Numerical Study Using Statistical and Quantum Approaches for Solving Energy and Navier Stokes Momentum Equations (PDEs)

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Abstract

Statistical and Quantum numerical method was implemented in this study to solve various cases in partial differential equations (PDEs) in engineering applications. One-dimensional with two lattices arrangements as well as two-dimensional with nine lattices arrangements is employed. The stability and the accuracy have been investigated either using statistical technique or using Euler’s method. The numerical limitations of using LBM method have been obtained and compared with those obtained by Euler’s method finite difference method. The main goal of this study is to investigate the ability of a statistical method in solving various ODEs or PDEs in energy and momentum equations and comparing them with those obtained by a classical numerical technique. The results show the ability of the statistical method for solving ODEs and PDE’s with more stable and accurate results. Therefore, the motivation of utilizing the statistical technique is the stability and it is easy for a complex fluid flow application.

Keywords

FDM, Technique, Stability, Analysis, Statistical, Quantum

1. Introduction

The Austrian physicist, Boltzmann is the first physicists who applied the statistical method for solving ODEs or PDEs. He had the greatest achievement in the development of statistical methodology, which based on the statistical and probability of behavior of a group of particles. This technique is quiet new tech-
nique and recently applied for various applications in order to predict macroscopic properties of matter such as the viscosity, thermal conductivity, and diffusion coefficient from the microscopic properties of atoms and molecules [1] [2] [3]. The probability of finding particles within certain range of velocities at a certain range of locations replaces tagging each particle as in molecular dynamic simulation. The statistical technique belongs to the molecular dynamics, filling the gap between the microscopic and macroscopic phenomenology. It generated from the lattice-gas cellular automata method [1]. The statistical technique which is known as the lattice Bhatnagar-Gross-Krook (BGK) method has been developed rapidly and applied for many studies. The nonlinear term in the lattice Boltzmann is approximated by BGK to become linear term, and this term is known as the collision term in the lattice BGK governing equation. The main idea of LBM is to embank the gap between micro-scale and macro-scale by not considering individual behavior of particles alone but behavior of a group of particles as a unit. The property of particle is represented by a distribution function. The distribution function acts as a representative for collection of particles. This scale is unknown as microscopic scale. In nature, the two immiscible fluids are multicomponent fluids. This type of technique is based on the interaction between each fluid molecule naturally as well as the interface region for multi-phase flow [4] [5] [6].

2. Mathematical Model

The statistical approach has been employed to predict macroscopic properties of matter such as the viscosity, thermal conductivity, and diffusion coefficient from the microscopic properties of atoms and molecules [7]. The probability of finding particles within certain range of velocities at a certain range of locations replaces tagging each particle as in molecular dynamics simulation. The Boltzmann transportation of single fluid has been modeled by several investigators including the present authors recently [4]. Statistical technique will be considered in the present study using one and two-dimensional with two and nine directional lattices arrangements. Statistical approach is a relatively recent technique that has been shown to be as accurate as traditional CFD methods having ability to be implemented to simulate complex flows. The statistical technique can be utilized for different arrangements which can give a more stable and accurate results [8] [9] [10]. The collision of particles takes place between the molecules; there will be a net difference between the numbers of molecules in the interval. The rate of change of the distribution function is expressed as:

\[
\frac{\partial S_k}{\partial t} + c_k \cdot \nabla S_k = \omega \left( S_k^{eq} - S_k \right) \quad \text{for} \quad k = 1, \ldots, m
\]

\[
\frac{\partial h_k}{\partial t} + c_k \cdot \nabla h_k = \omega \left( h_k^{eq} - h_k \right)
\]

Here \(k\) denotes the direction, \(c\) is the lattice discrete velocity and \(F\) is external forces applied. \(\omega \left( S_k^{eq} - S_k \right)\) and \(\omega \left( h_k^{eq} - h_k \right)\) denote the source or the colli-
sion term for each phase. Equation (1) is known as the BGK LB governing equation. \( \omega_1 = 1/\tau_1 \) and \( \omega_2 = 1/\tau_2 \) are the relaxation frequency and the \( \tau_1 \) and \( \tau_2 \) are the relaxation time of each phase. \( S_i^{eq} \) and \( h_i^{eq} \) are the equilibrium value of distribution function for each phase. They need to be selected carefully to ensure that each of the components obeys the Navier’s Stokes Law:

\[
\frac{S_i^{eq}}{w_i \rho_i} = \frac{h_i^{eq}}{w_i \rho_i} = \left[ 1 + \frac{3c_i \cdot V}{c_i^2} + 4.5 \left( \frac{c_i \cdot V}{c_i^4} \right)^2 - 1.5 \frac{V \cdot V}{c_i^2} \right]
\]

