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Numerical analysis of time integration errors for nonequilibrium radiation diffusion

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Abstract

Numerical analysis of time integration errors for nonequilibrium radiation diffusion is considered. Two first-order implicit time integration methods are studied. Asymptotic analysis and modified equation analysis are applied to both time integration methods. Numerical experiments are used to highlight the results of the analysis. Asymptotic analysis is used to highlight the source of temperature spiking when a hot radiation wave propagates into a cold material. Modified equation analysis is used to provide insight into the thermal wave speed coming from the two different first-order methods.

Keywords: Radiation diffusion; Asymptotic analysis; Modified equation analysis

1. Background

Nonequilibrium radiation diffusion systems are used to simulate problems in inertial confinement fusion [1], Z-pinch experiments [19], and astrophysical problems [20]. There has been a recent interest in putting forth new time integration methods for nonequilibrium radiation diffusion [8,17,2,14,16,18]. This activity has been motivated by the desire to potentially increase the accuracy of time integration of these systems by removing first-order linearization and operator splitting. There has also been some effort on applying numerical analysis to such problems [6,14]. Here we advance the effort of applying numerical analysis to time integration of nonequilibrium radiation diffusion with the goal of gaining insight. We will apply both modified equation analysis [5] and asymptotic analysis [12] to a pair of first-order time integration methods.

We study the following one-dimensional coupled system for the grey radiation energy density, E, and the material temperature, T, ignoring material conduction and material motion:

$$\frac{\partial E}{\partial t} - \frac{\partial}{\partial x}\left(D_r \frac{\partial E}{\partial x}\right) = c\sigma_a(B - E), \tag{1a}$$

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$$C_v \frac{\partial T}{\partial t} = -c\sigma_a(B - E), \tag{1b}$$

$$\sigma_a = \bar{\sigma}_a T^{-3}, \tag{2}$$

$$B = a_R T^4, \tag{3}$$

where D_r is the diffusion coefficient, c is the speed of light, σ_a is the macroscopic absorption cross section, C_v is the material heat capacity, $\bar{\sigma}$ is a parametric constant, and a_R is the radiation constant. We comment that all results in this study are directly applicable in more than one dimension. Eqs. (1a) and (1b) are a coupled partial differential equation (PDE) and ordinary differential equation (ODE) system. These equations (in some cases with certain material properties explicitly set to 1) were considered previously in [7,8,17,14]. Here we use Larsen's form for a flux-limited diffusion coefficient,

$$D_r(T, E) = \frac{c}{\sqrt{(3\sigma_a)^2 + \left(\frac{1}{E}\frac{\partial E}{\partial x}\right)^2}}, \tag{4}$$

which has certain desirable asymptotic properties that are later discussed [15]. Since the heat capacity is often a weak function of temperature, we henceforth assume for simplicity that it is equal to 1.

The coupled system (1) contains a dynamical time scale, in which the system evolves, and two normal mode time scales which combine to define the dynamical time scale. For the thermal wave problems we will consider the dynamical time scale as simply the time scale for the thermal wave propagation. The two normal mode time scales come from thermal equilibration (the reaction term) and radiation diffusion.

In the limit where thermal equilibration is much faster than radiation diffusion ($c\sigma_a \gg \frac{D_r}{\ell^2}$, with ℓ the gradient scale length of the solution) this system is said to be in its equilibrium limit. In that case $E = a_R T^4$ and the following equation provides a solution to the problem,

$$\frac{\partial(T + a_R T^4)}{\partial t} - \frac{\partial}{\partial x}\left(d_r \frac{\partial a_R T^4}{\partial x}\right) = 0, \tag{5a}$$

$$E = a_R T^4, \tag{5b}$$

$$d_r(T) = \frac{c}{3\sigma_a}. \tag{5c}$$

We will derive this analytic result shortly through the use of asymptotic analysis [12].

We will consider two methods of advancing the solution in time from time level n to time level $n+1$ over a time step Δt. Spatial discretization will be ignored for this discussion, and we focus on two methods which are first-order accurate in time.

A commonly used approach for time integration of this system is referred to as the linearly implicit (LI) method [7,8]. In the linearly implicit method (also called the semi-implicit (SI) method) we solve the two component system coupled but the nonlinearities are not converged within a time step. The transport coefficients, σ_a and D_r are evaluated at time level n, and B^{n+1} is approximated from a first-order Taylor series expansion at time level $n\left(B^{n+1} \approx B^n + \Delta t \frac{\partial B}{\partial t} = B^n + \Delta t \frac{\partial B}{\partial T}\frac{\partial T}{\partial t}\right)$. These approximations yield the following difference equations

$$\frac{E^{n+1} - E^n}{\Delta t} - \frac{\partial}{\partial x}\left(D_r^n \frac{\partial E^{n+1}}{\partial x}\right) = c\sigma_a^n(a_R(T^n)^4 + 4a_R(T^n)^3(T^{n+1} - T^n) - E^{n+1}), \tag{6a}$$

$$\frac{T^{n+1} - T^n}{\Delta t} = -c\sigma_a^n(a_R(T^n)^4 + 4a_R(T^n)^3(T^{n+1} - T^n) - E^{n+1}). \tag{6b}$$

This is a linear problem and requires no nonlinear iteration.

We will also consider an implicitly balanced (IB) method [6]. By implicitly balanced methods we mean that all nonlinearities are converged, and all fluxes and sources are evaluated at the same point in discrete time. The first-order accurate implicitly balanced time integration method is based on backward Euler time discretization and is

$$\frac{E^{n+1}-E^n}{\Delta t}-\frac{\partial}{\partial x}\left(D_r^{n+1}\frac{\partial E^{n+1}}{\partial x}\right)=c\sigma_{\mathrm{a}}^{n+1}(a_{\mathrm{R}}(T^{n+1})^4-E^{n+1}), \tag{7a}$$

$$\frac{T^{n+1}-T^n}{\Delta t}=-c\sigma_{\mathrm{a}}^{n+1}(a_{\mathrm{R}}(T^{n+1})^4-E^{n+1}). \tag{7b}$$

This method is nonlinear and thus requires some form of nonlinear iteration. As in [7,8] we use the Jacobian-free Newton–Krylov method to solve this system.

Both the LI and IB methods are consistent. They will both produce first-order time step convergence in the limit of small Δt. However, their performance can be different at larger Δt, and these methods are often used with larger Δt.

