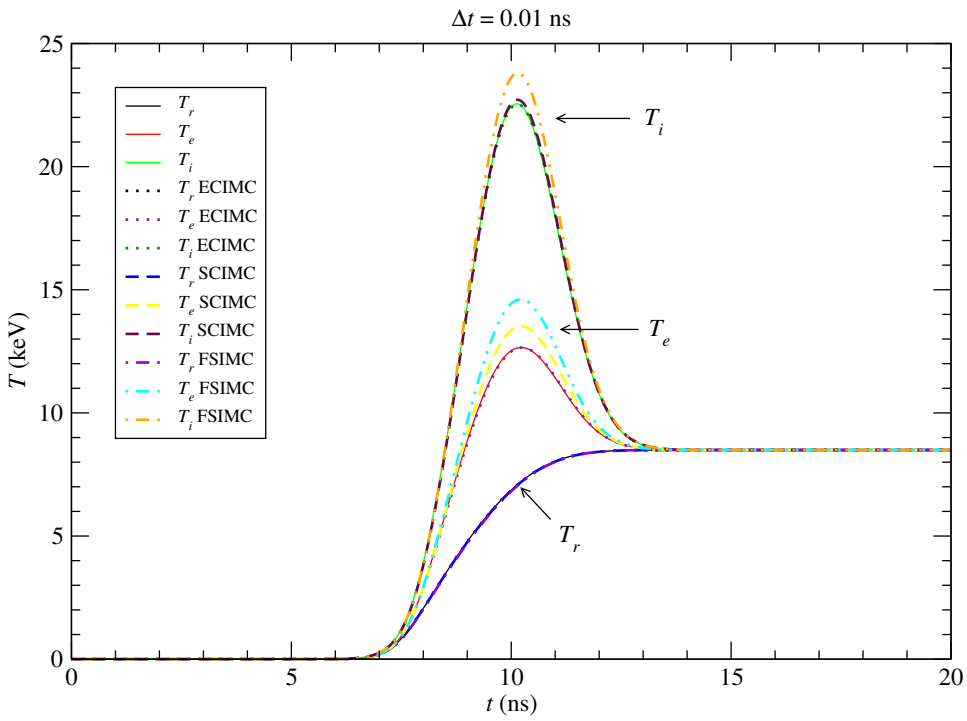
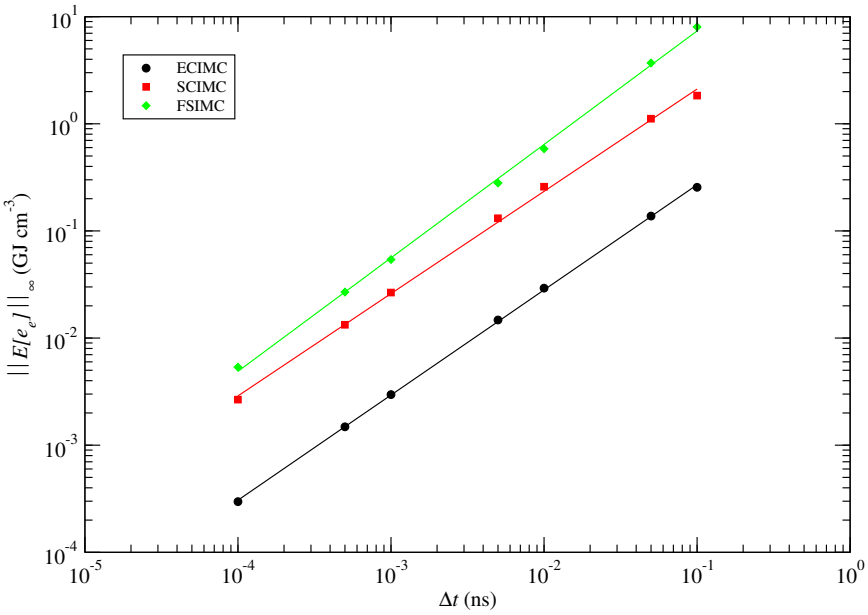


Figure 1. IMC solutions to the model problem. The timestep is a constant 0.01 ns. The errors in each method as a function of timestep are shown in Fig. 2.

