

Asymptotic Derivation of the Multigroup Modified Time-Dependent Simplified P_2 Equations

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Abstract

The multigroup modified time-dependent simplified P_2 (SP_2) equations are derived as the higher order asymptotic approximations to the multigroup time-dependent transport equation in a physical regime in which the conventional multigroup time-dependent diffusion equations are the leading-order asymptotic approximation. The derivation is performed in general three-dimensional geometry.

I. Introduction

The transport behavior of neutral particles, as well as charged particles in some important physics regimes, is given by the Boltzmann Equation.¹ For decades, many researchers have investigated various computational methods to solve this equation, such as discrete ordinates(S_N) method, Monte Carlo method and so on. These methods generally provide great accuracy but for many applications, especially time-dependent, multidimensional cases, such as reactor-core-disruptive problems, require too much computational time. To avoid this computational inefficiency, the time-dependent diffusion equation, which is known to be an asymptotic limit of the transport equation in an optically-thick scattering-dominant regimes,² has been widely-used to approximate the transport phenomena in reactor kinetics calculations.

The simplified P_N (SP_N) equations were originally proposed by Gelbard to deal with the large number and complexity of the general P_N equations.³ The SP_N equations abandon the requirement that the exact

transport solution is obtained as N goes to infinity. Instead, the goal is to obtain a relatively inexpensive approximation to the transport equation that contains most of the transport physics lacking in diffusion theory. Through the years, numerous studies have been performed to investigate the accuracy of the SP_N equations, and these equations are confirmed to provide approximate transport solutions that are significantly more accurate than diffusion solutions but with almost the same computational efforts.^{4,5} Nevertheless, the lack of theoretical foundation in the original derivation of the SP_N equations had been an obstruction to the widespread use of these equations.

Recent work by Larsen et al. provided the theoretical background to the SP_N equations.⁶⁻⁸ They dealt with the steady-state transport equation, and they showed that the SP_N equations are robust, high-order, asymptotic approximations to the transport equation in a physical regime in which the conventional diffusion equation is the leading-order approximation. In other words, SP_N theory contains higher-order asymptotic corrections to diffusion theory for the problems in which the diffusion equation is an asymptotic limit of the transport equation.

Building on earlier steady-state work, author and Miller obtained an interesting result by performing an asymptotic analysis for the time-dependent transport equation.^{9,10} We found that the *modified* time-dependent SP_2 equations are robust, high-order, asymptotic approximations to the time-dependent transport equation in a physical regime in which the conventional time-dependent diffusion equation is the leading-order approximation. We also confirmed that the time-dependent SP_2 equations contain high-order asymptotic approximation to the time-dependent transport equation. The implication is that there is a class of problems, perhaps very important physically, for which the time-dependent diffusion equation is not a good enough approximation to the time-dependent transport equation, but the time-dependent SP_2 (or modified time-dependent SP_2) equations are. Various numerical results in ref. [11] confirmed that, in many problems in which the conventional time-dependent diffusion equation is not sufficiently accurate, the time-dependent SP_2 equations can give considerably more accurate solutions than the time-dependent diffusion equation with almost the same computational efforts.

We previously derived the modified time-dependent SP_2 equations in monoenergetic, multidimensional transport problem and multigroup transport problem in planar geometry. In this paper, we derive the multigroup modified time-dependent SP_2 equations as the higher-order asymptotic approximations to the transport equation, in general three-dimensional geometry, in a physical regime in which the time-dependent diffusion equation is the leading-order approximation.

II. Asymptotic Derivation

The multigroup time-dependent transport equation can be written as

$$\frac{1}{v} \frac{\partial \mathbf{y}}{\partial t} + \hat{\Omega} \cdot \nabla \mathbf{y} + \mathbf{s}_t(\vec{r}) \mathbf{y}(\vec{r}, \hat{\Omega}, t) = \mathbf{s}_s(\vec{r}) \int \mathbf{y}(\vec{r}, \hat{\Omega}', t) d\hat{\Omega}' + Q(\vec{r}, t), \quad (1)$$

where

$$\begin{aligned} \mathbf{y}(\vec{r}, \hat{\Omega}, t) &= \text{angular flux (a } G \text{ vector)} \\ Q(\vec{r}, t) &= \text{source (a } G \text{ vector)} \\ \mathbf{s}_t(\vec{r}) &= \text{total cross section (a } G \times G \text{ diagonal matrix)} \\ \mathbf{s}_s(\vec{r}) &= \text{scattering cross section (a } G \times G \text{ matrix)} \\ G &= \text{number of energy groups.} \end{aligned}$$

