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Stability of explicit radiation-material coupling in radiative transfer calculations

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ABSTRACT

We show that explicit radiation-material coupling, which is essentially always stable for infrared radiative transfer is conditionally stable in the high energy density regime. A linearized stability analysis is first performed for a simple infinite-medium problem that yields both a criterion for unconditional stability, a time-step restriction that applies for conditional stability, and a time-step criterion that always applies for non-oscillatory solutions. This analysis is then extended to include space dependence with the result that the system is always conditionally stable, but with a time step restriction somewhat different from the infinite-medium case. Nonetheless, the time step restriction for non-oscillatory solutions remains the same. Computations are presented that confirm the predictions of our analysis, and conclusions are given.

1. Introduction

The purpose of this paper is to present a linearized stability analysis that is relevant to nonlinear radiative transfer calculations in the high energy density regime, i.e., with material temperatures on the order of one million degrees Kelvin. There are two primary ways to couple the radiation intensity to the material temperature in such calculations. We refer to one as explicit and the other as implicit. Explicit coupling requires less computational effort than implicit coupling, and in many instances it is the simplest and most efficient manner to couple the two fields. This is particularly so in the infrared transfer regime [1,2]. It is well-known from experience with Monte Carlo methods for radiative transfer in the stellar regime that implicit discretizations are needed to avoid instabilities when using time steps chosen on the basis of accuracy. Indeed, this was the motivation for the original development of the implicit Monte Carlo (IMC) method by Fleck and Cummings [3]. We were motivated to perform this study by a desire to quantify the stability properties of explicit coupling so as to demonstrate that it may or may not be a practical method in high energy density laboratory physics (HEDLP) simulations, depending upon the specific properties of the problem under consideration. Our analysis is related to stability analyses for the implicit Monte Carlo (IMC) method [4,5]. However, there is always one significant difference between our analysis and any IMC stability analysis: an exact treatment for the transport time and space derivatives is assumed for IMC whereas we assume a discrete treatment. An exact treatment is appropriate for IMC, but any practical deterministic method will require a discrete treatment. Thus we consider a form of radiation-material coupling that is related but distinct from that of IMC. Our analysis is first presented for the infinite-medium case. After considering the results of this case, we extend the analysis to the space-dependent case. Our overall analysis yields various time step restrictions that are a function of the material properties. In general, the restrictions become increasingly severe with decreasing heat capacity, increasing material temperature, and increasing cross sections (opacities). The restrictions related to cross sections cause explicit coupling to become impractical in the equilibrium-diffusion limit. Implicit coupling is always

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stable and is based upon a linearization of the temperature dependence of the Planckian. One can either iterate to achieve a truly implicit solution or terminate the iteration process after one solution of the linearized system. While one iteration is sufficient to achieve stability, solutions that are not nonlinearly converged have sometimes been observed to violate the thermodynamic maximum principle [6], and correcting this shortcoming is the subject of recent work [4,5,7]. The maximum principle is discussed in [8].

The remainder of the paper is organized as follows. First we give the equations of multifrequency radiative transfer. Then we describe the explicit and implicit coupling schemes. Next we perform a linearized stability analysis for a grey infinite-medium problem and discuss the implications of that analysis. We then extend that analysis to include spatial dependence and discuss its implications. Computational results are given next to validate our theoretical predictions. Finally, conclusions are given.

The equations of radiative transfer consist of an equation for the radiation intensity,

$$\frac{1}{c}\frac{\partial I}{\partial t}+\vec{\Omega}\cdot\vec{\nabla}I=\sigma_{\mathrm{a}}(B-I), \tag{1}$$

and an equation for the material temperature,

$$C_{\mathrm{v}}\frac{\partial T}{\partial t}=\int_0^\infty \sigma_{\mathrm{a}}(\phi-4\pi B)\,dv, \tag{2}$$

where $I(t,\vec{r},\vec{\Omega},v)$ is the radiation intensity (*energy*/(*area–time–steradians–frequency*), T is the material temperature, c is the speed of light, $\vec{\Omega}$ is the photon direction, v is the photon frequency, $\sigma_{\mathrm{a}}(\vec{r},v,T)$ is the total macroscopic cross section (*length*$^{-1}$), $\phi(t,\vec{r},E)$ is angular intensity integrated over all directions (*energy*/(*area–time–frequency*), $C_{\mathrm{v}}(\vec{r},T)$ is the material heat capacity (*energy*/*volume–temperature*), and $B(v,T)$ is the Planck function (*energy*/(*area–time–steradians–frequency*):

