Equivalence between kinetic method for fluid-dynamic equation and macroscopic finite-difference scheme

Pietro Asinari[(1)], Taku Ohwada[(2)]

[(1)]Department of Energetics, Politecnico di Torino, Torino 10129, Italy,
pietro.asinari@polito.it
[(2)]Department of Aeronatics and Astronautics, Graduate School of Engineering, Kyoto University, Kyoto 606-8501, Japan,
ohwada@kuaero.kyoto-u.ac.jp

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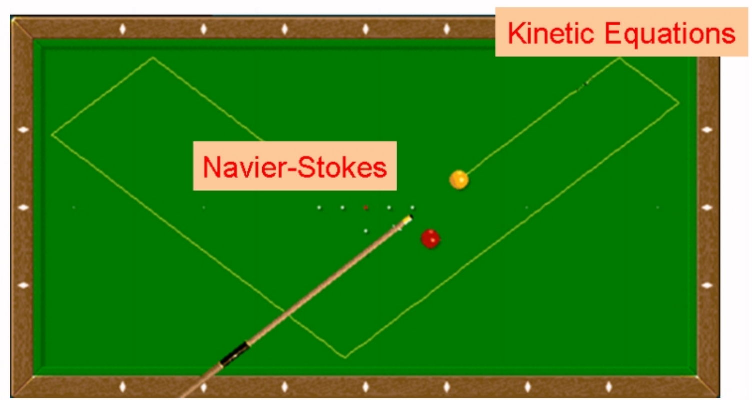
Outline of this talk

Playing billiards...

Some of the LBM models point to kinetic equations in order to solve fluidynamic equations in continuous regime. Does it worth the effort to do so ?



Motivation of this work

- The lattice Boltzmann method (LBM) for the incompressible Navier-Stokes (NS) equations and the gas kinetic scheme (GKS) for the compressible NS equations are based on kinetic theory of gases. In the latter case, however, it is clearly shown that the kinetic formulation is necessary only in the discontinuous reconstruction of fluid-dynamic variables for shock capturing.
- LBM yields solution of ICNS in the asymptotic passage for small Knudsen number and low Mach number (diffusion scaling). On the other hand, GKS for compressible NS does not require any asymptotic passage.
- Then, what is the key of the employment of kinetic theory in the incompressible computation? These schemes recover solutions of ICNS only asymptotically.

Outline Compass

The key idea of LKS

- By means of the tensorial notation, a simple lattice Boltzmann scheme can be expressed as

$$\boldsymbol{f}(\hat{t}+1,\hat{\boldsymbol{X}}) = \lambda\,\boldsymbol{f}_e(\hat{t},\hat{\boldsymbol{X}}-\hat{\boldsymbol{V}}) + (1-\lambda)\boldsymbol{f}(\hat{t},\hat{\boldsymbol{X}}-\hat{\boldsymbol{V}}), \quad (1)$$

  where $\hat{\boldsymbol{X}} = \mathbf{1}\otimes\hat{\boldsymbol{x}}^T$ and $\mathbf{1}\in\mathbb{R}^9$.
- If the dimensionless relaxation frequency λ in the simple LBM with the BGK model is set to unity, the macroscopic variables can be calculated without the velocity distribution function, and the scheme becomes very similar to the kinetic schemes, leading to Lattice Kinetic Scheme — LKS [Junk & Rao 1999, Inamuro 2002].
- Clearly it is possible to express LKS in terms of purely finite difference (FD) formulas on a compact stencil, without any reference to kinetic theory and this would be perfectly equivalent to the original scheme.

Operative formulas in FD-LKS: pressure update p^+

In this case, the updating rule becomes

$$\boldsymbol{f}_{LKS}(\hat{t}_c + 1, \hat{\boldsymbol{X}}_c) = \boldsymbol{f}_e(\hat{t}_c, \hat{\boldsymbol{X}}_c - \hat{\boldsymbol{V}}). \qquad (2)$$

Taking the hydrodynamic moments of Eq. (2) yields, for the pressure update in time,

$$\begin{aligned} p^+ = \quad & p - \frac{\delta t\, c^2}{3} \left[\delta_x u_x + \delta_y u_y + \frac{\delta x^2}{6} (\delta_x^2 \delta_y u_y + \delta_x \delta_y^2 u_x) \right] \\ & + \frac{\delta t^2\, c^2}{6} \left[\delta_x^2 p + \delta_y^2 p + \delta_x^2 (u_x^2) + \delta_y^2 (u_y^2) + 2\, \delta_x \delta_y (u_x u_y) \right] \\ & + \frac{\delta t^4\, c^4}{36} \delta_x^2 \delta_y^2 \left(p + u_x^2 + u_y^2 \right), \qquad (3) \end{aligned}$$