Integrating Eq. (1) over the whole angle, $\int d\hat{\Omega}$, and introducing

$$\mathbf{f}(\vec{r}, t) = \int \mathbf{y}(\vec{r}, \hat{\Omega}', t) d\hat{\Omega}' = \text{scalar flux (a } G \text{ vector),}$$

we obtain

$$\frac{1}{v} \frac{\partial \mathbf{f}}{\partial t} + \int \hat{\Omega}' \cdot \nabla \mathbf{y}(\vec{r}, \hat{\Omega}', t) d\hat{\Omega}' + [\mathbf{s}_t(\vec{r}) - \mathbf{s}_s(\vec{r})] \mathbf{f}(\vec{r}, t) = Q(\vec{r}, t). \quad (2)$$

And from Eqs. (1) and (2), we also obtain

$$\frac{1}{v} \frac{\partial \mathbf{y}}{\partial t} + \hat{\Omega} \cdot \nabla \mathbf{y} + \mathbf{s}_t(\vec{r}) \mathbf{y}(\vec{r}, \hat{\Omega}, t) = \frac{1}{v} \frac{\partial \mathbf{f}}{\partial t} + \mathbf{s}_t \mathbf{f}(\vec{r}, t) + \int \hat{\Omega}' \cdot \nabla \mathbf{y}(\vec{r}, \hat{\Omega}', t) d\hat{\Omega}'. \quad (3)$$

Introducing into Eqs. (2) and (3) the asymptotic scaling

$$\mathbf{s}_t \Rightarrow \frac{\mathbf{s}_t}{\epsilon}, \quad \mathbf{s}_s \Rightarrow \frac{\mathbf{s}_s}{\epsilon}, \quad Q = \epsilon Q, \quad v \Rightarrow \frac{v}{\epsilon}, \quad (4)$$

we obtain

$$\frac{\epsilon}{v} \frac{\partial \mathbf{f}}{\partial t} + \int \hat{\Omega}' \cdot \nabla \mathbf{y}(\vec{r}, \hat{\Omega}', t) d\hat{\Omega}' + \frac{1}{\epsilon} [\mathbf{s}_t(\vec{r}) - \mathbf{s}_s(\vec{r})] \mathbf{f}(\vec{r}, t) = \epsilon Q(\vec{r}, t), \quad (5)$$

and

$$\frac{\epsilon}{v} \frac{\partial \mathbf{y}}{\partial t} + \hat{\Omega} \cdot \nabla \mathbf{y} + \frac{\mathbf{s}_t(\vec{r})}{\epsilon} \mathbf{y}(\vec{r}, \hat{\Omega}, t) = \frac{\epsilon}{v} \frac{\partial \mathbf{f}}{\partial t} + \frac{\mathbf{s}_t}{\epsilon} \mathbf{f}(\vec{r}, t) + \int \hat{\Omega}' \cdot \nabla \mathbf{y}(\vec{r}, \hat{\Omega}', t) d\hat{\Omega}'. \quad (6)$$

We next introduce into Eq. (6) the expansion

$$\mathbf{y} = \mathbf{j}_0 + \epsilon \mathbf{j}_1 + \epsilon^2 \mathbf{j}_2 + \dots, \quad (7)$$

and equate the coefficients of different powers of ϵ to obtain the following equations:

$$O(\mathbf{e}^{-1}) \quad \mathbf{j}_0 = \mathbf{f},$$

$$O(\mathbf{e}^0) \quad \mathbf{j}_1 = -\frac{1}{\mathbf{s}_t} \hat{\Omega} \cdot \nabla \mathbf{f},$$

$$O(\mathbf{e}^1) \quad \mathbf{j}_2 = \left[\left\{ \frac{1}{\mathbf{s}_t} (\hat{\Omega} \cdot \nabla) \right\}^2 - \frac{1}{3} \left(\frac{1}{\mathbf{s}_t} \nabla \right)^2 \right] \mathbf{f},$$

$$O(\mathbf{e}^2) \quad \mathbf{j}_3 = \left[\frac{1}{v \mathbf{s}_t} \frac{\partial}{\partial t} \left(\frac{1}{\mathbf{s}_t} \hat{\Omega} \cdot \nabla \right) + \frac{1}{3} \left(\frac{1}{\mathbf{s}_t} \hat{\Omega} \cdot \nabla \right) \left(\frac{1}{\mathbf{s}_t} \nabla \right)^2 - \left\{ \frac{1}{\mathbf{s}_t} (\hat{\Omega} \cdot \nabla) \right\}^3 \right] \mathbf{f},$$

$$O(\mathbf{e}^3) \quad \mathbf{j}_4 = \left[-\frac{1}{v \mathbf{s}_t} \frac{\partial}{\partial t} \left\{ \left(\frac{1}{\mathbf{s}_t} \hat{\Omega} \cdot \nabla \right)^2 - \frac{1}{3} \left(\frac{1}{\mathbf{s}_t} \nabla \right)^2 \right\} + \left(\frac{1}{\mathbf{s}_t} \hat{\Omega} \cdot \nabla \right)^4 - \frac{1}{3} \left(\frac{1}{\mathbf{s}_t} \hat{\Omega} \cdot \nabla \right)^2 \left(\frac{1}{\mathbf{s}_t} \nabla \right)^2 - \frac{4}{45} \left(\frac{1}{\mathbf{s}_t} \nabla \right)^4 \right] \mathbf{f},$$

