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by Pranowo Pranowo

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Compact Finite Difference Method for Solving Discrete Boltzmann Equation

PRANOWO[1] & A. GATOT BINTORO[2]

[1] Senior Lecturer of Informatics Engineering, Atma Jaya University, Yogyakarta, Indonesia. (Email: pran@mail.uajy.ac.id)
[2] Lecturer of Industrial Engineering Atma Jaya University, Yogyakarta, Indonesia

ABSTRACT
Fourth compact finite difference (FD) method for solving two dimensional Discrete Boltzmann Equation (DBE) for simulation of fluid flows is proposed in this paper. The solution procedure is carried out in Eulerian framework. BGK (Bhatnagar–Gross–Krook) scheme is adopted to approximate the collison term. The convective terms are discretized using 4th compact finite difference method to improve the accuracy and stability. Te semidiscrete equations are updated using 4th order explicit Runge-Kutta method. Preliminary results of the method applied on the Taylor-Green vortex flows benchmark are presented. We compared the numerical results with other numerical results, i.e. explicit 2nd and 4th FD, and exact solutions. The comparisons showed excellent agreement.

KEYWORDS
Compact finite difference; Boltzmann; BGK; ; Taylor vortex

I.INTRODUCTION

In the last decade the lattice-Boltzmann method (LBM) has attracted much attention in the simulation of fluid dynamics problems. Unlike conventional computational fluid dynamics methods, which discretize the macroscopic governing equations directly, the LBM method solves the gas kinetic equation at the mesoscopic scale, i.e. the discrete Boltzmann equation with the Bhatnagar–Gross–Krook (BGK) relaxation for the collision operator. The BGK relaxation process allows the recovery of Navier Stokes equations through Chapman Enskog expansion for low Knudsen number.

In the gas kinetic theory, the evolution of the single-particle density distribution function $f(t,\mathbf{x},\mathbf{e})$ which represents the probability density of a particle with unit mass moving with velocity $\mathbf{e}$ at point $\mathbf{x}$ at time t, is governed by the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{e} \bullet \nabla f = -\frac{\left(f - f^{eq}\right)}{\tau} \qquad (1)$$

where f^{eq} is the equilibrium distribution and τ is relaxation time. After discretizing the velocity space $\mathbf{e}$ into various directions, the 2-D Boltzmann equation for the velocity distributon function f_i may be written as discrete Boltzmann equation.

$$\frac{\partial f_i}{\partial t} + \mathbf{e}_i \bullet \nabla f_i = -\frac{\left(f_i - f_i^{eq}\right)}{\tau} \qquad (2)$$

The discrete velocity $\mathbf{e}_i$ is expressed as:

$$\mathbf{e}_i = \begin{cases} (0,0) & , i = 1 \\ (\cos\theta_i, \sin\theta_i) & , \theta_i = (i-1)\frac{\pi}{4}, i = 2,3,4,5 \\ \sqrt{2}(\cos\theta_i, \sin\theta_i), \theta_i = (i-1)\frac{\pi}{4}, i = 6,7,8,9 & \end{cases}$$

$$\rho = \sum_{i=0}^{8} f_i \qquad (3a)$$

$$\rho u_j = \sum_{i=0}^{8} f_i e_{ij} \; ; \qquad (3b)$$

$$f_i^{eq} = \omega_i\left(\frac{e_i.u}{c_s^2} + \frac{(e_i.u)^2}{2c_s^4} - \frac{|u|^2}{2}\right)$$

with $\omega_1 = 4/9, \omega_2 = \omega_3 = \omega_4 = \omega_5 = 1/9$, and $\omega_6 = \omega_7 = \omega_8 = \omega_9 = 1/36$. The pressure can be calculated from $p = c_s^3 \rho$ with of sound velocity $c_s = 1/\sqrt{3}$ in lattice unit and the kinematic viscosity of fluid is $\nu = \frac{\tau}{3}$. .

