A Multilevel Quasidiffusion Method with Hybrid Temporal Discretization for Thermal Radiative Transfer Problems

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INTRODUCTION

Nonlinear thermal radiative transfer (TRT) problems describe the interaction of radiation and matter. They are defined by the radiative transfer (RT) equation for the specific intensity $I_\nu = I_\nu(\mathbf{r}, \mathbf{\Omega}, \nu, t)$

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \mathbf{\Omega}\cdot\mathbf{\nabla} I_\nu + \varkappa_\nu(T) I_\nu = \varkappa_\nu(T) B_\nu(T) \tag{1a}$$

coupled with the energy balance (EB) equation

$$\frac{\partial \varepsilon(T)}{\partial t} = \int_0^\infty \int_{4\pi} \varkappa_\nu(T)\Big(I_\nu - B_\nu(T)\Big) d\mathbf{\Omega} d\nu \,. \tag{1b}$$

Here $\mathbf{r}$ is the spatial position; $\mathbf{\Omega}$ is the unit vector in the direction of particle motion; ν is the photon frequency; t is time; $\varkappa_\nu$ is the opacity; T is the material temperature; ε is the material energy density; $B_\nu(T) = \frac{2h\nu^3}{c^2}\Big(e^{\frac{h\nu}{kT}} - 1\Big)^{-1}$ is the Planckian spectrum. To solve the TRT problem (1) we use the quasidiffusion (QD) method that is also known as the Variable Eddington Factor (VEF) method [1–6]. It is formulated by a multilevel system of equations consisting of the high-order RT equation for the intensity and low-order equations for the energy density and radiative flux. This system of equations is closed exactly by stable linear-fractional QD (Eddington) factors.

To approximate the differential equations of the multilevel QD method, one can use independent discretization of the high-order and low-order equations. This approach enables one to increase the accuracy of the solution by improving discretization of the low-order equations for the moments of the intensity. In this paper, we study the multilevel QD method for TRT problems in which the RT and low-order QD (LOQD) equations are approximated by temporal discretization schemes of different orders of accuracy. The time-dependent RT equation is approximated with the first order backward Euler scheme. The time-dependent multigroup LOQD equations are discretized by the second order Crank-Nicolson (C-N) method. Thus, we use a relatively inexpensive and robust temporal scheme for the high-dimensional part of the system of equations and enhance the numerical solution by applying a scheme of higher resolution to the part of the problem with reduced dimensionality.

Like the RT equation, the time-dependent LOQD equations are hyperbolic. If high-order schemes are used to discretize hyperbolic equations, then monotonicity of the numerical solution is not guaranteed. This can lead to oscillations in the solution and other unphysical behavior. To remove or reduce these oscillations, it is necessary to use a monotonization procedure. In the proposed numerical method, we apply the Limited-Trapezoidal (L-TRAP) scheme for monotonization of the second-order scheme for the time-dependent multigroup LOQD equations. The L-TRAP scheme was developed for hyperbolic conservation laws [7]. It has been shown that this scheme significantly reduces the oscillatory behavior of the solution.

MULTILEVEL QD METHOD

The multilevel QD method for multigroup TRT problems is formulated by the following equations [1, 3–6]:
(a) the high-order RT equation for the group intensity

$$\frac{1}{c}\frac{\partial I_g}{\partial t} + \mathbf{\Omega}\cdot\mathbf{\nabla} I_g + \varkappa_{E,g} I_g = \varkappa_{B,g} B_g \,, \tag{2}$$