$$B(v,T)=\frac{2hv^3}{c^2}\left[\exp\left(\frac{hv}{kT}\right)-1\right]^{-1}, \tag{3}$$

h is *Planck's constant* and k is *Boltzmann's constant*. The photon equation can include scattering, and other types of physics such as heat conduction can be included in the temperature equation. These complications do not significantly affect our analysis. At high-energy densities, the radiation equation is generally coupled to the Euler or Navier–Stokes equations to account for material acceleration due to radiation energy and/or momentum deposition. In this case, the material temperature appears in either the material internal energy equation or the total energy equation.

2. Radiation-material coupling

In this section we describe the two temporal discretization techniques used to treat the radiation-material coupling. We use first-order accurate discretizations for simplicity. It is straightforward to develop higher-order versions of these techniques.

2.1. Explicit coupling

The discretized equations with explicit radiation-material coupling are given by

$$\frac{1}{c\Delta t}\left(I^{n+1}-I^n\right)+\vec{\Omega}\cdot\vec{\nabla}I^{n+1}=\sigma_a^n\left(B^n-I^{n+1}\right), \tag{4}$$

$$\frac{C_v^n}{\Delta t}\left(T^{n+1}-T^n\right)=\int_0^\infty \sigma_a^n\left(\phi^{n+1}-4\pi B^n\right)\,dv, \tag{5}$$

where n is the time index and the time step advances the unknowns from t^n to t^{n+1}. Note that the radiation intensity is treated implicitly while the temperature dependencies of the material properties, σ and C_v, as well as the Planckian are treated explicitly. The great advantage of this type of coupling is that one can apply standard implicit transport solution techniques to first solve the transport equation and then apply standard explicit techniques to solve the temperature equation. One can easily include additional physics such as conduction or full fluid dynamics via an operator split approach. As we shall see, this coupling scheme can be unstable.

2.2. Implicit coupling

The discretized equations with implicit radiation-material coupling are given by

$$\frac{1}{c\Delta t}\left(I^{n+1}-I^n\right)+\vec{\Omega}\cdot\vec{\nabla}I^{n+1}=\sigma_a^n\left[B^n+\frac{\partial B^n}{\partial T}\left(T^{n+1}-T^n\right)-I^{n+1}\right], \tag{6}$$

$$\frac{C_v^n}{\Delta t}\left(T^{n+1}-T^n\right)=\int_0^\infty \sigma_a^n\left(\phi^{n+1}-4\pi B^n-4\pi\frac{\partial B^n}{\partial T}\left(T^{n+1}-T^n\right)-I^{n+1}\right)\,dv, \tag{7}$$

where the Planck function has been linearized. The temperature-dependent properties can also be linearized if desired. However, it has long been observed in the radiative transfer community that only the linearization of the Planck function is critical to stability. If these equations are iterated to nonlinear convergence, the main property gained (other than increased accuracy) is the preservation of the thermodynamic maximum principle. To our knowledge, the preservation of this property has not been formally proved, but it has been observed in practice. We will present some numerical results that support this conjecture. Larsen has performed an analysis for the partially linearized implicit Monte Carlo radiative transfer method which indicates a lack of the maximum principle for those equations [6].

3. An infinite-medium stability analysis

In this section we perform an infinite-medium linearized stability analysis for explicit coupling assuming a grey rather than multifrequency radiation approximation. The relevant equations are

$$\frac{\partial E}{\partial t}=\sigma_{\mathrm{a}}c(aT^4-E), \tag{8}$$

$$C_v \frac{\partial T}{\partial t} = \sigma_a c(E - aT^4), \tag{9}$$

where E (*energy/vol*) is the radiation energy density, i.e.,

$$E = \frac{1}{c}\int_0^\infty \phi \, dv, \tag{10}$$

and all other variables are as previously defined except that the cross section no longer depends upon photon frequency.

