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Time discrete scheme matched adaptive time step for particle transport equations

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A B S T R A C T

The conventional time discrete schemes seldom consider adaptive time step. Therefore some physical quantity for time variable exits numerical oscillation. The motivation in this paper is to provide a time discrete scheme which matches adaptive time step. The typical exponential method, diamond difference and modified time discrete scheme, second-order time evolution scheme are researched for adaptive time step. Some numerical results show that time differential curves (particle current especially) are very smooth for second-order time evolution scheme associated the exponential method.

1. Introduction

With the development of nuclear energy, the new fission-type reactor with complex structure, strong non-uniform medium, strong anisotropic property is given more and more attention. Furthermore, the nuclear device has more complicated characteristics, for example, width energy region, complicated dynamic state. Therefore, the time-dependent transport equations are studied to comprehend time behavior for neutron, photon, charged particle. To transport equation, some research take focus on space discrete schemes (Lathrop, 1969; Lewis and Miller, 1993). When we discuss the time-dependent equation, the time discrete scheme should be considered carefully. The reference McClarren (2008) gives the convergence property to radiation transport equation. To time discrete scheme, there are Backward Euler (Szilard and Pomraning, 1992) method with $O(\Delta t)$ and Crank–Nicolson method (McClarren, 2008) with $O(\Delta t^2)$. However, the Crank–Nicolson method produces numerical oscillation. The reference McClarren (2008) combines Backward Euler and Crank–Nicolson method to avoid numerical oscillation. The reference Olson (2009) constructs the second-order time evolution scheme (*SOTE*) to P_N equation for radiation transport equation which reduce the numerical oscillation.

Moreover, the finite volume method (*FVM*) is usually apply to time discrete scheme which solves particle transport equation on time interval $[t_{n+1/2}, t_{n+3/2}]$ (Morel and Wareing, 1996; Lathrop, 1969) to give numerical flux with $O(\Delta t^2)$ at t_{n+1}. However, these discrete schemes need to introduce extrapolation formula, for example, exponential extrapolation, diamond extrapolation. Furthermore these extrapolation formulas seldom consider time step change and produce numerical oscillation for adaptive time step. Time step is very important to time-dependent particle transport equations which impacts numerical precision and computing time. Time step is given by physical progress in a general way and time step change is very large (some magnitude difference) for the whole physical progress.

However, these simple extrapolation equations are not adapt to complex time-dependent progress for multi-media problem and numerical precision is very poor for adaptive time step problem. Therefore, some key physical quantities exit large oscillation. In the reference Hong et al. (2010a, b), we construct a modified time discrete scheme. Therefore the time differential curve of particle number is very smooth. Through profound research, the time differential curve of particle current for modified time discrete scheme still exits large oscillation which takes difficulty to physical research. Therefore, we study time discrete scheme matched adaptive time step to simulate time differential curve of different physical quantity in particular for particle current.

In this paper, we construct time discrete scheme for multi-media complex time-dependent progress and apply second-order time evolution to discrete ordinates (S_N) equation for one-dimensional spherical geometry particle transport equation.

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The remainder of this paper is organized as follows. In Section 2, some conventional time discrete schemes are presented. In Section 3, a modified time discrete scheme is presented. In Section 4, we introduce the second-order time evolution scheme. In Section 5, we provide some numerical results of different scheme for some problems. Finally, Section 6 will summarize the paper with an eye to the future.

2. Conventional time discrete scheme

The time-dependent particle transport equation may be written as follows in multi-group form:

$$\frac{1}{v_g}\frac{\partial\varphi_g}{\partial t}+\Omega\cdot\nabla\varphi_g+\sum\nolimits_g^{tr}\varphi_g = Q_g,\ \ g = 1,\cdots,G. \tag{1}$$

where φ_g is angular flux of $g'th$ group particle, v_g is velocity of $g'th$ group particle, Σ_g^{tr} is total macroscopic cross section of $g'th$ group particle, and Q_g is total source (including scatter source (Q_g^s), fission source (Q_g^f) and external source (S_g)).

$$Q_g = \frac{1}{4\pi}\left[Q_g^f+Q_g^s+S_g\right]. \tag{2}$$

In this paper, we focus on the conservative equation for 1-D spherical geometry transport equations in multi-group form:

$$\frac{1}{v_g}\frac{\partial\varphi_g}{\partial t}+\frac{\mu}{r^2}\frac{\partial(r^2\varphi_g)}{\partial r}+\frac{1}{r}\frac{\partial\left[(1-\mu^2)\varphi_g\right]}{\partial\mu}+\sum\nolimits_g^{tr}\varphi_g = Q_g. \tag{3}$$

With the following initial and boundary conditions:

$$\varphi_g(r,\mu,0) = \varphi_g^{(0)}(r,\mu), t = 0, 0\le r\le r_J. \tag{4}$$

$$\varphi_g(r_J,\mu,t) = 0, \mu\le 0. \tag{5}$$

Where r_J is the outermost boundary point.

To the spherical geometry transport equation, the finite volume method is a conventional method which involves extrapolation of angular, time, space variables. These extrapolations adopt same form or different form. Exponential method (*EM*) and diamond difference (*DD*) are classical extrapolations. Time step is large at flat stage and small at strenuous stage for physical progress. Therefore, adaptive time step is adopted in numerical calculation for practical physical problem.