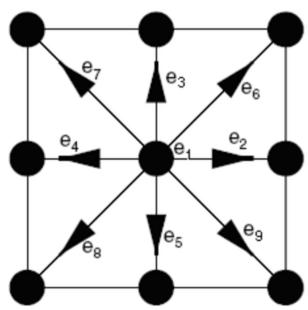

Figure 1. Velocities in 2-D Lattice Boltzmann model (D2Q9)

In Lattice Boltzmann method eq. (2) is solved in the form of

$$f_i(\mathbf{x}+\mathbf{e}_i, t+1) = f_i(\mathbf{x}, t) + -\frac{1}{\tau}\left(f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)\right) \tag{4}$$

using $\Delta x = \Delta y = \Delta t = 1$. The use of unit square mesh elements is restrictive. Several extension to the LBM have been developed to overcome this restriction. Reference [1] used finite difference method (FDM) with 2nd upwind discretization for convective terms. In ref. [1] the FDM is extended to curvilinear coordinates with non-uniform grids. Unfortunately the 2nd upwind makes the stencil longer, so it is not easy to handle the boundary condition. Reference [2] used FDM on non-uniform grids. They used implicit temporal discretization to improve the stability. Many modified FDM were proposed to improve the stability and numerical accuracy. Upwind FDM suffers from large dissipation error and standard 2nd suffers from large dispersion error. Spectral method [5] offers exact differentiation but suffers from low flexibility in treatment of boundary condition.

In this paper, the 4th order compact FDM is proposed to discretize the convective terms of eq. (2). The method is preffered due to high accuracy and flexibility [4]. For improving the stability, the 2nd explicit Runge Kutta method is used to integrate the semi-discrete equation.

II. DISCRETIZATION

The linear convective terms of equations (2) are discretized using 4th compact finite difference method:

$$\frac{1}{6}\left(\frac{\partial f_i}{\partial x}\right)_{k+1,l} + \frac{2}{3}\left(\frac{\partial f_i}{\partial x}\right)_{k,l} + \frac{1}{6}\left(\frac{\partial f_i}{\partial x}\right)_{k-1,l} = \frac{(f_i)_{k+1,l} - (f_i)_{i-k,l}}{2\Delta x} \tag{5a}$$

$$\frac{1}{6}\left(\frac{\partial f_i}{\partial y}\right)_{k,l+1} + \frac{2}{3}\left(\frac{\partial f_i}{\partial y}\right)_{k,l} + \frac{1}{6}\left(\frac{\partial f_i}{\partial y}\right)_{k,l-1} = \frac{(f_i)_{k,l+1} - (f_i)_{k,l-1}}{2\Delta y} \tag{5b}$$

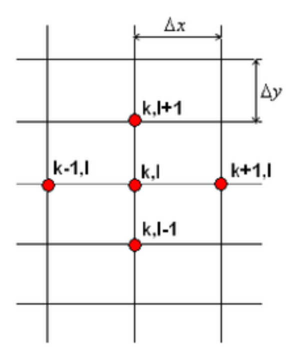

Figure 2. Finite Difference Stencil

After discretizing the convective terms using 4th compact FD, we obtain semi discrete equation of (2).

$$\frac{\partial f_i}{\partial t} = \mathbf{e}_i \bullet \nabla f_i - \frac{\left(f_i - f_i^{eq}\right)}{\tau} = L(f_i) \qquad (6)$$

Then the time update is performed using classical 4th explicit Runge Kutta method.

III. ANALYSIS OF DISCRETIZATION

The analysis of spatial and temporal discretization are given in this section. For simplicity, linear advective equation is takes as example.

8

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0, \quad x \in [0, 2\pi] \qquad (7)$$
$$u(x,0) = e^{ikx}$$

where a is velocity constant.