3.1. Linearization

Our first step is to linearize the equations about an arbitrary equilibrium solution, $E_0 = aT_0^4$. We begin by assuming that

$$E = E_0 + \delta E, \tag{11}$$

and

$$T = T_0 + \delta T. \tag{12}$$

Substituting from Eqs. (11) and (12) into Eqs. (8) and (9) and linearizing the temperature dependence of C_v, σ_a, and T^4, we get the following linearized system:

$$\frac{\partial \delta E}{\partial t} = \sigma_{a,0} c\left(4aT_0^3 \delta T - \delta E\right), \tag{13}$$

$$C_{v,0} \frac{\partial \delta T}{\partial t} = \sigma_{a,0} c\left(\delta E - 4aT_0^3 \delta T\right), \tag{14}$$

where

$$4\pi \int_0^\infty B \, dv = acT^4,$$

and $C_{v,0}$ and $\sigma_{a,0}$ are evaluated at T_0. Note that the temperature derivatives of C_v and σ_a do not appear in the linearized system because they generate second-order terms. This result is consistent with the fact that the transport community has long observed that lagging the temperature dependence of the cross sections does not affect stability. The experience of the community with this type of analysis for nonlinear transfer systems is that it yields surprisingly accurate results. Nevertheless, knowledge of the rigorous implications of this type of analysis is apparently lacking.

3.2. Discretization

We next apply a temporal discretization to our linearized system that corresponds to explicit coupling:

$$\frac{1}{\Delta t}\left(\delta E^{n+1} - \delta E^n\right) = \sigma_{a,0} c\left(4aT_0^3 \delta T^n - \delta E^{n+1}\right), \tag{15}$$

$$\frac{C_{v,0}}{\Delta t}\left(\delta T^{n+1} - \delta T^n\right) = \sigma_{a,0} c\left(\delta E^{n+1} - 4aT_0^3 \delta T^n\right), \tag{16}$$

where n is the time index, and $\Delta t = t^{n+1} - t^n$ is the time step. This system generates the following amplification matrix, **A**:

$$\begin{bmatrix} \delta E^{n+1} \\ \delta T^{n+1} \end{bmatrix} = \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{pmatrix} \begin{bmatrix} \delta E^n \\ \delta T^n \end{bmatrix}, \tag{17}$$

where

$$a_{1,1} = \frac{1}{1 + \sigma_{a,0} c \Delta t}, \tag{18a}$$

$$a_{1,2} = \frac{\sigma_{a,0} c \Delta t \; 4aT_0^3}{1 + \sigma_{a,0} c \Delta t}, \tag{18b}$$

$$a_{2,1} = \frac{\sigma_{a,0} c \Delta t}{C_{v,0}\left(1 + \sigma_{a,0} c \Delta t\right)}, \tag{18c}$$

$$a_{2,2} = 1 - \frac{\sigma_{a,0} c \Delta t \; 4aT_0^3}{C_{v,0}\left(1 + \sigma_{a,0} c \Delta t\right)}. \tag{18d}$$

4. Stability

The eigenvalues of **A** determine the stability of the system. In particular, the system is stable if the magnitudes of the eigenvalues are less than or equal to unity. The eigenvalues are given as follows:

$$\omega = \tfrac{1}{2}(a_{1,1} + a_{2,2}) \pm \tfrac{1}{2}\sqrt{(a_{1,1} + a_{2,2})^2 - 4(a_{1,1}a_{2,2} - a_{2,1}a_{1,2})}. \tag{19}$$

Evaluating these eigenvalues we get

$$\omega = \left\{1, \frac{C_{v,0} - \sigma_{a,0} c \Delta t (4aT_0^3)}{C_{v,0}(1 + \sigma_{a,0} c \Delta t)}\right\}. \tag{20}$$

It can be easily shown that the maximum value of $|\omega|$ occurs at either $\Delta t = 0$ or $\Delta t = \infty$ because the derivative of ω with respect to Δt is not zero for any positive, finite value of Δt. At $\Delta t = 0$ both eigenvalues are unity, and at $\Delta t = \infty$ we get

$$\lim_{\Delta t \to \infty} \omega = \left\{1, -\frac{4aT_0^3}{C_{v,0}}\right\}.$$

Thus, when

$$C_{v,0} \geq 4aT_0^3,$$

explicit coupling is unconditionally stable. We note that we can relate this condition to the parameter $\beta = 4aT^3/C_v$ [3]; specifically, explicit coupling is stable when $\beta < 1$. Explicit coupling is not, however, L stable [9] because neither eigenvalue goes to zero as $\Delta t \to \infty$. Furthermore, one of the eigenvalues in Eq. (20) is negative unless

$$\Delta t \leq \frac{C_{v,0}}{4\sigma_{a,0} acT_0^3}. \tag{21}$$

As a result we expect that numerical solutions using explicit coupling will oscillate around the true solution when the condition in Eq. (21) is not satisfied. We stress that this non-oscillatory condition applies independently of the unconditional stability of the method. It is important to note the non-oscillatory condition becomes increasingly restrictive as the opacity is increased. Thus as the optical thickness of a problem increases, the time step required to avoid oscillations approaches zero. This implies that explicit coupling has serious deficiencies in the diffusion limit.

