Second-order time evolution scheme for time-dependent neutron transport equation

Zhenying Hong, Guangwei Yuan, Xuedong Fu, Shulin Yang

Abstract—In this paper, the typical exponential method, diamond difference and modified time discrete scheme is researched for self adaptive time step. The second-order time evolution scheme is applied to time-dependent spherical neutron transport equation by discrete ordinates method. The numerical results show that second-order time evolution scheme associated exponential method has some good properties. The time differential curve about neutron current is more smooth than that of exponential method and diamond difference and modified time discrete scheme.

Keywords—exponential method, diamond difference, modified time discrete scheme, second-order time evolution scheme.

I. 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 characteristic, for example, width energy region, complicated dynamic state. Therefore, the time-dependent transport equation is studied to comprehend the time behavior for neutron, photon, charged particle. To transport equation, some research has focus on space discrete scheme[1], [8]. When we discuss the time-dependent equation, the time discrete scheme should be considered carefully. The reference[2] gives the convergence property to radiation transport equation. To time discrete scheme, there are Backward Euler method[3] with O(Δt) and Crank-Nicolson method with O(Δt^2). However, the Crank-Nicolson method can produce numerical oscillation. The reference[4] combines the Backward Euler and Crank-Nicolson method to avoid the numerical oscillation. The reference[6] constructs the second-order time evolution scheme[7] to Pn equation for radiation transport equation which reduces the numerical oscillation.

Moreover, the finite volume method (FVM) is usually applied to the time discrete scheme which solves the neutron transport equation on time interval [t_{n+1/2}, t_{n+3/2}],[5][9] to give the numerical flux with O(Δt^2) at t_{n+1}. However, these discrete schemes need to introduce extrapolation formula, for example, exponential extrapolation, diamond extrapolation. Furthermore these extrapolation formula seldom consider the time step change and produce numerical oscillation for adaptive time step. The time step is very important to time-dependent neutron transport equation which impacts the numerical precision and computing time. The time step is given by physical progress in a general way and the time step change is very large(such as some magnitudes) between the whole physical progress.

However, these simple extrapolation equations are not adapted to complex time-dependent progress for multi-media problem and the numerical precision is very poor for adaptive time step problem. Therefore, the key physical quantity exists large oscillation. In the reference[10], we construct modified time discrete scheme and the time differential curve of neutron number is very smooth. Through profound research, the time differential curve of neutron current for modified time discrete scheme still exists large oscillation which takes difficulty to physical analyse. Therefore, we study the time discrete scheme to give high numerical precision scheme to simulate time differential curve of different physical quantity in particular for neutron current.

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

The remainder of this paper is organized as follows. In Section 2, the modified time discrete scheme is presented. In Section 3, we introduce the second-order time evolution scheme. In Section 4, we provide numerical results for different scheme. In the final section, we offer a summary with some concluding remarks.

II. MODIFIED TIME DISCRETE SCHEME

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

\[ \frac{1}{v_g} \frac{\partial \varphi_g}{\partial t} + \Omega \cdot \nabla \varphi_g + \Sigma_{tr}^{g} \varphi_g = Q_g, \quad g = 1, \cdots, G. \] (1)

where \( \varphi_g \) is the angular flux of \( g-th \) group neutron, \( v_g \) is the velocity of \( g-th \) group neutron, \( \Sigma_{tr}^{g} \) is the total macroscopic cross section of \( g-th \) group neutron, and \( Q_g \) is the sum of scattering source(\( Q_s^g \)), fission source(\( Q_f^g \)) and external source(\( S_g \)).

\[ Q_g = \frac{1}{4\pi} \left[ Q_s^g + Q_f^g + S_g \right]. \] (2)

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

\[ \frac{1}{v_g} \frac{\partial \varphi_g}{\partial t} + \frac{\mu}{r^2} \frac{\partial}{\partial r} \left( r^2 \varphi_g \right) + \frac{1}{r} \frac{\partial}{\partial \mu} \left[ (1 - \mu^2) \varphi_g \right] + \Sigma_{tr}^{g} \varphi_g = Q_g. \] (3)
With the following initial and boundary conditions:

\[ \varphi_g(r, \mu, 0) = \varphi_g^{(0)}(r, \mu), t = 0, 0 \leq r \leq r_J. \]  

\[ \varphi_g(r_J, \mu, t) = 0, \mu \leq 0. \]  

Where \( r_J \) is the outermost boundary point.