2. Asymptotic analysis

Many multiphysics problems have expected behavior in certain, asymptotic limits. A classic example of this is the diffusion limit of the transport equation [11,10,15]. Here, if the collisional mean free path is small compared the gradient scale length of the problem, then the transport equation will be equivalent to the diffusion equation to lowest order. This can be shown on the analytic problem using asymptotic analysis [11,10,15]. This same analysis can be usefully applied to the discretized transport equation. Certain discretizations of the transport equation have been shown to preserve the discrete diffusion limit, while others do not. Discretizations of the transport equation which preserve the diffusion limit are generally essential for highly diffusive problems because accurate solutions with non-asymptotic preserving discretizations can only be assured with grids that resolve the collisional mean free path. This results in arbitrarily over-resolved grids because the diffusion length, which is the spatial scale length of diffusive solutions, becomes infinite relative to the collisional mean free path in the asymptotic diffusion limit. In contrast, asymptotic preserving discretizations of the transport equation yield accurate solutions in highly diffusive problems whenever the spatial variation of such solutions is well resolved by the grid.

The above discussion focuses on the spatial discretization of the transport equation. In the present work we "accept" the spatial discretization and perform asymptotic analysis of the thermal nonequilibrium diffusion model in time. This is similar to the recent work of Densmore and Larsen [3]. In this paper, we are not studying the issue related to resolving an initial transport layer within a diffusion model.

We will first perform the asymptotic analysis on our PDE/ODE nonequilibrium system, Eq. (1), to establish the asymptotic model in the continuum. Next we will apply the asymptotic analysis to the different time integration methods and establish if they satisfy the equilibrium solution. We desire methods which can obtain the proper equilibrium solution when it is appropriate, without needing to resolve the fast equilibration time scale.

2.1. Continuum analysis

To perform the asymptotic analysis, we must nondimensionalize the equations and identify which nondimensional parameters are small. Each quantity is nondimensionalized via the following substitutions:

$$x\to x_{\mathrm{ref}}x,\quad t\to t_{\mathrm{ref}}t,\quad T\to T_{\mathrm{ref}}T,$$
$$E\to a_{\mathrm{R}}T_{\mathrm{ref}}^4E,\quad \sigma_{\mathrm{a}}\to\sigma_{\mathrm{a_{ref}}}\sigma_{\mathrm{a}},\quad D_r\to\frac{c}{\sigma_{\mathrm{a_{ref}}}}D_r,$$

where $\sigma_{\mathrm{a_{ref}}}=\bar{\sigma}_{\mathrm{a}}T_{\mathrm{ref}}^{-3}$. The subscript "ref" represents a dimensional reference value for each quantity. Under this transformation, the system (1) can be rearranged to read

$$\frac{x_{\mathrm{ref}}}{ct_{\mathrm{ref}}}\frac{\partial E}{\partial t}-\frac{1}{x_{\mathrm{ref}}\sigma_{\mathrm{a_{ref}}}}\frac{\partial}{\partial x}\left(D_r\frac{\partial E}{\partial x}\right)=x_{\mathrm{ref}}\sigma_{\mathrm{a_{ref}}}\sigma_{\mathrm{a}}(T^4-E), \tag{8a}$$

$$\frac{x_{\mathrm{ref}}}{ct_{\mathrm{ref}}}\frac{\partial T}{\partial t}=-x_{\mathrm{ref}}\sigma_{\mathrm{a_{ref}}}\sigma_{\mathrm{a}}(T^4-E), \tag{8b}$$

where

$$D_r(T,E) = \frac{1}{\sqrt{(3\sigma_a)^2 + \left(\frac{1}{x_{\text{ref}}\sigma_{a_{\text{ref}}}}\frac{1}{E}\frac{\partial E}{\partial x}\right)^2}}. \tag{8c}$$

We now can identify the following two nondimensional parameters:

$$\frac{x_{\text{ref}}}{ct_{\text{ref}}}, \quad \frac{1}{x_{\text{ref}}\sigma_{a_{\text{ref}}}}.$$

The first parameter represents the ratio of the gradient length scale (x_{ref}) to the distance streaming photons travel within the dynamical time scale of interest (ct_{ref}). The second parameter is the ratio of the absorption mean free path ($\sigma_{a_{\text{ref}}}^{-1}$) to the gradient length scale. In the collision-dominated regime of interest here, we expect both of these parameters to be small, and therefore set

$$\frac{x_{\text{ref}}}{ct_{\text{ref}}} \sim \frac{1}{x_{\text{ref}}\sigma_{a_{\text{ref}}}} \sim \varepsilon \ll 1,$$

where ε is our asymptotic "smallness" parameter. See Refs. [3,12,15] for similar analysis of more complicated transport models. With $B = T^4$ our scaled nonequilibrium equations are,

$$\varepsilon^2\frac{\partial E}{\partial t} - \varepsilon^2\frac{\partial}{\partial x}\left(D_r\frac{\partial E}{\partial x}\right) = \sigma_a(B-E), \tag{9a}$$

$$\varepsilon^2\frac{\partial T}{\partial t} = -\sigma_a(B-E), \tag{9b}$$

where

$$D_r(T,E) = \frac{1}{\sqrt{(3\sigma_a)^2 + \varepsilon^2\left(\frac{1}{E}\frac{\partial E}{\partial x}\right)^2}} \tag{9c}$$

and $\sigma_a = 1/T^3$. Note that the sum of these equations gives the conservation statement

$$\frac{\partial(T+E)}{\partial t} - \frac{\partial}{\partial x}\left(D_r\frac{\partial E}{\partial x}\right) = 0, \tag{10}$$

which we will use frequently in our analysis.

Next, the variables are expanded in powers of ε as, for example,

$$E = E_0 + \varepsilon E_1 + \varepsilon^2 E_2 + \cdots$$

and similar expansions for T, B, D_r, d_r, and σ_a. We then substitute the expansions into the scaled equations and equate like powers of ε to complete the analysis. The $O(\varepsilon^0)$-equations for both Eqs. (9a) and (9b) give

$$E_0 = B_0 = T_0^4, \tag{11a}$$

while Eq. (10) becomes simply

$$\frac{\partial(T_0+B_0)}{\partial t} - \frac{\partial}{\partial x}\left(d_{r_0}\frac{\partial B_0}{\partial x}\right) = 0, \tag{11b}$$

where

$$d_{r_0} = \frac{1}{3\sigma_{a_0}}, \quad \sigma_{a_0} = T_0^{-3}. \tag{11c}$$

This system is simply a nondimensional version of the system (5).