Operative formulas in FD-LKS: velocity update u_x^+

and, for the velocity update in time,

$$\begin{aligned} u_x^+ = \quad & u_x + \delta t \Big[-\delta_x p - \delta_x(u_x^2) - \delta_y(u_x u_y) \\ & + \frac{c^2\,\delta t}{6}\,(3\,\delta_x^2 u_x + 2\,\delta_x\delta_y u_y + \delta_y^2 u_x) + \frac{c^2\,\delta t\,\delta x^2}{12}\,\delta_x^2\delta_y^2 u_x \Big] \\ & - \delta t\,\delta x^2 \left[\frac{1}{6}\,\delta_x\delta_y^2(p + u_x^2 + u_y^2) + \frac{1}{2}\,\delta_x^2\delta_y(u_x u_y) \right], \end{aligned} \qquad (4)$$

where $\delta_x^m \delta_y^n$ are pure FD formulas defined on compact stencils (D2Q9 and D3Q27). Actually there are some analogies with the high-order compact finite difference schemes [Spotz, 1995]. The previous formulas are exact (!!), in the sense that they can be used instead of the original LKS.

Improvements to FD-LKS: tunable viscosity FD-LKSν

- The viscosity in original LKS is fixed and it depends on the discretization. In order to overcome this shortcoming, it is possible to modify the definition of the local equilibrium in order to include terms coming from Chapman-Enskog expansion and to compute them by means of FD formulas on a larger stencil [Inamuro, 2002].
- Actually it is possible to implement the same idea on the original compact stencil too. In fact, the added terms to the local equilibrium, namely

$$\boldsymbol{f}_e^* = \boldsymbol{f}_e - \frac{\epsilon}{\lambda} \hat{\boldsymbol{V}} \cdot \hat{\nabla} \boldsymbol{f}_e^{(1)} + O(\epsilon^3), \tag{5}$$

  involve only first order derivatives, which can be computed with second order accuracy by usual stencils (D2Q9 and D3Q27).

Improvements to FD-LKS: semi-implicit FD-LKSν

- In the original LKS, the pressure and velocity updates are done at the same time, by means of the distribution function. However splitting of these steps in FD-LKS may lead to some advantages.
- Let us simplify the previous pressure update formula $p \rightarrow P$, namely

$$P^{+} = P - \frac{\delta t\, c^2}{3} \left[\delta_x u_x + \delta_y u_y + \frac{\delta x^2}{6} (\delta_x^2 \delta_y u_y + \delta_x \delta_y^2 u_x) \right]. \quad (6)$$

- In order to enhance the stability, it is possible to consider a semi-implicit formulation, namely
  - $\boldsymbol{u}^{+} = \boldsymbol{u} + \cdots$
  - $p^{+} = p - \delta t\, c^2/3\, \nabla \cdot \boldsymbol{u}^{+}$

Taylor-Green vortex flow test case

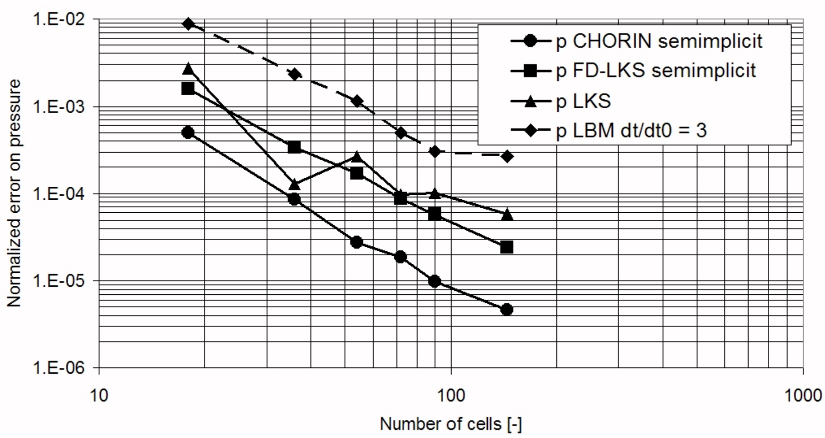
We have confirmed the validity of the above formulas for high order asymptotic computation of ICNS in the problem of 2D Taylor-Green test problem. We carried the computation for the case where the exact solution is given by

$$u_x = -\cos(\frac{\pi x}{3})\sin(\frac{\pi y}{3})\exp(-\frac{2\pi^2 \nu t}{9}), \tag{7}$$