In the case where the method is not unconditionally stable we can derive a condition on Δt for stability by solving for the value of the time step that yields eigenvalues of 1 and -1. This procedure gives the stability

Table 1
Constraints for the explicit coupling scheme.

Property	Constraint
Unconditional stability	$C_{v,0} \geq 4aT_0^3$
Conditional stability	$\Delta t \leq \frac{2C_{v,0}}{\sigma_{a,0}c(4aT_0^3 - C_{v,0})}$
Non-oscillatory solutions	$\Delta t \leq \frac{C_{v,0}}{4\sigma_{a,0}acT_0^3}$

condition

$$\Delta t \leq \frac{2C_{v,0}}{\sigma_{a,0}c(4aT_0^3 - C_{v,0})}.$$

Here we see that if the method is conditionally stable, the time step required for stability (like the time step required for non-oscillatory solutions) becomes increasingly restrictive as the opacity increases.

The results for our infinite-medium stability analysis are summarized in Table 1.

4.1. Infrared versus X-ray regimes

Substituting values for T_0 and $C_{v,0}$ from real problems we see that the stability constraints affect radiative transfer problems in the X-ray regime, as often encountered in high energy density physics [10], and not in infrared radiative transfer. As an example, we look at the infrared test problem in [2]. For this problem the material temperature would have to be at least 3.6×10^6 K or about 300 eV for the explicit method to be unstable. At this temperature, the spectrum of the material emission has its peak near a wavelength of 1 nm, which is well within the X-ray regime. Indeed, stability problems with explicit coupling is why implicit coupling schemes were investigated early in the development of computational X-ray radiative transfer techniques [3].

4.2. Effect of radiation diffusion

We can easily include the effect of radiation diffusion in our stability analysis. First, we replace Eq. (8) as follows:

$$\frac{\partial E}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial E}{\partial x}\right) + \sigma_a c(aT^4 - E), \tag{22}$$

where

$$D = \frac{c}{3\sigma_t}. \tag{23}$$

Next we proceed as in the infinite-medium case and linearize the equations about the equilibrium solution. This yields the following replacement for Eq. (13):

$$\frac{\partial \delta E}{\partial t} = \frac{\partial}{\partial x}\left(D_0\frac{\partial \delta E}{\partial x}\right) + \sigma_{a,0}c\left(4aT_0^3\delta T - \delta E\right), \tag{24}$$

where D_0 is evaluated at T_0. We next difference the diffusion term implicitly and replace Eq. (15) with:

$$\frac{1}{\Delta t}\left(\delta E^{n+1} - \delta E^n\right) = \frac{\partial}{\partial x}\left(D_0\frac{\partial \delta E^{n+1}}{\partial x}\right) + \sigma_{a,0}c\left(3aT_0^3\delta T^n - \delta E^{n+1}\right). \tag{25}$$

Next we assume an infinite homogeneous medium and make the following standard Fourier anzatz:

$$\delta E(x) = \delta E(\lambda)\exp i\lambda x, \tag{26}$$

$$\delta T(x) = \delta T(\lambda)\exp i\lambda x, \tag{27}$$

where i is the square root of -1 and $\lambda \in (-\infty, +\infty)$ is the Fourier spatial frequency. Substituting from Eqs. (26) and (27) into Eqs. (25) and (16), we obtain the following amplification matrix, **A**:

$$\begin{bmatrix} \delta E^{n+1}(\lambda) \\ \delta T^{n+1}(\lambda) \end{bmatrix} = \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{pmatrix} \begin{bmatrix} \delta E^n(\lambda) \\ \delta T^n(\lambda) \end{bmatrix}, \tag{28}$$

where

$$a_{1,1} = \frac{1}{1 + \lambda^2 D_0 \Delta t + \sigma_{a,0}c\Delta t}, \tag{29a}$$

