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Comparison of Statistical and Quantum Numerical Methodology for Solving Energy and Navier Stokes Momentum Equation

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Abstract. Statistical and Quantum numerical method are implemented in this study to solve various cases in partial differential equations (PDEs). One -dimensional with two lattices arrangements as well as two-dimensional with nine lattices arrangements are 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. Consequently, statistical technique is a powerful and promising numerical technique for scientists who are struggling for solving ODEs or PDEs. The next study will be extended to cover upwind scheme technique.

Keywords: FDM; Technique; Stability; Analysis; Statistical; Quantum

1. Introduction

The greatest scientist in statistical mechanics is Ludwig Eduard Boltzmann (1844-1906), the Austrian physicist. 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 (LBM). This technique is quiet new technique 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 [1-3]. 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 (LGCA) [1], The LBGK 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 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 embankment 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. LBM can take of the interaction between each fluid molecule naturally as well as the interface region for multi-phase flow [5-7].

2. Mathematical Model (Statistical (LBM) and Quantum (FDM) Approach)

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 [4]. 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 [5]. 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. LBM can be used for different arrangements such as D1Q2, D2Q4, D2Q9, D3Q15, D3Q19, or D3Q27 [8-10]. The collision of particles takes place

between the molecules; there will be a net difference between the numbers of molecules in the interval $drdc$. The rate of change of the distribution function is expressed as:

$$\begin{aligned} \frac{\partial S_k}{\partial t} + c_k \cdot \nabla S_k &= \omega(S_k^{eq} - S_k) \\ \frac{\partial h_k}{\partial t} + c_k \cdot \nabla h_k &= \omega(h_k^{eq} - h_k) \end{aligned} \quad \text{for } k=1, \dots, m \quad (1)$$

Here k denotes the direction, c is the lattice discrete velocity and F is external forces applied. $\omega(S_k^{eq} - S_k)$ and $\omega_2(h_k^{eq} - h_k)$ denote the source or the collision 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 τ_1 and τ_2 are the relaxation time of each phase S_k^{eq} and h_k^{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:

$$\frac{S_k^{eq}}{w_k \rho_1} = \frac{h_k^{eq}}{w_k \rho_2} = \left[1 + \frac{3c_k \cdot V}{c_s^2} + 4.5 \frac{(c_k \cdot V)^2}{c_s^4} - 1.5 \frac{V \cdot V}{c_s^2} \right] \quad (2)$$

Where c_k is the discrete velocities vector, V is the bulk fluid velocity and w_k is the weight factor.

$$c_k = \begin{cases} (0,0) & k = 1 \\ c \left(\left[\frac{\sin(k-1)\pi}{2}, \left[\frac{\cos(k-1)\pi}{2} \right] \right) & k = 2,3,4,5 \\ c \left(\sqrt{2} \left[\frac{\cos(2k-11)\pi}{4}, \sqrt{2} \left[\frac{\sin(2k-11)\pi}{4} \right] \right) & k = 6,7,8,9 \end{cases} \quad (3)$$

$$w_k = \begin{cases} \frac{1}{2} & k = 1 \\ \frac{1}{2} & k = 2 \end{cases} \quad w_k = \begin{cases} \frac{4}{9} & k = 1 \\ \frac{4}{36} & k = 2,3,4,5 \\ \frac{1}{9} & k = 6,7,8,9 \end{cases}$$

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

$$\rho = \sum_{k=1}^Q S_k \quad (4)$$

$$\theta = \sum_{k=1}^Q h_k \quad (5)$$

Solving of Navier 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 concerns [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 have been solved using statistical and quantum approach. The stability and accuracy have been investigated for various number of nodes/ lattices. The table 1 shows the three study cases which are selected for comparison purposes between statistical approach and quantum approach.