We generally take Eq. (3) in the intervals $[t_{n+1/2}, t_{n+3/2}]$ to solve flux at t_{n+1}. However, the time step between t_{n+1} and $t_{n+3/2}$ should be dynamic given by physical progress. The time step is unknown for interval $t_{n+3/2}$ to t_{n+1} when introduce time extrapolation.

The nature of particle transport equation determines the order of numerical solution procedure. The upwind scheme must be employed. In order to compute $\varphi_{k+1/2}^{n+1}$, the extrapolation formula about $\varphi_{k+1/2}^{n+3/2}$ is introduced to close discrete equation. In this paper, we introduce two kinds of extrapolation formulas in the following form.

The extrapolation formula of exponential method for time variable is as follows:

$$\left(\varphi_{k+\frac{1}{2}}^{n+1}\right)^2 = \varphi_{k+\frac{1}{2}}^{n+\frac{3}{2}}\varphi_{k+\frac{1}{2}}^{n+\frac{1}{2}}. \tag{6}$$

The extrapolation formula of diamond difference method for time variable is as follows

$$2\varphi_{k+\frac{1}{2}}^{n+1} = \varphi_{k+\frac{1}{2}}^{n+\frac{3}{2}}+\varphi_{k+\frac{1}{2}}^{n+\frac{1}{2}}. \tag{7}$$

For the sake of simplicity representation, we omit the detailed derivation for these conventional time discrete schemes.

3. Modified time discrete scheme

If taking exponential extrapolation or diamond extrapolation for time variable, the extrapolation flux will exit deviation when time step has great change (sometimes magnitude difference). We will adopt modified time discrete scheme (Hong et al., 2010a, b). The modified extrapolation formula ($\tilde{\varphi}_{k+1/2}^{n+1/2}$) for different time discrete scheme is described as follows.

The modified exponential method (*MEM*) is:

$$\tilde{\varphi}_{k+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{\left(\varphi_{k+\frac{1}{2}}^{n}\right)^{\frac{\tilde{\Delta}t_{n+1}+\tilde{\Delta}t_n}{\tilde{\Delta}t_n}}}{\left(\varphi_{k+\frac{1}{2}}^{n-\frac{1}{2}}\right)^{\frac{\tilde{\Delta}t_{n+1}}{\tilde{\Delta}t_n}}}. \tag{8}$$

The modified diamond difference (*MDD*) is:

$$\tilde{\varphi}_{k+\frac{1}{2}}^{n+\frac{1}{2}} = \varphi_{k+\frac{1}{2}}^{n}\frac{\tilde{\Delta}t_{n+1}+\tilde{\Delta}t_n}{\tilde{\Delta}t_n}-\varphi_{k+\frac{1}{2}}^{n-\frac{1}{2}}\frac{\tilde{\Delta}t_{n+1}}{\tilde{\Delta}t_n} \tag{9}$$

Where $\tilde{\Delta}t_n = t_n\text{-}t_{n-1}$.

We will take the step scheme if Eq. (9) exits negative flux. These modified time schemes are very simple and are easy to embed some large-scale application programs.

4. Second-order time evolution scheme

To consider time step change in the whole physical progress adequately, we apply second-order time evolution scheme to time-dependent spherical geometry particle transport equation by discrete ordinates method. *SOTE* considers adaptive time step for the whole physical progress and has no use for extrapolation of time variable.

Now, we deduce discrete scheme for particle transport equation by *SOTE*. *SOTE* takes three-level backward difference and the specific equation is as followed (Olson, 2007, 2009):

$$\varphi_g^{n+1}(r,\mu) = \beta\varphi_g^{n}(r,\mu)+(1-\beta)\varphi_g^{n-1}(r,\mu)+\gamma\Delta t_{n+1}\frac{\partial\varphi_g(r,\mu)}{\partial t}. \tag{10}$$

Where

$$\beta = \frac{(1+\rho)^2}{1+2\rho}, \gamma = \frac{1+\rho}{1+2\rho}, \rho = \frac{t_{n+1}-t_n}{t_n-t_{n-1}} \tag{11}$$

To constant the time step problem, $\rho = 1$, $\beta = 4/3$, $\gamma = 2/3$.

The Eq. (10) is rewritten as follows:

$$\frac{\partial\varphi_g(r,\mu)}{\partial t} = \frac{\varphi_g^{n+1}(r,\mu)-\beta\varphi_g^{n}(r,\mu)-(1-\beta)\varphi_g^{n-1}(r,\mu)}{\gamma\Delta t_{n+1}}. \tag{12}$$

Taking Eq. (12) to Eq. (3), we get the time discrete equation:

$$\frac{\varphi_g^{n+1}(r,\mu)-\beta\varphi_g^{n}(r,\mu)-(1-\beta)\varphi_g^{n-1}(r,\mu)}{\gamma\Delta t_{n+1}v_g}+\frac{\mu}{r^2}\frac{\partial\left(r^2\varphi_g^{n+1}\right)}{\partial r} + \sum\nolimits_g^{tr}\varphi_g^{n+1} = Q_g^{n+1}. \tag{13}$$

Divide the intervals $0\le r\le r_J$, $-1\le\mu\le 1$, $0\le t\le T$ by