(b) the multigroup LOQD (MLOQD) equations for the group energy densities (E_g) and fluxes ($\mathbf{F}_g$)

$$\frac{\partial E_g}{\partial t} + \mathbf{\nabla}\cdot\mathbf{F}_g + c\varkappa_{E,g} E_g = 4\pi\varkappa_{B,g} B_g \,, \tag{3}$$

$$\frac{1}{c}\frac{\partial \mathbf{F}_g}{\partial t} + c\mathbf{\nabla}\cdot(\mathfrak{f}_g E_g) + \varkappa_{ros,g}\mathbf{F}_g = 0 \,, \tag{4}$$

$$\varkappa_{E,g} = \big\langle \varkappa_\nu, B(T_r)\big\rangle_g \,, \quad \varkappa_{B,g} = \big\langle \varkappa_\nu, B(T)\big\rangle_g \,, \tag{5}$$

$$(\varkappa_{ros,g})^{-1} = \Big\langle \varkappa_\nu^{-1}, \frac{\partial B}{\partial T}(T_r)\Big\rangle_g \,, \tag{6}$$

$$\big\langle \varkappa_\nu, w(T^*)\big\rangle_g = \int_{\nu_g}^{\nu_{g+1}} \varkappa_\nu(T) w_\nu(T^*) d\nu \Big/ \int_{\nu_g}^{\nu_{g+1}} w_\nu(T^*) d\nu \,,$$

where T_r is the effective temperature of radiation,

$$f_{g,\beta\gamma} = \int_{4\pi} \Omega_\beta \Omega_\gamma I_g d\mathbf{\Omega} \Big/ \int_{4\pi} I_g d\mathbf{\Omega} \,, \quad \beta,\gamma = x, y \tag{7}$$

are components of the group QD (Eddington) tensor $\mathfrak{f}_g$,
(c) the effective grey LOQD (GLOQD) equations for the radiation energy density (E) and flux ($\mathbf{F}$) coupled with the EB equation

$$\frac{\partial E}{\partial t} + \mathbf{\nabla}\cdot\mathbf{F} + c\bar{\varkappa}_E E = c\bar{\varkappa}_B a_R T^4 \,, \tag{8}$$

$$\frac{1}{c}\frac{\partial \mathbf{F}}{\partial t} + c\mathbf{\nabla}\cdot(\bar{\mathfrak{f}} E) + \bar{\varkappa}_{ros}\mathbf{F} + \bar{\boldsymbol{\eta}} E = 0 \,, \tag{9}$$

$$\frac{\partial \varepsilon}{\partial t} = c\bar{\varkappa}_E E - c\bar{\varkappa}_B a_R T^4 \,, \tag{10}$$

where $\bar{\varkappa}_E$, $\bar{\varkappa}_B$, $\bar{\mathfrak{f}}$, and $\bar{\varkappa}_{ros}$ are grey quantities averaged with the group solution. $\bar{\boldsymbol{\eta}}$ is a compensation term [4–6].

We consider TRT problems in 2D Cartesian geometry on orthogonal spatial grids. The modified subcell step method is used to discretize the RT equation in space [6, 8]. The MLOQD equations are discretized in space by a second-order accurate finite volume scheme. The discretization of the GLOQD equations is algebraically consistent with the discretization of

the MLOQD equations. To approximate the multilevel QD method in time, we apply the first-order fully implicit (backward Euler) scheme for temporal discretization of the RT, MLOQD and EB equations. The group opacities and Planckian emission terms are approximated implicitly. This method is referred to as the *first-order scheme*. In another method, we use (a) the first-order fully implicit discretization of the RT equation and (b) the C-N scheme of the second-order accuracy to approximate the MLOQD and EB equations. It is referred to as the *hybrid scheme*. A third variant of the temporal discretization is the hybrid scheme in which a monotonization procedure is applied to the C-N scheme. This method is referred to as the *monotonized hybrid scheme*.

MONOTONIZATION PROCEDURE

The spatially discretized MLOQD equations have the following general form:

$$\frac{dE_g}{dt} = L_{0,g}[E_g, \mathbf{F}_g, T]\,, \quad \frac{1}{c}\frac{d\mathbf{F}_g}{dt} = \mathbf{L}_{1,g}[E_g, \mathbf{F}_g, T]\,, \quad (11)$$

$$L_{0,g}[E_g, \mathbf{F}_g, T] = \boldsymbol{\nabla}\cdot\mathbf{F}_g + c\varkappa_{E,g}E_g - 4\pi\varkappa_{B,g}B_g\,, \quad (12)$$

$$\mathbf{L}_{1,g}[E_g, \mathbf{F}_g, T] = c\boldsymbol{\nabla}\cdot(\mathfrak{f}_g E_g) + \varkappa_{ross,g}\mathbf{F}_g\,. \quad (13)$$