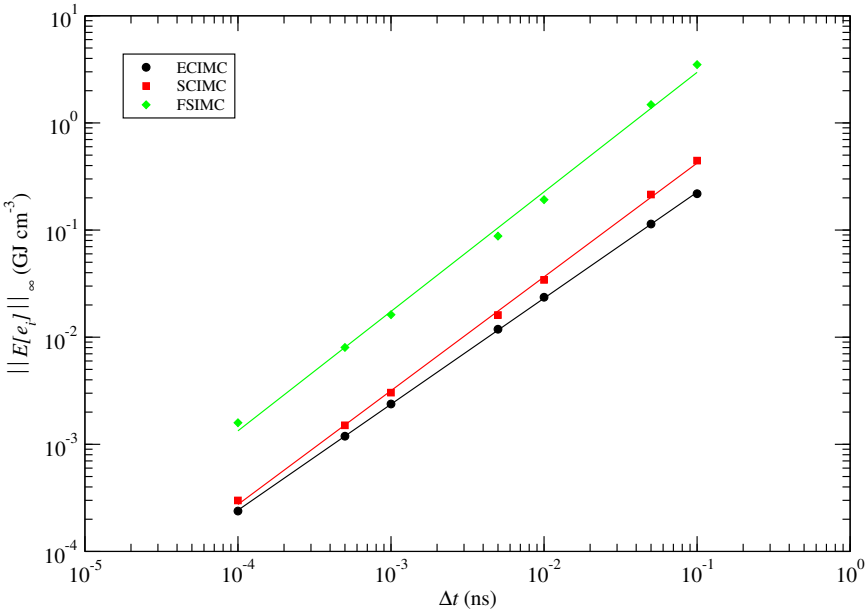
most accurate, followed by SCIMC. Using the MEA solutions in Eqs. (37)-(41) we can quantify the errors that hamper the accuracy of the SCIMC and FSIMC methods relative to the ECIMC method.

For each IMC method the first-order MEA solution adequately represents the IMC solution. This indicates that we can expect first-order convergence for each method. Plotting the L_∞ norms for electron and ion energies for this problem in Figure 2, we see that the methods do indeed converge to first-order. If the methods did not show first-order convergence, we would have to include higher-order terms in the modified equations to represent the additional errors. Also, the results in Fig. 2 show that the ECIMC method is approximately ten times more accurate than the SCIMC and FSIMC methods for $\Delta t = 0.01$ ns when calculating the electron energy.

We can now use MEA to calculate the errors for each method. Figure 3 shows the absolute values of the error terms for the model problem for each IMC method. Analyzing the error terms in Eqs. (39)-(41) and the results shown in Fig. 3, we see that the SCIMC and FSIMC methods have $\xi_2 \sim \xi_4$. Furthermore, the ECIMC method has very small contributions in the ξ_2 and ξ_4 terms. Labeling the error terms for the



(a) Electron Energy



(b) Ion Energy

Figure 2. L_∞ error norms for electron and ion energies. The continuous lines are log-log fits to the data. As indicated by MEA, the methods show first order convergence.