To spherical transport equation, the finite volume method (FVM) is the typical method which involves the extrapolation of angular, time, space variables. These extrapolation can adopt the same form and also adopt different form for specific physical problems. The classical extrapolations are exponential method(EM), diamond difference(DD). The time discrete scheme should considered for adaptive time step. The time step can be large at flat stage for physical progress and be small at strenuous stage for physical progress. Therefore, the adaptive time step is adopted in numerical calculation for practical physical problem.

We general 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 time extrapolation is introduced. If taking exponential extrapolation or diamond extrapolation for time variable, the extrapolation flux can exist deviation when the time step has great change(sometimes magnitude difference ). The modified time discrete scheme can be adopted[10].

The modified equation( \( \varphi_g^{n+\frac{1}{2}} \) ) for different time discrete scheme is described as follows.

The modified exponential method(MEM) is

\[ \varphi_g^{n+\frac{1}{2}} = \left( \frac{2 \Delta t_{n+1}}{2 \Delta t_{n} + \Delta t_{n+1}} \right)^{\alpha} \varphi_g^{n} + \left( \frac{2 \Delta t_{n}}{2 \Delta t_{n} + \Delta t_{n+1}} \right)^{\alpha} \varphi_g^{n+1}. \]  

The modified diamond difference(MDD) is

\[ \varphi_g^{n+\frac{1}{2}} = \frac{\varphi_g^{n}(\Delta t_{n+1} + \Delta t_{n})}{\Delta t_{n}} - \frac{\varphi_g^{n+1}(\Delta t_{n+1})}{\Delta t_{n}} \]  

Where \( \Delta t_{n} = t_{n+1} - t_{n-1} \), \( \Delta t_{n+1} = t_{n+1} - t_{n} \). There may appear negative flux for MDD, therefore we take step scheme for this case. The MEM, MDD is very simple and is easy to embed the flux old program.

III. SECOND-ORDER TIME EVOLUTION SCHEME

To consider the time step change in the whole physical progress adequately, we apply the second-order time evolution(SOTE) scheme to time-dependent spherical neutron transport equation by discrete ordinates(Sn) method. The SOTE considers the case of adaptive time step for the whole physical progress and needs not to introduce exponential extrapolation or diamond extrapolation.

Now, we deduce the discrete scheme for neutron transport equation by SOTE. The SOTE take three-level backward difference and the specific equation is as followed[7,8]:

\[ \frac{\partial \varphi_g}{\partial t}(r, \mu) = \frac{1}{r^2} \frac{\partial \varphi_g}{\partial r}(r, \mu) + \frac{2}{r} \varphi_g + \Sigma_g' \varphi_g = Q_g. \]  

Where \( \beta = \frac{(1 + \gamma)^2}{\gamma - 2}, \gamma = \frac{1 + \rho}{\gamma - 2}, \rho = \frac{\eta_{n+1} - \eta_{n}}{\eta_{n+1} - \eta_{n-1}}. \) To constant time step problem, \( \rho = 1, \beta = \frac{1}{2}, \gamma = \frac{3}{2}. \)

The Eq.(8) is rewritten as follows:

\[ \varphi_g^{n+1}(r, \mu) - \beta \varphi_g^{n}(r, \mu) - (1 - \beta)\varphi_g^{n-1}(r, \mu) = \gamma \Delta t_{n+1} \]  

Taking Eq.(9) to Eq.(8), we get the time discrete equation:

\[ \frac{\partial \varphi_g}{\partial t}(r, \mu) = \frac{\partial \varphi_g}{\partial r}(r, \mu) + \frac{2}{r} \varphi_g + \Sigma_g' \varphi_g = Q_g. \]  