Matching solely the $O(\varepsilon^0)$ asymptotic behavior is insufficient. Larsen et al. [12] showed that the equilibrium diffusion model matches the asymptotics of the full transport equation through $O(\epsilon^1)$, and Morel [15] showed that the nonequilibrium diffusion model, with the flux-limited diffusion coefficient (9c), similarly matches the asymptotics of the full transport equation through $O(\epsilon^1)$. Consequently, we must ensure our time discretizations maintain this asymptotic behavior. The $O(\varepsilon^1)$-terms for of Eqs. (9a) and (9b) give

$$E_1 = B_1 = 4T_0^3 T_1. \tag{12a}$$

Eq. (10) yields

$$\frac{\partial(T_1 + B_1)}{\partial t} - \frac{\partial}{\partial x}\left(d_{r_1}\frac{\partial B_0}{\partial x}\right) - \frac{\partial}{\partial x}(d_{r_0}\frac{\partial B_1}{\partial x}) = 0 \tag{12b}$$

where

$$d_{r_1} = -d_{r_0}\frac{\sigma_{a_1}}{\sigma_{a_0}}, \quad \sigma_{a_1} = -3\sigma_{a_0}\frac{T_1}{T_0}. \tag{12c}$$

This completes the analysis of the continuum model.

2.2. Discrete analysis

Next we wish to apply the analysis above to our time discretizations. This will tell us if the asymptotic solution resulting from the time discretization of the nonequilibrium system will produce a numerical answer which is equivalent to the time discretization of the equilibrium equation. If this is the case, then when the equilibrium equation applies, we should be able to use time steps which are large relative to $(c\sigma_a)^{-1}$. Following similar arguments as in Ref. [13], we refer to such methods as *asymptotic preserving*. Non-asymptotic preserving methods must always use a time step which resolves the equilibration process. In other words, since the equilibration time goes to zero as ϵ goes to zero, non-asymptotic preserving methods require a time step that goes to zero as epsilon goes to zero. This can clearly lead to arbitrarily small time steps in highly asymptotic problems. In contrast, asymptotic preserving methods require a time step that depends only upon the temporal variation of the asymptotic solution, and is therefore independent of ϵ to leading order.

2.2.1. Implicitly balanced method

It is straightforward to show that the leading order asymptotic terms of the implicitly balanced (IB) time integration method, Eq. (7), satisfy

$$\frac{(T_0 + B_0)^{n+1} - (T_0 + B_0)^n}{\Delta t} - \frac{\partial}{\partial x}\left(d_{r_0}^{n+1}\frac{\partial B_0^{n+1}}{\partial x}\right) = 0, \tag{13a}$$

$$E_0^{n+1} = B_0^{n+1} = (T_0^{n+1})^4. \tag{13b}$$

This system is a first-order accurate time discretization of the system, Eq. (11). Next, we check the $O(\varepsilon^1)$ terms, which yield

$$\frac{(T_1 + B_1)^{n+1} - (T_1 + B_1)^n}{\Delta t} - \frac{\partial}{\partial x}\left(d_{r_1}^{n+1}\frac{\partial B_0^{n+1}}{\partial x}\right) - \frac{\partial}{\partial x}\left(d_{r_0}^{n+1}\frac{\partial B_1^{n+1}}{\partial x}\right) = 0, \tag{14a}$$

where

$$E_1^{n+1} = B_1^{n+1} = 4(T_0^{n+1})^3 T_1^{n+1}. \tag{14b}$$

This is a first-order accurate time discretization of the system in Eq. (12). Therefore, the IB method matches the asymptotic behavior of the analytic equation through $O(\varepsilon^1)$ terms, and thus is asymptotic preserving.

2.2.2. Linearly implicit method

The result for the linearly implicit (LI) method, Eq. (6), is more interesting. The scaled discrete problem is

$$\varepsilon^2\frac{E^{n+1} - E^n}{\Delta t} - \varepsilon^2\frac{\partial}{\partial x}\left(D_r^n\frac{\partial E^{n+1}}{\partial x}\right) = \sigma_a^n\left(B^n + \frac{\partial B}{\partial T}(T^{n+1} - T^n) - E^{n+1}\right), \tag{15a}$$

and

$$\varepsilon^2\frac{T^{n+1} - T^n}{\Delta t} = -\sigma_a^n\left(B^n + \frac{\partial B}{\partial T}(T^{n+1} - T^n) - E^{n+1}\right), \tag{15b}$$

while the discrete conservation statement is

$$\frac{(T+E)^{n+1}-(T+E)^{n}}{\Delta t}-\frac{\partial}{\partial x}(D_r^n\frac{\partial E^{n+1}}{\partial x})=0. \tag{16}$$

The $O(\varepsilon^0)$-equations of Eq. (15) produce

$$E_0^{n+1}=B_0^n+\left(\frac{\partial B_0}{\partial T_0}\right)^n(T_0^{n+1}-T_0^n), \tag{17}$$

while Eq. (16) becomes

$$\frac{(T_0+E_0)^{n+1}-(T_0+E_0)^{n}}{\Delta t}-\frac{\partial}{\partial x}\left(d_{r_0}^n\frac{\partial E_0^{n+1}}{\partial x}\right)=0, \tag{18}$$

Not surprisingly, Eq. (17) differs from Eq. (13b). If the LI method is asymptotic preserving, then this difference must be within the order-of-accuracy of the methods (both are $O(\Delta t)$-methods). To show this, we begin with the following expansion:

$$B_0^{n+1}=B_0^n+\left(\frac{\partial B_0}{\partial T_0}\right)^n\delta T_0^n+\left(\frac{\partial^2 B_0}{\partial T_0^2}\right)^n(\delta T_0^n)^2+O((\delta T_0^n)^3), \tag{19}$$

where $\delta T_0^n=T_0^{n+1}-T_0^n$. Eq. (17) may then be written as

$$E_0^{n+1}=B_0^{n+1}-\left(\frac{\partial^2 B_0}{\partial T_0^2}\right)^n(\delta T_0^n)^2+O((\delta T_0^n)^3). \tag{20}$$

But $\delta T_0^n=O(\Delta t)$ and therefore,

$$E_0^{n+1}=B_0^{n+1}+O((\Delta t)^2). \tag{21}$$

Consequently, the LI method satisfies Eq. (11a) to within the order-of-accuracy of the method. Note that this is a weaker result than that for the IB method, in that the IB method satisfies Eq. (11a) exactly at each time level. We stress that the $O((\Delta t)^2)$ error appearing in Eq. (21) is independent of ϵ. If it were an increasing function of ϵ, the LI method would not be asymptotic preserving.

