Progress in Nuclear Energy 52 (2010) 315–320

Contents lists available at ScienceDirect

Progress in Nuclear Energy

journal homepage: www.elsevier.com/locate/pnucene

Oscillation of numerical solution for time-dependent particle transport equations

Zhenying Hong*[1], Guangwei Yuan, Xuedong Fu

Institute of Applied Physics and Computational Mathematics, Department 6, NO.2. Fenghaodong Road, Haidian District, Beijing 100094, China

Keywords:
Transport equations
Oscillation of numerical solution
Exponential method
Diamond difference
Linear discontinuous finite element method

ABSTRACT

In this paper, the oscillating problem of numerical solution for time-dependent particle transport equations is investigated. The influence of numerical scheme on this oscillating phenomenon is analysed for a kind of particular particle transport equations with a small perturbation and spherical geometric time-dependent particle transport equation. The numerical experiments show that linear discontinuous finite element method can yield more accurate results and improve the oscillating numerical solution for the derivative of flux with respect to time.

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1. Introduction

The transport equations used in radiation shielding and nuclear reaction system, as well as medicine realm, are linearized version of the equation originally developed by Boltzmann for the kinetic theory of gases. In general, analytical solutions to particle transport equations cannot be found for multi-group approximation problems with non-uniform medium. In the past years, many approximate methods for solving certain types of particle transport problems have been developed. Instead of directly solving this equation, approximations to the particle transport equations, such as the discrete ordinates (S_N) (Lewis and Miller, 1993; Coelho, 2002; Siewert, 2000) and spherical harmonics (P_N) (Frank et al., 2007; Sahni and Sharma, 2004; Klose and Larsen, 2006) equations, have been made to overcome the constraints. The S_N method, which is employed in solving neutral particle transport equations, has emerged in the last decade as one of the most popular methods, providing a good compromise between computational accuracy and efficiency. The S_N method is based on the numerical solution of the particle transport equations along a set of discrete directions spanning the total solid angle range of 4π, replacing the integrals over direction by numerical quadratures. Up to now attention has been focused on the time-independent particle transport problems. But, with the increase of practical requirements, the physics problems discussed now become more sophisticated than before, for example, complex structure, non-uniform medium, anisotropic property, broad-energy region, sophisticated physical condition, movement station etc. Therefore, it is essentially necessary to study more advanced numerical method, and pay more attention on time-dependent transport equations. Moreover, the discretization methods for angular variable should be studied for curvilinear geometry transport equations (Lathrop, 2000).

The goal of numerical method is to accurately approximate the transport equations by a discrete system of algebraic equations and to efficiently solve the resulting discrete system. Moreover, a good numerical method should rationally simulate physical properties of mathematical models, and do not introduce non-physical deviation. One of the focus for solving nuclear radiation problems is to obtain accurate estimates of certain physical quantities at some spatial points within the physical system considered. In particular, for photonics problems accurate estimates of the exiting partial current on the outer boundary of the system are required. However, the differential of the exiting partial current with respect to time variable shows character of violent oscillatory, when exponential method (EM) and diamond difference (DD) method are used to discretize particle transport equations. Therefore, based such discretization methods, it is difficult to perform physical and mathematical analysis properly.

The exponential method and diamond difference method are typical discrete schemes for finite volume method to solving transport equations. The diamond difference method is simple and it is easy to be applied to solve transport equations. However, a disadvantage of the DD method is that it can produce non-physical oscillating solutions (Klose and Larsen, 2006). The exponential method is more sophisticated than diamond difference method and is a nonlinear, positive numerical scheme. The extended short-characteristics (ESC) method (Dedner and Vollmöller, 2002) that combines the finite element and the short-characteristics approaches can inhibit the oscillating of flux. But we focus on differential property of flux with respect to time in

* Corresponding author.
E-mail addresses: zyhong@iapcm.ac.cn (Z. Hong), yuan_guangwei@iapcm.ac.cn (G. Yuan), xdfu@iapcm.ac.cn (X. Fu).

[1] Supported by the Special Funds for Major State Basic Research Projects 2005CB321703, Science Foundation of CAEP(2008A0202008).

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doi:10.1016/j.pnucene.2009.07.002

different numerical schemes. Discontinuous finite element methods have been applied to transport equations in a variety of different settings (Wareing et al., 2001; Adams, 2001; Morel and Wareing, 1996; Machorro, 2007), and we hope to choice a suitable numerical method with higher order accuracy. There are two kinds of discontinuous finite element method for transport equations, one is partial variable finite element method and the other full variable finite element method. In this paper, we consider partial variable finite element method, namely apply linear discontinuous finite element method (LD) to spatial variable and diamond difference method to other variables. As for angular variable, we apply the S_N method. The LD method uses basis function of finite element and weighted function to give system of linear algebraic equations about flux on edge of cell, which is different from the extrapolation used by exponential method and diamond difference method.

In this paper, we consider firstly one kind of particular transport equations with analytic solution and then spherical geometry transport equations. Moreover, we analyse the oscillating phenomenon about numerical solution.