The exact solution of eq. (7) is easily computed, and we have

$$u(x,t) = e^{i(kx-\omega t)} \quad . \qquad (8)$$

where k is the wave number and ω is angular frequency. From the exact solution, we obtained the exact dispersion relation: $\omega = ak$. By subtituting the local solution $\mathbf{u}^i(x,t) = \mathbf{U}^i e^{i(k^* x^i - \omega t)}$ to eq. (6), we obtain the numerical dispersion relation [5]:

$$ik^*\Delta x = i\left(\frac{1.5\sin(k\Delta x)}{1 + \frac{2}{4}\cos(k\Delta x)}\right) \qquad (9)$$

From the eq. (9), it can be seen that numerical dispersion relation of 4th compact FD has no imaginair components, so it can be concluded that 4th compact FD is conservative and has no dissipation error. For acceptable dispersion error $\left|k^*\Delta x - k\Delta x\right| \le 10^{-2}$, we found that $k^*\Delta x = 1.0893$. Therefore, the spatial grid points per wavelength (PPW) is $PPW = 2\pi/1.0893 = 5.7683$. From the right term of eq. (9) the eigenvalues of 4th compact FD can be calculated and they are purely imaginary, covering $(-1.732\, a/\Delta x, +1.732\, a/\Delta x)$

(8)

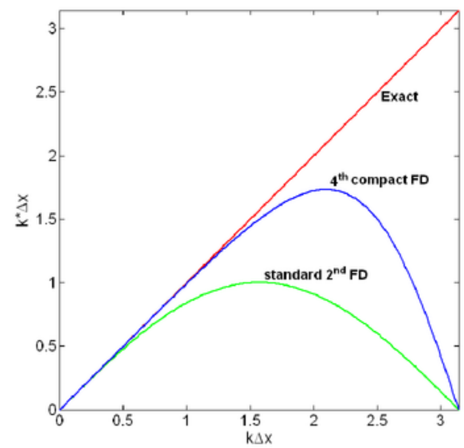

Figure 3. Dispersion error

The stability of 2nd explicit Runge-Kutta scheme can be analyzed by considering eq. (6),

$$\frac{\partial f_i}{\partial t} = L(f_i) \qquad (10)$$

where L is the residual terms which contains the spatial terms of the governing equations. By subtituting $f_i = \bar{f}_i(t)e^{kx}$ into eq. (6), we obtain

$$\frac{\partial \bar{f}_i}{\partial t} = \lambda \bar{f} \qquad (11)$$

Where $\bar{f}$ is the Fourier coefficient, $i = \sqrt{-1}$, and λ is complex number. The left terms of eq. (11) is expanded by using 4th explicit Runge-Kutta scheme to obtain the amplification factor:

$$G = \frac{\bar{f}_i^{n+1}}{\bar{f}_i^{n}} = 1 + (\lambda \Delta t) + \frac{1}{2}(\lambda \Delta t)^2 \qquad (12)$$

The stability condition requires that the amplification factor must be bounded,

$$|G| \le 1 \qquad (13)$$

The stability region in complex plane can be seen in figure 4. The eigenvalues of 4[th] RK in imaginary axis are covering $(-2.828, +2.828)\Delta t$, the stability condition of the fully discrete equation is

$$CFL = \frac{a\Delta t}{\Delta x} \le 2.828/1.732 \qquad (14)$$
$$CFL \le 1.6328$$

CFL is Courant Friedrichs Lewy number.

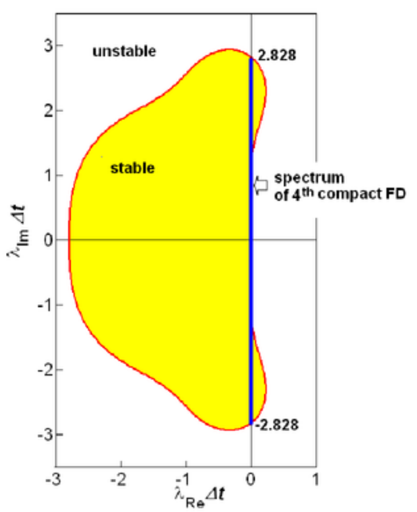

Figure 4. The stability region in complex plane

IV. NUMERICAL RESULTS

The performance of numerical is tested by application to 2 benchmark problems. The first problem to be solved is 1-D linear convection problem [3]:

$$\frac{\partial u}{\partial t} + 2\pi \frac{\partial u}{\partial x} = 0, \quad x \in [0, 2\pi]$$
$$u(x,0) = e^{\sin(x)}$$

with periodic boundary condition

The exact solution to above equation is a right-moving wave of the form:

$$u(x,t) = e^{\sin(x - 2\pi t)}$$

We compare the results with explicit 2[nd] and 4[th] order FD. We take constant $\Delta t = 5e-3$ and $\Delta x = 0.0982, \Delta x = 0.0491, \Delta x = 0.0245$.