Let us consider the θ-weighted method for Eq. (11). The discretized MLOQD equations are given by

$$E_g^{n+1} - E_g^n = \tau^n\left(\theta L_{0,g}^{n+1} + (1-\theta)L_{0,g}^n\right), \quad (14a)$$

$$\mathbf{F}_g^{n+1} - \mathbf{F}_g^n = c\tau^n\left(\theta \mathbf{L}_{1,g}^{n+1} + (1-\theta)\mathbf{L}_{1,g}^n\right), \quad (14b)$$

where n is the index of the time level, and τ^n is the n-th time step. For this method, θ is a specified parameter. When $\theta = 1$, this scheme is equivalent to the backward Euler method which is the first-order accurate in time. When $\theta = \frac{1}{2}$, it becomes the C-N method which is second-order accurate.

The L-TRAP scheme is applied to the MLOQD equations (14) [7]. This method restricts θ such that a monotonicity condition is not violated. We define

$$s_{0,g}^{n+\frac{1}{2}} = \frac{1}{\tau^n}\left(E_g^{n+\frac{1}{2}} - E_g^n\right)\,, \quad s_{1,\alpha,g}^{n+\frac{1}{2}} = \frac{1}{c\tau^n}\left(F_{g,\alpha}^{n+\frac{1}{2}} - F_{g,\alpha}^n\right)\,, \quad (15)$$

$$E_g^{n+\frac{1}{2}} = E_g^n + \tau^n L_{0,g}^{n+1}\,, \quad F_{g,\alpha}^{n+\frac{1}{2}} = F_{g,\alpha}^n + \tau^n L_{1,g,\alpha}^{n+1}\,, \quad (16)$$

where $F_{g,\alpha}^n = \mathbf{F}_g^n\cdot\mathbf{e}_{n,\alpha}$, $\mathbf{e}_{n,\alpha}$ is the face normal, $\alpha = L, R, T, B$ is the index of the cell face. A parameter, r_{ij}, is defined for each cell in the domain with $\theta_{ij} = 1 - 0.5r_{ij}$. The monotonization scheme checks whether $L_{0,g}^n$, $L_{0,g}^{n+\frac{1}{2}}$ and $L_{1,\alpha,g}^n$, $L_{1,\alpha,g}^{n+\frac{1}{2}}$ are within the intervals $[0, 2s_{g,0}^{n+\frac{1}{2}}]$ and $[0, 2s_{p,\alpha,g}^{n+\frac{1}{2}}]$, respectively. If these conditions are met, then θ is set to $\frac{1}{2}$. If one or both quantities are of opposite sign, they can be non-monotonic and therefore θ is set to 1. If neither condition is met, this is a case where the derivative has the same sign but is too large. The minimum r_{ij} that still preserves monotonicity is selected. The algorithm of the L-TRAP scheme is defined as

if $L^{n+\frac{1}{2}}(L^{n+\frac{1}{2}} - 2s^{n+\frac{1}{2}}) \le \epsilon$ *and* $L^n\left(L^n - 2s^{n+\frac{1}{2}}\right) \le \epsilon$ **then**
  $r_{ij} = 1$
else if $L^{n+\frac{1}{2}} \le -\tilde{\epsilon}(s^{n+\frac{1}{2}} + \epsilon)$ *or* $L^n \le -\tilde{\epsilon}(s^{n+\frac{1}{2}} + \epsilon)$ **then**
  $r_{ij} = 0$
else
  $r_{ij} = \min\left[\frac{2s^{n+\frac{1}{2}}}{L^n + \epsilon}, \frac{2s^{n+\frac{1}{2}}}{L^{n+\frac{1}{2}} + \epsilon}, 1\right]$
end

Note that we omitted subscripts in the algorithm. The parameters ϵ and $\tilde{\epsilon}$ are set to a small value that prevents breaking the condition due to small changes in the solution.

