

MASTER

Time-dependent simplified Pn equations in two dimensions

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Time-Dependent Simplified P_N Equations in Two Dimensions

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Abstract

Radiotherapy has been used in medicine for more than 100 years, the radiative transport equation plays a very important role in radiotherapy mathematically. The steady-state simplified P_N approximation to the radiative transport equation has been successfully applied to many problems involving radiation. In this work, we use asymptotic analysis to derive the time-dependent SP_N equations. And also three numerical test cases are given, including Marshak wave and Lattice problem.

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Chapter 1

Introduction

This introduction is based on [6] and several internet sources, see [7], [8], [9], [10].

In 1895, Wilhelm Conrad Röntgen in Würzburg (Germany) discovered X-rays. In the same year, Emil Grubbe (Chicago) attempted to treat a local relapse of breast carcinoma by using X-rays. In 1896, First use of X-Rays for stomach cancer is done by Victor Despeignes (Lyon - France). Since then, it has been more than 100 years. People have been trying to use the radiation to treat disease all the time, and there has been a lot of progress. It has already become a science called radiotherapy. Only in 1990, over 500,000 individuals in the United States received radiation cancer therapy, the number is even bigger all over the world.

Radiotherapy is the safe use of controlled doses of radiation (emitted by high-energy photons and electrons, such as X-rays and similar rays) to treat disease, especially cancer. Usually it is given by pointing an X-ray machine to the part of the body which should be treated. It can also be given by drinking liquid, having an injection or by having a radioactive implant into the human body. Radiotherapy is commonly used along with other treatment such as chemotherapy (taking drugs to treat cancer), and surgery to remove a tumor (an abnormal tissue).

The human body is made up of millions of cells, which can grow and divide up to form more cells. If radiation is directed at cells in the body, it will damage them and stop them from growing and dividing. However, healthy cells have the ability to repair themselves from damage (of course, this ability has limits), while diseased cells are destroyed. So the object of radiotherapy is: (i) to deliver a sufficiently strong dose (energy deposited per unit mass) to the tumor to make sure that it is controlled, and (ii) to deliver a sufficiently weak dose to make sure that complications (complication is a secondary disease, an accident, or a negative reaction occurring during the course of an illness and usually aggravating the illness, it is also called side effect) will not occur in the surrounding healthy tissue.

The basic procedures to use the radiation of high-energy particles are: outline the tu-

mor and important nearby organs and obtain three-dimensional images, usually this is done by CT (Computerized Tomography) or MRI (Magnetic Resonance Imaging) scans and the images will be shown on computer screen. Then the dosimetrist (the dosimetrist is a member of the radiation oncology team who has knowledge of the overall characteristics and clinical relevance of radiation oncology treatment machines and equipment) visualizes the geometry of the tumor in relation to nearby organs. After that the dosimetrist selects a set of beams (high-energy rays) which is eventually used to do the operation to kill the tumor. The dosimetrist should also consider geometrical uncertainties (patient motion and tumor volume) and biology uncertainties (organ tolerance differences and patient tolerance differences for radiation) and other factors.

Generally, the rays will be emitted into human body in different direction, penetrate the human body and intersect at the tumor part to make sure the cancer is killed and no complications (side effects) occur in the healthy issue.

To understand the radiation process in the radiotherapy, we need to understand the physical process and give the mathematical model to study. The mathematical model is given by time-dependent radiative transport equation. Since the radiation process is three-dimensional and we need consider time, space and velocity, then we have a seven dimensional equation. It is very hard to tackle it both theoretically and computationally.

In order to study the radiative transport equation, we can simplify it. One way is to study planar transport equation first, then go to 3-D problem. Another way is to study time-independent transport equation first, then go to time-dependent problem.

In this work, we will give the corresponding Boltzmann transport equation and the time-dependent SP_N equations from P_N equations, then explicitly explain how to derive the SP_N equations via asymptotic analysis in Chapter 2. In Chapter 3 we will use Marshak's Method to computer the boundary and initial conditions for SP_1, SP_3, SSP_3 equations. In the following Chapter 4, we will give the numerical method to solve the SP_N equations and the main idea to make the Matlab code. And in Chapter 5, we will investigate three test cases, compare the numerical results with the corresponding benchmark. In the end, conclusion and future work will be given in Chapter 6.

Chapter 2

SP_N equations

To derive the SP_N equations, we need to look at the Boltzmann transport equation which is stated in the following.

2.1 The Boltzmann transport equation

Consider a convex, open, bounded domain Z in \mathbb{R}^3 , and assume that Z has a boundary with outward normal vector n . The direction of particle motion is given by $\Omega \in S^2$, where S^2 is the unit sphere in three dimensions. Define

$$\Gamma = \partial Z \times S^2 \quad \text{and} \quad \Gamma^- = \{(x, \Omega) \in \Gamma : n(x) \cdot \Omega < 0\}. \quad (2.1.1)$$

The transport of mono-energetic particles that undergo isotropic scattering (isotropy is the property which is independent of direction) in a medium is modeled by the linear Boltzmann equation [1]

$$\frac{1}{v} \partial_t \psi(t, x, \Omega) + \Omega \cdot \nabla_x \psi(t, x, \Omega) + \sigma_t(x) \psi(t, x, \Omega) = \frac{\sigma_s(x)}{4\pi} \int_{S^2} \psi(t, x, \Omega') d\Omega' + \frac{q(t, x)}{4\pi} \quad (2.1.2)$$

where q is an isotropic source term.

For the boundary condition, we have

$$\psi(t, x, \Omega) = \psi_b(t, x, \Omega) \quad \text{on } \Gamma^-, \quad (2.1.3)$$

which describes the ingoing characteristics, and for the initial condition, we have

$$\psi(0, x, \Omega) = \psi_0(x, \Omega) \quad (2.1.4)$$

Here, $\psi(t, x, \Omega) \cos \theta dA dt d\Omega$ is the number of particles at point x and time t that move with velocity v during dt through an area dA into a solid angle $d\Omega$ around Ω , and θ is the angle between Ω and dA . The total cross section $\sigma_t(x)$ is the sum of the absorption cross section $\sigma_a(x)$ and the total scattering cross section $\sigma_s(x)$.

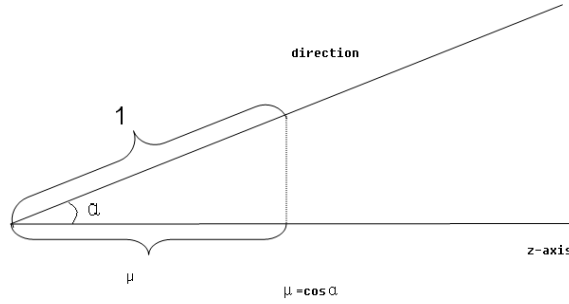
2.2 The steady-state SP_N equations

Generally, the Boltzmann transport equations we have given in the above doesn't have an explicit solution ψ , so we need to approximate the solution with the functions which are easy to handle. One way to do this is using a infinite function series instead of ψ . Plug the series into the equation, take finite terms of the series to approximate the solution. Of course, the more terms we take, the higher precision we expect. For the infinite function series, we often take orthogonal functions so that we could calculate the corresponding coefficients easily. Here we will take the Legendre polynomials to approximate the solution.

In 1-D case, the steady-state (if a system is in steady state then the recently behavior of the system will keep the same in the future) transfer equation is

$$\mu \partial_z \psi(z, \mu) + \sigma_t(z) \psi(z, \mu) - \frac{\sigma_s(z)}{2} \int_{-1}^1 \psi(z, s) ds = \frac{q(z)}{2} \quad (2.2.1)$$

where ψ is a function only depends on z and μ is the cosine of the angle between direction and z -axis.



Apparently, $\mu \in [-1, 1]$. Denote P_l the l th Legendre polynomial on $[-1, 1]$.

Remark 2.2.1. Legendre polynomials P_n , sometimes called Legendre functions of the first kind, are solutions to the Legendre differential equation. They are orthogonal over $[-1, 1]$, which is

$$\int_{-1}^1 P_m(\mu) P_n(\mu) d\mu = \frac{2}{2n+1} \delta_{m,n} \quad (2.2.2)$$

where $\delta_{m,n}$ is the Kronecker delta. And also have the following property:

$$\mu P_m = \frac{1}{2m+1} [(m+1)P_{m+1} + mP_{m-1}] \quad (2.2.3)$$

The P_N approximation assume ψ as a summation of a finite number of Legendre polynomial ψ_l , which is

$$\psi(z, \mu) = \sum_{l=0}^N \psi_l(z) \frac{2l+1}{2} P_l(\mu). \quad (2.2.4)$$

where $l = 0, 1, \dots, N$. Moreover, we assume N is odd. If we apply the P_N approximation (2.2.4) to (2.2.1) and use the formula (2.2.3), we have for $l = 0, 1, \dots, N$

$$\begin{aligned} \sum_{l=0}^N \frac{1}{2} [(l+1)P_{l+1}(\mu) + lP_{l-1}(\mu)] \partial_z \psi_l(z) + \sigma_t(z) \sum_{l=0}^N \psi_l(z) \frac{2l+1}{2} P_l(\mu) = \\ \frac{\sigma_s(z)}{2} \int_{-1}^1 \sum_{l=0}^N \psi_l(z) \frac{2l+1}{2} P_l(s) ds + \frac{q(z)}{2} \end{aligned} \quad (2.2.5)$$

Collect the items of P_l , we have for $l = 0$

$$\frac{1}{2} \partial_z \psi_1(z) P_0(\mu) + \frac{1}{2} \sigma_t(z) \psi_0(z) P_0(\mu) = \frac{\sigma_s(z)}{2} \int_{-1}^1 \psi_0(z) \frac{1}{2} P_0(s) ds + \frac{q(z)}{2} \quad (2.2.6)$$

using $P_0(\mu) = 1$, we have

$$\frac{1}{2} \partial_z \psi_1(z) + \frac{1}{2} \sigma_t(z) \psi_0(z) = \frac{1}{2} \sigma_s(z) \psi_0(z) + \frac{1}{2} q(z) \quad (2.2.7)$$

which is

$$\partial_z \psi_1(z) + \sigma_t(z) \psi_0(z) = \sigma_s(z) \psi_0(z) + q(z) \quad (2.2.8)$$

For $l \neq 0$, we have

$$\frac{1}{2} [(l+1)P_l(\mu) \partial_z \psi_{l+1}(z) + lP_l(\mu) \partial_z \psi_{l-1}(z)] + \sigma_t(z) \psi_l(z) \frac{2l+1}{2} P_l(\mu) = 0 \quad (2.2.9)$$

which is

$$\partial_z \left[\frac{l+1}{2l+1} \psi_{l+1}(z) + \frac{l}{2l+1} \psi_{l-1}(z) \right] + \sigma_t \psi_l(z) = 0 \quad (2.2.10)$$

Combine (2.2.8) and (2.2.10), we obtain

$$\partial_z \left(\frac{l+1}{2l+1} \psi_{l+1} + \frac{l}{2l+1} \psi_{l-1} \right) + \sigma_t \psi_l = \sigma_s \delta_{0,l} \psi_l + \delta_{0,l} q \quad (2.2.11)$$

where $\psi_{-1} = \psi_{N+1} = 0$ and δ is Kronecker delta function.