and so on. Introducing these moments into Eq. (7), we obtain an asymptotic expansion for \mathbf{y} in terms of \mathbf{f} . Applying this expansion into Eq. (5), we finally obtain the equation for \mathbf{f} , as follows:

$$\frac{\mathbf{e}}{v} \frac{\partial \mathbf{f}}{\partial t} - \nabla \cdot \left[\frac{\mathbf{e}}{3} \left(\frac{1}{\mathbf{s}_t} \nabla \right) - \frac{\mathbf{e}^3}{3} \left(\frac{1}{\mathbf{s}_t} \nabla \right) \left\{ \frac{1}{v \mathbf{s}_t} \frac{\partial}{\partial t} - \frac{4}{15} \left(\frac{1}{\mathbf{s}_t} \nabla \right)^2 \right\} + O(\mathbf{e}^5) \right] \mathbf{f} + \frac{1}{\mathbf{e}} \{ \mathbf{s}_t(\bar{r}) - \mathbf{s}_s(\bar{r}) \} \mathbf{f}(\bar{r}, t) = \mathbf{e} Q(\bar{r}, t). \quad (8)$$

If we delete the terms of $O(\mathbf{e}^3)$ and higher in Eq. (8) and reapply the definition of the scaling [Eq. (4)] in reverse into the resulting equation, we obtain

$$\frac{1}{v} \frac{\partial \mathbf{f}}{\partial t} - \nabla \cdot \frac{1}{3 \mathbf{s}_t} \nabla \mathbf{f} + \{ \mathbf{s}_t(\bar{r}) - \mathbf{s}_s(\bar{r}) \} \mathbf{f}(\bar{r}, t) = Q(\bar{r}, t). \quad (9)$$

These are the conventional multigroup time-dependent diffusion equations.

We next delete the terms of $O(\mathbf{e}^5)$ and higher in Eq. (8) and introduce Eqs. (4) and (9) into the resulting equation to obtain

$$\left(\frac{1}{v \mathbf{s}_t} \frac{\partial}{\partial t} - \frac{4}{15} \frac{1}{\mathbf{s}_t} \nabla \cdot \frac{1}{\mathbf{s}_t} \nabla \right) \left[\frac{1}{v} \frac{\partial \mathbf{f}}{\partial t} + (\mathbf{s}_t - \mathbf{s}_s) \mathbf{f} - Q \right] + \frac{1}{v} \frac{\partial \mathbf{f}}{\partial t} - \nabla \cdot \frac{1}{3 \mathbf{s}_t} \nabla \mathbf{f} + \{ \mathbf{s}_t(\bar{r}) - \mathbf{s}_s(\bar{r}) \} \mathbf{f}(\bar{r}, t) = Q(\bar{r}, t). \quad (10)$$

These are the multigroup modified time-dependent SP_2 equations, which can be obtained by neglecting the time-derivative term of the second moment of angular flux, $\partial \mathbf{y}_2 / \partial t$, in the multigroup time-dependent SP_2 equations.¹¹ Note that in the leading-order approximation, the resulting equations are not the time-dependent SP_l equations but the time-dependent diffusion equations. In the steady-state problem, the diffusion equations are the same as the SP_l equations; however, in the time-dependent problem, the time-dependent diffusion equations are obtained from the time-dependent SP_l equations by neglecting the time-derivative term of the first moment of angular flux, $\partial \mathbf{y}_1 / \partial t$.

III. Discussion

We have derived the multigroup modified time-dependent SP_2 equations as the higher order asymptotic approximations to the multigroup time-dependent transport equation in a physical regime in which the conventional multigroup time-dependent diffusion equations are the leading-order asymptotic approximation. The derivation has been performed in general three-dimensional geometry with isotropic scattering only. In succession to this paper, we plan to extend our study to the fully general three-dimensional multigroup transport problems with anisotropic scattering. This work provides a theoretical foundation for the multigroup modified time-dependent SP_2 equations. Various numerical results in ref. [11] confirmed that, in many problems in which the conventional time-dependent diffusion equation is not sufficiently accurate, the time-dependent SP_2 equations can give considerably more accurate solutions than the time-dependent diffusion equation with almost the same computational efforts. For future work, we need to test a benchmark problem to validate the advantages of using the multigroup modified time-dependent SP_2 equations to solve more realistic three-dimensional reactor problems. We also plan to analyze the higher order, time-dependent SP_N equations (or modified time-dependent SP_N equations) by using asymptotic and numerical approaches.

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