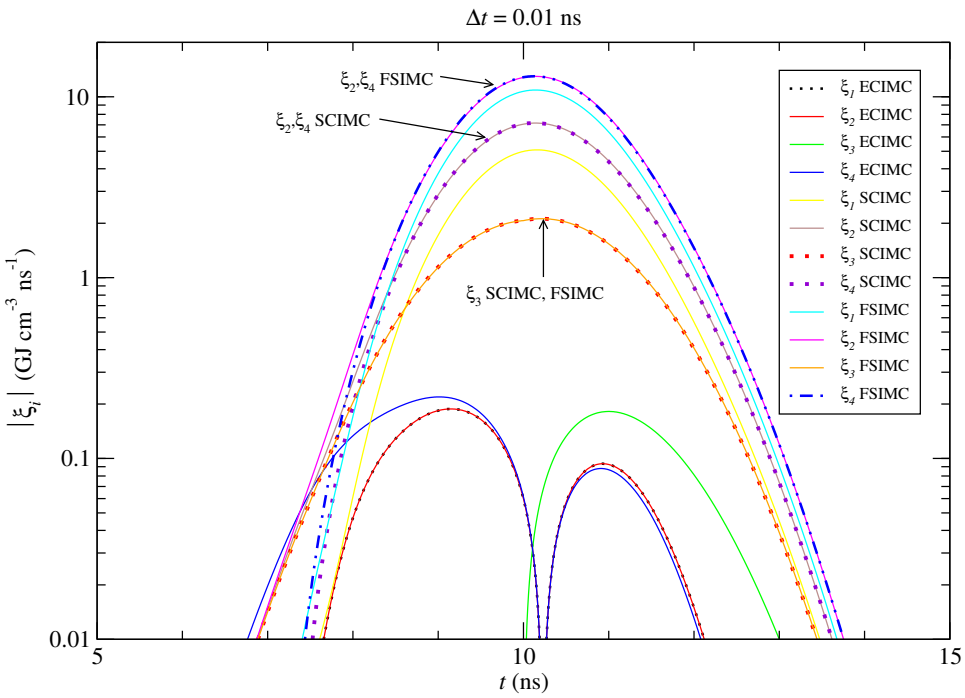


Figure 3. Error terms generated by MEA for the model problem.

SCIMC method as follows

$$\Delta t \frac{C_{ve}}{4\tau^2}\left(\frac{C_{ve}}{C_{vi}}+1\right)(T_i - T_e)\,, \tag{A}$$

$$\Delta t \sigma c \beta \frac{C_{ve}}{2\tau}(T_i - T_e)\,, \tag{B}$$

$$-\frac{1}{\beta}\frac{C_{ve}}{\tau}\frac{\partial \beta}{\partial T_e}(T_e - T_e^n)(T_i - T_e)\,, \tag{C}$$

$$\frac{1}{\beta}\frac{\partial \beta}{\partial T_e}\sigma c(T_e - T_e^n)(\phi - E)\,, \tag{D}$$

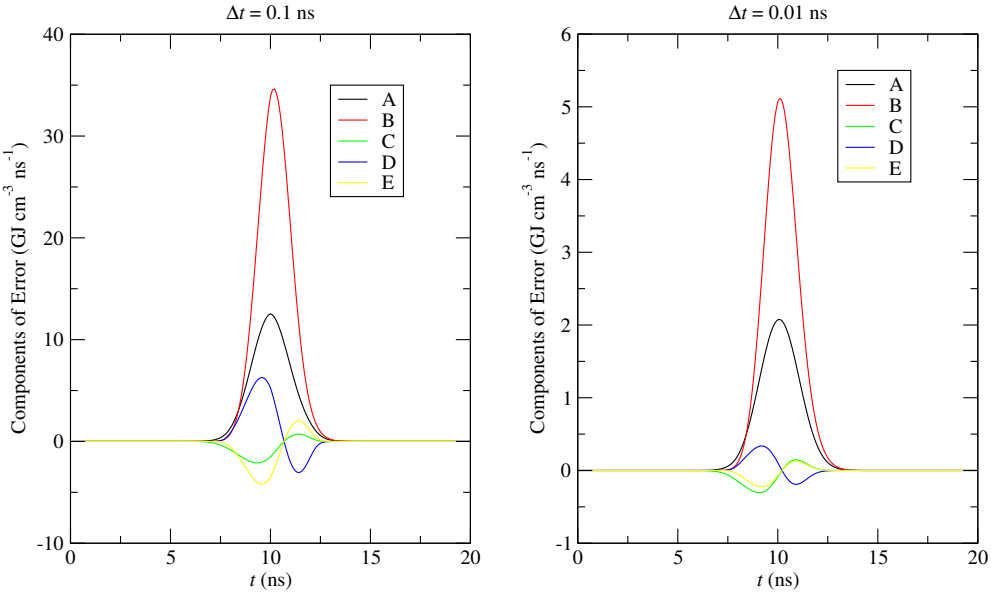
$$c\frac{\partial \sigma}{\partial T_e}(T_e - T_e^n)(\phi - E)\,, \tag{E}$$

we conclude that the T_e and ϕ equations are dominated by the A and B error terms. Figure 4 shows the magnitude of the error terms in Eqs. (40a–d) for $\Delta t = 0.1$ and $\Delta t = 0.01$ ns. Clearly the error is dominated by the A and B terms. These terms do not exist in the ECIMC method, and the B term is twice as large in the FSIMC method. Because the B term is the largest source of error it accounts for the improved accuracy in the ECIMC and SCIMC methods. Error terms C, D, and E contain time-derivatives of σ and β. These terms become significant when the opacity and temperature are rapidly varying. In the model problem they do not significantly impact the total error.