STUDY CASES (FOR COMPARISON PURPOSES)

Table1. Investigated Cases: diffusion heat energy equations and momentum equations (Navier Stokes equation)

CASE (1)	1D Diffusion Energy Equation	$\frac{\partial T}{\partial t} = \alpha \left[\frac{\partial^2 T}{\partial x^2} \right] \quad (6)$ <p><i>BCs are taken as: at $x = 0$, $T(x=0) = 100^\circ C$ & at $x = 3m$, $T(x=3m) = 20^\circ C$</i></p>
CASE (2)	1D Energy Equation with heat source	$\frac{\partial T}{\partial t} = \alpha \left[\frac{\partial^2 T}{\partial x^2} \right] + \frac{Q_s}{C_p} \quad (7)$ <p><i>BCs are taken as: at $x = 0$, $T(x=0) = 100^\circ C$ & at $x = 3m$, $T(x=3m) = 20^\circ C$, and $Q_s = 100 W/m^2$</i></p>
CASE (3)	Navier Stokes Equation in x&y direction (Momentum Equation)	$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$ $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + g_x \quad (8)$ $\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + g_y$ <p><i>BCs are taken as: Upper: $u = \nu Re/L$ lower and left and right BCs are no-slip boundary conditions.</i></p>

STATISTICAL & QUANTUOM APPROCH DESCRTIZATION

The normalization parameters in this study are: $X = \frac{x}{L}$, $Y = \frac{y}{H}$, $\theta = \frac{T - T_c}{T_h - T_c}$, $U = \frac{\nu Re_L}{Lu}$, $G = \frac{Q_s L^2}{C_p (T_h - T_c)}$

Explicit Method of Case (1):

$$\frac{\theta^{t+1}(i) - \theta^t(i)}{\Delta t} = \alpha \frac{\theta^t(i+1) - 2\theta^t(i) + \theta^t(i-1)}{\Delta x^2} \quad (9)$$

$$\theta^{t+1}(i) = \left(1 - \frac{2\Delta t}{\Delta x^2} \alpha \right) \theta^t(i) + \frac{2\Delta t}{\Delta x^2} \alpha \frac{[\theta^t(i+1) + \theta^t(i-1)]}{2} \quad (10)$$

The equation (1) can be expnaded for one-dimentional and two directional lattices as:

$$h_k(x + \Delta x, t + \Delta t) = (1 - \omega) h_k(x, t) + \omega h_k^{eq}(x, t) \quad (11)$$

Where

$$h_k^{eq}(x, t) = \frac{[\theta^t(i+1) + \theta^t(i-1)]}{2} \text{ and } \omega = \frac{2\Delta t}{\Delta x^2} \alpha \quad (12)$$

Explicit Method of Case (2):

$$\theta^{t+1}(i) = \left(1 - \frac{2\Delta t}{\Delta x^2} \alpha \right) \theta^t(i) + \frac{2\Delta t}{\Delta x^2} \alpha \frac{[\theta^t(i+1) + \theta^t(i-1)]}{2} + \Delta t G_s \quad (13)$$

$$\theta^{t+1} = \frac{\Delta t}{\Delta x^2} \alpha [\theta^t(i+1) - 2\theta^t(i) + \theta^t(i-1)] + \theta^t(i) + \Delta t G_s \quad (14)$$

Now, the equation (1) can be expanded for one-dimensional and two directional lattices as:

$$h_k(x + \Delta x, t + \Delta t) = (1 - \omega)h_k(x, t) + \omega h_k^{eq}(x, t) + \Delta t w(i)G_s \quad (15)$$

Where:

$$h_k^{eq}(x, t) = \frac{[\theta^t(i+1) + \theta^t(i-1)]}{2} \text{ and } \omega = \frac{2\Delta t}{\Delta x^2} \alpha \quad (16)$$

Explicit Method of Case (3):

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

$$u = \frac{\partial \psi}{\partial y}, v = -\frac{\partial \psi}{\partial x} \quad \varphi = \frac{\partial v}{\partial y} - \frac{\partial u}{\partial x} \quad (17)$$

$$\frac{\partial \varphi}{\partial t} + \frac{\partial \psi}{\partial y} \frac{\partial \varphi}{\partial x} - \frac{\partial \psi}{\partial x} \frac{\partial \varphi}{\partial y} = \frac{1}{Re_L} \left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} \right) \quad (18)$$

$$\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) = -\varphi$$

Using central difference scheme in order to linearize the equation (18) leads to:

$$\begin{aligned} & \psi^{t+1}(i, j+1) - 2\psi^{t+1}(i, j) + \psi^{t+1}(i, j-1) \\ & = -\Delta y^2 \varphi^t(i, j) - \frac{\Delta y^2}{\Delta x^2} [\psi^{t+\frac{1}{2}}(i+1, j) - 2\psi^{t+\frac{1}{2}}(i, j) + \psi^{t+\frac{1}{2}}(i-1, j)] \end{aligned} \quad (19)$$