This monotonization procedure adds a stage for evaluating $E_g^{n+\frac{1}{2}}$ and $F_{g,\alpha}^{n+\frac{1}{2}}$ before solving the MLOQD equations. It also makes the temporal scheme nonlinear. However, the multilevel QD method is a nonlinear one originally. The nonlinearity of the algorithm does not significantly affect iterations for solving nonlinear multilevel system of equations.

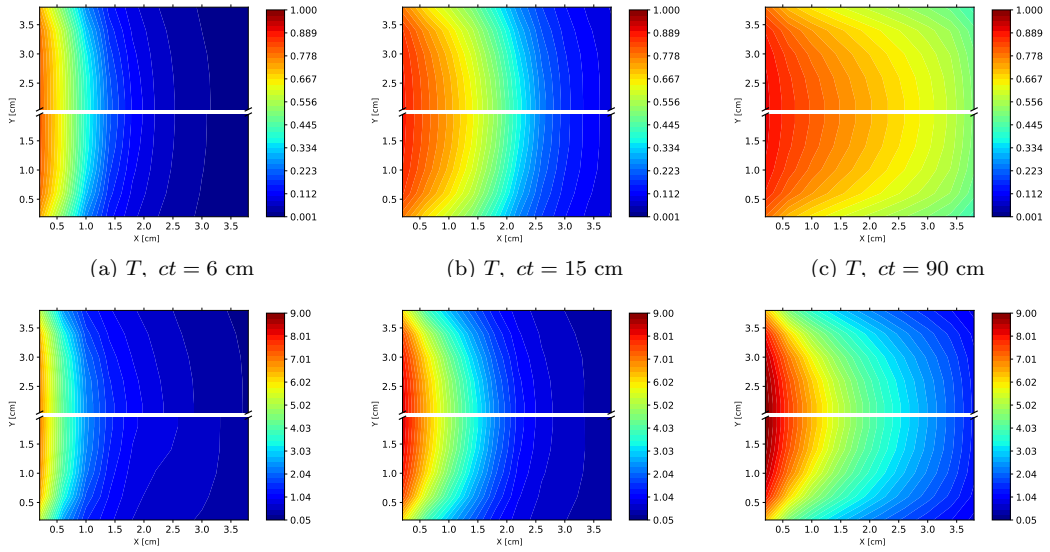
NUMERICAL RESULTS

To demonstrate the performance of each time discretization scheme, we present computational results of a Fleck-Cummings test problem [9]. A square 4×4 cm domain is made of one material with the opacity of the material given by $\varkappa_\nu(T) = \frac{27}{\nu^3}\left(1 - e^{-\frac{\nu}{T}}\right)$, where ν and T are in units of keV. There is incoming radiation with the Planckian spectrum at T_b=1 keV at the left boundary. The rest of boundaries are vacuum. The initial temperature in the domain is T_0=10^{-3} keV. The initial distribution of radiation is $I_\nu|_{t=0} = B_\nu(T_0)$. The material energy is given by $\varepsilon(T) = c_v T$, where $c_v = 0.5917 a_R T_b^3$. The spatial mesh is uniform with 10×10 square cells. We use 17 groups and a quadruple-range quadrature with 36 angles/octant. The parameters of convergence criteria for transport iterations are equal to 10^{-6}.

Figures 1 and 2 show numerical solutions obtained by each of three methods at different instants of time with the constant time step $\tau = 2\times10^{-2}$ ns. There are no oscillations in T and E obtained by the hybrid scheme, but at $ct = 6$ cm, we notice that the energy density has a change in sign of the second derivative before the front (See Fig. 1d). It is caused by non-monotonicity of E_g in some groups. This behavior is illustrated in Figures 3a and 3c, where E_g computed by the hybrid scheme are shown for groups $g = 13$ (7 keV $\le \nu \le$ 9 keV) and $g = 16$ (15 keV$\le \nu \le$ 20 keV). The matter is optically thin in these groups. The optically thick groups do not show this behavior and the intermediate groups are mildly affected but the oscillations are not as drastic. The L-TRAP monotonization procedure corrects the shape of the solution of the time-dependent MLOQD equations. Figures 3b and 3d show the solution of the monotonized hybrid scheme in these groups. The effect on the energy density

can be seen in Figure 2d.