Error terms C, D, and E will generally be small because of the following limits,

$$\lim_{\sigma\to\infty}(\phi - E) = 0\,, \tag{43}$$

$$\lim_{\tau\to 0}(T_i - T_e) = 0\,. \tag{44}$$



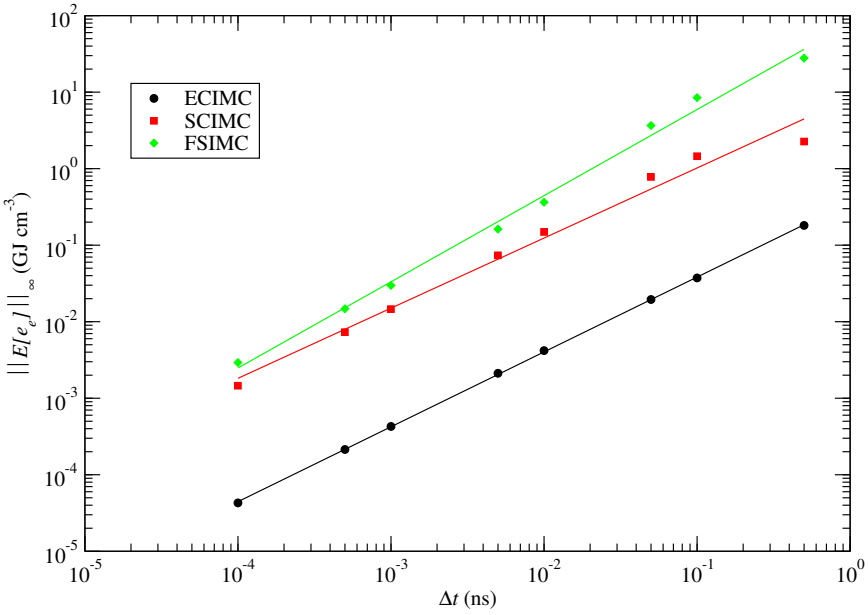
(a) $\Delta t = 0.1$ ns (b) $\Delta t = 0.01$ ns

Figure 4. Components of error for the SCIMC method in the model problem. The A and B components dominate the error; however, as the timestep increases the other terms contribute.

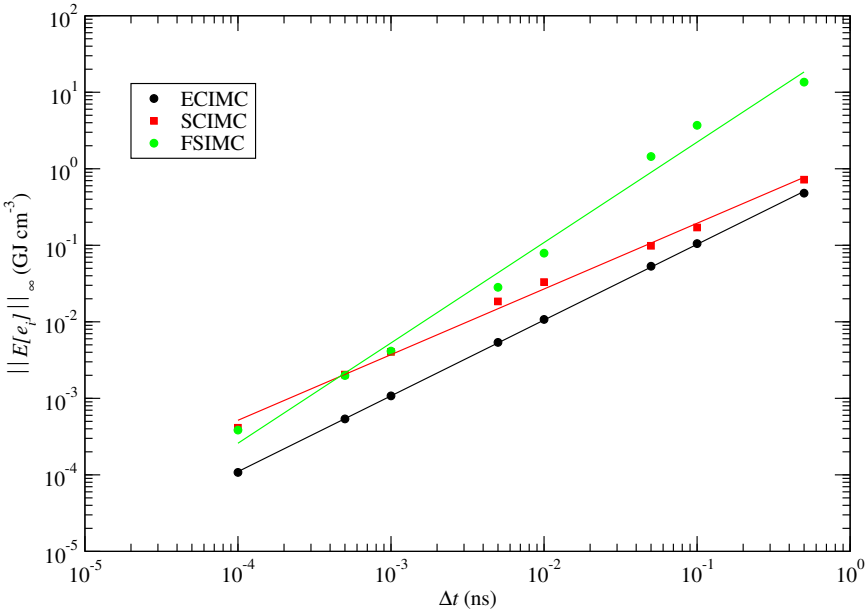
When the problem becomes optically thick, error terms D and E vanish. Similarly, when the electrons and ions are tightly coupled C goes to zero. Error term B is not bounded in this manner. This term is proportional to σ, and there is no corresponding radiation-electron coupling term to limit the error when the problem becomes thick. Thus, B represents a source of unbounded error when the electrons and ions are out of equilibrium.