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

$$S_k(x + \Delta x, t + \Delta t) = (1 - \omega)S_k(x, t) + \omega S_k^{eq}(x, t) \quad (20)$$

Where:

$$\begin{aligned} S_k^{eq}(x, t) &= \frac{[U^t(i+1, j) - 2U^t(i, j) + U^t(i-1, j)]}{\Delta x^2} \text{ and } \omega = \frac{2\Delta t}{\Delta x^2} \alpha \\ S_k^{eq}(y, t) &= \frac{[U^t(i, j+1) - 2U^t(i, j) + U^t(i, j-1)]}{\Delta y^2} \text{ and } \omega = \frac{2\Delta t}{\Delta y^2} \alpha \end{aligned} \quad (21)$$

3. Results and Discussions

The **Fig1a.** illustrates the solution of one-dimensional energy equation using statistical and quantum approach with absent of heat source. Statistical approach (LBM) can be derived from the extension of quantum approach, FDM, as shown in eq. (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. The **Fig1b.** shows the case (2) with heat source applied to the energy equation as shown in eq.(13). 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 **Fig2a,b,c,** and **d.** The normalized horizontal velocity and streamlines are plotted for both numerical techniques

which have the same velocity and streamlines profile.

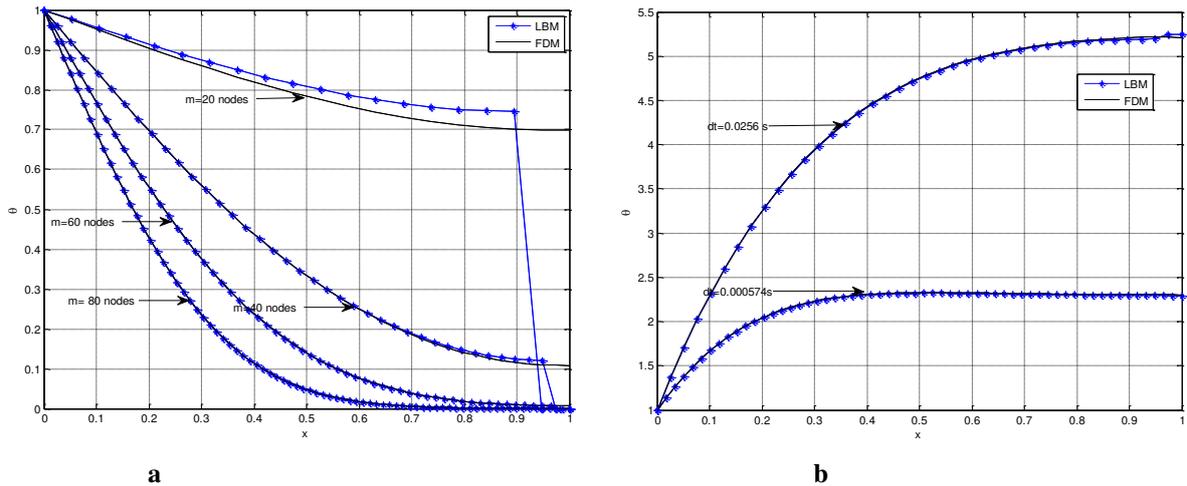


Fig1a. A Stability study of case (1) for various Number of Nodes/Lattices and **b.** A Study of case (2) for various time step using Statistical Approach (**LBM**) & Quantum Approach (**FDM**)