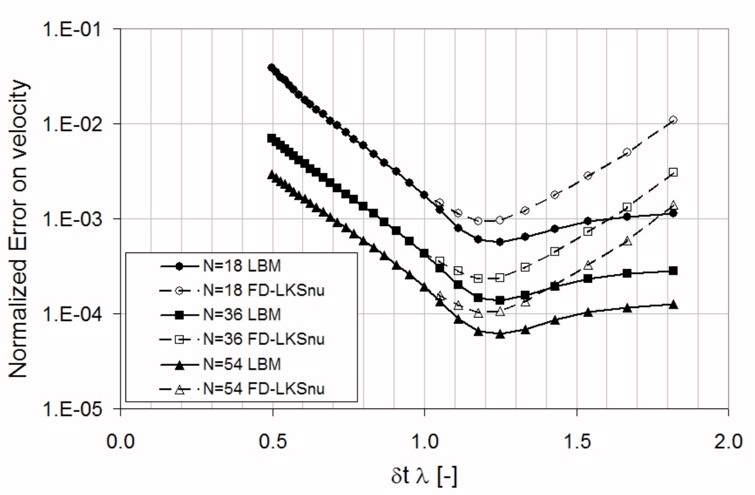
$$u_y = \cos(\frac{\pi y}{3})\sin(\frac{\pi x}{3})\exp(-\frac{2\pi^2 \nu t}{9}), \tag{8}$$

$$P = -\frac{1}{4}[\cos(\frac{2\pi x}{3}) + 1]\cos(\frac{2\pi y}{3})\exp(-\frac{4\pi^2 \nu t}{9}). \tag{9}$$

Taylor-Green vortex flow test case: advantages of semi-implicit formulation for FD-LKSν



Taylor-Green vortex flow test case: comparison between FD-LKSν and LBM



Outline Compass

Asymptotic analysis of LBM

The solution of LBM for small ϵ (both Knudsen and Mach number in diffusive scaling) is investigated in the form of an asymptotic regular expansion. Concerning the coefficients of the expansions for the macroscopic moments,...

1. the leading coefficients $\boldsymbol{u}^{(1)}$ and $p^{(2)}$ are given by the incompressible Navier-Stokes (ICNS) system of equations,

$$\nabla \cdot \boldsymbol{u}^{(1)} = 0, \tag{10}$$

$$\partial_t \boldsymbol{u}^{(1)} + \nabla \boldsymbol{u}^{(1)} \boldsymbol{u}^{(1)} + \nabla p^{(2)} = \omega_1/3\, \nabla^2 \boldsymbol{u}^{(1)}; \tag{11}$$

2. the next PDE system for coefficients for $\boldsymbol{u}^{(2)}$ and $p^{(3)}$ is given by the homogeneous (linear) Oseen system, which admits null solutions, if proper initial and boundary conditions are considered;
3. then the next PDE system for coefficients $\boldsymbol{q}^{(3)}$ and $p^{(4)}$ is given by the Burnett-like system...

Recovered macroscopic equations

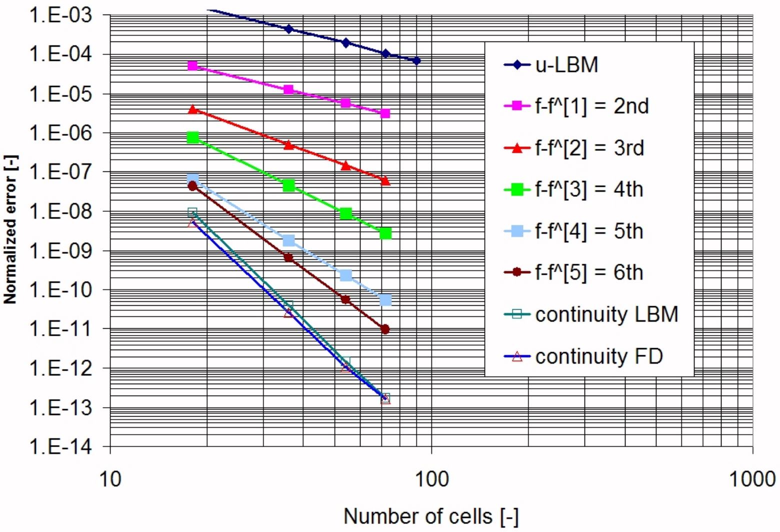
- Let us define the following approximation $f^{[k]} = \sum_{i=0}^{k} \epsilon^i f^{(i)}$.
- According to the selected regular expansion, by definition $f - f^{[k]} = O(\epsilon^{k+1})$.
- Then we use the previous approximations in order to derive macroscopic equations approximating the behavior of the numerical scheme, namely