Take $N = 1$ and $N = 5$ as an example, from (2.2.11) for $N = 1$ we have

$$\partial_z \psi_1 + \sigma_t \psi_0 = \sigma_s \psi_0 + q \quad (2.2.12a)$$

$$\partial_z \frac{1}{3} \psi_0 + \sigma_t \psi_1 = 0 \quad (2.2.12b)$$

Also for $N = 5$, we have

$$\partial_z \psi_1 + \sigma_t \psi_0 = \sigma_s \psi_0 + q \quad (2.2.13a)$$

$$\partial_z \left(\frac{2}{3} \psi_2 + \frac{1}{3} \psi_0 \right) + \sigma_t \psi_1 = 0 \quad (2.2.13b)$$

$$\partial_z(\frac{3}{5}\psi_3 + \frac{2}{5}\psi_1) + \sigma_t\psi_2 = 0 \quad (2.2.13c)$$

$$\partial_z(\frac{4}{7}\psi_4 + \frac{3}{7}\psi_2) + \sigma_t\psi_3 = 0 \quad (2.2.13d)$$

$$\partial_z(\frac{5}{9}\psi_5 + \frac{4}{9}\psi_3) + \sigma_t\psi_4 = 0 \quad (2.2.13e)$$

$$\partial_z(\frac{5}{11}\psi_4) + \sigma_t\psi_5 = 0 \quad (2.2.13f)$$

Then we have P_1 equations and P_5 equations. In the following, we will derive the SP_1 equation and SP_5 equations.

Solve ψ_1 from (2.2.12b), then plug into (2.2.12a) we obtain

$$-\partial_z\frac{1}{3\sigma_t}\partial_z\psi_0 = q + (\sigma_s - \sigma_t)\psi_0 = q - \sigma_a\psi_0 \quad (2.2.14)$$

which is SP_1 equation.

From (2.2.13b), (2.2.13d) and (2.2.13f), we know

$$\psi_1 = -\frac{1}{\sigma_t}\partial_z(\frac{2}{3}\psi_2 + \frac{1}{3}\psi_0) \quad (2.2.15a)$$

$$\psi_3 = -\frac{1}{\sigma_t}\partial_z(\frac{4}{7}\psi_2 + \frac{3}{7}\psi_0) \quad (2.2.15b)$$

$$\psi_5 = -\frac{1}{\sigma_t}\partial_z(\frac{5}{11}\psi_4) \quad (2.2.15c)$$

Plug (2.2.15a), (2.2.15b), (2.2.15c) into (2.2.13a), (2.2.13c), (2.2.13e), we obtain

$$\partial_z[-\frac{1}{\sigma_t}\partial_z(\frac{2}{3}\psi_2 + \frac{1}{3}\psi_0)] = (\sigma_s - \sigma_a) + q = -\sigma_t + q \quad (2.2.16a)$$

$$\partial_z[-\frac{1}{\sigma_t}\partial_z(\frac{12}{35}\psi_4 + \frac{11}{21}\psi_2 + \frac{2}{15}\psi_0)] + \sigma_t\psi_2 = 0 \quad (2.2.16b)$$

$$\partial_z[-\frac{1}{\sigma_t}\partial_z(\frac{39}{77}\psi_4 + \frac{12}{63}\psi_2)] + \sigma_t\psi_4 = 0 \quad (2.2.16c)$$

Which are SP_5 equations.

To obtain the other SP_N equations, use the same idea as above, solve every second equation for the odd order and insert the result into the equations above and below, then we can obtain a system of second-order partial differential equations.

On the other hand, the steady-state SP_N equations have been derived from

$$\Omega \cdot \nabla_x \psi(x, \Omega) + \frac{1}{\varepsilon} \sigma_t \psi(x, \Omega) = (\frac{\sigma_t}{\varepsilon} - \varepsilon \sigma_a) \frac{1}{4\pi} \int_{S^2} \psi(x, \Omega') d\Omega' + \varepsilon \frac{q(x)}{4\pi}$$

via asymptotic analysis in [2], where all quantities are assumed to be $O(1)$ except for the scalar parameter ε , which is assumed to be small. In the following part, we will derive the time-dependent SP_N equations via asymptotic analysis.

2.3 Time-dependent SP_N equations via asymptotic analysis

To derive the time-dependent SP_N equations via asymptotic analysis, we need to do the so-called parabolic scaling: space-derivatives are scaled by a small parameter ε and the time-derivative is scaled by ε^2 . Then we write the transport equation as

$$\varepsilon^2 \frac{1}{v} \partial_t \psi + \varepsilon \Omega \cdot \nabla_x \psi + \sigma_t \psi = (\sigma_t - \varepsilon^2 \sigma_a) \frac{1}{4\pi} \phi + \varepsilon^2 \frac{q}{4\pi} \quad (2.3.1)$$

where $\psi = \psi(t, x, \Omega)$, $\phi(t, x) = \int_{S^2} \psi(t, x, \Omega) d\Omega$ and $q = q(t, x)$.

In the following, we assume that σ_a and σ_t are constant, which means the system is homogeneous. For simplicity, we rewrite (2.3.1) as

$$(1 + \varepsilon \Omega \cdot X + \varepsilon^2 T) \psi = S \quad (2.3.2)$$

where

$$X = \frac{1}{\sigma_t} \nabla_x, \quad T = \frac{1}{v \sigma_t} \partial_t \quad \text{and} \quad S = (1 - \varepsilon^2 \frac{\sigma_a}{\sigma_t}) \frac{\phi}{4\pi} + \varepsilon^2 \frac{q}{4\pi \sigma_t} \quad (2.3.3)$$

In the following, we use two auxiliary results:

Remark 2.3.1. A Neumann series is a series of the form

$$\sum_{n=0}^{\infty} T^n$$

where T is an operator. If the Neumann series converges ($\|T\| < 1$) in the operator norm, then we have

$$(I - T)^{-1} = \sum_{n=0}^{\infty} T^n$$

In the following, we use Neumann's series to expand the inverse of the operator in (2.3.2). Although the operator is not bounded here and the series is not necessarily convergent, we just do it formally. Then we obtain the following equation:

$$\begin{aligned} \psi &= (1 + \varepsilon \Omega \cdot X + \varepsilon^2 T)^{-1} S \\ &= (1 - (\varepsilon \Omega \cdot X + \varepsilon^2 T) + (\varepsilon \Omega \cdot X + \varepsilon^2 T)^2 - (\varepsilon \Omega \cdot X + \varepsilon^2 T)^3 + (\varepsilon \Omega \cdot X + \varepsilon^2 T)^4 \\ &\quad - (\varepsilon \Omega \cdot X + \varepsilon^2 T)^5 + (\varepsilon \Omega \cdot X + \varepsilon^2 T)^6) S + O(\varepsilon^7) \\ &= \left\{ 1 - (\Omega \cdot X) \varepsilon + [-T + (\Omega \cdot X)^2] \varepsilon^2 + [2(\Omega \cdot X)T - (\Omega \cdot X)^3] \varepsilon^3 + \right. \\ &\quad [(T - 3(\Omega \cdot X)^2)T + (\Omega \cdot X)^4] \varepsilon^4 + (-3(\Omega \cdot X)T^2 + 4(\Omega \cdot X)^3T + (\Omega \cdot X)^5) \varepsilon^5 \\ &\quad \left. + (-T^3 + 6(\Omega \cdot X)^2T^2 - 5(\Omega \cdot X)^4T + (\Omega \cdot X)^6) \varepsilon^6 \right\} S + O(\varepsilon^7) \end{aligned} \quad (2.3.4)$$

Lemma 1

$$\int_{S^2} (\Omega \cdot X)^n d\Omega = [1 + (-1)^n] \frac{2\pi}{n+1} X^n = [1 + (-1)^n] \frac{2\pi}{n+1} (X \cdot X)^{\frac{n}{2}} \quad (2.3.5)$$

Proof: Take rotation R ($\|R\| = 1$) such that $Rx = \|x\|(0, 0, 1)^T$, then we have

$$\int_{S^2} (\Omega \cdot X)^n d\Omega = \int_{S^2} (R\Omega \cdot \|x\|(0, 0, 1)^T)^n dR\Omega$$

Denote $\Omega' = R\Omega$ and set $\Omega' = (\sqrt{1 - \mu'^2} \cos \theta', \sqrt{1 - \mu'^2} \sin \theta', \mu')$, where $\mu' \in [-1, 1]$ and $\theta' \in [0, 2\pi]$, then we have $d\Omega' = d\mu' d\theta'$ and

$$\begin{aligned} \int_{S^2} (\Omega \cdot X)^n d\Omega &= \int_0^{2\pi} \int_{-1}^1 \|x\|^n \mu'^n d\mu' d\theta' \\ &= \|x\|^n \cdot \begin{cases} 0 & n \text{ is odd} \\ \frac{4\pi}{n+1} & n \text{ is even} \end{cases} \\ &= [1 + (-1)^n] \frac{2\pi}{n+1} X^n \\ &= [1 + (-1)^n] \frac{2\pi}{n+1} (X \cdot X)^{\frac{n}{2}} \quad \square \end{aligned}$$

Integrate the both sides of the equation (2.3.4) and use the formula (2.3.5). Then we obtain

$$\begin{aligned} \phi &= \int_{S^2} \psi d\Omega \\ &= 4\pi \left\{ 1 + \left(\frac{1}{3}X^2 - T\right)\varepsilon^2 + \left(T^2 + \frac{1}{5}X^4 - TX^2\right)\varepsilon^4 + \right. \\ &\quad \left. \left(\frac{1}{7}X^6 + 2T^2X^2 - T^3 - TX^4\right)\varepsilon^6 \right\} S + O(\varepsilon^8) \end{aligned} \quad (2.3.6)$$