Next we must check whether the LI method satisfies Eq. (11b) in the asymptotic limit. Using the relation (20),

$$\begin{aligned}E_0^{n+1}-E_0^n&=B_0^{n+1}-B_0^n+\left(\frac{\partial^2 B_0}{\partial T_0^2}\right)^n(\delta T_0^n)^2-\left(\frac{\partial^2 B_0}{\partial T_0^2}\right)^{n-1}(\delta T_0^{n-1})^2+O((\delta T_0)^3)\\&=B_0^{n+1}-B_0^n+O((\Delta t)^3).\end{aligned} \tag{22}$$

Insert this expression, along with (21), into Eq. (18) to obtain

$$\frac{(T_0+B_0)^{n+1}-(T_0+B_0)^{n}}{\Delta t}-\frac{\partial}{\partial x}\left(d_{r0}^n\frac{\partial B_0^{n+1}}{\partial x}\right)=O((\Delta t)^2). \tag{23}$$

Note that unlike the implicitly balanced result (see Eq. (13a)), (23) treats the diffusion coefficient explicitly. Nevertheless, this is a first-order accurate discretization of (11b) and therefore, the LI method is asymptotic preserving through $O(\varepsilon^0)$.

Next we must check the $O(\varepsilon^1)$ terms. We obtain

$$E_1^{n+1}=B_1^n+\left(\frac{\partial B_0}{\partial T_0}\right)^n(T_1^{n+1}-T_1^n)+\left(\frac{\partial B_1}{\partial T_1}\right)^n(T_0^{n+1}-T_0^n) \tag{24}$$

and

$$\frac{(T_1+E_1)^{n+1}-(T_1+E_1)^{n}}{\Delta t}-\frac{\partial}{\partial x}\left(d_{r_1}^n\frac{\partial E_0^{n+1}}{\partial x}\right)-\frac{\partial}{\partial x}\left(d_{r_0}^n\frac{\partial E_1^{n+1}}{\partial x}\right)=0, \tag{25}$$

Using the same arguments that led to Eqs. (21) and (22), we obtain

$$E_1^{n+1} = B_1^{n+1} + \mathrm{O}((\Delta t)^2) \tag{26}$$

and

$$E_1^{n+1} - E_1^n = B_1^{n+1} - B_1^n + \mathrm{O}((\Delta t)^3), \tag{27}$$

so that (25) becomes

$$\frac{(T_1 + B_1)^{n+1} - (T_1 + B_1)^n}{\Delta t} - \frac{\partial}{\partial x}\left(d_{r_1}^n \frac{\partial B_0^{n+1}}{\partial x}\right) - \frac{\partial}{\partial x}\left(d_{r_0}^n \frac{\partial B_1^{n+1}}{\partial x}\right) = \mathrm{O}((\Delta t)^2). \tag{28}$$

This is a first-order accurate time discretization of the system (12a). Therefore, the LI method is asymptotic preserving through $\mathrm{O}(\varepsilon^1)$.

2.2.3. Summary of the asymptotic analysis

From our asymptotic analysis, we can conclude the following:

- Both the IB and LI methods yield asymptotic discretizations that are asymptotic preserving through $\mathrm{O}(\epsilon)$.
- However, the IB method has the advantage that at each time level, it *exactly* satisfies the equilibrium condition $E = B$. We refer to this property as *equilibrium-exact*. We anticipate that because of the equilibrium-exact property, in cases where
  – the time-level-n solution is far from equilibrium, or
  – the temporal history of the relaxation process is unimportant(i.e. near equilibrium conditions),
  the IB method will allow larger time steps than the LI method, while maintaining accuracy. Our numerical results will demonstrate this advantage of the IB method, which we attribute to its equilibrium-exact property. Note, however, that we have no formal proof that equilibrium-exact methods generally allow for larger time steps.
- In the asymptotic limit, the IB method treats its diffusion coefficient implicitly, whereas the LI method treats it explicitly. Both are first-order accurate, but this is another reason that the IB method may be more robust and allow larger time steps.

3. Modified equation analysis

In this section we will focus on semi-discrete in time modified equation analysis (MEA), as was done in [6]. It should be pointed out that MEA can be used for either accuracy or stability analysis [5,21]. For an excellent discussion on the use of MEA, including the impacts of initial and boundary conditions one should consult [4].

3.1. Implicitly balanced methods

To apply MEA to Eqs. (7a) and (7b), we require Taylor series to eliminate T^n and E^n,

$$T^n = T^{n+1} - \Delta t T_t^{n+1} + \frac{\Delta t^2}{2} T_{tt}^{n+1} - \frac{\Delta t^3}{6} T_{ttt}^{n+1} + \mathrm{O}(\Delta t^4), \tag{29}$$

$$E^n = E^{n+1} - \Delta t E_t^{n+1} + \frac{\Delta t^2}{2} E_{tt}^{n+1} - \frac{\Delta t^3}{6} E_{ttt}^{n+1} + \mathrm{O}(\Delta t^4). \tag{30}$$

After Eqs. (29) and (30) are substituted into Eqs. (7a) and (7b), the equations are manipulated resulting in the original PDE/ODE system on the left hand side, and an additional right hand side which is the modification of our original system.

The resulting modified equations for the first-order IB method are:

$$\left[\frac{\partial E}{\partial t} - \frac{\partial}{\partial x}\left(D_r \frac{\partial E}{\partial x}\right) - c\sigma_{\mathrm{a}}(a_{\mathrm{R}} T^4 - E)\right]^{n+1} = \frac{\Delta t}{2} E_{tt} + \mathcal{O}(\Delta t^2), \tag{31}$$

and

$$\left[\frac{\partial T}{\partial t} + c\sigma_{\mathrm{a}}(a_{\mathrm{R}}T^4 - E)\right]^{n+1} = \frac{\Delta t}{2}T_{tt} + \mathcal{O}(\Delta t^2). \tag{32}$$

This is the equation system the first-order IB numerical time integration is actually solving.

3.2. Linearized implicit method

When applying MEA to the LI method, in addition to Eqs. (29) and (30), we will need expansions for coefficients which have been linearized (or fixed at time level n). This includes $D_r^n, \sigma_{\mathrm{a}}^n$, and B^n,

$$D_r^n = D_r^{n+1} - \Delta t \frac{\partial D_r}{\partial T}\frac{\partial T}{\partial t} - \Delta t \frac{\partial D_r}{\partial E}\frac{\partial E}{\partial t} + \mathcal{O}(\Delta t^2),$$
$$\sigma_{\mathrm{a}}^n = \sigma_{\mathrm{a}}^{n+1} - \Delta t \frac{\partial \sigma_{\mathrm{a}}}{\partial T}\frac{\partial T}{\partial t} + \mathcal{O}(\Delta t^2),$$
$$B^n = B^{n+1} - \Delta t \frac{\partial B}{\partial T}\frac{\partial T}{\partial t} + \mathcal{O}(\Delta t^2).$$