$$< (f^{[k]} - f_e^{[k]}) >= \partial_{\hat{t}} \hat{\rho}^{[k]} + \mathrm{Eq}_{\hat{\rho}}^{[k]}(\rho^{[k]}) = 0, \quad (12)$$

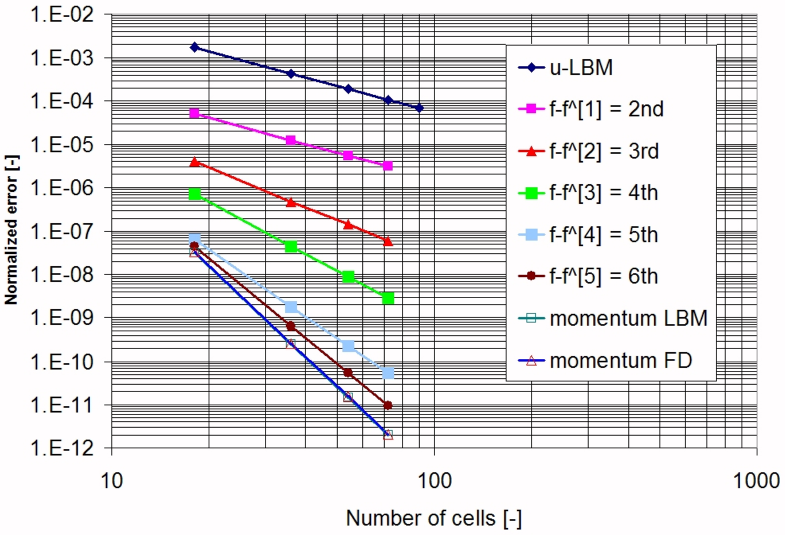
$$< \hat{\boldsymbol{V}} (f^{[k]} - f_e^{[k]}) >= \partial_{\hat{t}} \hat{\boldsymbol{u}}^{[k]} + \mathrm{Eq}_{u}^{[k]}(\hat{\boldsymbol{u}}^{[k]}) = 0, \quad (13)$$

where $< \cdot >$ means the discrete moment computing.
- It is possible to prove that $\partial_{\hat{t}} \hat{\rho} + \mathrm{Eq}_{\rho}^{[k]}(\hat{\rho}) = O(\epsilon^{k+3})$ and $\partial_{\hat{t}} \hat{\boldsymbol{u}} + \mathrm{Eq}_{u}^{[k]}(\hat{\boldsymbol{u}}) = O(\epsilon^{k+2})$, if ρ and $\boldsymbol{u}$ are numerical solutions of LBM scheme.

Taylor-Green vortex flow: continuity equation $O(\epsilon^{5+3})$



Taylor-Green vortex flow: momentum equation $O(\epsilon^{5+2})$



Basic idea of FD-LBM

- Passing to the macroscopic scaling yields

$$\partial_t \rho + \text{Eq}_\rho^{[5]}(\rho) = O(\epsilon^4) \to 0, \quad (14)$$

$$\partial_t \boldsymbol{u} + \text{Eq}_u^{[5]}(\boldsymbol{u}) = O(\epsilon^4) \to 0, \quad (15)$$

- This means that consistency at least up to fifth order, i.e. at least an approximation $f^{[5]}$, is required in order to solve the same equations for both the leading physical quantities and the leading error (FD-LKSν is an approximation of LBM based on $f^{[3]}$ only).
- We define FD-LBM the FD approximation of LBM based on $f^{[5]}$, which requires a larger stencil (D2Q25 and D3Q125)
- Unfortunately FD-LBM is usually quite unstable and this proves that there is no point in proceeding further in searching a FD approximation of LBM.