(2)

where \( c_k \) is the discrete velocities vector, \( V \) is the bulk fluid velocity and \( w_k \) is the weight factor.

\[
\begin{align*}
  c_k &= \begin{cases} 
  (0,0) & k = 1 \\
  \frac{\sin(k-1)\pi}{2}, \frac{\cos(k-1)\pi}{2} & k = 2, 3, 4, 5 \\
  \sqrt{2} \frac{\cos(2k-11)\pi}{4}, \sqrt{2} \frac{\sin(2k-11)\pi}{4} & k = 6, 7, 8, 9 
  \end{cases} \\
  w_k &= \begin{cases} 
  \frac{4}{9} & k = 1 \\
  \frac{4}{36} & k = 2, 3, 4, 5 \\
  \frac{1}{9} & k = 6, 7, 8, 9 
  \end{cases} \\
  w_k &= \begin{cases} 
  \frac{1}{2} & k = 1 \\
  \frac{1}{2} & k = 2 
  \end{cases}
\end{align*}
\]

(3)

The momentum statistical technique assigns the directional velocities to the particles, in D2Q9 model, the particle at the origin is at rest and the remaining particles move in different directions with different speed \([11]\). Each velocity vector is a lattice per unit step. These velocities are very convenient in that all x and y-components are either 0 or ±1. Mass of particle is taken as unity uniformly throughout the flow domain. The macroscopic fluid density is governed by conservation of mass for each phase (Table 1)

\[
\rho = \sum_{k=1}^{q} S_k
\]

(4)

**Table 1.** Investigated Cases: diffusion heat energy equations and momentum equations (Navier Stokes equation).

| CASE (1) | 1D Diffusion Energy Equation |
|----------|------------------------------|
|          | \( \frac{\partial T}{\partial t} = \alpha \left[ \frac{\partial^2 T}{\partial x^2} \right] \) |
|          | BCs are taken as: at \( x = 0 \), \( T(x = 0) = 100^\circ C \) \& at \( x = 3 \text{ m} \), \( T(x = 3 \text{ m}) = 20^\circ C \) |

| CASE (2) | 2D Energy Equation |
|----------|------------------|
|          | \( \frac{\partial T}{\partial t} = \alpha \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] \) |
|          | BCs are taken as: at \( x = 0 \), \( T(y = 0) = 100^\circ C \) \& at \( x = 3 \text{ m} \), \( T(y = H) = 100^\circ C \) |
CASE (3) Navier Stokes Equation in x & y direction (Momentum Equation)

\[
\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial x} + \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + g_x
\]

(7)

\[
\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial y} + \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + g_y
\]

(8)

BCs are taken as: Left: \( u = vRe/D \), lower and upper BCs are no-slip boundary conditions.

\[
\theta = \sum_{k=1}^{Q} h_k
\]

(10)

Solving of Naiver stokes equation is one of challenging problem in fluid behavior applications. The different methodologies have been developed. The stability and the accuracy of these methodologies are the most researchers concern [12]. The geometry of a problem and the type of the interaction fluid need different simulation tools [13]. In this part of study, the diffusion heat transfer equation as well as the momentum equation for a single-phase fluid flow has been solved using statistical and quantum approach. The stability and accuracy have been investigated for various number of nodes/lattices. Table 1 shows the three study cases which are selected for comparison purposes between statistical approach and quantum approach.

**Study Cases (For Comparison Purposes)**

**Explicit Method of Case (3):**

The combining of vorticity formulation and stream function formulation with Equation (8) lead to:

\[
u = \frac{\partial \psi}{\partial y}, v = -\frac{\partial \psi}{\partial x}, \phi = \frac{\partial v}{\partial y} - \frac{\partial u}{\partial x}
\]

(11)

\[
\frac{\partial \phi}{\partial t} + \frac{\partial \psi}{\partial x} \frac{\partial \phi}{\partial x} - \frac{\partial \psi}{\partial y} \frac{\partial \phi}{\partial y} = \frac{1}{Re} \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right)
\]

(12)

\[
\left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) = -\phi
\]

(13)

Using central difference scheme in order to linearize the Equation (12) leads to:

\[
\psi^{i+1} (i, j+1) - 2\psi^{i+1} (i, j) + \psi^{i+1} (i, j-1) - \Delta x^2 \frac{\Delta^2 \psi^{i+1} (i, j) - 2\psi^{i+1} (i, j) + \psi^{i+1} (i-1, j)}{2\Delta x^2}
\]

