Faculty of Computer Science and Information Technology

LATTICE BOLTZMANN METHOD FOR GENERAL CONVECTION-DIFFUSION EQUATION BY USING MULTIPLE RELAXATION MODEL AND BOUNDARY SCHEMES

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Bachelor of Computer Science with Honours (Computational Science)

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ABSTRACT

Due to the multidimensionality, nonlinearity and the coupling with other physical fields of convection-diffusion equation, the traditional numerical method faces some complication in terms of universality and efficiency. In the past years, Lattice Boltzmann (LB) methods has been adapted to convection-diffusion equations due to its efficient approach for hydrodynamics simulation and this method is simple in formulation, easy for parallelization and can be used extendedly to high dimensional problems directly. Therefore, a model is proposed in order to solve the nonlinear convection-diffusion equation and the model used is the Multiple-Relaxation-Time model. This model provides great flexibility in tuning the relaxation of individual movement and it is the most stable model although some might say that the model is difficult to deal with. The model mimics the traditional method and additionally, these models are able to be developed further into third-order models which will be left for future.

ABSTRAK

Disebabkan dengan multidimensi, ketidaklineran dan gandingan dengan medan fizikal yang lain yang terdapat di dalam persamaan penyebaran konveksi, kaedah berangka tradisional telah menghadapi beberapa kesulitan dari segi universal dan kecekapan. Dalam tahun-tahun lepas, kaedah kekisi Boltzmann telah diguna pakai dalam persamaan penyebaran konveksi kerana mempunyai pendekatan yang cekap untuk simulasi hidrodinamik dan kaedah ini mudah dari segi formulasi, keselarian dan boleh digunakan secara meluas untuk masalah dimensi tinggi secara langsung. Oleh itu, satu model telah dicadangkan untuk menyelesaikan persaaman penyebaran konveksi tidak linear.

CHAPTER 1: INTRODUCTION

1.1 Overview

Convection diffusion equation is a combination of two equation, diffusion equation and convection (advection) equation. This equation describes physical phenomena where energy, particles or other physical quantities are transferred inside a physical system due to two processes which is diffusion and convection.

The convection diffusion equations are as follow:

$$\frac{\partial x}{\partial t} = \nabla \cdot (D\nabla x) - \nabla \cdot (\vec{v}x) + F,$$

where:

- $\boldsymbol{x}$ is the variable of interest (species concentration for mass transfer, temperature of heat transfer),
- $\boldsymbol{D}$ is the diffusivity (diffusion coefficient), such as mass diffusivity for particle motion or thermal diffusivity for heat transport,
- $\vec{\boldsymbol{v}}$ is the velocity field that the quantity is moving with.
- $\boldsymbol{F}$ describes the source/sinks of the quantity $\boldsymbol{x}$**.** For heat transport, $\boldsymbol{F > 0}$ might occur if thermal energy is being gained by friction.

- $\boldsymbol{\nabla}$ represent gradient while $\boldsymbol{\nabla} \cdot$ represent divergence. In this equation, $\boldsymbol{\nabla x}$ represent concentration gradient.

This equation can be divided into three parts:

a) $\boldsymbol{\nabla} \cdot (\boldsymbol{D\nabla x})$ describes diffusion. The net diffusion is proportional to Laplacian of concentration. The net diffusion is proportional to the Laplacian of concentration is the diffusivity, $\boldsymbol{D}$ is a constant.

b) $-\boldsymbol{\nabla} \cdot (\boldsymbol{\vec{v}x})$ describes convection/advection.

c) $\boldsymbol{F}$ represents the source term; describes the creation or destruction of a quantity. $\boldsymbol{F}$ may be a function of $\boldsymbol{x}$ and of other parameters. Often there are several quantities, each with its own convection diffusion equation, where the destruction of one quantity entails the creation of another.

This class of partial differentiation equation has been extensively investigated numerically. Some traditional numerical method of solving convection-diffusion equations includes finite element, finite volume and finite difference methods.

1.2 Problem Statement

Due to the multidimensionality, nonlinearity and the coupling with other physical fields of convection diffusion equation, the traditional method faces some complication in terms of universality and efficiency. In the past years, Lattice Boltzmann (LB) methods has been adapted to convection diffusion equations due to its efficient approach for hydrodynamics simulation and although this method is simple in formulation, easy for parallelization and can be used extendedly to high dimensional problems directly, there are still some limitation in the implementation and may be not be satisfied for some special cases.

1.3 Scope

The scope for this research is to simulate mathematical modelling of convection diffusion equation by using Lattice Boltzmann method.