Therefore, using the Neumann series again, we have

$$\begin{aligned} 4\pi S &= \left\{ 1 + \left(\frac{1}{3}X^2 - T\right)\varepsilon^2 + \left(T^2 + \frac{1}{5}X^4 - TX^2\right)\varepsilon^4 + \right. \\ &\quad \left. \left(\frac{1}{7}X^6 + 2T^2X^2 - T^3 - TX^4\right)\varepsilon^6 \right\}^{-1} + O(\varepsilon^8) \\ &= \left\{ 1 - A + A^2 - A^3 \right\} \phi + O(\varepsilon^8) \\ &\quad \text{where } A = \left(\frac{1}{3}X^2 - T\right)\varepsilon^2 + \left(T^2 + \frac{1}{5}X^4 - TX^2\right)\varepsilon^4 + \left(\frac{1}{7}X^6 + 2T^2X^2 - T^3 - TX^4\right)\varepsilon^6 \\ &= \left\{ 1 - \left(\frac{1}{3}X^2 - T\right)\varepsilon^2 - \left(T^2 + \frac{1}{5}X^4 - TX^2\right)\varepsilon^4 - \left(\frac{1}{7}X^6 + 2T^2X^2 - T^3 - TX^4\right)\varepsilon^6 \right. \\ &\quad \left. + \left(\frac{1}{3}X^2 - T\right)^2\varepsilon^4 + 2\left(\frac{1}{3}X^2 - T\right)\left(T^2 + \frac{1}{5}X^4 - TX^2\right)\varepsilon^6 - \left(\frac{1}{3}X^2 - T\right)^3\varepsilon^6 \right\} + O(\varepsilon^8) \\ &= \left\{ 1 + \left(-\frac{1}{3}X^2 + T\right)\varepsilon^2 + \left(-\frac{4}{45}X^4 + \frac{1}{3}TX^2\right)\varepsilon^4 + \right. \\ &\quad \left. \left(-\frac{44}{945}X^6 - \frac{1}{3}T^2X^2 + \frac{4}{15}TX^4\right)\varepsilon^6 \right\} \phi + O(\varepsilon^8) \end{aligned} \quad (2.3.7)$$

From (2.3.3) the definition of S , we have

$$(1 - \varepsilon^2 \frac{\sigma_a}{\sigma_t})\phi + \varepsilon^2 \frac{q}{\sigma_t} = \left\{ 1 + (-\frac{1}{3}X^2 + T)\varepsilon^2 + (-\frac{4}{45}X^4 + \frac{1}{3}TX^2)\varepsilon^4 + \right. \\ \left. (-\frac{44}{945}X^6 - \frac{1}{3}T^2X^2 + \frac{4}{15}TX^4)\varepsilon^6 \right\} \phi + O(\varepsilon^8)$$

Minus ϕ from both sides and multiply $\frac{\sigma_t}{\varepsilon^2}$, we get

$$-\sigma_a\phi + q = \sigma_t T\phi - \frac{\sigma_t}{3}X^2 \left[\phi - \varepsilon^2 T\phi + \frac{4}{15}\varepsilon^2 X^2\phi + \right. \\ \left. \frac{44}{315}\varepsilon^4 X^4\phi + \varepsilon^4 T^2\phi - \frac{4}{5}\varepsilon^4 TX^2\phi \right] + O(\varepsilon^6) \quad (2.3.8)$$

In order to get the SP_N approximation, we just neglect the high orders of ε . In the following, we will explicitly give SP_1 and SP_3 approximations.

2.3.1 SP_1 approximation

From (2.3.8), neglect terms of order $O(\varepsilon^2)$, we have

$$-\sigma_a\phi + q = \sigma_t T\phi - \frac{\sigma_t}{3}X^2\phi \quad (2.3.9)$$

Remark 2.3.2. (2.3.9) gives the classical diffusion (SP_1) equation

$$\frac{1}{v}\partial_t\phi = \frac{1}{3\sigma_t}\nabla_x^2\phi - \sigma_a\phi + q \quad (2.3.10)$$

Obviously, this is a parabolic equation.

2.3.2 SP_3 approximation

In order to derive the SP_3 approximation and get a parabolic PDE system, we need to isolate the terms with first-order time and second-order space derivative (which the parabolic means). Here we introduce $\alpha \in [0, 1]$ to split the term TX^2 into two parts so that we can use it with time terms T and second order space terms X^2 . Therefore, from (2.3.8) we have

$$\begin{aligned} -\sigma_a\phi + q &= \sigma_t T\phi - \frac{\sigma_t}{3}X^2 \left\{ \phi + \left[-\frac{4}{5}\alpha\varepsilon^4 TX^2\phi + \frac{4}{15}\varepsilon^2 X^2\phi + \frac{44}{315}\varepsilon^4 X^4\phi \right] \right. \\ &\quad \left. + \left[-\varepsilon^2 T\phi + \varepsilon^4 T^2\phi - \frac{4}{5}(1-\alpha)\varepsilon^4 TX^2\phi \right] \right\} \\ &= \sigma_t T\phi - \frac{\sigma_t}{3}X^2 \left\{ \phi + \left[1 + \frac{11}{21}\varepsilon^2 X^2 - 3\alpha\varepsilon^2 T \right] \frac{4}{15}\varepsilon^2 X^2\phi \right. \\ &\quad \left. - \left[1 - \varepsilon^2 T + \frac{4}{5}(1-\alpha)\varepsilon^2 X^2 \right] \varepsilon^2 T\phi \right\} + O(\varepsilon^6) \end{aligned} \quad (2.3.11)$$

Using Neumann's series again, from (2.3.11) we have

$$\begin{aligned} -\sigma_a\phi + q &= \sigma_t T\phi - \frac{\sigma_t}{3}X^2\left\{\phi + \left[1 - \frac{11}{21}\varepsilon^2X^2 + 3\alpha\varepsilon^2T\right]^{-1}\frac{4}{15}\varepsilon^2X^2\phi\right. \\ &\quad \left.- \left[1 + \varepsilon^2T - \frac{4}{5}(1 - \alpha)\varepsilon^2X^2\right]^{-1}\varepsilon^2T\phi\right\} + O(\varepsilon^6) \end{aligned} \quad (2.3.12)$$

Define

$$\phi_2 = \frac{1}{2}\left[1 - \frac{11}{21}\varepsilon^2X^2 + 3\alpha\varepsilon^2T\right]^{-1}\left(\frac{4}{15}\varepsilon^2X^2\phi\right) \quad (2.3.13a)$$

$$\zeta = \left[1 + \varepsilon^2T - \frac{4}{5}(1 - \alpha)\varepsilon^2X^2\right]^{-1}(\varepsilon^2T\phi) \quad (2.3.13b)$$

Then (2.3.12) becomes

$$\sigma_t T\phi = \frac{\sigma_t}{3}X^2[\phi + 2\phi_2 - \zeta] - \sigma_a\phi + q \quad (2.3.14)$$

From (2.3.13a) and (2.3.13b), we have

$$\begin{aligned} \left[1 - \frac{11}{21}\varepsilon^2X^2 + 3\alpha\varepsilon^2T\right]\phi_2 &= \frac{2}{15}\varepsilon^2X^2\phi \\ 3\alpha\varepsilon^2T\phi_2 &= \frac{2}{15}\varepsilon^2X^2\phi + \frac{11}{21}\varepsilon^2X^2 - \phi_2 \\ 3\alpha\sigma_t T\phi_2 &= \frac{\sigma_t}{3}X^2\left[\frac{2}{5}\phi + \frac{11}{7}\phi_2\right] - \frac{\sigma_t}{\varepsilon^2}\phi_2 \end{aligned} \quad (2.3.15)$$

and

$$\begin{aligned} \left[1 + \varepsilon^2T - \frac{4}{5}(1 - \alpha)\varepsilon^2X^2\right]\zeta &= \varepsilon^2T\phi \\ \varepsilon^2T\zeta - \varepsilon^2T\phi &= \frac{4}{5}(1 - \alpha)\varepsilon^2X^2 - \zeta \\ \sigma_t T(\zeta - \phi) &= \frac{\sigma_t}{3}X^2\left[\frac{12}{5}(1 - \alpha)\zeta\right] - \frac{\sigma_t}{\varepsilon^2}\zeta \end{aligned} \quad (2.3.16)$$

Combine (2.3.14), (2.3.15) and (2.3.16), we have a parabolic system

$$\sigma_t T\phi = \frac{\sigma_t}{3}X^2[\phi + 2\phi_2 - \zeta] - \sigma_a\phi + q \quad (2.3.17a)$$

$$3\alpha\sigma_t T\phi_2 = \frac{\sigma_t}{3}X^2\left[\frac{2}{5}\phi + \frac{11}{7}\phi_2\right] - \frac{\sigma_t}{\varepsilon^2}\phi_2 \quad (2.3.17b)$$

$$\sigma_t T(\zeta - \phi) = \frac{\sigma_t}{3}X^2\left[\frac{12}{5}(1 - \alpha)\zeta\right] - \frac{\sigma_t}{\varepsilon^2}\zeta \quad (2.3.17c)$$

Diagonalize the left side of (2.3.17), plug (2.3.17a) into (2.3.17c) and use the definition (2.3.3), we get the following system

$$\frac{1}{v}\partial_t\phi = \frac{1}{3\sigma_t}\nabla_x^2[\phi + 2\phi_2 - \zeta] - \sigma_a\phi + q \quad (2.3.18a)$$

$$\frac{1}{v}\partial_t\phi_2 = \frac{1}{3\sigma_t}\nabla_x^2\left[\frac{2}{15\alpha}\phi + \frac{11}{21\alpha}\phi_2\right] - \frac{1}{3\alpha}\frac{\sigma_t}{\varepsilon^2}\phi_2 \quad (2.3.18b)$$

$$\frac{1}{v}\partial_t\zeta = \frac{1}{3\sigma_t}\nabla_x^2\left[\phi + 2\phi_2 + \frac{7-12\alpha}{5}\zeta\right] - \sigma_a\phi + q - \frac{\sigma_t}{\varepsilon^2}\zeta \quad (2.3.18c)$$

Remark 2.3.3. For the linear system

$$\frac{\partial u}{\partial t} + A\Delta u = B(u_0 - u)$$

which is the same form as we derived in (2.3.18), where $u, u_0 \in \mathbb{R}^n$ and A, B are $n \times n$ matrices. If one of the eigenvalues of A is negative, then the problem is ill-posed. If there is a pair of conjugate complex eigenvalues, then we do not have a maximum principle, for the details, see [1]. Then we can not expect the solution to be positive.