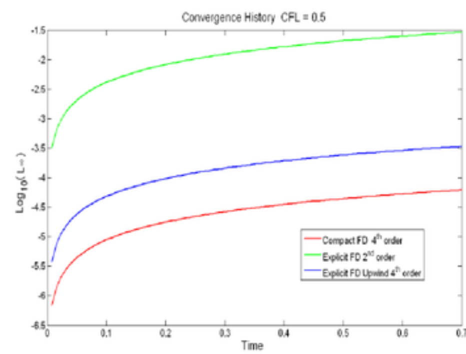

Figure 5. Convergence History for linear convection problem

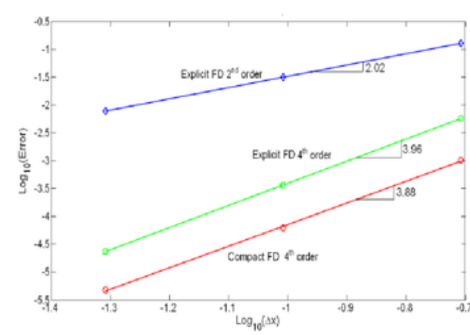

Figure 6. Accuracy Order

From figure 5, we can see that 4[th] compact FD has the lowest error among the r methods. The accuracy orders are in a good agreement with theoritical results.

The second problem to be solved is 2-D decaying Taylor –Green vortex flow problem [5]. The Taylor-Green vortex flow has the following analytic solutions to incompressible Navier-Stokes equation in 2-D:

$$u_x(x,y,t) = -U_0 \cos(k_x x)\sin(k_y y) e^{-(k_x+k_y)^2 t}$$

$$u_y(x,y,t) = \frac{k_x}{k_y} U_0 \cos(k_y y)\sin(k_x x) e^{-(k_x+k_y)^2 t}$$

$$p(x,y,t) = -\frac{U_0^2}{4}\left(\cos(2k_x x) + \left(\frac{k_x}{k_y}\right)^2 \sin(2k_y y)\right) e^{-(k_x+k_y)^2 t} - 1$$

where U_0 is initial velocity amplitude, k_x and k_y are the wave number in x dan y direction.

We use 2-D system of size 32 × 32 with periodic boundary condition in both directions. The simulation parameters are $U_0 = 0.01$, $k_x = k_y = 2$, $\Delta t = 0.005$, and $\tau = 0.0018$. The initial condition of velocity distributon function f_i actually are unknown, it is not easy how to generate consistent initial condition of f_i. Research for generating consistent initial condition of f_i is still in progress [6]. In this paper, we use a simple approach, we use the equilibrium distribution function f_i^{eq} to intialize f_i.

Figure 7 and 8 show the computed results for velocity field and density at $t = 2$.

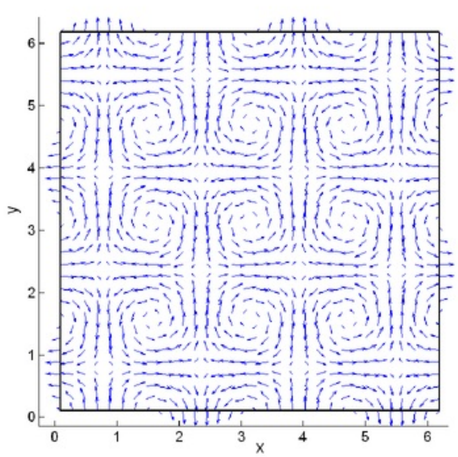

Figure 7. Velocity fields at t=2

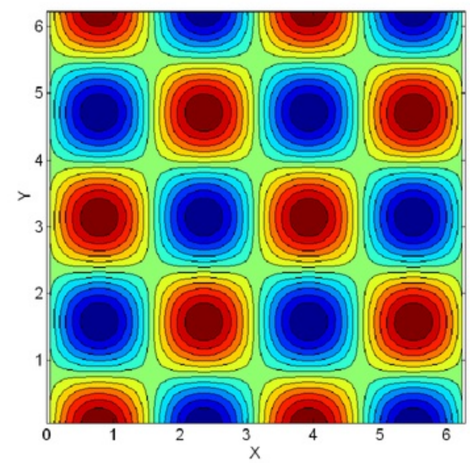

Figure 8. Density distribution at t=2.