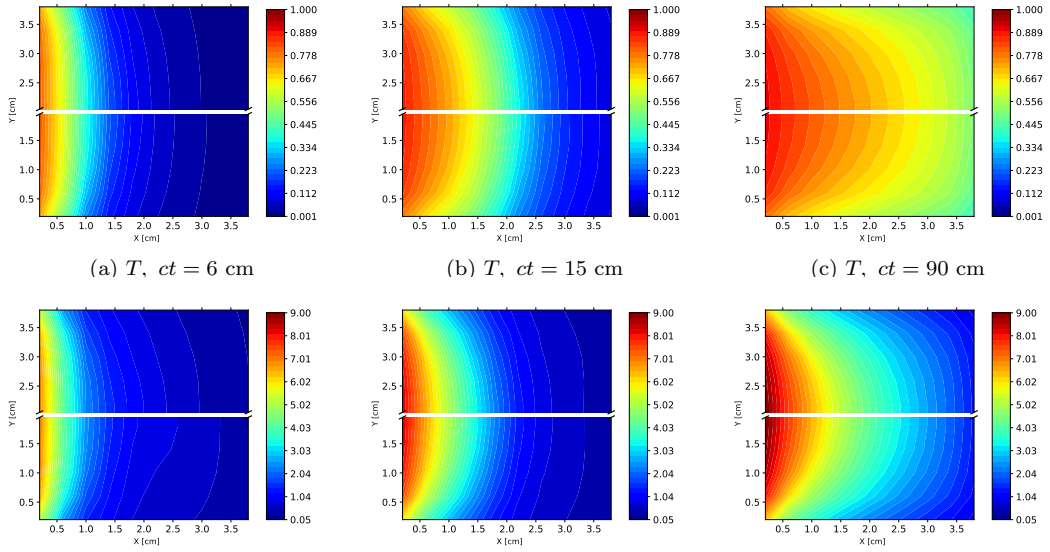
Analysis of the convergence rates of the solution with the time step refinement showed that the hybrid method converges with the first order. To evaluate the accuracy of the hybrid scheme we use the reference numerical solution obtained on the same spatial and angular mesh with a small time step $\tau = 7.8125 \times 10^{-5}$ ns. Figure 4 shows comparison of the solution computed with $\tau = 2{\times}10^{-2}$ ns with the reference solution at different instants of time. These results show that the hybrid scheme has higher accuracy than the first-order scheme. The monotonized hybrid scheme performs similarly to the first-order scheme at the early stages of the test problem when there is a need to correct the solution to preserve its monotonicity. Its accuracy approaches the accuracy of the hybrid scheme at the later stages.



(a) T, $ct = 6$ cm (b) T, $ct = 15$ cm (c) T, $ct = 90$ cm

(d) E, $ct = 6$ cm (e) E, $ct = 15$ cm (f) E, $ct = 90$ cm

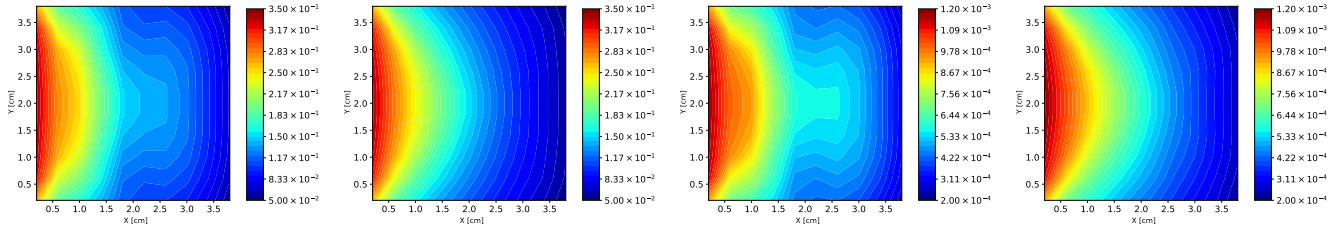
Figure 1: Temperature (in keV) and energy density ($E{\times}10^{-13}\frac{erg}{cm^3}$) computed by means of the first-order scheme (top-half) and the hybrid scheme (bottom-half) with $\tau{=}2{\times}10^{-2}$ ns.