Remark 2.3.4. For the system (2.3.18), the matrix

$$A = \frac{1}{3\sigma_t} \begin{bmatrix} 1 & 2 & -1 \\ \frac{2}{15\alpha} & \frac{11}{21\alpha} & 0 \\ 1 & 2 & \frac{7-12\alpha}{5} \end{bmatrix}$$

For approximately $\alpha > 0.9$, one eigenvalue of A has a negative real part. For $0 < \alpha < 0.9$ we have one positive real eigenvalue and two conjugate complex eigenvalues with positive real part. So to obtain a well-posed system, we must take $0 < \alpha < 0.9$, the calculation is taken from [1].

2.3.3 SSP_3 approximation

From the definition of (2.3.13b), we don't know the physical meaning of ζ . But we know $\zeta = 0$ is in steady-state. To simplify the SP_3 system, we can take $\zeta = 0$ in system (2.3.18) and have a new system

$$\frac{1}{v}\partial_t\phi = \frac{1}{3\sigma_t}\nabla_x^2[\phi + 2\phi_2] - \sigma_a\phi + q \quad (2.3.19a)$$

$$\frac{1}{v}\partial_t\phi_2 = \frac{1}{3\sigma_t}\nabla_x^2\left[\frac{2}{15\alpha}\phi + \frac{11}{21\alpha}\phi_2\right] - \frac{1}{3\alpha}\frac{\sigma_t}{\varepsilon^2}\phi_2 \quad (2.3.19b)$$

which we call SSP_3 (simplified-simplified P_3) equations.

Remark 2.3.5. For the system (2.3.19), the matrix

$$A = \frac{1}{3\sigma_t} \begin{bmatrix} 1 & 2 \\ \frac{2}{15\alpha} & \frac{11}{21\alpha} \end{bmatrix}$$

the eigenvalues of A are $(105\alpha + 55 + \sqrt{11025\alpha^2 + 210\alpha + 3025})/(210\alpha)$ and $(105\alpha + 55 - \sqrt{11025\alpha^2 + 210\alpha + 3025})/(210\alpha)$. Then we can see for $0 < \alpha < 1$, the eigenvalues are positive and we have a well-posed system.

Remark 2.3.6. In our test cases in Chapter 5, we take $\alpha = 2/3$, the reason is given in [1].

Chapter 3

Boundary and initial conditions

In this part, we will explicitly derive the boundary conditions for SP_1 , SP_3 and SSP_3 equations.

3.1 Boundary condition for SP_1

Here, we use Marshak's method [3], i.e. ignore the tangential derivative near the boundary and equate ingoing half fluxes

$$\int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi d\Omega = \int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi_b d\Omega \quad (3.1.1)$$

Use (2.3.4), the left side of (3.1.1) can be written as

$$\int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi d\Omega = \left\{ -1 - \frac{2}{3} \varepsilon (n \cdot X) \right\} \pi S + O(\varepsilon^2) \quad (3.1.2)$$

Proof of 3.1.2

Take rotation R ($\|R\| = 1$) such that $Rn = (0, 0, 1)^T$, then we have

$$\begin{aligned} \int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi d\Omega &= \int_{n \cdot \Omega < 0} (n \cdot \Omega) [1 - (\Omega \cdot X) \varepsilon] S d\Omega + O(\varepsilon^2) \\ &= \left\{ \int_{n \cdot \Omega < 0} (n \cdot \Omega) d\Omega - \varepsilon (n \cdot X) \int_{n \cdot \Omega < 0} (\Omega \cdot \Omega) d\Omega \right\} S + O(\varepsilon^2) \\ &= \left\{ \int_{Rn \cdot R\Omega < 0} (Rn \cdot R\Omega) dR\Omega - \varepsilon (n \cdot X) \int_{Rn \cdot R\Omega < 0} (R\Omega \cdot R\Omega) dR\Omega \right\} S + O(\varepsilon^2) \end{aligned}$$

Denote $\Omega' = R\Omega$ and set $\Omega' = (\sqrt{1-\mu'^2}\cos\theta', \sqrt{1-\mu'^2}\sin\theta', \mu')$, where $\mu' \in [-1, 1]$ and $\theta' \in [0, 2\pi]$, then we have $d\Omega' = d\mu'd\theta'$ and

$$\begin{aligned} \int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi d\Omega &= \left\{ \int_{Rn \cdot \Omega' < 0} (Rn \cdot \Omega') d\Omega' - \varepsilon(n \cdot X) \int_{Rn \cdot \Omega' < 0} (\Omega' \cdot \Omega') d\Omega' \right\} S + O(\varepsilon^2) \\ &= \left\{ \int_0^{2\pi} \int_{-1}^0 \mu' d\mu' d\theta' - \varepsilon(n \cdot X) \int_0^{2\pi} \int_{-1}^0 \mu'^2 d\mu' d\theta' \right\} S + O(\varepsilon^2) \\ &= \left\{ -1 - \frac{2}{3}\varepsilon(n \cdot X) \right\} \pi S + O(\varepsilon^2) \quad \square \end{aligned}$$

From (2.3.7) we have

$$\pi S = \frac{1}{4}\phi + O(\varepsilon^2) \quad (3.1.3)$$

Then we have

$$\frac{1}{4} \left\{ -1 - \frac{2}{3}\varepsilon(n \cdot X) \right\} \phi = \int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi_b d\Omega \quad (3.1.4)$$

Using $X = \frac{1}{\sigma_t} \nabla_x$, we get the boundary condition for SP_1 equation:

$$n \cdot \nabla_x \phi = \frac{\sigma_t}{\varepsilon} \left(\frac{3}{2} l_1 - \frac{3}{2} \phi \right) \quad (3.1.5)$$

where

$$l_1 = -4 \int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi_b d\Omega \quad (3.1.6)$$

3.2 Boundary conditions for SP_3

Use the same way that we derived boundary condition for SP_1 equations, we have

$$\int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi d\Omega = \int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi_b d\Omega \quad (3.2.1a)$$

$$\int_{n \cdot \Omega < 0} P_3(n \cdot \Omega) \psi d\Omega = \int_{n \cdot \Omega < 0} P_3(n \cdot \Omega) \psi_b d\Omega \quad (3.2.1b)$$

where P_3 is Legendre polynomial and $P_3(\mu) = \frac{1}{2}(5\mu^3 - 3\mu)$.

Use (2.3.4), we have

$$\begin{aligned} \int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi d\Omega &= \left\{ -1 - \frac{2}{3}\varepsilon(n \cdot X) + \varepsilon^2 \left[-\frac{1}{2}(n \cdot X)^2 + T \right] + \right. \\ &\quad \left. \varepsilon^3 \left[\frac{4}{3}(n \cdot X)T - \frac{2}{5}(n \cdot X)^3 \right] \right\} \pi S + O(\varepsilon^4) \end{aligned} \quad (3.2.2)$$

$$\begin{aligned} \int_{n \cdot \Omega < 0} P_3(n \cdot \Omega) \psi d\Omega &= \left\{ \frac{1}{4} + \varepsilon^2 \left[-\frac{1}{12}(n \cdot X) - \frac{1}{4}T \right] \right. \\ &\quad \left. - \frac{4}{35}\varepsilon^3(n \cdot X)^3 \right\} \pi S + O(\varepsilon^4) \end{aligned} \quad (3.2.3)$$

Proof of 3.2.2 and 3.2.3

Use the result and the same notation we have in the proof of 3.1.2 and use $n \cdot n = 1$, we have

$$\begin{aligned}
\int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi d\Omega &= \int_{n \cdot \Omega < 0} (n \cdot \Omega) \{1 - (\Omega \cdot X)\varepsilon + [-T + (\Omega \cdot X)^2]\varepsilon^2 \\
&\quad + [2(\Omega \cdot X)T - (\Omega \cdot X)^3]\varepsilon^3\} S d\Omega + O(\varepsilon^4) \\
&= \left\{-1 - \frac{2}{3}\varepsilon(n \cdot X) + \varepsilon^2 T + \frac{4}{3}\varepsilon^3 T(n \cdot X)\right\} \pi S + \\
&\quad \int_{n \cdot \Omega < 0} (n \cdot \Omega) [(\Omega \cdot X)^2 \varepsilon^2 - (\Omega \cdot X)^3 \varepsilon^3] S d\Omega + O(\varepsilon^4) \\
&= \left\{-1 - \frac{2}{3}\varepsilon(n \cdot X) + \varepsilon^2 T + \frac{4}{3}\varepsilon^3 T(n \cdot X)\right\} \pi S + \\
&\quad \int_{n \cdot \Omega < 0} (n \cdot \Omega) [(n \cdot X)^2 (\Omega \cdot \Omega)^2 \varepsilon^2 - (n \cdot X)^3 (\Omega \cdot \Omega)^3 \varepsilon^3] S d\Omega + O(\varepsilon^4) \\
&= \left\{-1 - \frac{2}{3}\varepsilon(n \cdot X) + \varepsilon^2 T + \frac{4}{3}\varepsilon^3 T(n \cdot X)\right\} \pi S + \\
&\quad \int_0^{2\pi} \int_{-1}^0 \{\varepsilon^2 (n \cdot X)^2 \mu'^3 - \varepsilon^3 (n \cdot X)^3 \mu'^4\} S d\mu' d\theta' + O(\varepsilon^4) \\
&= \left\{-1 - \frac{2}{3}\varepsilon(n \cdot X) + \varepsilon^2 \left[-\frac{1}{2}(n \cdot X)^2 + T\right] + \right. \\
&\quad \left. \varepsilon^3 \left[\frac{4}{3}(n \cdot X)T - \frac{2}{5}(n \cdot X)^3\right]\right\} \pi S + O(\varepsilon^4)
\end{aligned}$$

$$\begin{aligned}
\int_{n \cdot \Omega < 0} P_3(n \cdot \Omega) \psi d\Omega &= \int_{n \cdot \Omega < 0} \frac{1}{2} [5(n \cdot \Omega)^3 - 3(n \cdot \Omega)] \{1 - (\Omega \cdot X)\varepsilon + [-T + (\Omega \cdot X)^2]\varepsilon^2 \\
&\quad + [2(\Omega \cdot X)T - (\Omega \cdot X)^3]\varepsilon^3\} S d\Omega + O(\varepsilon^4) \\
&= \frac{1}{2} \int_0^{2\pi} \int_{-1}^0 \{(5\mu'^3 - 3\mu')(1 - \varepsilon^2 T) - (n \cdot X)\varepsilon(5\mu'^4 - 3\mu'^2) + \\
&\quad \varepsilon^2 (n \cdot X)^2 [5\mu'^5 - 3\mu'^3] + \varepsilon^3 [2T(n \cdot X)(5\mu'^4 - 3\mu'^2) \\
&\quad - (n \cdot X)^3 (5\mu'^6 - 3\mu'^4)]\} d\mu' d\theta' S + O(\varepsilon^4) \\
&= \left\{\frac{1}{4} + \varepsilon^2 \left[-\frac{1}{12}(n \cdot X) - \frac{1}{4}T\right] - \frac{4}{35}\varepsilon^3 (n \cdot X)^3\right\} \pi S + O(\varepsilon^4) \quad \square
\end{aligned}$$