$$a_{1,2} = \frac{\sigma_{a,0}c\Delta t 4aT_0^3}{1 + \lambda^2 D_0 \Delta t + \sigma_{a,0}c\Delta t}, \tag{29b}$$

$$a_{2,1} = \frac{\sigma_{a,0}c\Delta t}{C_{v,0}\left(1 + \lambda^2 D_0 \Delta t + \sigma_{a,0}c\Delta t\right)}, \tag{29c}$$

$$a_{2,2} = 1 - \frac{\sigma_{a,0}c\Delta t\ 4aT_0^3\left(1 + \lambda^2 D_0 \Delta t\right)}{C_{v,0}\left(1 + \lambda^2 D_0 \Delta t + \sigma_{a,0}c\Delta t\right)}. \tag{29d}$$

When spatial diffusion is taken into account, we obtain two eigenvalues for each value of λ and thus for the corresponding Fourier mode. We first note that the system obtained for $\lambda = 0$ is the infinite-medium system. Thus our infinite-medium analysis applies to the space-dependent case as well, so the presence of diffusion does not mitigate in any way the time-step restrictions that we have derived. The question naturally arises as to whether diffusion results in more stringent requirements. To address this question we compute the eigenvalues obtained in the limit as $\lambda \to \infty$. We have numerically investigated the behavior of the eigenvalues with λ, and it appears that the largest magnitude eigenvalue occurs in the limit as $\lambda \to \infty$ if the system is oscillatory or unstable. We cannot prove that this is the case, but we present computational results that support this conjecture. It is easily seen that the radiation energy density is completely attenuated in this limit:

$$\delta E^{n+1} = 0, \tag{30}$$

resulting in the following equation for the temperature:

$$\frac{C_{v,0}}{\Delta t}\left(\delta T^{n+1} - \delta T^n\right) = -\sigma_{a,0}c4aT_0^3\delta T^n, \tag{31}$$

Thus the eigenvalue associated with δE is zero and the eigenvalue associated with δT follows directly from Eq. (31):

$$\omega = 1 - \frac{\sigma_{a,0}c\Delta t 4aT_0^3}{C_{v,0}}. \tag{32}$$

It can be seen from Eq. (32) that the system is always conditionally stable. Stability requires that

$$\Delta t \le \frac{2C_{v,0}}{\sigma_{a,0}c4aT_0^3}, \tag{33}$$

while a non-oscillatory solution requires that

$$\Delta t \le \frac{C_{v,0}}{\sigma_{a,0}c4aT_0^3}. \tag{34}$$

Comparing Eqs. (33) and (34) with the results given in Table 1, we find that the stability condition in the high-frequency limit is more stringent than the stability conditions for the infinite-medium case, but the conditions are essentially the same when $C_{v,0} \ll 4aT_0^3$. Furthermore, and most importantly, the non-oscillatory conditions are identical for both cases. Thus if one desires non-oscillatory solutions, the impact of spatial diffusion on the time-step restriction is null. Finally, we note that the high-frequency limit is never reached but only approached in practice in the limit as the spatial mesh is increasingly refined. We show evidence of this effect in our computational results.

5. Numerical results

The results obtained above can be readily demonstrated using numerical results on gray, infinite-medium problems. In such a problem we set an initial material temperature and radiation energy density, and the two fields relax to equilibrium. In these infinite medium problems we will compare explicit coupling, implicit coupling, and the exact solution as derived by Mosher [11]. The code to compute the Mosher solutions was supplied by Gentile [12]. We computed all of our infinite-medium numerical solutions using MATLAB. For convenience we express the radiation energy density in terms of a radiation temperature:

$$T_r = \sqrt[4]{\frac{E}{a}}.$$

In the gray case the linearized implicit method is written as [3,13]

$$E^{n+1} = \frac{E^n + \Delta t f \sigma_a c a T^4}{1 + \Delta t f \sigma_a c},$$

$$T^{n+1} = T^n + \frac{c\Delta t f \sigma_a}{C_v}(E - aT^4),$$

where

$$f = \frac{1}{1 + \beta \sigma_a c \Delta t}.$$

The first problem we solve was used previously by Densmore and Larsen [14] in their analysis of coupling schemes for Monte Carlo methods for radiative transfer. In this problem the material has a constant heat capacity of $C_v = 0.01\ \mathrm{GJ/cm^3}$ and constant opacity of $\sigma_a = 100\ \mathrm{cm^{-1}}$. The material temperature is initially 0.4 keV and the radiation temperature is 0.5 keV. We measure time in units of nanoseconds and distance in centimeters; this makes $c = 29.98$ cm/ns and $a = 0.01372\ \mathrm{GJ/cm^3\ keV^{-1}}$. This material will have $C_v > 4aT^3$ as long as $T < 0.567$ keV. In Figs. 1 and 2 we show results for this problem using