Other scope includes:

i) To use MATLAB to simulate the model

1.4 Objective

The main objective of this research is to

i. To validate the accuracy of the proposed model and boundary schemes.

ii. To simulate the model by using MATLAB software.

1.5 Brief Methodology

1 Identify the problem

The first step in this project is to identify the problems. In this project, we know that the traditional method that has been used to solve convection diffusion equation is not enough and even though Lattice Boltzmann method has been adapted to solve convection diffusion equation we still need a modification in solving the problem such as Bhatnagar-Gross and Krook model (BGK) but it cannot be used in solving special convection diffusion equation due to the assumptions and integration of the models. So, we try to identify the suitable model for solving the special convection diffusion equation and will focus on the factor model.

2 Define goals and objective

The goal of the problem will be aimed as the objectives for this project. So, for this case we would like to study more on the Lattice Boltzmann method for general convection diffusion equation. The problem is then solved using suitable method.

3 Characterize the model

All the assumptions of this model will be listed where the quality of interest for this project is clear and the equation model could be explained. Also, all the rules are fixed based on the chosen equation model to solve the modelling for MRT model.

4 Define rules for the model

The mathematical model that will be used in this research includes Partial Differential Equation, Convection Diffusion Equation, and Lattice Boltzmann Model.

5 Solve and simulate the model

In this model, MATLAB plays an important role. This software allows us to analyse data, algorithm development and model creation. MATLAB also allows us to do some calculation and model simulation.

6 Analyse the model

Result of the simulation will be analysed once the model has been simulated.

7 Comparison of model

In this phase, the data from the model that has been chosen will be compared with the result produced by the model.

1.6 Significant of Project

Based on the outcome of the research, we would like to understand the convection diffusion equation using Lattice Boltzmann by focusing numerical analysis.

1.7 Project Schedule

Refer to Appendix A

1.8 Expected Outcome

In this research, a relationship between Lattice Boltzmann method and convection-diffusion equation will be set up through the comprehension of each parameters in the model. This will be obtained by using MRT model and simulation using MATLAB software.

CHAPTER 2: LITERATURE REVIEW

2.1 Introduction

In this chapter, we will focus on the literature review that are related to our studies. Different articles and journals are used as a source of review in order to gain knowledge about this topic and for better understanding in order to proceed with our research. The chapter review will deal with other sources that are mainly related to the Lattice Boltzmann Method for general convection- diffusion equation.

Lattice Boltzmann methods (LBM) is a class of computational fluid dynamics (CFD) methods for fluid simulation. Instead of solving the Navier–Stokes equations directly, a fluid density on a lattice is simulated with streaming and collision (relaxation) processes. The method is versatile as the model fluid can straightforwardly be made to mimic common fluid behaviour like vapour/liquid coexistence, and so fluid systems such as liquid droplets can be simulated. Also, fluids in complex environments such as porous media can be straightforwardly simulated, whereas with complex boundaries other CFD methods can be hard to work with.

The Lattice Boltzmann Model is relatively a new approach for simulating fluid flows and modelling complex physics in fluids. Compared to the traditional computational fluid dynamic approach, the Lattice Boltzmann Method is simpler in terms of programming intrinsically parallel and easier to incorporate complicated boundary like those in porous media. (Shi, 2009) and it also has been developed as an efficient numerical scheme for solving other problems which includes diffusion reaction equation, wave equation, traffic flow and image analysis. (Zhang, 2001)

2.2 Problems with the Existing Lattice Boltzmann Method

Xiang (2013) stated that although Lattice Boltzmann Methods has a number of advantages such as algorithmic simplicity, fully parallel computation and easy implementation for complex boundary condition, it cannot get the simulation result as accurate as possible and even fails to complete the numerical simulation for wider range of computation due to the numerical instability with small kinetic viscosity or the dimensionless relaxation time is close to a critical value. It is found out that the Lattice Boltzmann Method also can only be applied on a regular mesh. (Wang et al, 2015). The time step is also tied up with the mesh spacing in Lattice Boltzmann Method.

Chai (2013) says that based on a collision operator, the models of Lattice Boltzmann Method is divided into three types which are:

a) The single-relaxation time model (known as Bhatnagar-Gross-Krook (BGK) model)
b) The two-relaxation-time model
c) Multiple-relaxation-time model

According to Luo (2011), the difference of each model resides in their collision terms.

2.3 Single-Relaxation Time Model (BGK Model)

The single-relaxation time model is the simplest model in terms of the appearance and thus is the most popular one. However, the model has several inherent deficiencies which includes numerical instability and inaccurate boundary locations. In terms of the equilibrium of the models, there is an integration related to the convection term of the convection-diffusion equation. This integration may or may not be analytically obtained for some convection terms so that the models cannot be used directly. Also, more storage space is needed for discretizing the time derivative in the source terms, which requires special treatments for initializations as well. Peng (2016) also added that the lattice Boltzmann equation with Single-Relaxation-Time Model is less stable due to the fixed Prandtl number (the ratio of kinematic viscosity to thermal diffusivity) and fixed ratio between the kinematic and bulk viscosities.