Divide the intervals \( 0 \leq r \leq r_J, -1 \leq \mu \leq 1, 0 \leq t \leq T \) by

\[ 0 = t_0 < t_\frac{1}{2} \cdots < t_{k-\frac{1}{2}} = \frac{1}{2}\left(t_{k-1} + t_{k}\right). \]

By integrating Eq.(10) on intervals \( t_{k+1}^{n+1} \), \( \mu_{m-\frac{1}{2}} \leq \mu \leq \mu_{m+\frac{1}{2}} \), we get:

\[ \varphi_g^{n+1}(r, \mu) = \varphi_g^{n+1}(r, \mu_{m-\frac{1}{2}}) \]

\[ = \frac{\mu_m}{V_{n+1}^{k+\frac{1}{2}}} \left[ A_k^{n+1} + \frac{\alpha_m^{n+1}}{V_g^{k+\frac{1}{2}}} + \frac{\alpha_m^{n+1}}{V_g^{k+\frac{3}{2}}} \right]. \]

Where

\[ V_{n+1}^{k+\frac{1}{2}} = \left[ \Sigma_{tr,n+1}^{r,n+1} \varphi_g^{n+1} + \Sigma_{tr,n+1}^{r,n+1} \varphi_g^{n+1} \right], \]

\[ A_k^{n+1} = (r_{n+1}^{k+1})^2, A_k^{n+1} = (r_{n+1}^{k+1})^2, \]

\[ \alpha_m^{n+1} = (1 - \mu^2) m_{n+1} + r_{n+1}^{k+1} = \mu_{m+\frac{1}{2}} - \mu_{m-\frac{1}{2}}. \]

To \( \mu = -1 \), the Eq.(3) is:

\[ 1 \frac{\partial \varphi_g}{\partial t} + \frac{1}{r^2} \frac{\partial \varphi_g}{\partial r}(r, \mu) + \frac{2}{r} \varphi_g + \Sigma_g' \varphi_g = Q_g. \]
Therefore, to \( \mu_m = -1 \), the discrete equation is:

\[
\varphi_{n+1}^{g,m,k} = \beta \varphi_{n}^{g,m,k} - (1 - \beta) \varphi_{n-1}^{g,m,k} - \gamma \Delta t_{n+1} v g \frac{(A_{k+1} - A_{k}) \varphi_{n}^{g,m,k} + (A_{k+1} - A_{k-1}) \varphi_{n+1}^{g,m,k} + \gamma \Delta t_{n+1} v g \frac{A_{k+1} - A_{k}}{A_{k+1} - A_{k-1}} \alpha_m}{2V_{n+1} \mu_m}
\]

To \( \mu_m < 0 \), we take Eq.(17), Eq.(18) to Eq.(14) or Eq.(16) and to \( \mu_m > 0 \), we take Eq.(17), Eq.(19) to Eq.(14). Through rearrangement, we get:

\[
a \left( \varphi_{n+1}^{g,m,k} \right)^2 + b \varphi_{n+1}^{g,m,k} + c = 0.
\]

To \(-1 < \mu_m < 0\):

\[
a = -\frac{\mu_m A_{k+1}^{n+1}}{\sqrt{V_{n+1}^{g,m,k} v g} \alpha_m + \frac{1}{\gamma \Delta t_{n+1} v g}},
\]

\[
b = \frac{\alpha_m}{\gamma \Delta t_{n+1} v g} + \frac{\gamma \Delta t_{n+1} v g}{\sqrt{V_{n+1}^{g,m,k} v g} \alpha_m + \frac{1}{\gamma \Delta t_{n+1} v g}} - \frac{\beta \varphi_{n+1}^{g,m,k} + (1 - \beta) \varphi_{n-1}^{g,m,k}}{\gamma \Delta t_{n+1} v g}.
\]