(14)

Now, the Equation (1) can be expanded for two-dimensional lattices as:

\[
S_x (x+\Delta x, t+\Delta t) = (1-\omega)S_x (x, t) + \omega S_x^\alpha (x, t)
\]

(15)

where:

\[
S_x^\alpha (x, t) = \frac{U' (i+1, j) - 2U' (i, j) + U' (i-1, j)}{\Delta X^2} \text{ and } \omega = \frac{2\Delta}{\Delta X^2} \alpha
\]

(16)

\[
S_y^\alpha (y, t) = \frac{U' (i, j+1) - 2U' (i, j) + U' (i, j-1)}{\Delta Y^2} \text{ and } \omega = \frac{2\Delta}{\Delta Y^2} \alpha
\]
3. Results and Discussions

**Figure 1(a)** illustrates the solution of one-dimensional energy equation using statistical and quantum approach with absent of heat source. Statistical approach can be derived from the extension of quantum approach, FDM, as shown in Equation (1). This technique can be applied for more distribution functions to get more accurate results and more numerical stability. Therefore, the extension study will apply two-dimensional and three-dimensional lattices arrangement. The statistical approach is a conditional numerical technique, which has been employed in a few years ago. **Figure 1(b)** shows the case (2) with heat source applied to the energy equation, as shown in Equation (5). The results show strong agreement between the classical and statistical numerical method either in heat diffusion equations (case (1 & 2)) or in the momentum Navier Stokes equations as shown in **Figures 2(a)-(d)**. The normalized temperature profiles of the fluid flow in a heated duct with a single strainer are plotted for both numerical techniques which show strong agreement.

![Figure 1](image-url)

**Figure 1.** (a) A Stability study of case (1) for various Number of Nodes/Lattices and (b) A Study of case (2) for various time step using Statistical Approach (LBM) & Quantum Approach (FDM).
Figure 2. The normalized temperature profile plotted for \( \text{Re} = 100 \) using statistical technique (a) for single strainer, (b) for a double strainers and quantum technique (FDM) for (c) for a single strainer, (d) for double strainers.

4. Conclusion

The three investigated cases have shown identical results; therefore, the statistical approach will become the most popular and powerful numerical technique in the coming years. The stability and the accuracy have been employed either using statistical approach or using Euler’s method (quantum approach). The numerical limitations of using statistical method have been obtained and compared with those obtained by Euler’s finite difference method. All the results are exactly the same. Consequently, the statistical approach is able to solve linear and nonlinear ODEs and PDE’s with more stable and accurate results. Consequently, statistical approach is a powerful and promising numerical technique for scientists who are struggling for solving nonlinear ODEs or PDEs.

Declarations

Ethics approval and consent to participate.

Consent for Publication

Not applicable.

Availability of Data and Materials

Availability of data and materials data sharing requested from the correspondence author of this article.
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Author Contributions

The author developed two numerical codes for statistical and quantum numerical approach, and selected three cases for comparison purposes.

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Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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List of Abbreviations

| Symbol | Unit | Description |
|--------|------|-------------|
| S      | [-]  | Distribution function of fluid flow |
| c      | [-]  | Lattice discrete velocity in x-and-y components |
| w      | [-]  | Weigh Factor |
| $V_{1,2}$ | [lu/ts] | Total velocity of fluid 1 & 2 per unit lattice-time step |
| r      | [-]  | Position vector |
| t      | [s]  | Time |
| n      | [-]  | Dimensionless relaxation time |
| $\rho$ | [-]  | Macrscopic density |
| BCs    |      | Boundary conditions |
| $\omega$ | [-] | Relaxation frequency |
| $S_{eq}$ | [-] | Local equilibrium distribution function |
| $\Delta t$ | [-] | Time step |
| $g_{cf}$ | [m/s$^2$] | Gravitational acceleration |
| Re     | [-]  | Reynolds Number |
| $\Delta x$ | [-] | Distance between two adjacent lattice nodes |
| PDEs   | [-]  | Partial Differential Equations |
| ODEs   | [-]  | Ordinary Differential Equations |

Special Characters:

| Symbol | Unit | Description |
|--------|------|-------------|
| $\nu$ | [m$^2$/s] | Kinematic Viscosity |
| $\alpha$ | [m$^2$/s] | Thermal diffusivity |

Subscripts:

| Symbol | Description |
|--------|-------------|
| M      | Lattice nodes in x-direction |
| N      | Lattice nodes in y-direction |