From (2.3.7), we know

$$\pi S = \frac{1}{4} \left(\phi + \varepsilon^2 T \phi - \frac{1}{3} \varepsilon^2 X^2 \phi \right) + O(\varepsilon^4) \quad (3.2.4)$$

And from the definition (2.3.13) we get

$$\phi_2 = \frac{2}{15} \varepsilon^2 X^2 \phi + O(\varepsilon^4) \quad \text{and} \quad \zeta = \varepsilon^2 T \phi + O(\varepsilon^4) \quad (3.2.5)$$

Now we assume ϕ is constant on the boundary, that is we set $\zeta = 0$ on the boundary. Plug (3.2.4) into (3.2.2) and (3.2.3), using (3.2.5), up to $O(\varepsilon^4)$, we obtain

$$\begin{aligned}
-4 \int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi_b d\Omega &= \left\{ -1 - \frac{2}{3} \varepsilon (n \cdot X) + \varepsilon^2 \left[-\frac{1}{2} (n \cdot X)^2 + T \right] + \right. \\
&\quad \left. \varepsilon^3 \left[\frac{4}{3} (n \cdot X) T - \frac{2}{5} (n \cdot X)^3 \right] \right\} \cdot \left(\phi + \varepsilon^2 T \phi - \frac{1}{3} \varepsilon^2 X^2 \phi \right) \\
&= \phi + \varepsilon^2 T \phi - \frac{1}{3} \varepsilon^2 X^2 \phi - \varepsilon^2 T \phi + \frac{1}{2} \varepsilon^2 X^2 \phi \\
&\quad + \frac{2}{3} \varepsilon (n \cdot X) (\phi + \varepsilon^2 T \phi - \frac{1}{3} \varepsilon^2 X^2 \phi) - \varepsilon^3 \left[\frac{4}{3} (n \cdot X) T - \frac{2}{5} (n \cdot X)^3 \right] \phi \\
&= \phi + \frac{1}{6} \varepsilon^2 X^2 \phi + \frac{2}{3} (n \cdot X) \left[\phi + \frac{4}{15} \varepsilon^2 X^2 \phi - \varepsilon^2 T \phi \right] \\
&= \phi + \frac{5}{4} \phi_2 + \frac{2}{3} \varepsilon (n \cdot X) (\phi + 2\phi_2 - \zeta) \\
16 \int_{n \cdot \Omega < 0} P_3(n \cdot \Omega) \psi_b d\Omega &= \left\{ 1 + \varepsilon^2 \left[-\frac{1}{3} (n \cdot X)^2 - T \right] - \frac{16}{35} \varepsilon^3 (n \cdot X)^3 \right\} \left(\phi + \varepsilon^2 T \phi - \frac{1}{3} \varepsilon^2 X^2 \phi \right) \\
&= \phi + \varepsilon^2 T \phi - \frac{1}{3} \varepsilon^2 X^2 \phi - \varepsilon^2 T \phi - \frac{1}{3} \varepsilon^2 (n \cdot X)^2 \phi - \frac{16}{35} \varepsilon^3 (n \cdot X)^3 \phi \\
&= \phi - 5 \cdot \frac{2}{15} \varepsilon^2 X^2 \phi - \frac{24}{7} (n \cdot X) \varepsilon \cdot \frac{2}{15} \varepsilon^2 X^2 \phi \\
&= \phi - 5\phi_2 - \frac{24}{7} \varepsilon (n \cdot X) \phi_2
\end{aligned}$$

which are

$$\phi + \frac{5}{4} \phi_2 + \frac{2}{3} \varepsilon (n \cdot X) (\phi + 2\phi_2 - \zeta) = l_1 \quad (3.2.6)$$

$$\phi - 5\phi_2 - \frac{24}{7} \varepsilon (n \cdot X) \phi_2 = l_2 \quad (3.2.7)$$

where

$$l_1 = -4 \int_{n \cdot \Omega < 0} (n \cdot \Omega) \psi_b d\Omega, \quad l_2 = 16 \int_{n \cdot \Omega < 0} P_3(n \cdot \Omega) \psi_b d\Omega \quad (3.2.8)$$

Then we have the boundary conditions for SP_3 equations

$$\varepsilon(n \cdot X)\phi = -\frac{25}{12}\phi + \frac{25}{24}\phi_2 + \frac{3}{2}l_1 + \frac{7}{12}l_2 \quad (3.2.9a)$$

$$\varepsilon(n \cdot X)\phi_2 = \frac{7}{24}\phi - \frac{35}{24}\phi_2 - \frac{7}{24}l_2 \quad (3.2.9b)$$

$$\zeta = 0 \quad (3.2.9c)$$

Remark 3.2.1. From (3.2.9), neglect the $\zeta = 0$, we get the boundary conditions for SSP_3 equations.

3.3 Initial conditions

For a specific physical problem, the initial condition can be easily calculated. Since the physical meaning of ϕ_2 and ζ is not obvious, it is not so clear that which initial conditions should be given. But in many cases, the initial conditions are steady states. Then, the time-dependent SP_N equations become the steady-state SP_N equations. Thus the initial value for ζ should be 0. For ϕ_2 , we could also set it be zero, the reason is given in [1].

Chapter 4

Numerical method

In this part, we are going to give the methods which solve the SP_1, SSP_3, SP_3 equations numerically. The general form of these equations is:

$$\frac{\partial u}{\partial t} = \nabla D(x, y) \nabla u + f(u) \quad (4.0.1)$$

where $D(x, y)$ is a function of x, y , $f(u)$ is a function of u .

4.1 Discretization

We will do the discretization in 2-D followed by method of lines:

Take $Z = (0, 1) \times (0, 1)$ as an example, we cover it with a rectangular grid with grid sizes Δx in the x direction and Δy in the y direction, with $M + 2$ and $N + 2$ lines respectively, i.e, we have $M^2 N^2$ interior points, we label them as shown in Figure 4.1. And also we have four boundaries conditions (left, right, upper and lower) to be decided.

Define:

$$\begin{aligned} u_{i,j} &= u(i\Delta x, j\Delta y), \quad D(i, j) = D(i\Delta x, j\Delta y), \\ D_{i+1/2,j} &= \frac{1}{2}(D_{i+1,j} + D_{i,j}), \quad D_{i,j+1/2} = \frac{1}{2}(D_{i,j+1} + D_{i,j}) \end{aligned} \quad (4.1.1)$$

We write the equation (4.0.1) as

$$\begin{aligned} \frac{du}{dt} &= \frac{D_{i+1/2,j}(u_{i+1,j} - u_{i,j}) - D_{i-1/2,j}(u_{i,j} - u_{i-1,j})}{(\Delta x)^2} + \\ &\quad \frac{D_{i,j+1/2}(u_{i,j+1} - u_{i,j}) - D_{i,j-1/2}(u_{i,j} - u_{i,j-1})}{(\Delta y)^2} + f(u_{i,j}) \end{aligned}$$

Define U as:

$$U = (u_{1,1}, \dots, u_{M,1} | u_{1,2}, \dots, u_{M,2} | \dots | u_{1,N}, \dots, u_{M,N})^T \quad (4.1.2)$$

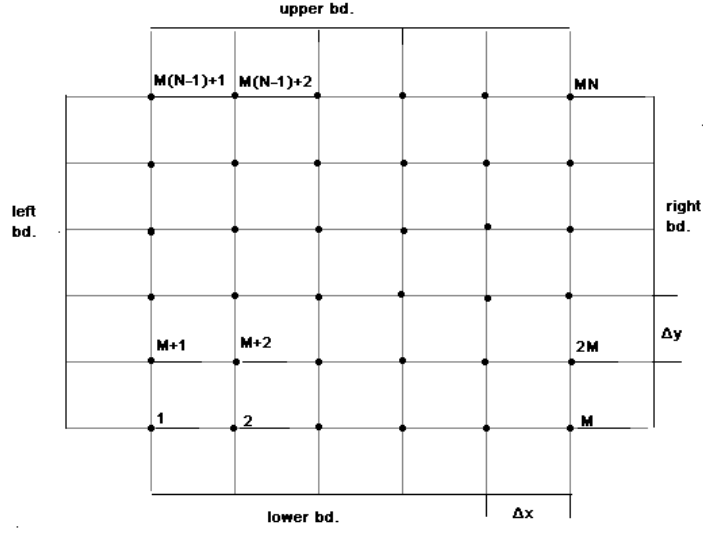


Figure 4.1: Discretization

Then we can obtain an ODE:

$$\frac{dU}{dt} = F(U) \quad (4.1.3)$$

On the other hand, if we have a system like

$$\begin{aligned} \frac{\partial u_1}{\partial t} &= \nabla a_1(x, y) \nabla g_1(u_1, u_2, \dots, u_n) + f_1(u_1, u_2, \dots, u_n) \\ \frac{\partial u_2}{\partial t} &= \nabla a_2(x, y) \nabla g_2(u_1, u_2, \dots, u_n) + f_2(u_1, u_2, \dots, u_n) \\ &\dots\dots\dots \\ \frac{\partial u_n}{\partial t} &= \nabla a_n(x, y) \nabla g_n(u_1, u_2, \dots, u_n) + f_n(u_1, u_2, \dots, u_n) \end{aligned}$$

where $a_i(x, y), i = 1, 2, \dots, n$ are functions of x, y and $g_i, i = 1, 2, \dots, n$ are linear combinations of $u_i, i = 1, 2, \dots, n$.