(a) T, $ct = 6$ cm (b) T, $ct = 15$ cm (c) T, $ct = 90$ cm

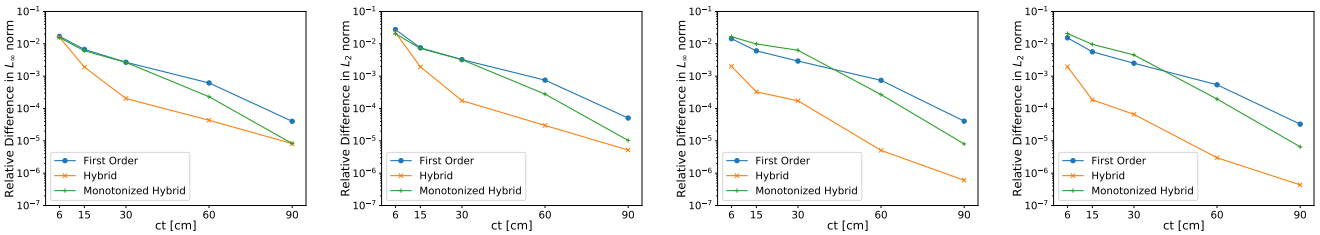
(d) E, $ct = 6$ cm (e) E, $ct = 15$ cm (f) E, $ct = 90$ cm

Figure 2: Temperature (in keV) and energy density ($E{\times}10^{-13}\frac{erg}{cm^3}$) computed by means of the monotonized hybrid scheme (top-half) and the hybrid scheme (bottom-half) with $\tau{=}2{\times}10^{-2}$ ns.



(a) $g = 13$, hybrid scheme (b) $g = 13$, monotonized hybrid scheme (c) $g = 16$, hybrid scheme (d) $g = 16$, monotonized hybrid scheme

Figure 3: Group energy densities ($E_g \times 10^{-13} \frac{erg}{cm^3}$) computed by the hybrid and monotonized hybrid schemes at ct=6 cm.



(a) $||E - E_{ref}||_{L_\infty}/||E_{ref}||_{L_\infty}$ (b) $||E - E_{ref}||_{L_2}/||E_{ref}||_{L_2}$ (c) $||T - T_{ref}||_{L_\infty}/||T_{ref}||_{L_\infty}$ (d) $||T - T_{ref}||_{L_2}/||T_{ref}||_{L_2}$

Figure 4: The norm of difference of the solution computed with $\tau = 2 \times 10^{-2}$ ns compared to the reference solution.

CONCLUSION

We developed a hybrid temporal discretization scheme for the multilevel QD method for solving TRT problems. It is based on the first-order fully implicit scheme for the high-order time-dependent radiative transfer equation and the second-order scheme for the time-dependent multigroup low-order QD equations. The discretization of the grey LOQD equations is consistent with the scheme for the MLOQD equations. Thus, it is approximated with the same temporal scheme as the MLOQD equations. The numerical results showed that the developed hybrid time-integration scheme for the multilevel QD method is first order accurate. However, it generates more accurate solution than the uniform first-order scheme based on the fully implicit (backward Euler) method. To address the natural issue of non-monotonicity of a high-order scheme for hyperbolic time-dependent LOQD equations, we apply the monotonization procedure based on the L-TRAP scheme. The resulting nonlinear monotonized hybrid scheme demonstrates good performance. More studies are necessary to further analyze the properties of the proposed schemes.

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