At this point, one could inquire about variants of the FSIMC method when electron-ion conduction is not required for a given problem. In that case, an alternative form of the FSIMC method could be derived that splits the electron-ion coupling from the IMC in a single step. MEA analysis of this system shows that the errors are identical to the ECIMC method except that the $\Delta t \sigma c \beta \frac{C_{ve}}{\tau}(T_i - T_e)$ term is present in the alternate FSIMC scheme. Thus, the MEA shows that splitting the coupling equations from the IMC simulation will always give this source of unbounded error.

In Fig. 2 we demonstrated that first-order convergence is obtained for all three IMC methods up to timesteps of 0.1 ns. However, the B error term that is present in the SCIMC and FSIMC methods is an unbounded function of σ. In the model problem the opacity was defined, $\sigma = 0.5/T_e^2$. In Fig. 5 L_∞ error norms are shown for the model problem with $\sigma = 100/T_e^2$. Here we see that the SCIMC and FSIMC methods are no longer first order, and second-order error terms are required in the modified equations in order to match the discrete solutions. When calculating the ion energy, SCIMC begins to lose first-order convergence around $\Delta t = 10^{-2}$ ns, and FSIMC loses first-order convergence around $\Delta t = 5 \times 10^{-3}$ ns. These methods fail first-order convergence because the timescale represented by the coefficient in the B error term is no longer resolved. Since $B \propto \sigma$ the timesteps must be small in thick problems to achieve first-order convergence using the SCIMC and FSIMC methods. Conversely, when the problem is very thick



(a) Electron Energy



(b) Ion Energy

Figure 5. L_∞ error norms for electron and ion energies with $\sigma_o = 100$. The continuous lines are log-log fits to the data. Because the B term is unbounded, the SCIMC and FSIMC methods can lose first-order convergence when they do not respect the timescales required by the B error term.

the D and E error terms are zero because $(\phi - E) = 0$. Therefore the ECIMC method maintains first-order convergence independent of σ.

4. CONCLUSIONS

We have analyzed three IMC methods for performing $3T$ transport calculations. Using MEA we have shown that, for the simplified system in Eqs. (36a–c), the ECIMC method has the smallest number of error terms. Also, we have demonstrated that ECIMC is the most accurate of the three methods on a model problem. All of the IMC methods presented in this work are first-order accurate in time. However, the SCIMC and FSIMC methods have more significant timestep constraints due to the presence of unbounded error terms that result from the splitting. These terms are proportional to σ; thus, we can expect that the timestep constraints will be more severe in the SCIMC and FSIMC methods in thick problems. The ECIMC error terms are bounded so it maintains first-order convergence as long as the dynamic timescale of the problem is respected.

In problems where the effects of conduction can be ignored, the ECIMC method is the obvious choice. The only other realistic competitor would be a variant of the FSIMC method in which the electron-ion coupling was calculated in a single solve. However, MEA shows that the unbounded error term B is still present in this scheme. When conduction can be neglected, ECIMC is the most accurate method.

Solving the conduction separate from the radiation and coupling equations is a scheme that we have not analyzed. The physical accuracy of separating the electron-ion conduction from the coupling is an open question. An advantage of this approach is that the unbounded errors that result from splitting the coupling from the radiation solve can be avoided while the conduction is still treated implicitly. The drawback is that there is no feedback between the electron-ion conduction and coupling. We will investigate these issues in a future study.

While we have not performed detailed performance analysis, we can state that the ECIMC method is the least expensive scheme from the standpoint of number-of-operations. Both the SCIMC and FSIMC methods require two inversions of the parabolic conduction operator. SCIMC requires one sweep of the mesh to solve the final part of the electron-ion coupling. FSIMC requires this sweep plus an additional sweep to solve split the first part of the electron-ion coupling. When Newton's method, or another nonlinear iteration scheme, is used to solve these splits, multiple iterations per cell will be required on the block-diagonal matrix that constitutes the final electron-ion coupling split. Monte Carlo performance analysis on these methods will be the topic of a future paper.

Finally, we have not analyzed the effects that conduction has on the proposed IMC methods. The splittings proposed in this paper impose error from the treatment of conduction. Nonetheless, these additional errors do not invalidate the analysis of errors resulting from the electron-ion coupling splits and linearization of the radiation equation. Therefore, we feel justified in analyzing the errors in the linearization and splitting schemes that we have proposed in this paper while neglecting conduction. We will investigate problems with conduction using fully implemented Monte Carlo solvers in a future study.

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