Define a new U :

$$U = (U_1 | U_2 | \dots | U_n)^T \quad (4.1.4)$$

where $U_i = (u_{i1,1}, \dots, u_{iM,1} | u_{i1,2}, \dots, u_{iM,2} | \dots | u_{i1,N}, \dots, u_{iM,N})$ and we can still obtain an ODE

$$\frac{dU}{dt} = F(U) \quad (4.1.5)$$

4.2 Implementation

When we make the Matlab code, we first use command 'reshape' to convert U to a $M \times N$ matrix, then use command 'diff' to include the boundaries, after that use 'reshape' to transform the matrix back to a vector, we give one example here to show how the code is made.

```
1/(3*sigma_t)*(reshape(1/dx^2*diff([ul1;reshape(z1,m,n);ur1],2,1),2,1) +  
1/dy^2*diff([ud1,reshape(z1,m,n),uu1],2,2),m*n,1)
```

Then use the ODE solvers which we have in Matlab (see table 4.1) to solve the equations.

| <i>solver</i> | <i>Numerical method</i> | <i>Type of problem</i> | <i>Order</i> | <i>Tolerance</i> |
|---------------|-------------------------|------------------------|--------------|------------------|
| ode45 | Runge-Kutta | nonstiff | Medium | Low |
| ode23 | Runge-Kutta | nonstiff | Low | High |
| ode15s | Difference | stiff | Variable | Low |
| ode23s | Modified Rosenbrock | stiff | Low | High |

Table 4.1: Solvers of Matlab

It is very convenient to use these solvers, but when we want to know the solution of large time and high space resolution, since our hardware is not good enough, it takes too much time (like 10 hours, 12 hours or even more for one equation), even the memory is not enough for the large time and high space resolution. So we need to make our own solver to solve the equations. In the following test cases, we use the explicit Euler scheme to get the solution at large time and high resolution.

Chapter 5

Test case

After we finish the code, we need to validate the code, here we give three test cases to validate the code.

In all of the following test problems, the physical medium is described by the absorption cross section σ_a and the total cross section σ_t , propagation speed c , density ρ and heat capacity c_v . And l_1, l_2 are what we have defined in Chapter 3.

5.1 Marshak Wave

This test case was taken from [4]. This problem corresponds to an initially cold, homogeneous, infinite and isotropically scattering medium with an internal radiation source. It is a 1-D problem. Also here, we have an energy equation coupled with the radiation equation. The corresponding radiative transport equation and the coupled energy equation are given by

$$\begin{aligned} \left(\frac{1}{v} \frac{\partial}{\partial t} + \mu \frac{\partial}{\partial z}\right) I(z, \mu, t) &= \sigma_a(T) \left[\frac{1}{2} a T^4(z, t) - I(z, \mu, t) \right] + \\ &\sigma_s(T) \left[\frac{1}{2} \int_{-1}^1 I(z, \mu', t) d\mu' - I(z, \mu, t) \right] + Q(z, \mu, t) \end{aligned} \quad (5.1.1a)$$

$$\frac{1}{v} c_v(T) \frac{\partial T(z, t)}{\partial t} = \sigma_a(T) \left[\int_{-1}^1 I(z, \mu', t) d\mu' - a T^4(z, t) \right] \quad (5.1.1b)$$

where z is the spatial variable, μ is the cosine of the angle between the photon direction and z -axis (as we shown in Chapter 2), t is the time variable. I is the photon intensity, T is temperature; Q is the radiation source, σ_a is the absorption cross section and σ_s is the scattering cross section; c_v is the heat capacity, a is the radiation constant.

Use the asymptotic analysis in Chapter 2, we give the problem setting and SP_N equations in the following.

5.1.1 Setting

The setting is one-dimensional in space ($x \in \mathbb{R}$ or x in a large interval $[-L, L]$), with time $t \in [0, 10]$.

We have $v = 1, \sigma_a = \sigma_t = 1$ and $\sigma_s = 0$. And we have a source

$$Q = \begin{cases} \frac{1}{2x_0} & 0 \leq t \leq t_0, -x_0 \leq x \leq x_0, \\ 0 & \text{otherwise} \end{cases} \quad (5.1.2)$$

with $x_0 = 0.5$ and $t_0 = 10$.

This is a $1 - D$ problem, but we will view it as $2 - D$ problem, the trick is: we solve it in the domain $[-L, L] \times [-M, M]$ and choose M big enough. Since the solution is symmetric, in order to compute the solution more cheaply, we do it in the domain $[0, L] \times [-M, M]$. The corresponding SP_N equations are given as follows.

5.1.2 SP_N equations

SP_1 equations

The equations are

$$\begin{aligned} \frac{\partial}{\partial t} \phi &= \nabla_x \frac{1}{3\sigma_t} \nabla_x \phi + \sigma_a (B - \phi) + Q \\ \frac{\partial}{\partial t} B &= \sigma_a (\phi - B) \end{aligned}$$

with boundary condition

$$\begin{aligned} \frac{1}{3\sigma_t} \frac{\partial}{\partial n} \phi &= -\frac{1}{2} \phi \quad \text{for } x = L \\ \frac{\partial}{\partial n} \phi &= 0 \quad \text{for } x = 0, y = \pm M \end{aligned}$$

and initial condition

$$\phi(0, x) = B(0, x) = 0$$

SSP_3 equations

The equations are

$$\begin{aligned} \frac{\partial}{\partial t} \phi &= \nabla_x \frac{1}{3\sigma_t} \nabla_x [\phi + 2\phi_2] + \sigma_a (B - \phi) + Q \\ \frac{\partial}{\partial t} \phi_2 &= \nabla_x \frac{1}{3\sigma_t} \nabla_x \left[\frac{2}{15\alpha} \phi + \frac{11}{21\alpha} \phi_2 \right] - \frac{1}{3\alpha} \sigma_t \phi_2 \\ \frac{\partial}{\partial t} B &= \sigma_a (\phi - B) \end{aligned}$$

Here we set $\alpha = 2/3$. The boundary conditions for $x = L$ are

$$\begin{aligned}\frac{\partial}{\partial n}\phi &= 3\sigma_t\left(-\frac{25}{36}\phi + \frac{25}{72}\phi_2\right) \\ \frac{\partial}{\partial n}\phi_2 &= 3\sigma_t\left(\frac{7}{72}\phi - \frac{35}{72}\phi_2\right)\end{aligned}$$

And the boundary conditions for $x = 0, y = \pm M$ are

$$\frac{\partial}{\partial n}\phi = \frac{\partial}{\partial n}\phi_2 = 0$$

and we have the initial conditions

$$\phi(0, x) = \phi_2(0, x) = B(0, x) = 0$$

SP_3 equations

The equations are

$$\begin{aligned}\frac{\partial}{\partial t}\phi &= \nabla_x \frac{1}{3\sigma_t} \nabla_x [\phi + 2\phi_2 - \zeta] + \sigma_a(B - \phi) + Q - \frac{5}{12 - 12\alpha}\zeta + \frac{5}{12 - 12\alpha}\sigma_t\zeta \\ \frac{\partial}{\partial t}\phi_2 &= \nabla_x \frac{1}{3\sigma_t} \nabla_x \left[\frac{2}{15\alpha}\phi + \frac{11}{21\alpha}\phi_2\right] - \frac{1}{3\alpha}\sigma_t\phi_2 \\ \frac{\partial}{\partial t}\zeta &= \nabla_x \frac{1}{3\sigma_t} \nabla_x \left[\phi + 2\phi_2 + \frac{7 - 12\alpha}{5}\zeta\right] + \sigma_a(B - \phi) + Q - \frac{5}{12 - 12\alpha}\zeta - \frac{7 - 12\alpha}{12 - 12\alpha}\sigma_t\zeta \\ \frac{\partial}{\partial t}B &= \sigma_a(\phi - B)\end{aligned}$$

Here we set $\alpha = 2/3$. The boundary conditions for $x = L$ are

$$\begin{aligned}\frac{\partial}{\partial n}\phi &= 3\sigma_t\left(-\frac{25}{36}\phi + \frac{25}{72}\phi_2\right) \\ \frac{\partial}{\partial n}\phi_2 &= 3\sigma_t\left(\frac{7}{72}\phi - \frac{35}{72}\phi_2\right) \\ \zeta &= 0\end{aligned}$$

And the boundary conditions for $x = 0, y = \pm M$ are

$$\frac{\partial}{\partial n}\phi = \frac{\partial}{\partial n}\phi_2 = \frac{\partial}{\partial n}\zeta = 0$$

and we have the initial conditions

$$\phi(0, x) = \phi_2(0, x) = \zeta(0, x) = B(0, x) = 0$$

5.1.3 Numerical results

For the numerical results, we take $L = 10$ and $M = 100$ and we are interested in ϕ as a function of x at three different time $t = 1, 3.16, 10$.

In the following, we give a table to compare the values at different time (1, 3.16, 10) for the SP_N equations and the transport equation, see Table 5.1. The values for the transport equation are taken from Table 1, [4].

| $x \setminus t$ | 1.0000 | 3.1623 | 10.000 | $x \setminus t$ | 1.0000 | 3.1623 | 10.000 |
|-----------------|---------|--------|--------|-----------------|--------|--------|--------|
| 0.0100 | 0.5029 | 0.9577 | 1.8621 | 0.0100 | 0.5371 | 1.0722 | 2.1027 |
| 0.1000 | 0.4981 | 0.9507 | 1.8533 | 0.1000 | 0.5320 | 1.0631 | 2.0902 |
| 0.1778 | 0.4859 | 0.9333 | 1.8315 | 0.1778 | 0.5191 | 1.0402 | 2.0589 |
| 0.3162 | 0.4381 | 0.8664 | 1.7475 | 0.3162 | 0.4654 | 0.9501 | 1.9372 |
| 0.4500 | 0.3742 | 0.7788 | 1.6386 | 0.4500 | 0.3866 | 0.8280 | 1.7763 |
| 0.5000 | 0.3415 | 0.7350 | 1.5844 | 0.5000 | 0.3435 | 0.7650 | 1.6950 |
| 0.5623 | 0.2904 | 0.6658 | 1.4979 | 0.5623 | 0.2762 | 0.6664 | 1.5663 |
| 0.7500 | 0.1946 | 0.5237 | 1.3089 | 0.7500 | 0.1659 | 0.4822 | 1.3040 |
| 1.0000 | 0.1051 | 0.3648 | 1.0705 | 1.0000 | 0.0844 | 0.3078 | 1.0088 |
| 1.3335 | 0.0404 | 0.2122 | 0.7945 | 1.3335 | 0.0363 | 0.1702 | 0.7092 |
| 1.7783 | 0.0108 | 0.1037 | 0.5386 | 1.7783 | 0.0134 | 0.0873 | 0.4650 |
| 3.1623 | | 0.0064 | 0.1226 | 3.1623 | 0.0002 | 0.0103 | 0.1160 |
| 5.6234 | | | 0.0044 | 5.6234 | | 0.0001 | 0.0080 |
| $x \setminus t$ | 1.0000 | 3.1623 | 10.000 | $x \setminus t$ | 1.0000 | 3.1623 | 10.000 |
| 0.0100 | 0.6179 | 1.1519 | 2.1619 | 0.0100 | 0.6431 | 1.2005 | 2.2358 |
| 0.1000 | 0.6119 | 1.1430 | 2.1505 | 0.1000 | 0.6359 | 1.1887 | 2.2194 |
| 0.1778 | 0.5975 | 1.1221 | 2.1240 | 0.1778 | 0.6196 | 1.1691 | 2.1834 |
| 0.3162 | 0.5424 | 1.0434 | 2.0245 | 0.3162 | 0.5619 | 1.0718 | 2.0645 |
| 0.4500 | 0.4315 | 0.8911 | 1.8352 | 0.4500 | 0.4471 | 0.9095 | 1.8607 |
| 0.5000 | 0.3815 | 0.8247 | 1.7537 | 0.5000 | 0.3580 | 0.7990 | 1.7319 |
| 0.5623 | 0.3089 | 0.7286 | 1.6355 | 0.5623 | 0.2537 | 0.6668 | 1.5750 |
| 0.7500 | 0.1445 | 0.4825 | 1.3060 | 0.7500 | 0.1143 | 0.4468 | 1.2740 |
| 1.0000 | 0.0563 | 0.3141 | 1.0438 | 1.0000 | 0.0365 | 0.2754 | 0.9878 |
| 1.3335 | 0.0032 | 0.1571 | 0.7385 | 1.3335 | 0.0029 | 0.1453 | 0.7082 |
| 1.7783 | -0.0050 | 0.0553 | 0.4510 | 1.7783 | | 0.0597 | 0.4502 |
| 3.1623 | | 0.0012 | 0.0964 | 3.1623 | | 0.0012 | 0.0967 |
| 5.6234 | | | 0.0040 | 5.6234 | | | 0.0038 |