To \( \mu_m > 0 \):

\[
a = \frac{\mu_m A_{k+1}^{n+1}}{\sqrt{V_{n+1}^{g,m,k} v g} \alpha_m + \frac{1}{\gamma \Delta t_{n+1} v g}},
\]

\[
b = \frac{1}{\gamma \Delta t_{n+1} v g} + \frac{\gamma \Delta t_{n+1} v g}{\sqrt{V_{n+1}^{g,m,k} v g} \alpha_m + \frac{1}{\gamma \Delta t_{n+1} v g}} - \frac{\beta \varphi_{n+1}^{g,m,k} + (1 - \beta) \varphi_{n-1}^{g,m,k}}{\gamma \Delta t_{n+1} v g}.
\]

We can know that the above equations are not closed and should introduce the extrapolation relation for angular variable and space variable. In this paper, we introduce the exponential extrapolation and diamond extrapolation to angular and space variable which are named SOTE EM, SOTE DD respectively.

The exponential extrapolation for angular variable and space variable is given as follows:

\[
\varphi_{n+1}^{g,m,k+\frac{1}{2}} = \left( \frac{n+\frac{1}{2}}{n+1} \right)^{\frac{1}{2}} \varphi_{n+1}^{g,m,k-\frac{1}{2}}
\]

\[
\varphi_{n+1}^{g,m,k} = \left( \frac{n+\frac{1}{2}}{n+1} \right)^{\frac{1}{2}} \varphi_{n+1}^{g,m,k+\frac{1}{2}}
\]

\[
\varphi_{n+1}^{g,m,k+\frac{1}{2}} = \left( \frac{n+\frac{1}{2}}{n+1} \right)^{\frac{1}{2}} \varphi_{n+1}^{g,m,k-\frac{1}{2}}
\]

Based on Eq.(20), the flux \( \varphi \) is written as:

\[
\varphi_{n+1}^{g,m,k+\frac{1}{2}} = \varphi_{n+1}^{g,m,k} - \beta (1 - \beta) \varphi_{n-1}^{g,m,k}
\]

Furthermore, diamond extrapolation to angular variable and space variable is:

\[
\varphi_{n+1}^{g,m,k+\frac{1}{2}} = \frac{\varphi_{n+1}^{g,m,k} - \varphi_{n}^{g,m,k}}{f \varphi_{n+1}^{g,m,k} - (f - 1) \varphi_{n}^{g,m,k} + \frac{1}{2} f \varphi_{n-1}^{g,m,k}}
\]

(36)

\[
\varphi_{n+1}^{g,m,k+\frac{1}{2}} = \varphi_{n+1}^{g,m,k} - (f - 1) \varphi_{n+1}^{g,m,k+1}
\]

(37)

\[
\varphi_{n+1}^{g,m,k+\frac{1}{2}} = (f - 1) \varphi_{n+1}^{g,m,k+1}
\]

(38)

Where \( f = 1 \) is step scheme extrapolation. \( f = 2 \) is diamond extrapolation.
We take Eq. (36), Eq. (37) to Eq. (14), then we get the discrete equation for \(-1 < \mu_m < 0\). Similarly, we take Eq. (36), Eq. (38) to Eq. (14), then we get the discrete equation for \(\mu_m > 0\). And we take Eq. (36), Eq. (38) to Eq. (16), we get the discrete equation for \(\mu_m = -1\). Through rearrangement, we get:

\[
\phi_{g,m,k+\frac{1}{2}}^{n+1} = \left(\phi_{g,m,k+\frac{1}{2}}^{n} + b + c\right)/a. \tag{39}
\]