Using these along with the Taylor series for T^n and E^n, substituting into Eq. (6) and rearranging, produces the modified equations for the linearized implicit (LI) method,

$$\begin{aligned}\left[\frac{\partial E}{\partial t} - \frac{\partial}{\partial x}\left(D_r\frac{\partial E}{\partial x}\right) - c\sigma_{\mathrm{a}}(B - E)\right]^{n+1} &= \frac{\Delta t}{2}E_{tt} - \Delta t\frac{\partial}{\partial x}\left(\left[\frac{\partial D_r}{\partial T}\frac{\partial T}{\partial t}\right]\frac{\partial E}{\partial x}\right) - \Delta t\frac{\partial}{\partial x}\left(\left[\frac{\partial D_r}{\partial E}\frac{\partial E}{\partial t}\right]\frac{\partial E}{\partial x}\right) \\ &\quad + \Delta t c\frac{\partial \sigma_{\mathrm{a}}}{\partial T}\frac{\partial T}{\partial t}[B^{n+1} - E^{n+1}] + \mathcal{O}(\Delta t^2),\end{aligned} \tag{33}$$

and

$$\left[\frac{\partial T}{\partial t} + c\sigma_{\mathrm{a}}(B - E)\right]^{n+1} = \frac{\Delta t}{2}T_{tt} + \Delta t\frac{\partial c\sigma_{\mathrm{a}}}{\partial T}\frac{\partial T}{\partial t}[B^{n+1} - E^{n+1}] + \mathcal{O}(\Delta t^2). \tag{34}$$

This system has new terms as compared to that resulting from the first order IB system (Eqs. (31) and (32)). It is interesting to note that the terms which come from the expansion of B^{n+1} are collected in the $\mathcal{O}(\Delta t^2)$ expression. Again, when the LI method is used to time integrate Eq. (1), the resulting solution is the solution to Eqs. (33) and (34).

4. Numerical experiments

4.1. Supporting asymptotic analysis

First we consider thermal equilibration in an ODE system, ignoring radiation diffusion in Eq. (1). Next we consider the solution of the two component spatial solution (PDE/ODE system). Finally we consider the spatial solution to the actual equilibrium problem. In all cases we have set $a_{\mathrm{R}} = c = 1$.

Consider the ODE problem with σ_{a} constant and equal to 1. This gives us the following for the LI method,

$$\frac{E^{n+1} - E^n}{\Delta t} = ([(T^n)^4 + 4(T^n)^3(T^{n+1} - T^n)] - E^{n+1}), \tag{35}$$
$$\frac{T^{n+1} - T^n}{\Delta t} = -([(T^n)^4 + 4(T^n)^3(T^{n+1} - T^n)] - E^{n+1}). \tag{36}$$

For the IB method we have

$$\frac{E^{n+1} - E^n}{\Delta t} = ((T^{n+1})^4 - E^{n+1}), \tag{37}$$
$$\frac{T^{n+1} - T^n}{\Delta t} = -((T^{n+1})^4 - E^{n+1}). \tag{38}$$

Thus, for this simplified problem the only difference between the IB and LI methods is the linearization of T^4. For time steps larger than the equilibration time scale (σ_a^{-1}, or 1 in this case) we expect the solution $E = T^4$.

We simulate this problem with initial conditions of $E = 2$ and $T^4 = 0.1$, and with time steps of $\Delta t = 1, 2.5, 5$ for IB and $\Delta t = 0.5, 1, 2.5, 5$ for LI. For the ODE system, and these initial conditions, $T^4 > E$ is not a solution of the continuum system at any time. Fig. 1 shows the solutions coming from the IB method. Recall that the implicitly balanced method was shown to have the property of *equilibrium-exact*. Here we see correct physical trends, even for large time steps. Near equilibrium is observed in one time step and clear equilibrium in two time steps when $\Delta t > \sigma_a^{-1}$. Next we consider the LI method. Recall that it was shown that this approach was *asymptotic preserving*, but not *equilibrium-exact*. Fig. 2 shows the solutions and a different behavior is observed. There is erroneous temperature spiking, and clear equilibrium is obtained only after four time steps. When the time step is less than the equilibrium time scale, ($\Delta t = 0.5$) physically correct trends are observed. The fact that the asymptotic analysis produced different results for the IB and LI methods provides an expectation of such behavior. This behavior results directly from the linearization of T^4, and it has also been analyzed by Larsen and Mercier [9].

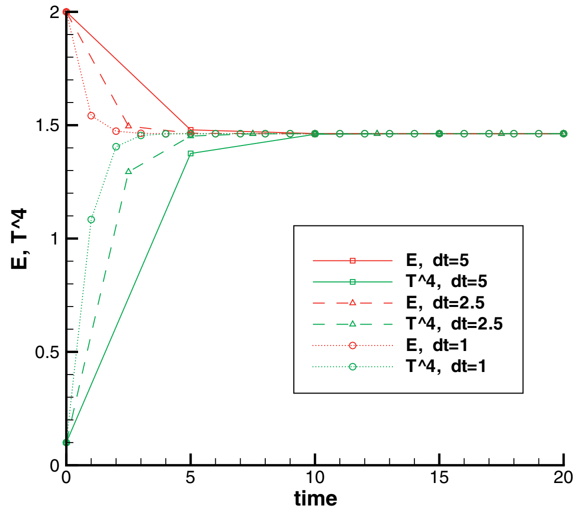

Fig. 1. Implicitly balanced solutions.

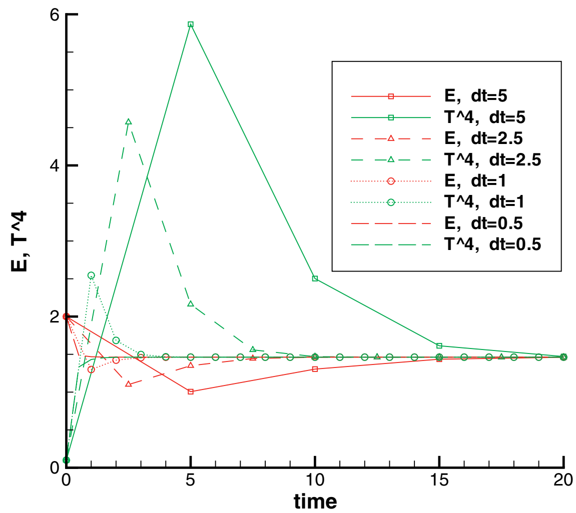

Fig. 2. Linearized implicit solutions.

Finally, the potential for erroneous results is directly related to the initial spread between E and T. This can be seen in Fig. 3 where the initial conditions are $E = 1$ and $T^4 = 0.5$ and the overall behavior of the solutions is much better, although erroneous temperature spiking still occurs for $\Delta t = 2.5$ and $\Delta t = 5$.