Numerical and exact solutions of vertical velocity for t = 2 and t = 150 are compared in figure 8, showing excellent agreement.

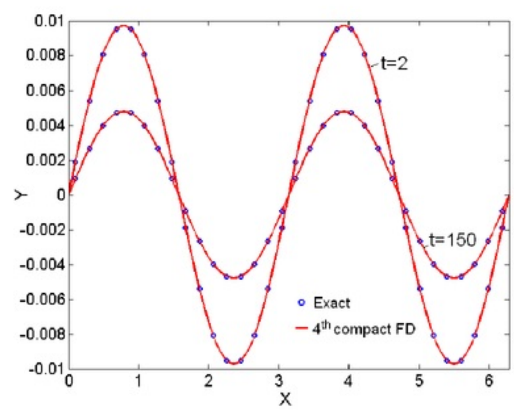

Figure 8. Comparison of vertical velocity at t= 2 and t=150

We compared the vertical velocity error of 4th compact FD with explicit 2nd and 4th FD, the comparisons show that 4th compact FD much more accurate than 2nd and slightly more accurate than explicit 4th FD. Figure 9a and 9b show the comparisons.

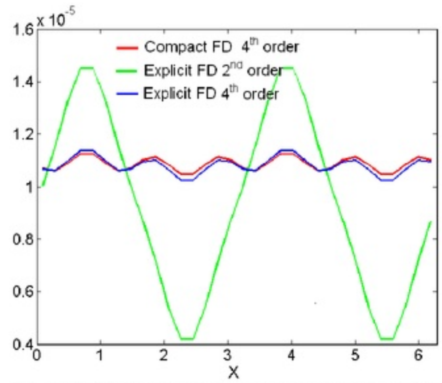

Figure 9a. Vertical velocity error at t=2 and y=3.043

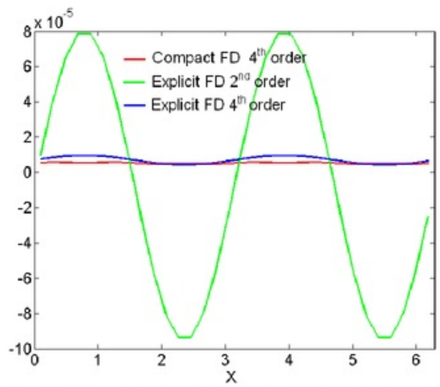

Figure 9b. Vertical velocity error at t=150 and y= 3.043

Figure 10 shows the evolution of averaged error for 4th compact FD, 2nd and explicit 4th FD schemes. It can be seen that the averaged error of 4th compact FD and explicit 4th FD are almost equal and the the averaged error of 2nd FD scheme is higher than others.

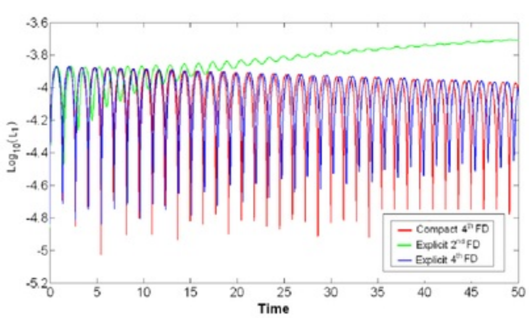

Figure 10. Convergence history of Taylor-Green vortex problem

V. CONCLUSIONS

In this paper, we have presented a 4th compact finite difference method for solving two dimensional Discrete Boltzmann Equation. The proposed method has been verified for the 1-D convective equations and Taylor-Green vortex flows benchmark. The excellent agreement with exact solution and results of 2nd and explicit 4th FD shows the excellent accuracy and stability of the proposed method.

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PAGE 1

PAGE 2

PAGE 3

PAGE 4

PAGE 5

PAGE 6