Table 5.1: the value of ϕ , from left to right, up to down, they are from SP_1, SSP_3, SP_3 , transport equation respectively.

Compare the values at three different times (1,3,16,10) from the table, we can see for $x < 0.5$, the values calculated by SP_1, SSP_3, SP_3 equations are all smaller than the transport equation. SP_1 is about 20% smaller, SSP_3 is about 16%, SP_3 is about 5%. For $x > 0.5$ most of the values calculated by SP_1, SSP_3, SP_3 equations are bigger than the transport equation, the values calculated by SP_3 equations has the smallest error. So the SP_3 is best approximation among SP_1, SSP_3, SP_3 . Also we see there is a negative value calculate by SP_3 equations at $x = 1.7783$, which is due to the maximum principle is not satisfied.

Here, we also give three figures to compare the numerical results between SP_1, SSP_3, SP_3 equations and transport equation, see Figure 5.1, 5.2, 5.3. From the three figures, we can see that when $x < 0.5$, the plot computed by SP_1, SSP_3, SP_3 equations are lower than the transport equation; when $x > 0.5$, the plot computed by SP_1, SSP_3, SP_3 equations are a litter higher than the transport equation. The larger the x is, the smaller the error is. Also we can clearly see that the plot computed by SP_3 equations is the closest approximation among SP_1, SSP_3, SP_3 equations, which is our expectation.

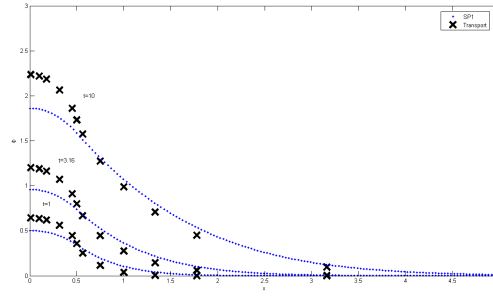


Figure 5.1: SP_1 and Transport equation

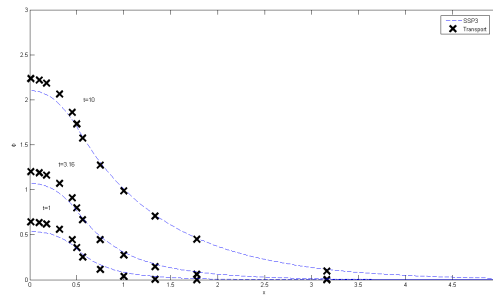


Figure 5.2: SSP_3 and Transport equation

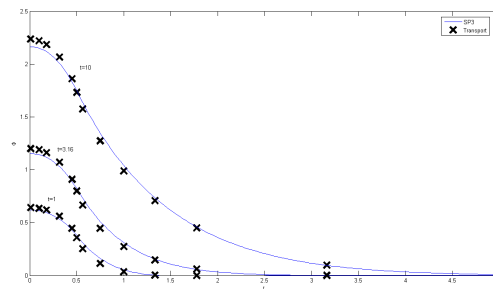


Figure 5.3: SP_3 and Transport equation

5.2 Marshak Wave 2

In this test case, we use the same SP_N equations we have given in Case Marshak wave. We use the same initial conditions, but different setting and boundary conditions.

5.2.1 Setting

Here, we take $v = 10$, $Q = 0$, $\sigma_a = 4$, $\sigma_t = 20$, $\sigma_s = 16$, and we consider $x \in [0, 1]$.

5.2.2 Boundary conditions

For the left boundary we take $\psi_b = \frac{50}{2\pi}$ and the right boundary we take $\psi_b = 0$. Use the definition of l_1, l_2 and the proofs in Chapter 3, we can get that $l_1 = l_2 = 100$ for the left boundary and $l_1 = l_2 = 0$ for the right boundary. In the following we will give the boundary conditions for SP_1, SSP_3, SP_3 equations.

Boundary conditions for SP_1

$$\begin{aligned}\frac{1}{3\sigma_t} \frac{\partial}{\partial n} \phi &= -\frac{1}{2} \phi \quad \text{for } x = L \\ \frac{\partial}{\partial n} \phi &= \frac{3}{2} \sigma_t (l_1 - \phi) \quad \text{for } x = 0 \\ \frac{\partial}{\partial n} \phi &= 0 \quad \text{for } y = \pm M\end{aligned}$$

Boundary conditions for SSP_3

The boundary conditions for $x = 0$ are

$$\begin{aligned}\frac{\partial}{\partial n} \phi &= 3\sigma_t \left(-\frac{25}{36} \phi + \frac{25}{72} \phi_2 + \frac{1}{2} l_1 + \frac{7}{36} l_2 \right) \\ \frac{\partial}{\partial n} \phi_2 &= 3\sigma_t \left(\frac{7}{72} \phi - \frac{35}{72} \phi_2 - \frac{7}{72} l_2 \right)\end{aligned}$$

The boundary conditions for $x = L$ are

$$\begin{aligned}\frac{\partial}{\partial n} \phi &= 3\sigma_t \left(-\frac{25}{36} \phi + \frac{25}{72} \phi_2 \right) \\ \frac{\partial}{\partial n} \phi_2 &= 3\sigma_t \left(\frac{7}{72} \phi - \frac{35}{72} \phi_2 \right)\end{aligned}$$

And the boundary conditions for $y = \pm M$ are

$$\frac{\partial}{\partial n} \phi = \frac{\partial}{\partial n} \phi_2 = 0$$

Boundary conditions for SP_3

The boundary conditions for $x = 0$ are

$$\begin{aligned}\frac{\partial}{\partial n}\phi &= 3\sigma_t\left(-\frac{25}{36}\phi + \frac{25}{72}\phi_2 + \frac{1}{2}l_1 + \frac{7}{36}l_2\right) \\ \frac{\partial}{\partial n}\phi_2 &= 3\sigma_t\left(\frac{7}{72}\phi - \frac{35}{72}\phi_2 - \frac{7}{72}l_2\right) \\ \zeta &= 0\end{aligned}$$

The boundary conditions for $x = L$ are

$$\begin{aligned}\frac{\partial}{\partial n}\phi &= 3\sigma_t\left(-\frac{25}{36}\phi + \frac{25}{72}\phi_2\right) \\ \frac{\partial}{\partial n}\phi_2 &= 3\sigma_t\left(\frac{7}{72}\phi - \frac{35}{72}\phi_2\right) \\ \zeta &= 0\end{aligned}$$

And the boundary conditions for $y = \pm M$ are

$$\frac{\partial}{\partial n}\phi = \frac{\partial}{\partial n}\phi_2 = \frac{\partial}{\partial n}\zeta = 0$$

5.2.3 Numerical results

First, let's check if the asymptotic analysis is valid. Take $t' = 0.1t$, $x' = x$, $\sigma'_t = \frac{1}{20}\sigma_t$ and $\sigma'_s = \frac{1}{16}\sigma_s$, then we have

$$\frac{1}{10} \cdot 0.1\partial_{t'}\psi + \Omega\nabla_{x'} + 20\sigma'_t\psi = \frac{16\sigma'_s}{4\pi} \int_{S^2} \psi d\Omega'$$

compare to (2.3.1), we know the assumption is satisfied for $t = 10$.

According to the setting, the radiation will propagate through the medium from left to right. Here we will compare the results computed by SP_1, SSP_3, SP_3 equations at time $t = 1$ and $t = 10$. The results are shown in Figure 5.4 and Figure 5.5. For $t = 1$, we can see the plots computed by SP_1 and SSP_3 are almost the same, but the plot computed by SP_3 are higher. For $t = 10$, we can see the three plots are almost the same, which is our expectation.

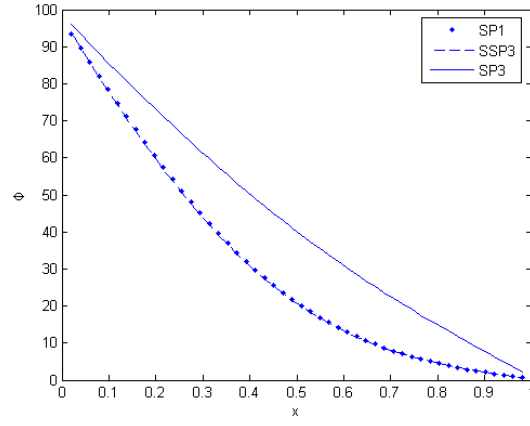


Figure 5.4: Comparison among SP_1 , SSP_3 and SP_3 at $t = 1$

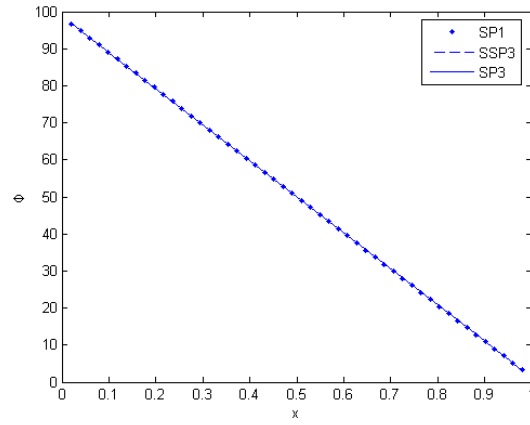


Figure 5.5: Comparison among SP_1 , SSP_3 and SP_3 at $t = 10$

5.3 Lattice Problem

This test case was taken from [5]. In this case, there is a source in the middle of the area and there are several obstacles surround the source.