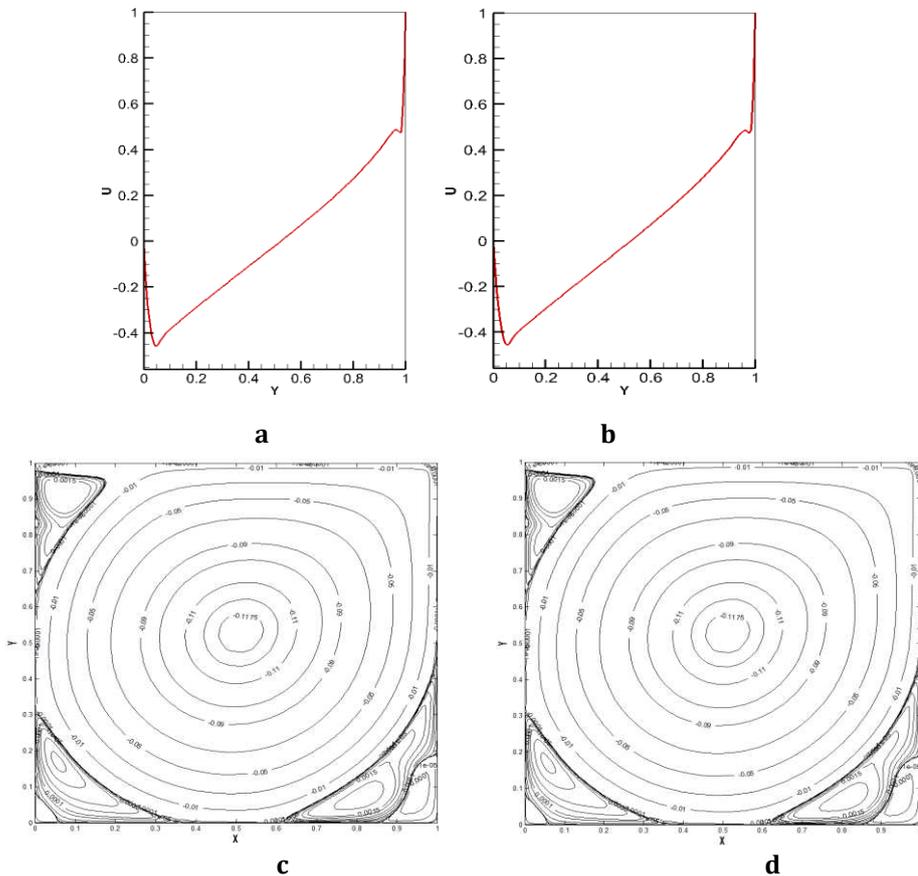


Fig2a. The normalized horizontal velocity statistical technique at $Y=0.5$, **2b.** quantum technique (FDM) at $Y=0.5$ of $R=10\ 000$, **2c.** The streamlines contour of $Re=10000$ using statistical technique, and **2d.** The streamlines contour of $Re=10000$ using quantum technique (FDM)

4. Conclusion

In conclusion, the three investigated cases show identical results, as shown in **Fig 2a,2b,2c, and 2d**. 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, as shown in **Fig1a and 1b**. All the results are exactly the same. 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. Finally, this type of

study will be extended to cover upwind scheme technique with three-dimensional geometrical problems.

List of Abbreviations

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 fluid1&2 per unit lattice-time step
\mathbf{r}	[-]	Position vector
t	[s]	Time
τ_l	[-]	Dimensionless relaxation time
ρ	[-]	Macroscopic density
BCs		Boundary conditions
ω	[-]	Relaxation frequency
S^{eq}	[-]	Local equilibrium distribution function
Δt	[-]	Time step
$g_{x,y}$	[m/s ²]	Gravitational acceleration
Re	[-]	Reynolds Number
Δx	[-]	Distance between two adjacent lattice nodes
$PDEs$	[-]	Partial Differential Equations
$ODEs$	[-]	Ordinary Differential Equations
Special Characters		
ν	[m ² /s]	Kinematic Viscosity
α	[m ² /s]	Thermal diffusivity
Subscripts		
M		Lattice nodes in x-direction
N		Lattice nodes in y-direction

Declarations

Ethics approval and consent to participate

Not applicable

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.

Competing interests

The author declare that they have no competing interests

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Author Contributions

The author generated and built the codes for solving three different cases for comparison purposes.

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