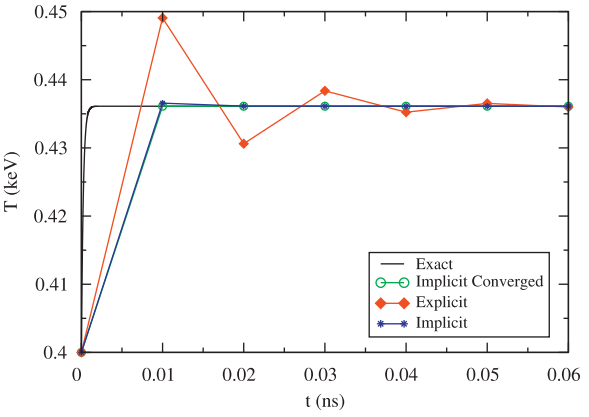

Fig. 1. Material temperature for a problem with $T_{r,0} = 0.5$ keV, $T_0 = 0.4$ keV, $\sigma_a = 100\ \mathrm{cm^{-1}}$, and $C_v = 0.01\ \mathrm{GJ/cm^3}$ using a time step of $\Delta t = 0.01$ ns. In this problem $C_v > 4aT_0^3$ so any sized time step is stable.

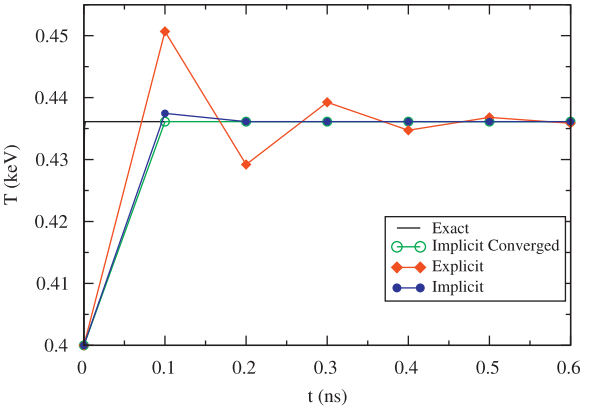

Fig. 2. Material temperature for a problem with $T_{r,0} = 0.5$ keV, $T_0 = 0.4$ keV, $\sigma_a = 100\ \mathrm{cm^{-1}}$, and $C_v = 0.01\ \mathrm{GJ/cm^3}$ using a time step of $\Delta t = 0.1$ ns. In this problem $C_v > 4aT_0^3$ so any sized time step is stable.

different values of Δt. In these figures we see that for large time step sizes the explicit method does remain stable, though it does oscillate about the equilibrium solution: to avoid oscillations Δt must be less than 0.5 ps. Indeed, both the explicit and implicit methods show some oscillation for this problem because the time step is coarse compared to the fast transient seen in the exact solution, but the implicit oscillations are minimal. It can also be seen from Figs. 1 and 2 that the minor implicit oscillations are completely eliminated when the nonlinearities are fully converged.

Next we will exercise all the stability properties of explicit coupling using an infinite medium problem with the same material properties as above, except the material and radiation will be near equilibrium initially. We set $T_r = 0.649$ keV and $T = 0.65$ keV initially. Therefore, for this problem $C_v < 4aT^3$ and we can expect unstable results. In Fig. 3 we show results for this problem. Using the formulas from Table 1 we compute that a time step above 1.31×10^{-3} ns will be unstable, and a time step below 2.214×10^{-5} ns will lead to a non-oscillatory solution. The numerical results confirm these predictions: (1) the time step just above the stability condition does lead

to a divergent solution, (2) the time step between the oscillatory threshold and the stability condition is stable but (highly) oscillatory, and (3) for a time step below the oscillatory threshold given in Eq. (21) the solution approaches equilibrium monotonically. One interesting feature of the explicit solution is that even though the time step is small enough to avoid oscillations, the solution goes to equilibrium faster than the exact solution