2.4 Two-Relaxation-Time Model

The two-relaxation-time model is a type of model which allows only two most important relaxation rates in the Lattice Boltzmann Model, and assumptions on smallness of the derivatives of convection and diffusion have been made to derive the correct microscopic equation. Although this model provides more flexibility and control compared to single-relaxation-time model, the model itself is limited and it cannot cure all deficiencies of the single-relaxation-time model. There are still truncation errors in in this model and they can be large for certain simulations. (Krüger, 2016)

2.5 Multiple-Relaxation-Time Model

As for the multiple-relaxation-time model, it is the most general form derived from the linearized collision model within the theoretical framework of the Lattice Boltzmann Model and its kinetic theory. It includes all the possible degrees of freedom to optimise the Lattice Boltzmann Model, and it has been proven that Multiple-Relaxation-Time model is more superior over the Single-Relaxation-Time model in terms of efficiency, stability and computational efficiency. This model has the largest number of parameters to tune accuracy and stability and also allows us to choose the bulk viscosity independently of the shear viscosity. (Krüger, 2016).

2.6 Convection

Convection is the gradient of concentration of pollutant which corresponds to distances and it is expressed in terms of $u\frac{\partial c}{\partial x}$, where u is the flow velocity and can be constant. This term is considered as one-dimensional concentration gradient. Both advection and diffusion move the pollutant from one place to another, but each accomplishes this in different ways. That is; advection moves in one way (i.e., in the flow direction downstream) while diffusion spreads out (i.e., regardless of a stream flow direction). Another important property is that advection is represented by first-order derivate, which means that if x is replaced by $-x$ the term changes signs; this is the anti-symmetric, while by observing, diffusion term is introducing the symmetry property where if x is replaced by – x then the term does not change sign (Sobey, 1983).

2.7 Diffusion

Diffusion can be said as a fundamental transport process in environmental fluid mechanics. The difference between diffusion and convection is that diffusion is random in nature and does not follow a fluid particle). Diffusion has two primary properties: it is random in nature, and transport occurs from regions of high concentration to low concentration, with an equilibrium state of uniform concertation. In convection-diffusion equation, the term $-D\,\frac{\partial^L c}{\partial x^2}$ is the one-dimensional diffusive flux equation. It is important to note that diffusive flux is a vector quantity and since the concertation is expressed in units of $\frac{M}{L^3}$ it has units of $\frac{M}{L^2T}$. To compute the total mass flux rate *m*, the diffusive flux rate must be integrated over a surface area (Sobey, 1983)

2.8 Summary

A lattice Boltzmann model for convection-diffusion equation with nonlinear convection and isotropic diffusion terms are proposed through selecting equilibrium distribution function properly. The model can be applied to the common real and complex-valued nonlinear evolutionary equations, such as the nonlinear Schrödinger equation, complex Ginzburg-Landau equation, Burgers-Fisher equation, nonlinear heat conduction equation, and sine-Gordon equation, by using a real and complex-valued distribution function and relaxation time. Detailed simulations of these equations are performed, and it is found that the numerical results agree well with the analytical solutions and the numerical solutions reported in previous studies.

Two main approaches build the anisotropic diffusion coefficients either from the anisotropic anti-symmetric collision matrix or from the anisotropic symmetric equilibrium distribution. We combine and extend existing approaches for all commonly used velocity sets, prescribe most general equilibrium and build the diffusion and numerical-diffusion forms, then derive and compare solvability conditions, examine available anisotropy and stable velocity magnitudes in the presence of advection. Besides the deterioration of accuracy, the numerical diffusion dictates the stable velocity range.

A modified lattice Boltzmann model with multiple relaxation times (MRT) for the convection-diffusion equation (CDE) is proposed. By modifying the relaxation matrix, as well as choosing the corresponding equilibrium distribution function properly, the present model can recover the CDE with anisotropic diffusion coefficient with no deviation term even when the velocity vector varies generally with space or time through the Chapman-Enskog analysis. This model is firstly validated by simulating the diffusion of a Gaussian hill, which demonstrates it can handle the anisotropic diffusion problem correctly. Then it is adopted to calculate the longitudinal dispersion coefficient of the Taylor-Aris dispersion. Numerical results show that the present model can further reduce the numerical error under the condition of non-zero velocity vector, especially when the dimensionless relaxation time is relatively large.