To \(-1 < \mu_m < 0\):

\[
a = \frac{1}{v_g \Delta t_{n+1}} - f \mu_m A_{k+1}^{n+1} + \frac{f \left(A_{k+1}^{n+1} - A_{k}^{n+1}\right) \alpha_{m+\frac{1}{2}}}{2V_{k+\frac{1}{2}} V_m} + \frac{f \left(A_{k+1}^{n+1} - A_{k}^{n+1}\right) \alpha_{m-\frac{1}{2}}}{2V_{k-\frac{1}{2}} V_m} + f \lambda_{g,k}^{n+1} + \lambda_{g,k}^{n+1} + \lambda_{f,g_{,r,n+1}}^{n+1} + \lambda_{f,g_{,r,n-1}}^{n+1}. \tag{40}
\]

\[
b = -\mu_m \frac{1}{v_g + \frac{1}{2}} \left(\alpha_{m+\frac{1}{2}} - 1\right) A_{k+1}^{n+1} + \left(\alpha_{m-\frac{1}{2}} - 1\right) A_{k}^{n+1} \phi_{g,m,k+\frac{1}{2}}^{n+1}. \tag{41}
\]

To \(\mu_m > 0\):

\[
a = \frac{1}{v_g \Delta t_{n+1}} + f \mu_m A_{k+1}^{n+1} \frac{v_{g+\frac{1}{2}}}{V_{k+\frac{1}{2}}} + \frac{f \left(A_{k+1}^{n+1} - A_{k}^{n+1}\right) \alpha_{m+\frac{1}{2}}}{2V_{k+\frac{1}{2}} V_m} + \frac{f \left(A_{k+1}^{n+1} - A_{k}^{n+1}\right) \alpha_{m-\frac{1}{2}}}{2V_{k-\frac{1}{2}} V_m} + f \lambda_{g,k}^{n+1} + \lambda_{g,k}^{n+1} + \lambda_{f,g_{,r,n+1}}^{n+1} + \lambda_{f,g_{,r,n-1}}^{n+1}. \tag{42}
\]

\[
b = -\mu_m \frac{1}{v_g + \frac{1}{2}} \left(\alpha_{m+\frac{1}{2}} - 1\right) A_{k+1}^{n+1} + \left(\alpha_{m-\frac{1}{2}} - 1\right) A_{k}^{n+1} \phi_{g,m,k+\frac{1}{2}}^{n+1}. \tag{43}
\]

To \(\mu_m = -1\):

\[
a = \frac{1}{v_g \Delta t_{n+1}} + A_{k+1}^{n+1} + \left(f - 1\right) A_{k}^{n+1} \frac{v_{g+\frac{1}{2}}}{V_{k+\frac{1}{2}}} + \frac{f \lambda_{g,k}^{n+1} + \lambda_{g,k}^{n+1} + \lambda_{f,g_{,r,n+1}}^{n+1} + \lambda_{f,g_{,r,n-1}}^{n+1}}{2V_{k+\frac{1}{2}} V_m}. \tag{44}
\]

\[
b = \frac{1}{v_g} \left(\alpha_{m+\frac{1}{2}} - 1\right) A_{k+1}^{n+1} + \left(\alpha_{m-\frac{1}{2}} - 1\right) A_{k}^{n+1} \phi_{g,0,k+\frac{1}{2}}^{n+1}. \tag{45}
\]

\[
c = \frac{1}{v_g} \left(\alpha_{m+\frac{1}{2}} - 1\right) A_{k+1}^{n+1} + \left(\alpha_{m-\frac{1}{2}} - 1\right) A_{k}^{n+1} \phi_{g,0,k+\frac{1}{2}}^{n+1}. \tag{46}
\]

Therefore, we get the SOTE_EM and SOTE-DD by combining SOTE for time variable with EM or DD for other variable. The discrete equation for SOTE_EM is a nonlinear equation and the discrete equation for SOTE_DD is a linear equation.

IV. NUMERICAL RESULTS

We define the undermentioned physical quantity to describe different differential curve for time variable.

\[
J = \int_{\Omega > 0} d\Omega \psi(r_j, \Omega, E, t). \tag{49}
\]

This physical quantity \(J\) gives the information about outflux at outermost boundary, which denotes the outflux current of system particle. The influx is zero for taking void boundary condition.

\[
N = 4\pi \int_E dE \int_V r^2 dr \frac{\psi(r, E, t)}{V}. \tag{50}
\]

This physical quantity \(N\) gives the information about flux at center cell, which denotes the total number of system neutron.

\[
\lambda_{edge} = \frac{dJ}{dt} \lambda_{center} = \frac{dN}{dt}. \tag{51}
\]

denotes the derivative of outflux current and total number of system neutron respectively.

