Lattice Boltzmann from the perspective of classic kinetic theory

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LBGK: The conventional wisdom

- The lattice BGK Equation

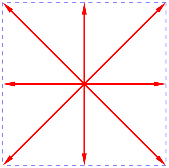
$$f_i(\mathbf{x}+\mathbf{e}_i, t+1) - f_i(\mathbf{x}, t) = -\frac{1}{\tau}\left[f - f^{(eq)}\right]$$

- Equilibrium distribution function

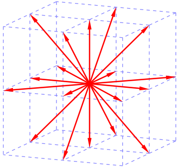
$$f_i^{(eq)} = w_p \rho \left\{1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{1}{2}\left[\frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{c_s^4} - \frac{u^2}{c_s^2}\right]\right\}$$

- Velocities on a lattice
- Navier-Stokes with sound speed $c_s^2 = 1/3$

D2Q9



D2Q19



Recovery of Navier-Stokes

- Single-relaxation-time collision model.
- $f^{(eq)}$ ensures Chapman-Enskog yields Navier-Stokes
- Cartesian lattice [1]:

$$f_i^{(eq)} = w_p \rho \left\{ 1 + \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{1}{2} \left[\frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{c_s^4} - \frac{u^2}{c_s^2} \right] \right\}$$

- Hexagonal lattice [2]:

$$f_i^{(eq)} = w_p \rho \left\{ \delta + |\mathbf{e}_i|(1 - 2\delta) + D\frac{\mathbf{e}_i \cdot \mathbf{u}}{c^2} + \frac{1}{2} \left[D(D+2)\frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{c^4} - D\frac{u^2}{c^2} \right] \right\}$$

- Most of the lattice artifacts eliminated.
- CFD applications for near-incompressible isothermal flows.

[1] Qian *et al*, *Europhys. Lett.*, **17**, 479, (1992)

[2] Chen *et al*, *Phys. Rev. A*, **45**, R5339, (1992)

Lattice Boltzmann BGK: Issues

- Not exactly Navier-Stokes, Viscosity depend on velocity [3]
- Thermal model numerically unstable
  more velocities help, but "one does not know off hand by what criterion to determine the additional velocities" [4]
- Lattice dependent: macroscopic equations obtained through tedious discrete-velocity Chapman-Enskog analysis.
- Not clear how to extend beyond Navier-Stokes
- Is it a lucky accident?

[3] Qian & Orszag, *Europhys. Lett.*, **21**, 255, (1993)

[4] McNamara *et al*, *J. Stat. Phys.*, **87**, 1111, (1997)

LBGK: Link to kinetic theory

- Abe [5] and He [6] derived the D2Q9 models by noticing that the LBGK equilibrium distribution is the Taylor expansion of the Maxwellian in velocity, evaluated on abscissas of Gauss-Hermite quadrature:

$$f^{(eq)} = \frac{\rho}{(2\pi RT)^{D/2}} \exp\left(-\frac{\xi^2}{2RT}\right)\left[1 + \frac{\boldsymbol{\xi}\cdot\mathbf{u}}{RT} + \frac{(\boldsymbol{\xi}\cdot\mathbf{u})^2}{2(RT)^2} - \frac{u^2}{2RT}\right]$$

- Abe also approximated the distribution by essentially:

$$f = \frac{\rho}{(2\pi RT)^{D/2}} \exp\left(-\frac{\xi^2}{2RT}\right)\left[a_0 + \mathbf{a}_1\cdot\boldsymbol{\xi} + (\mathbf{a}_2\cdot\boldsymbol{\xi})^2\right]$$

- The lowest terms of a Hermite expansion.
- Similar to Grad moment expansion theory.

[5] Abe, *J. Comp. Phys.*, **131**, *241, (1997)*

[6] He & Luo, *Phys. Rev. E*, **55**, R6333, (1997)

LB via Hermite expansion [7]

Lattice Boltzmann scheme derived from kinetic theory based on two observations:

- Only interested in the leading moments of the distribution. Huge complexity reduction from a 3-dimensional function to a handful of scalars.
- For finite Hermite expansion, leading moments and discrete function values are isomorphic.