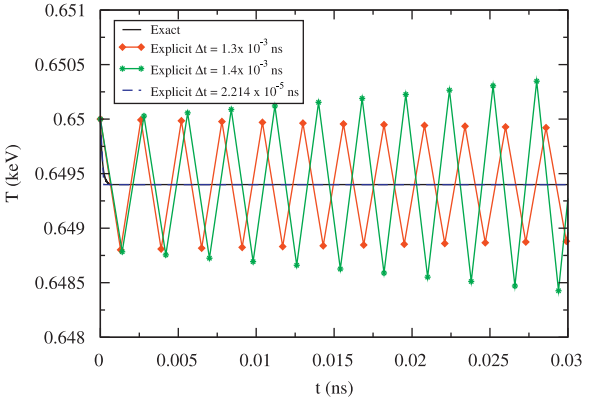

Fig. 3. Material temperature for a problem with $T_{r,0} = 0.649$ keV, $T_0 = 0.65$ keV, $\sigma_a = 100\ \mathrm{cm}^{-1}$, and $C_v = 0.01\ \mathrm{GJ/cm}^3$ using several different time step sizes. In this problem $C_v < 4aT_0^3$, the maximum stable time step is $\Delta t \approx 1.31 \times 10^{-3}$ ns, and the maximum non-oscillatory time step is $\Delta t \approx 2.214 \times 10^{-5}$ ns.

because the time steps are still too large from the point of view of accuracy. Thus ensuring a non-oscillatory solution does not ensure accuracy.

We can extend the infinite medium problems to a one-dimensional diffusion case. To do this we consider the spatial domain $x = [0,1]$ and set the material properties to be the same as those used in the above problems. The space-dependent equations were discretized using a standard cell-centered diffusion discretization [15] and solved using MATLAB. For initial conditions we set

$$T_r(x,0) = \begin{cases} 0.5\ \text{keV}, & x \in [0.3,0.7], \\ 1\ \text{eV} & \text{otherwise}, \end{cases} \tag{35}$$

and

$$T(x,0) = \begin{cases} 0.4\ \text{keV}, & x \in [0.3,0.7], \\ 1\ \text{eV} & \text{otherwise}; \end{cases} \tag{36}$$

we also use vacuum boundary conditions implemented via the Marshak treatment.

In Fig. 4 we show results for this problem at 0.1 ns using both the implicit and explicit coupling schemes with different numbers of computational cells in the domain and $\Delta t = 0.01$ ns. We remind the reader that for the infinite medium version of this problem explicit coupling is unconditionally stable. At $N_x = 20$ the explicit and implicit solutions are coincident on the scale of the plot. As the number of cells is increased, oscillations appear in the explicit scheme: at $N_x = 40$ small