Outline Compass

Artificial compressibility method revisited

- In the discussion of semi-implicit FD-LKSν, we derived a simplified version of the operative formula for the pressure update P^+, namely Eq. (6), where the time rate of change of the pressure is ruled by the divergence of the numerical velocity field (nearly incompressible).
- Let us introduce the Artificial Compressibility System (ACS):

$$bk \frac{\partial P}{\partial t} + \frac{\partial u_i}{\partial x_i} = 0, \tag{16}$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial P}{\partial x_i} = \nu \frac{\partial^2 u_i}{\partial x_j^2}, \tag{17}$$

where b and k are positive constants $b \sim O(1)$ and $k \ll 1$. ACS involves the acoustic mode and the sound speed C_s is given by $(bk)^{-1/2}$.

Diffusive mode: part 1

ACS involves the diffusive mode, where

$$u_i \sim \frac{\partial u_i}{\partial x_j} \sim \frac{\partial u_i}{\partial t} \sim O(1), \qquad P \sim \frac{\partial P}{\partial x_i} \sim \frac{\partial P}{\partial t} \sim O(1). \tag{18}$$

Regular asymptotic analysis yields

$$u_i = \tilde{u}_i^{(0)} + \tilde{u}_i^{(1)} k + \tilde{u}_i^{(2)} k^2 + \cdots, \qquad P = \tilde{P}^{(0)} + \tilde{P}^{(1)} k + \tilde{P}^{(2)} k^2 + \cdots,$$

$$\frac{\partial \tilde{u}_i^{(0)}}{\partial t} = \mathcal{N}_i(\tilde{u}_k^{(0)}, \tilde{P}^{(0)}; \nu); \qquad \frac{\partial \tilde{u}_i^{(0)}}{\partial x_i} = 0, \tag{19}$$

$$\frac{\partial \tilde{u}_i^{(1)}}{\partial t} = \mathcal{L}_i(\tilde{u}_k^{(1)}, \tilde{P}^{(1)}; \tilde{u}_k^{(0)}, \nu); \qquad \frac{\partial \tilde{u}_i^{(1)}}{\partial x_i} = -b\frac{\partial \tilde{P}^{(0)}}{\partial t}, \tag{20}$$

$$\frac{\partial \tilde{u}_i^{(2)}}{\partial t} = \mathcal{L}_i(\tilde{u}_k^{(2)}, \tilde{P}^{(2)}; \tilde{u}_k^{(0)}, \nu) + \tilde{u}_j^{(1)} \frac{\partial \tilde{u}_i^{(1)}}{\partial x_j}; \qquad \frac{\partial \tilde{u}_i^{(2)}}{\partial x_i} = -b\frac{\partial \tilde{P}^{(1)}}{\partial t}, \tag{21}$$

....

Diffusive mode: part 2

where

$$\mathcal{N}_i(u_k, P; \nu) \equiv -u_j \frac{\partial u_i}{\partial x_j} - \frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2}, \tag{22}$$

$$\mathcal{L}_i(u_k, P; v_k, \nu) \equiv -v_j \frac{\partial u_i}{\partial x_j} - u_j \frac{\partial v_i}{\partial x_j} - \frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2}. \tag{23}$$

- The leading term $O(1)$ is consistent with ICNS.
- The inhomogeneous Oseen-type $O(k)$ is the intrinsic error. Since $M^2 \sim k$ (M Mach number), there are two cases:
  1. in time-dependent cases, the error is $O(M^2)$, because inhomogeneous Oseen unchanges;
  2. in steady cases, the error is $O(M^4)$, because $O(k)$ inhomogeneous Oseen becomes homogeneous and the latter may admit null solutions, if proper initial and boundary conditions are considered.

Numerical realization of incompressible trajectory

- There are two time-step restrictions in the case of explicit schemes, namely
  1. Acoustic mode: $\Delta t \lesssim \Delta x / C_s$, where $C_s = (bk)^{-1/2}$;
  2. Diffusive mode: $\Delta t \lesssim (\Delta x)^2/\nu$.

  Obviously smaller k (M^2), more accurate results are recovered. However, the previous constraints imply a smaller time step.
- The following compromise is suggested: $\Delta x = \epsilon$, $k \sim \epsilon^2$, $\Delta t \sim \epsilon^2$, which is equivalent to LBM.
- From the numerical point of view, the solution of ACS should move along the incompressible trajectory of ICNS as smoothly as possible.