The remainder of this paper is organized as follows. In Section 2, the difference scheme for time-dependent particle transport equation is presented. In Section 3, we provide numerical results for one kind of particular transport and 1-D spherical geometry transport equations. In the final section, we offer a summary with some concluding remarks.

2. The difference scheme for time-dependent particle transport equations

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

$$\frac{1}{v_g}\frac{\partial \varphi_g}{\partial t} + \Omega \cdot \nabla \varphi_g + \Sigma_g^{tr}\varphi_g = Q_g, \quad g = 1, \ldots, G \tag{1}$$

where φ_g is the angular flux of g-th group particle, v_g is the velocity of g-th group particle, Σ_g^{tr} is the total macroscopic cross section of g-th group particle, and Q_g is the sum of scattering source, fission source and external source

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

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

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

With the following initial and boundary conditions:

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

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

We will study the phenomenon of oscillation of numerical solution, and the performance of different numerical scheme to transport equations with a small perturbation. To make statement clear, we consider at first the following particular transport problems:

$$\begin{aligned} &\frac{\partial \varphi}{\partial t} + \frac{\partial \varphi}{\partial x} = \alpha\varphi \quad x \in [0,1], \quad t > 0 \\ &\varphi(x,0) = f(x) \quad x \ge 0 \\ &\varphi(0,t) = g(t) \quad t \ge 0 \end{aligned} \tag{6}$$

where α is a given constant, $f(x)$ and $g(t)$ are given functions satisfying consistency condition $f(0) = g(0)$.

The analytic solution of the above problem is:

$$\varphi(x,t) = \begin{cases} e^{\alpha t} f(x-t) & x \ge t \\ e^{\alpha x} g(t-x) & x \le t \end{cases} \tag{7}$$

Let the initial condition be continuous, but the boundary condition be discontinuous:

$$f(x) = e^x, \tag{8}$$

$$g(t) = e^{-t} + \varepsilon\delta(t-t_0), t_0 \ne 0, \delta(t-t_0) = \begin{cases} 1 & t = t_0 \\ 0 & t \ne t_0 \end{cases} \tag{9}$$

where ε is a given perturbation constant.

By using finite volume method and integrating Eq. (6) on intervals $[t^{n+3/2}, t^{n+1/2}] \times [x_k, x_{k+1}]$, we get:

$$\int_{t^{n+1/2}}^{t^{n+3/2}}\int_{x_k}^{x_{k+1}}\left(\frac{\partial\varphi}{\partial t} + \frac{\partial\varphi}{\partial x}\right)\mathrm{d}x\mathrm{d}t = \int_{t^{n+1/2}}^{t^{n+3/2}}\int_{x_k}^{x_{k+1}}\alpha\varphi\mathrm{d}x\mathrm{d}t \tag{10}$$

Through rearrangement, Eq. (10) can used to give the discrete scheme as follows:

$$\frac{\varphi_{k+1/2}^{n+3/2} - \varphi_{k+1/2}^{n+1/2}}{\Delta t} + \frac{\varphi_{k+1}^{n+1} - \varphi_k^{n+1}}{\Delta x} = \alpha\varphi_{k+1/2}^{n+1} \tag{11}$$

where cell-centered unknowns $\varphi_{k+1/2}$ and cell-node unknowns φ_k are introduced, and $\Delta x_k = x_{k+1} - x_k$. Since the number of unknowns is larger than the number of equations, the extrapolation relation about unknown variables $\varphi_{k+1/2}^{n+3/2}, \varphi_{k+1}^{n+1}$ must be introduced to close the discrete system of equations. In this paper, two kinds of extrapolation formulas are discussed which lead to the so-called exponential method and diamond difference method. For discontinuous finite element method, there is not need to introduce such extrapolation relation.

(i) Exponential method

The extrapolation formula of exponential method is as follows:

$$\left(\varphi_{k+1/2}^{n+1}\right)^2 = \left(\varphi_{k+1/2}^{n+3/2}\right)\left(\varphi_{k+1/2}^{n+1/2}\right) = \left(\varphi_{k+1}^{n+1}\right)\left(\varphi_k^{n+1}\right) \tag{12}$$

The specific form of unknown quantity flux $\varphi_{k+1/2}^{n+1}$ is obtained by Eq. (11).

$$\varphi_{k+1/2}^{n+1} = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \tag{13}$$

where

$$a = \frac{\Delta x_k}{\varphi_{k+1/2}^{n+1/2}} + \frac{\Delta t}{\varphi_k^{n+1}}, \quad b = -\alpha\Delta t\Delta x_k, \quad c = -\varphi_{k+1/2}^{n+1/2}\Delta x_k - \varphi_k^{n+1}\Delta t$$

(ii) Diamond difference method

The extrapolation formula of diamond difference method is as follows:

$$\varphi_{k+1/2}^{n+1} = \frac{1}{2}\left(\varphi_{k+1/2}^{n+3/2} + \varphi_{k+1/2}^{n+1/2}\right) = \frac{1}{2}\left(\varphi_{k+1}^{n+1} + \varphi_k^{n+1}\right) \tag{14}$$

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