[7] Shan & He, *Phys. Rev. Lett.*, **80**, 65, (1998); Shan *et al J Fluid Mech*, **550**, 413 (2006)

Outline

Hermite polynomials

- Eigen-function of a Sturm-Liouville equation:

$$H_n''(x) - xH_n'(x) + nH_n(x) = 0.$$

- Explicitly:

$$H_n(x) = \frac{(-1)^n}{\omega(x)} \frac{d^n \omega(x)}{dx^n} \quad \text{where} \quad \omega(x) = \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{x^2}{2}\right]$$

- First few polynomials:

$$H_0(x) = 1, \quad H_1(x) = x, \quad H_2(x) = x^2 - 1, \quad H_3(x) = x^3 - 3x, \cdots$$

Properties

- Orthogonality

$$\int_{-\infty}^{\infty} \omega(x) H_n(x) H_m(x) dx = n! \delta_{nm}$$

- Generalized Fourier expansion:

$$f(x) = \omega(x) \sum_{n=0}^{\infty} \frac{1}{n!} a_n H_n(x) \quad \text{where} \quad a_n = \int_{-\infty}^{\infty} f(x) H_n(x) dx$$

for all "square-integrable" functions:

$$\int_{-\infty}^{\infty} \omega(x) |f(x)|^2 dx$$

In higher dimensions [8]

- The D-dimensional Hermite polynomials:

$$\mathcal{H}^{(n)}(\boldsymbol{\xi}) = \frac{(-1)^n}{\omega(\boldsymbol{\xi})}\nabla^n\omega(\boldsymbol{\xi}) \quad \text{where} \quad \omega(\boldsymbol{\xi}) = \frac{1}{(\sqrt{2\pi})^D}\exp\left[-\frac{\xi^2}{2}\right]$$

- $\mathcal{H}^{(n)}(\boldsymbol{\xi})$: rank-$n$ tensor and degree-n polynomial in $\boldsymbol{\xi}$

$$\mathcal{H}^{(0)}(\boldsymbol{\xi}) = 1, \quad \mathcal{H}^{(1)}(\boldsymbol{\xi})_i = \xi_i, \quad \mathcal{H}^{(2)}(\boldsymbol{\xi})_{ij} = \xi_i\xi_j - \delta_{ij}, \quad \cdots$$

- Hermite expansion in multi-dimensions:

$$f(\boldsymbol{\xi}) = \omega(\boldsymbol{\xi})\sum_{n=0}^{\infty}\frac{1}{n!}\mathbf{a}^{(n)}\mathcal{H}^{(n)}(\boldsymbol{\xi}) \quad \text{where} \quad \mathbf{a}^{(n)} = \int f(\boldsymbol{\xi})\mathcal{H}^{(n)}(\boldsymbol{\xi})d\boldsymbol{\xi}$$

- Expansion coefficients are the moments

$$\mathbf{a}^{(0)} \equiv \rho, \quad \mathbf{a}^{(1)} \equiv \rho\mathbf{u}, \quad \mathbf{a}^{(2)} \equiv \mathbf{P} + \rho\mathbf{uu} - \rho\boldsymbol{\delta}, \quad \mathbf{a}^{(3)} \equiv \mathbf{Q} + \cdots$$

[8] Grad *Commun Pure Appl Maths*, **2**, 331

Grad 13-moment system

Hermite (moment) expansion of Boltzmann equation [9]

- State variable: leading moments: ρ, $\mathbf{u}$, $\mathbf{P}$, $\mathbf{q}$. (or more)
- Hermite coefficients correspond to the moments
- Projection into a subspace spanned by leading polynomials
- Spectral method in velocity space
- Closure at an higher level.
- Complicated PDE in space-time, hard to compute

[9] Grad *Commun Pure Appl Maths*, **2**, 325

Outline

"Isomorphism" between moments and discrete velocities

- Gauss-Hermite quadrature:

$$\int \omega(\xi)p(\xi)d\xi = \sum_{i=1}^{d} w_i p(\xi_i), \quad \text{for polynomial } p$$

- Moments of a finite Hermite expansion:

$$\int f(\xi)\xi^m d\xi = \int \omega(\xi)\left[\frac{f(\xi)}{\omega(\xi)}\xi^m\right]d\xi$$

- Integrand is a polynomial with an order $\leq n+m$.
- In a finite Hermite space, moments and discrete-velocity distribution functions are isomorphic.
- Recovering LB:

$$\rho = \sum_{i=1}^{d} f_i, \quad \rho\mathbf{u} = \sum_{i=1}^{d} f_i\xi_i, \quad \cdots, \quad \text{where} \quad f_i \equiv \frac{w_i f(\xi_i)}{\omega(\xi_i)}$$