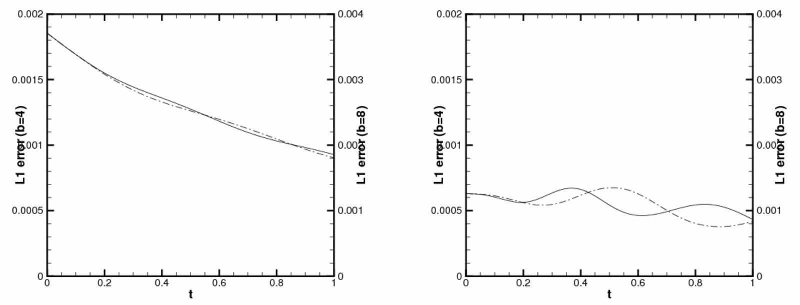
Asymptotic analysis of the finite-difference scheme

- Asymptotic analysis of finite-difference scheme can be done according to the recipe of Junk and Yang.
- Due to the discretization error, the equation systems for $(u_i^{(m)}, P^{(m)})$ $m \geq 1$ may be altered, according to the considered scheme.
  1. 1^{st} order accurate in time: discretization error appears in the equation system for $(u_i^{(1)}, P^{(1)})$ and the error of numerical solution is $O(k) = O(\epsilon^2)$.
  2. 2^{nd} order accurate in time and 4^{th} order accurate in space: the equation system for $(u_i^{(1)}, P^{(1)})$ is NOT altered. This means the leading error of numerical solution is linear in b. The leading error can be canceled out by combining two solutions for different values of b. Then, 2^{nd} order accuracy in time and 4^{th} order accuracy in space are expected.

Initialization

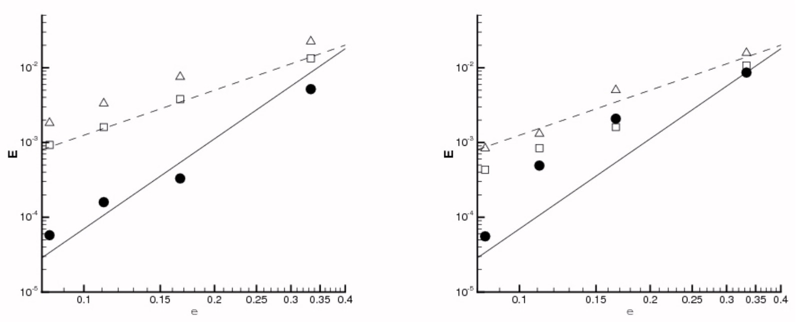
- The initial data for ICNS are: for u_i a divergence free field and for P a solution of the Poisson equation.
- However, this is not appropriate when ACS is employed. The divergence free velocity field means that the time derivative of P is zero in ACS and the incompatible initial condition activates the acoustic mode of ACS.
- In order to launch the solution of ACS along the trajectory of ICNS smoothly, special initial data for the error term $(u_i^{(m)}, P^{(m)})$ $(m = 1, 2, \cdots)$ should be chosen. For example, the initial data for $u_i^{(1)}$ should satisfy the second equation in (20), which requires the information of time derivative of pressure for ICNS.

Time evolution of L^1 error



These figures show the time evolution of L_1 error of the numerical solution for the case of $\nu = 0.2$ ($\epsilon = 1/12$ and $\Delta t = \epsilon^2/8$). It is seen from these figures that the error is nearly proportional to b. The acoustic mode is activated by the initial impact and is seen as small oscillations in these figures.

Convergence rate



The symbols △ and □ indicate the results for $b = 4$ and $b = 8$, respectively. The symbol • indicate the result generated as the linear combination of these two cases. The solid line indicates the fourth order convergence rate and the dashed line indicates the second order one.

Conclusions

1. FD methods based on asymptotic solution of LBM:
   - semi-implicit compact FD-LKSν is a pure FD scheme which represents a feasible alternative of LBM on the same compact lattice (D2Q9 and D3Q27);
   - proceeding further ($f^{[k]}$ for $k \geq 4$) in searching a FD approximation of LBM is usually hopeless in most of the cases, because of stability issues.
2. FD methods based on an extension of artificial compressibility method:
   - ACM is another feasible alternative of LBM, which eventually allows one to achieve higher accuracies (2^{nd} order accuracy in time and 4^{th} order accuracy in space) if larger stencils (D2Q25 and D3Q27) are used and proper linear combinations of intermediate results are considered.
3. Future work: implementation of boundary condition and high-accuracy compact scheme.