5.3.1 Setting

This problem is a checkerboard of highly scattering and highly absorbing regions distributed on a lattice. The spatial domain of this problem is shown in Figure 5.6.

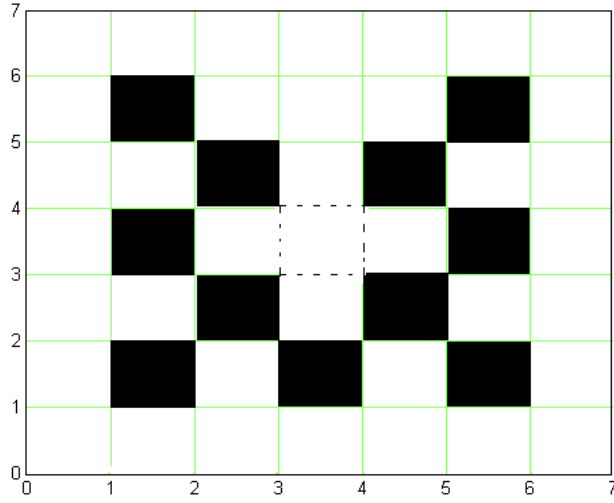


Figure 5.6: Lattice problem

The square $Z = [0, 7] \times [0, 7]$ is divided into the central region $Z_c = [3, 4] \times [3, 4]$ (dashed square), the absorbing region Z_a (black squares) and the bulk region Z_b (rest). The scattering cross sections vary with space

$$\sigma_t(x) = \sigma_a(x) = \begin{cases} 10, & x \in Z_a \\ 1, & \text{otherwise} \end{cases}$$

There is a unit source in the central region:

$$Q(x) = \begin{cases} 1, & x \in Z_c \\ 0, & \text{otherwise} \end{cases}$$

5.3.2 SP_N equations

SP_1 equations

The equations are

$$\frac{\partial}{\partial t}\phi = \nabla_x \frac{1}{3\sigma_t} \nabla_x \phi - \sigma_a \phi + Q$$

with boundary condition

$$\frac{1}{3\sigma_t} \frac{\partial}{\partial n} \phi = -\frac{1}{2} \phi$$

and initial condition

$$\phi(0, x) = 0$$

SSP_3 equations

The equations are

$$\begin{aligned} \frac{\partial}{\partial t}\phi &= \nabla_x \frac{1}{3\sigma_t} \nabla_x [\phi + 2\phi_2] - \sigma_a \phi + Q \\ \frac{\partial}{\partial t}\phi_2 &= \nabla_x \frac{1}{3\sigma_t} \nabla_x \left[\frac{2}{15\alpha} \phi + \frac{11}{21\alpha} \phi_2 \right] - \frac{1}{3\alpha} \sigma_t \phi_2 \end{aligned}$$

Here we set $\alpha = 2/3$. The boundary conditions are

$$\begin{aligned} \frac{\partial}{\partial n} \phi &= 3\sigma_t \left(-\frac{25}{36} \phi + \frac{25}{72} \phi_2 \right) \\ \frac{\partial}{\partial n} \phi_2 &= 3\sigma_t \left(\frac{7}{72} \phi - \frac{35}{72} \phi_2 \right) \end{aligned}$$

and we have the initial conditions

$$\phi(0, x) = \phi_2(0, x) = 0$$

SP_3 equations

The equations are

$$\begin{aligned} \frac{\partial}{\partial t}\phi &= \nabla_x \frac{1}{3\sigma_t} \nabla_x [\phi + 2\phi_2 - \zeta] - \sigma_a \phi + Q - \frac{5}{12 - 12\alpha} \zeta + \frac{5}{12 - 12\alpha} \sigma_t \zeta \\ \frac{\partial}{\partial t}\phi_2 &= \nabla_x \frac{1}{3\sigma_t} \nabla_x \left[\frac{2}{15\alpha} \phi + \frac{11}{21\alpha} \phi_2 \right] - \frac{1}{3\alpha} \sigma_t \phi_2 \\ \frac{\partial}{\partial t}\zeta &= \nabla_x \frac{1}{3\sigma_t} \nabla_x \left[\phi + 2\phi_2 + \frac{7 - 12\alpha}{5} \zeta \right] - \sigma_a \phi + Q - \frac{5}{12 - 12\alpha} \zeta - \frac{7 - 12\alpha}{12 - 12\alpha} \sigma_t \zeta \end{aligned}$$

Here we set $\alpha = 2/3$. The boundary conditions are

$$\begin{aligned}\frac{\partial}{\partial n}\phi &= 3\sigma_t\left(-\frac{25}{36}\phi + \frac{25}{72}\phi_2\right) \\ \frac{\partial}{\partial n}\phi_2 &= 3\sigma_t\left(\frac{7}{72}\phi - \frac{35}{72}\phi_2\right) \\ \zeta &= 0\end{aligned}$$

and we have the initial conditions

$$\phi(0, x) = \phi_2(0, x) = \zeta(0, x) = 0$$

5.3.3 Numerical results

Here, we concern about the value of ϕ which is a function of space at time $t = 3.2$. Please see the Figure 5.7 , 5.8 and 5.9. The color map is proportional to the logarithm of ϕ . They are given by solving the SP_1, SSP_3, SP_3 equations respectively.

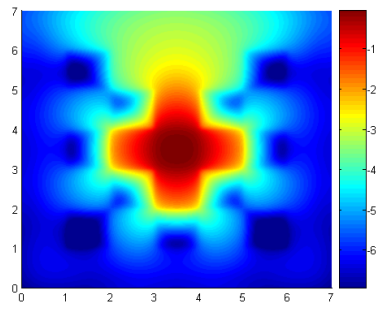


Figure 5.7: Lattice SP1

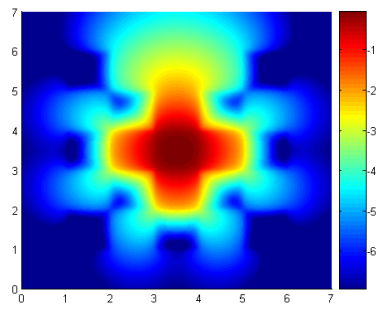


Figure 5.8: Lattice SSP3

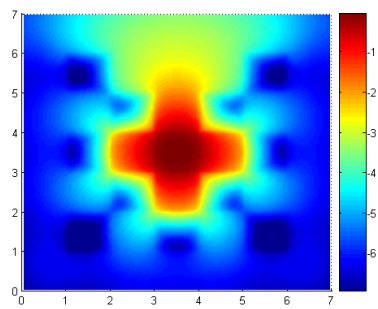


Figure 5.9: Lattice SP3

Compared to the numerical results in Figure 5, [5] (which we can consider it as a benchmark of Lattice problem), we can see that these three figures are all better than the upper left figure (a) which is calculated from P_1 approximation. But they are worse than the other three figures, the reason is due to the resolution is not high as shown in Figure 5, [5] and the approximation is not good enough. One of the figures is computed from P_{15} approximation and one of the figures is computed by implicit Monte-Carlo method which consists of 36 million particles.

First, look at these three figures, compare the mushroom shape in the upper middle with the benchmark, we can see these three figures in the left and right sides have more scattering than the benchmark, which maybe due to the lower approximation. According to this criterion, we can see the figure computed by SSP_3 is better than the other two figures.

Second, look at the six smaller mushroom shapes in the left, right and lower, compare with the benchmark, the mushroom should go deeper to the boundary, which we see here the figure computed by SSP_3 equations are deeper than the other two figures.

Third, the temperature of the six corners in the six smaller mushroom shapes should be higher, and the shape should be sharper. But in these three figures, we can only see very small sharp corners and the temperature is not high enough compared to the benchmark.

So we say the SSP_3 equations in this case is the best approximation among these three approximations. And also from the figures we can see that the figures computed by SP_3 is a little better than SP_1 .

Chapter 6

Conclusion and future work

In this work, we have derived the Simplified P_N equations for time-dependent problems via asymptotic analysis. And we explicitly derived the boundary conditions for SP_1, SSP_3, SP_3 equations. We give three test cases here. According to the numerical results, for the Marshak Case, the SP_3 give the best and quite close approximation compared to the transport equation; for Marshak Case 2, which is designed to satisfy the assumption of the asymptotic analysis. We see the solutions for SP_1, SSP_3 and SP_3 are very close at a large time, which is our expectation; for the Lattice Case, the SSP_3 give the best approximation, but still not so close to the benchmark due to the lower approximation and lower resolution. So we can try high-order approximation (like SP_7, SP_{11} and so on) and high resolution, especially for Lattice Case. Also we can try other numerical methods (like Monte-Carlo method) to solve the equations.

Bibliography

- [1] Martin Frank, Axel Klar, Edward W.Larsen, Shugo Yasuda *Time-dependent simplified P_N approximation to the equations of radiative transfer*, J. Comput. Phys. 226 (2007), 2289-2305.
- [2] E.W.Larsen, J.E.Morel, J.M.McGhee, *Asymptotic derivation of the multigroup P_1 and simplified P_N equations with anisotropic scattering*, Nucl. Sci. Eng. 123 (1996), 328.
- [3] R.E.Marshak, *Note on the spherical harmonic method as applied to Milne problem for a sphere*, Phys. Rev. 71 (1947), 443-446.
- [4] B.Su and G.L.Olson, *An analytical benchmark for non-equilibrium radiative transfer in an isotropically scattering medium*, Ann. Nucl. Energy 24 (1997), 1035-1055.
- [5] T.A.Brunner and J.P.Holloway, *Two-dimensional time dependent Riemann solvers for neutron transport*, J. Comput. Phys. 210 (2005), 386-399.
- [6] Edward W.Larsen, *The nature of transport calculations used in radiation oncology*, Transport Theory and Statistical Phys. 26 (1997), 739.
- [7] http://www.oncoprof.net/Generale2000/g08_Radiotherapie/Index/g08-gb_idx02.html, 31 December 2006.
- [8] http://en.wikipedia.org/wiki/Radiation_therapy, 21 November 2007.
- [9] <http://www.nhsdirect.nhs.uk/articles/article.aspx?articleId=309>, 22 October 2007.
- [10] <http://www.cancerbackup.org.uk/Treatments/Radiotherapy/Generalinformation/Whatisit>, 20 November 2007.