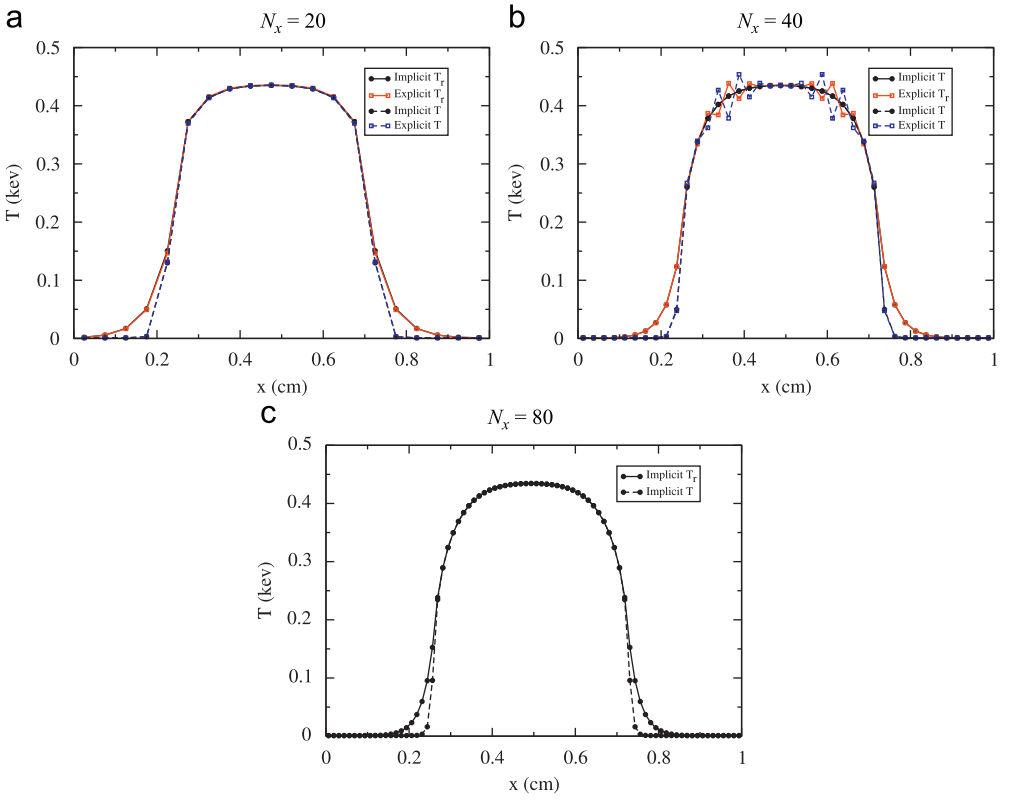

Fig. 4. Diffusion solutions as a function of number of computational cells, N_x, at $t = 0.1$ ns using $\Delta t = 0.01$ ns. With $N_x = 80$ the explicit coupling scheme was unstable to the point of its solution being off the scale of the plot.

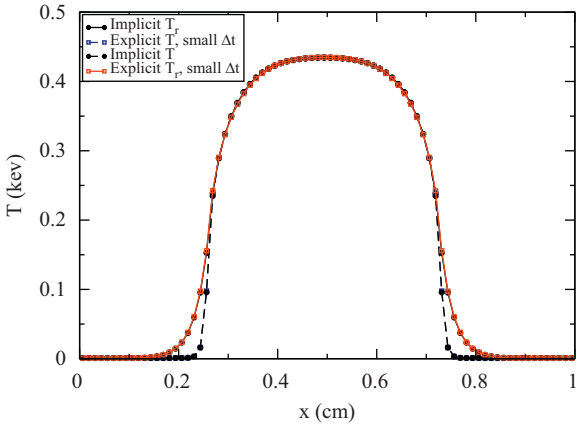

Fig. 5. Diffusion solutions with $N_x = 80$ at $t=0.1$ ns using $\Delta t = 0.01$ ns for implicit coupling and $\Delta t = 4.8077 \times 10^{-4}$ ns for explicit coupling. The explicit timestep is 0.98 of the maximum time step for non-oscillatory solutions.

oscillations appear in the solution and the solution is highly unstable at $N_x = 80$. At $N_x = 80$ the oscillations grew to be approximately 10^{69} keV. These results support the theory which indicates that diffusion is always conditionally stable when using explicit coupling. As we refine the mesh higher values of λ can be supported in the solution and we approach the stability condition for $\lambda \to \infty$ given by Eq. (33).

In Fig. 5 we show results for the previous problem using $N_x = 80$ at $t=0.1$ ns using $\Delta t = 0.01$ ns for implicit coupling and $\Delta t = 4.8077 \times 10^{-4}$ ns for explicit coupling. The explicit timestep is 0.98 of the maximum time step for non-oscillatory solutions given by Eq. (34). It can be seen that the explicit solutions show no sign of oscillations and are in excellent agreement with the implicit solutions. Thus, as expected, the criterion for non-oscillatory solutions does not appear to be dependent upon the spatial resolution.

6. Conclusions

Our theoretical and computational results indicate that explicit radiation-material coupling can yield highly oscillatory results even when it is unconditionally stable, and the criterion for non-oscillatory behavior becomes increasingly restrictive as the opacity increases. In addition, if the scheme is conditionally stable, the time-step for stability also becomes increasingly restrictive as the opacity increases. These properties lead us to conclude that explicit coupling is not a viable technique for highly diffusive problems. Although this scheme is routinely used in the infrared regime, it is clear that one must be very cautious when applying this scheme in the high energy density laboratory physics regime. The material temperatures are orders of magnitude higher than in the infrared regime and the maximum time steps for stable and non-oscillatory solutions vary as T^{-3}, although this effect can be mitigated to varying degrees by the typical decrease of opacity with temperature. If one chooses to use implicit coupling, stability will always be obtained with physically reasonable time steps, but oscillations are possible unless the nonlinearities are converged. In the future it would be useful to derive time step criteria for avoiding oscillations with implicit coupling when the nonlinearities are not converged.

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