With this information in hand let us consider a thermal wave with the full nonlinear model. We consider the region $0 \leqslant x \leqslant 1$ using 50 uniform finite volumes. The wave is driven by a fixed value of E on the left boundary, $E(x = 0, t) = 1$. The initial conditions are $E(x,t = 0) = (T(x,t = 0))^4 = 1.0 \times 10^{-4}$. We have chosen $\epsilon = 0.1$ (consistent with multiplying the equilibration terms by a factor of 100) with the goal of generating a near equilibrium solution. The time step is ramped up over the first eight time steps to its stated asymptotic value, Δt. The first eight time steps are: $0.1\Delta t$, $0.1\Delta t$, $0.2\Delta t$, $0.2\Delta t$, $0.3\Delta t$, $0.3\Delta t$, $0.4\Delta t$, $0.4\Delta t$. This was done to remove the issue of the early fast transient on the left boundary resulting from the discontinuity between the initial condition and the boundary condition (this is not a transport initial layer).

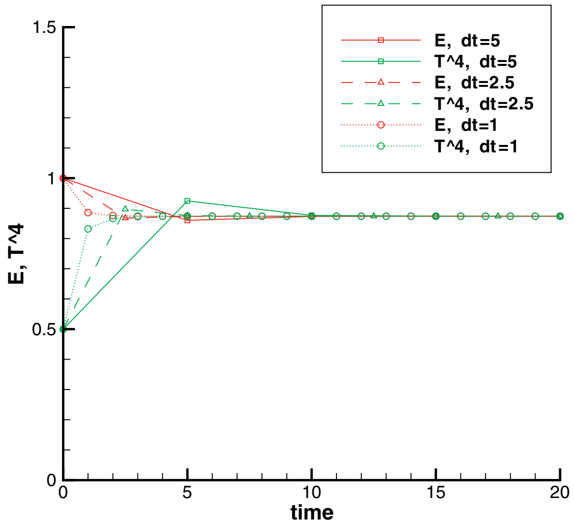

Fig. 3. Linearized implicit solutions for $E_0 = 1$ and $T_o^4 = 0.5$.

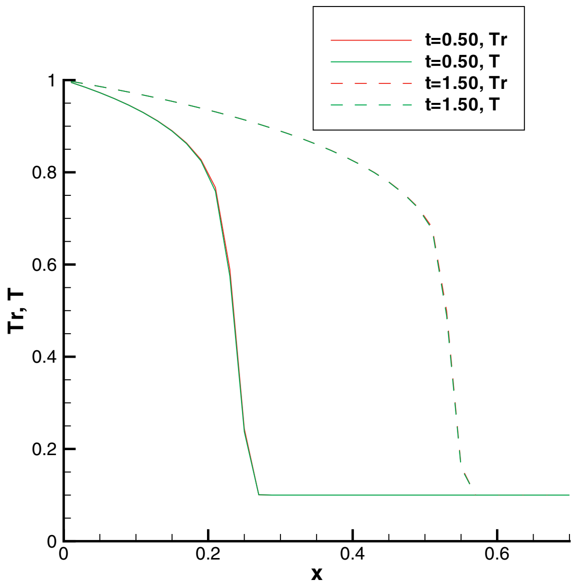

Fig. 4. Implicitly balance solutions at $t = 0.5$ and 1.5, with $\Delta t = 0.05$.

Fig. 4 shows results for the IB method with a time step of $\Delta t = 0.05$. This method should satisfy the asymptotic solution. Here $T_r \approx T$ (or $E \approx T^4$), but it is very important to note that $T \leqslant T_r$. For this set of initial conditions and boundary conditions, in the continuum system, it is not possible for for $T > T_r$. Fig. 5 shows results for the LI method. While we do see that $T_r \approx T$, we clearly have $T > T_r$ which is not a possible solution in the continuum. Fig. 6 show that the error in the LI method grows rapidly when we double the time step, while the IB method maintains $T_r > T$. This deficiency of the LI method is indicated by the asymptotic analysis and is also consistent with the findings of Larsen and Mercier [9]. This is not a transport initial layer issue, but rather an issue of linearizing T^4.

Fig. 7 shows that $T_r > T$ for both methods with $\Delta t = 0.005$, and that the solutions of the IB and LI methods become much closer. When comparing the LI and IB solutions in Figs. 6 and 7 we see that the wave from the

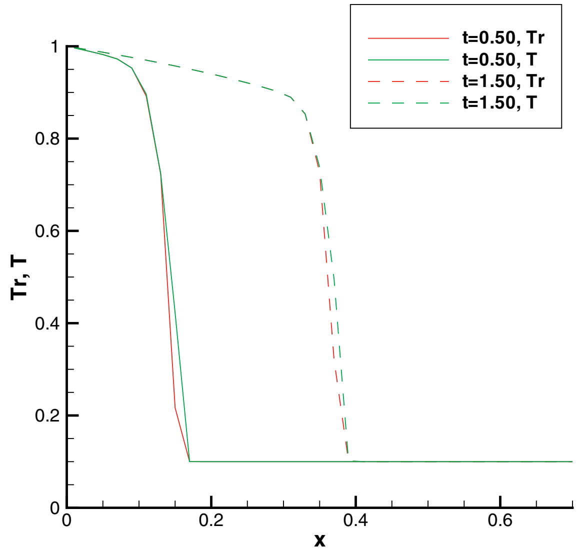

Fig. 5. Linearized implicit solutions at $t = 0.5$ and 1.5, with $\Delta t = 0.05$.

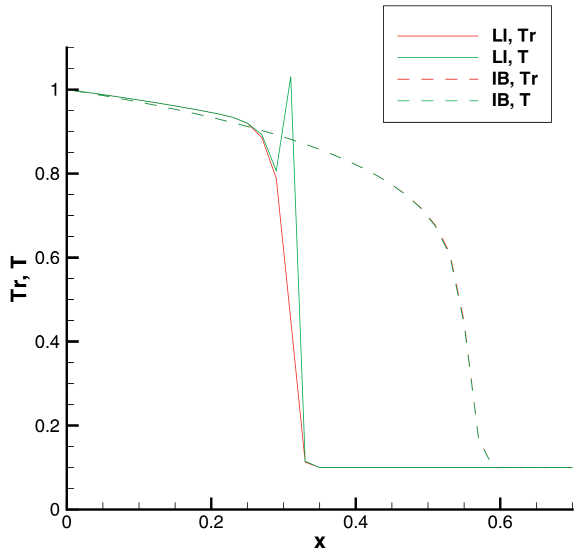

Fig. 6. LI and IB solutions at $t = 1.5$, with $\Delta t = 0.1$.