The problem discussed in this paper is about spherical geometry multi-group time-dependent problem including two media. The isotropic scattering source is employed. The discrete angular takes \(S_4\) and the end time is \(0.1\mu s\). The self-adaptive time step is shown in Table I. We adopt the original EM, DD and the modified time discrete scheme and second-order time evolution scheme. To analyse the computing effectiveness, we also take constant time step \((10^{-4}\mu s)\) to this problem.

<table>
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<th>time interval</th>
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<th>0.0001</th>
<th>0.01</th>
<th>0.0001</th>
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<tbody>
<tr>
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<td>0.018</td>
<td>0.08</td>
<td>0.1</td>
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</table>

The numerical results of neutron number for EM, MEM, SOTE_EM are showed in Fig.1 and the corresponding \(\lambda_{center}\), outermost current \(J\), \(\lambda_{edge}\) are given in Fig.2, Fig.3, Fig.4 respectively. Fig.5 gives the iterative number for EM, MEM, SOTE_EM. The numerical results of neutron number for DD, MDD, SOTE_DD are showed in Fig.6 and the corresponding \(\lambda_{center}\), outermost current \(J\), \(\lambda_{edge}\) are given in Fig.7, Fig.8, Fig.9 respectively. Fig.10 gives the iterative number for DD, MDD, SOTE_DD.

From these figures, the physical quantity of the neutron number, outermost current \(J\), \(\lambda_{center}\), \(\lambda_{edge}\) for original method(EM, DD) is more different to constant time step when the time step has great change. However the physical quantity to the MEM and MDD, SOTE_EM, SOTE_DD is approach to the constant time step results and the \(\lambda_{center}\) which reflects the differential property of neutron number is smooth. However the \(\lambda_{center}\), \(\lambda_{edge}\) of EM, DD exists large oscillation for adaptive time step. The shortcoming of MEM, MDD, SOTE_DD is that the \(\lambda_{edge}\) has large oscillation. To SOTE_EM, the physical quantity of neutron number, outermost current \(J\), \(\lambda_{center}\), \(\lambda_{edge}\) is very good and the corresponding curve especially for \(\lambda_{edge}\) is very smooth.

To computing time, the iteration number of the MEM, MDD is the smallest. The iteration number of SOTE_DD
is failure for some time point which the given max iteration number is 2000. The weakness of $SOTE_{EM}$ is that the computing time is larger than that of $MEM,MDD$.

V. Conclusion

According the character of time discrete for adaptive time step, we study the typical $EM, DD$ and corresponding modified time discrete scheme. We apply second-order time evolution scheme for time-dependent neutron transport equation and construct $SOTE_{EM}, SOTE_{DD}$. The modified scheme is simple and the iteration number is lower than others. To $MEM,MDD$, the neutron number, out-current at outermost boundary, $\lambda_{center}$ are smooth. However, there has oscillating for $\lambda_{edge}$. Whereas, the second-order time evolution scheme associated exponential method($SOTE_{EM}$) has some good properties. The differential curve including $\lambda_{edge}$ on time about neutron current is more smooth than that of exponential method and diamond difference and modified time discrete scheme. The shortcoming of $SOTE_{EM}$ is that the iteration number is more than other schemes and we will take acceleration method such as taking effective iterative initial value[11] to decrease the iteration number.
Fig. 6. Neutron number for DD, MDD and SOTE-DD

Fig. 7. \( \lambda \) center for DD, MDD and SOTE-DD

Fig. 8. Neutron current for DD, MDD and SOTE-DD

Fig. 9. \( \lambda \) edge for DD, MDD and SOTE-DD

Fig. 10. iteration for for DD, MDD and SOTE-DD

REFERENCES