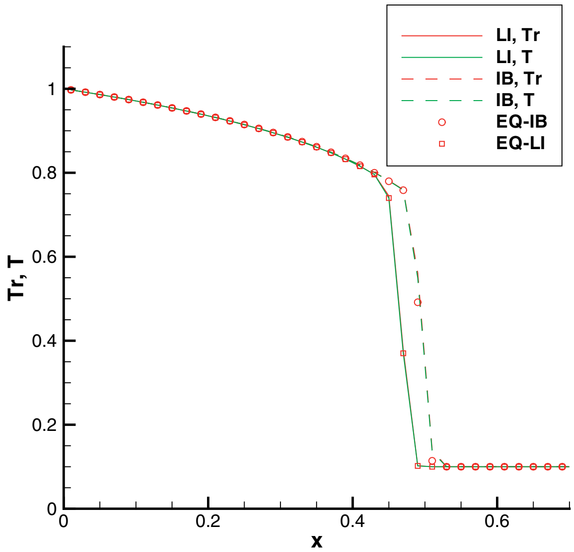

Fig. 7. LI and IB solutions $t = 1.5$, with $\Delta t = 0.005$, along with comparison to their respective asymptotic equations.

LI solution is slow compared to the wave from the IB solution. This has been observed previously in Ref. [7], and we will return to this issue in the next section.

We also consider the numerical solution of the equation resulting from the asymptotic analysis in the IB method Eq. (13) and LI method Eq. (18). The IB method is the circles and the LI method is the squares in Fig. 7. We see that both methods are consistent with the solution of their respective asymptotic solution for $\epsilon = 0.1$.

Finally, Figs. 8 and 9 show that both methods become independent of ϵ as ϵ is reduced (although different from each other). Such independence of ϵ is the essence of asymptotic preservation.

4.2. Supporting modified equation analysis

The results in this section are an extension of the study in Ref. [6]. First we will look at the coupled ODE system, ignoring radiation diffusion, and use $\sigma_a = T^{-3}$. Again, the IB method will be compared with the LI

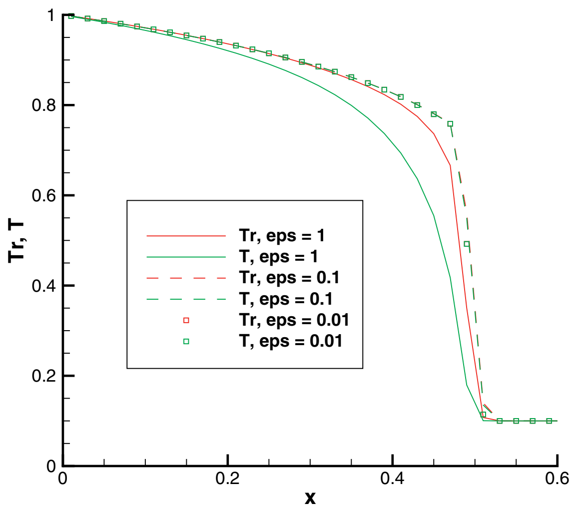

Fig. 8. IB solutions $t = 1.5$, with $\Delta t = 0.005$, for various ϵ.

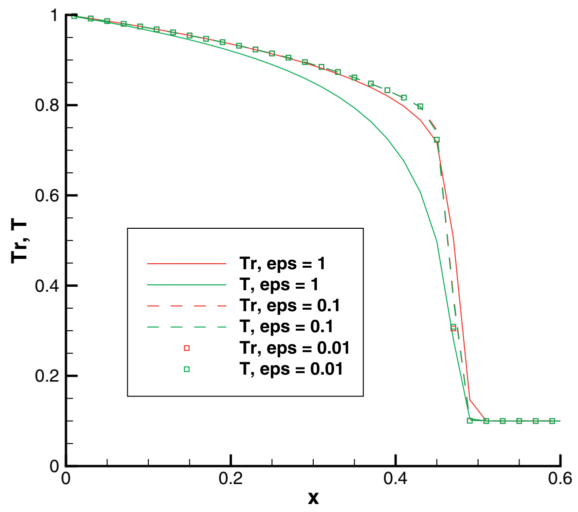

Fig. 9. LI solutions $t = 1.5$, with $\Delta t = 0.005$, for various ϵ.

method. To make isolating our point easier we will only linearize σ_a in the LI method here (T^4 will be iterated). To order Δt, the modified equations for this specific LI method, ignoring radiation diffusion are,

$$\left[\frac{\partial E}{\partial t} - \sigma_a(T^4 - E)\right] = \frac{\Delta t}{2}E_{tt} + \Delta t\frac{\partial \sigma_a}{\partial T}\frac{\partial T}{\partial t}[T^4 - E], \tag{39}$$

and

$$\left[\frac{\partial T}{\partial t} + \sigma_a(T^4 - E)\right] = \frac{\Delta t}{2}T_{tt} + \Delta t\frac{\partial \sigma_a}{\partial T}\frac{\partial T}{\partial t}[T^4 - E]. \tag{40}$$

The first-order implicitly balanced solution of

$$\frac{\partial E}{\partial t} - \sigma_a(T^4 - E) = \Delta t\frac{\partial \sigma_a}{\partial T}\frac{\partial T}{\partial t}[T^4 - E], \tag{41}$$

and

$$\frac{\partial T}{\partial t} + \sigma_a(T^4 - E) = \Delta t\frac{\partial \sigma_a}{\partial T}\frac{\partial T}{\partial t}[T^4 - E], \tag{42}$$

which we will call LI-MEA, should give the same result as the LI method, assuming that the first-order expansion,

$$\sigma_a^{n+1} = \sigma_a^n + \Delta t\frac{\partial \sigma_a}{\partial T}\frac{\partial T}{\partial t}$$

is accurate. If this is the case, the additional terms on the right hand side of Eqs. (41) and (42) define the difference between the LI and the IB solutions to this ODE system.

For initial conditions of $E = 2.0$, $T^4 = 0.1$, the results are in Figs. 10 and 11 for $\Delta t = 0.1$ and $\Delta t = 0.05$, respectively. It is clear the the terms in LI-MEA do define the difference between LI and IB. It is also clear that the accuracy of the expansion is better at $\Delta t = 0.05$. Thus the MEA can help us to understand the impact of linearizing σ_a in a problem like this. When using the LI method, the accuracy of the expansion of σ_a would be a sensible time step control. Simply using an allowed change in T may be less defensible [8].

Finally, we revisit the speed of the thermal wave issue which was seen in comparing Fig. 4 through Fig. 7. The LI method uses D_r^n while the IB method uses D_r^{n+1}. Ignoring flux limiting for the moment we have, to first order,

$$D_r^n = D_r^{n+1} - \Delta t \frac{\partial D_r}{\partial T} \frac{\partial T}{\partial t}.$$

We know that

$$\frac{\partial D_r}{\partial T} \propto T^2.$$

In the problem we are simulating $\frac{\partial T}{\partial t} > 0$. Thus $D_r^{n+1} > D_r^n$, and this is why LI is slower than IB. Again, as D_r^{n+1} approaches D_r^n we would expect the two solution to come together. Fig. 12 shows the two solutions at $t = 1.5$ with $\Delta t = 0.001$ and the two solutions are quite close. As has been shown in Ref. [8], second order methods for this problem are significantly more accurate. The specific second order method considered in [8] used $D_r^{n+\frac{1}{2}}$ to advance the solution from t^n to t^{n+1}. The position of the front for this second order method was in between

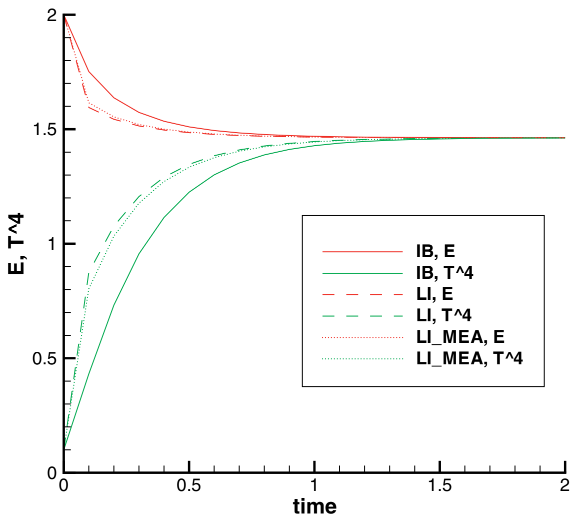

Fig. 10. Comparison of IB, LI, and LI-MEA for $\Delta t = 0.1$.

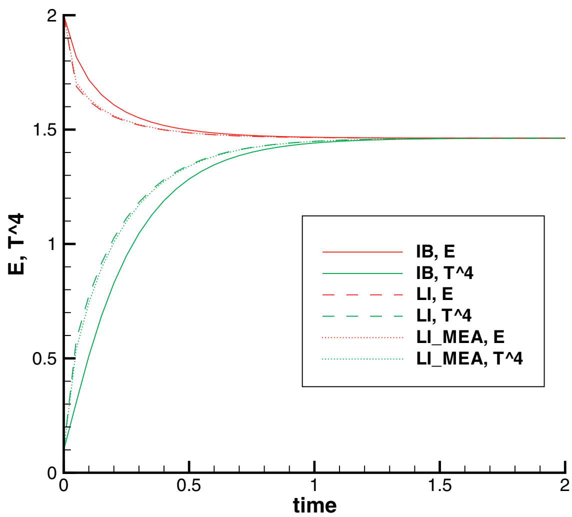

Fig. 11. Comparison of IB, LI, and LI-MEA for $\Delta t = 0.05$.

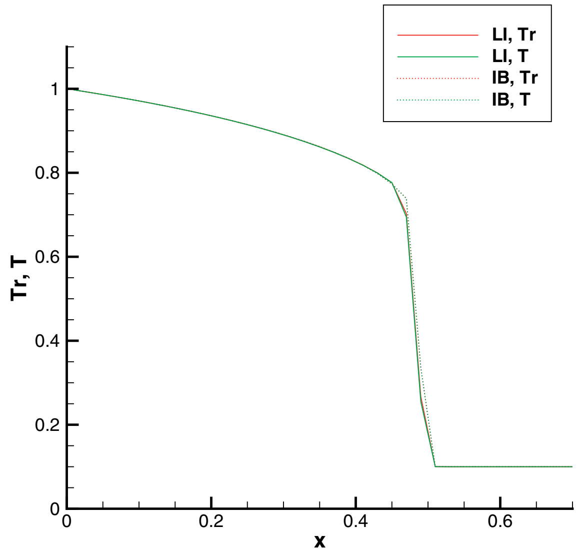

Fig. 12. LI and IB solutions $t = 1.5$, with $\Delta t = 0.001$.

that of the LI and IB methods when the same time step size was used. The MEA shows us that this results from the fact that and $D_r^{n+1} > D_r^{n+\frac{1}{2}} > D_r^n$.

5. Conclusions

Numerical analysis of time integration errors for nonequilibrium radiation diffusion has been considered. Two first-order implicit time integration methods have been studied. The implicitly balanced method (IB) iterates the nonlinearities within a time step, while the linearized implicit (LI) method does not. Asymptotic analysis and modified equation analysis have been applied to both time integration methods, and numerical experiments have been used to highlight the results of the analysis.

Using asymptotic analysis, it has been shown that the IB method preserves the asymptotic equilibrium solution exactly ($E = T^4$). The LI method has been shown to preserve the asymptotic equilibrium solution, while not exactly preserving $E = T^4$. Numerical experiments have demonstrated that with large enough time steps the LI method can produce erroneous answers when the equilibrium answer is expected. This is related to the violation of a so-called maximum principle as discussed by Larsen and Mercier [9], and it is not related to a transport layer being modeled by diffusion. The analysis of Larsen and Mercier applies to linearization of the Planck function with a full multifrequency transport treatment rather than a grey nonequilibrium diffusion approximation, but their results must nonetheless be expected to be qualitatively if not quantitatively relevant to our calculations.

Using modified equation analysis we have been able to extract the terms which represent the first-order difference between the IB and LI solutions. We have used this analysis to demonstrate why the LI method will equilibrate a cold material field and a warm radiation field at a different rate than will be done with the IB method. We have also used this analysis to explain why the progress of a one-dimensional thermal wave using the LI method will always be slower than the progress simulated with the IB method.

The computational cost of the LI versus IB methods has not been addressed in this study. A brief comparison for nonequilibrium radiation diffusion was given in Ref. [14]. There, it was demonstrated that although IB can take a larger time step than LI-type methods and maintain design accuracy, these larger time steps come at the cost of increased Newton iterations per time step and thus increased computational cost per time step. In this study, at time steps where the LI method shows significant nonphysical behavior (see Fig. 6), the IB method results, although well-behaved, do have significant error. For example, the front position predicted by the IB method in Fig. 6 is approximately 20% ahead of the time-step converged position (compare with

Fig. 12). Nevertheless, in terms of robustness, the ability of the IB method to maintain a physical solution at large time steps is a definite advantage. In the end, a reliable time step control is needed for either method to ensure the methods operate with desired accuracy. Time step control and a detailed computational cost comparison should be a focus of future work.

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