Outline

BGK projected into low-dimensional subspace

- Second-order Hermite expansion of Maxwellian:

$$f^{(0)}(\boldsymbol{\xi}) = \rho\omega \left\{1 + \mathbf{u}\cdot\boldsymbol{\xi} + \frac{1}{2}\left[(\mathbf{u}\cdot\boldsymbol{\xi})^2 - u^2 + (\theta - 1)(\xi^2 - D)\right]\right\}$$

  - No assumption of small Mach number
  - Temperature included
- Second-order Hermite expansion of the body force $(\mathbf{g}\cdot\nabla_\xi f)$:

$$F(\boldsymbol{\xi}) = -\rho\omega\left[\mathbf{g}\cdot\boldsymbol{\xi} + (\mathbf{g}\cdot\boldsymbol{\xi})(\mathbf{u}\cdot\boldsymbol{\xi}) - \mathbf{g}\cdot\mathbf{u}\right]$$

- Discrete-velocity distribution solved from projected BGK

Outline

Chapman-Enskog

With BGK, CE approximation is essentially:

$$f^{(1)} \cong -\tau \left[\frac{\partial}{\partial t} + \boldsymbol{\xi} \cdot \nabla + \mathbf{g} \cdot \nabla_\xi \right] f^{(0)}$$

Hermite expansion coefficients of $f^{(1)}$:

$$\mathbf{a}_1^{(n)} = -\tau \left[\frac{\partial \mathbf{a}_0^{(n)}}{\partial t} + \nabla \mathbf{a}_0^{(n-1)} + \nabla \cdot \mathbf{a}_0^{(n+1)} - \mathbf{g}\mathbf{a}_0^{(n-1)} \right].$$

- First n moments of $f^{(1)}$ given by first n+1 moments of $f^{(0)}$.
- First n moments of $f^{(k)}$ given by first n+k moments of $f^{(0)}$.

Same as continuum BGK iff leading moments of $f^{(0)}$ matches!

Summary

- LBGK approximates continuum BGK (Not near-incompressible NS)
- Accuracy:
  Let Q be quadrature precision, N: truncation order of $f^{(0)}$. To recover the dynamics of the first M moments:

  $$N \geq M \quad \text{and} \quad Q \geq M + N \quad \Rightarrow \quad Q \geq 2M.$$

  Can't use Maxwellian in LBGK
- many problems due to insufficient truncation
- Analogous to pseudo-spectral method (moment method analogous to spectral)

Outline

Galilean invariance

- Galilean invariance restored in pressure, but not in viscosity.
- Also known as the "cubic" dependency on velocity (Ma). [10]
- Efforts in correcting the "cubic" error [11]
- Root cause: insufficient truncation and lattice accurary. [12]
- Correct viscosity: $Q \geq 6$; thermal diffusivity: $Q \geq 8$.
- DxQx: $N = 2$ or 3 and $Q = 5$. Not enough for $M = 3$.

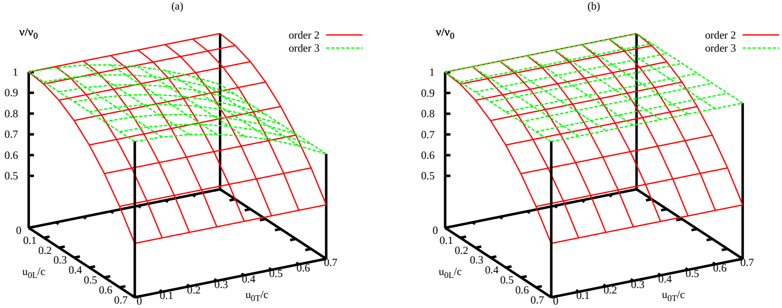
[10] Qian & Orszag *Europhys Lett*, **21**, 255, (1993)

[11] Chen *et al Phys Rev E*, **50**, 2776, (1994); Qian & Zhou *Europhys Lett*, **42**, 359, (1998); Házi & Kávrán *J. Phys A*, **39**, 3127 (2006)

[12] Nie *et al*, *Europhys Lett*, **81**, 34005, (2008)

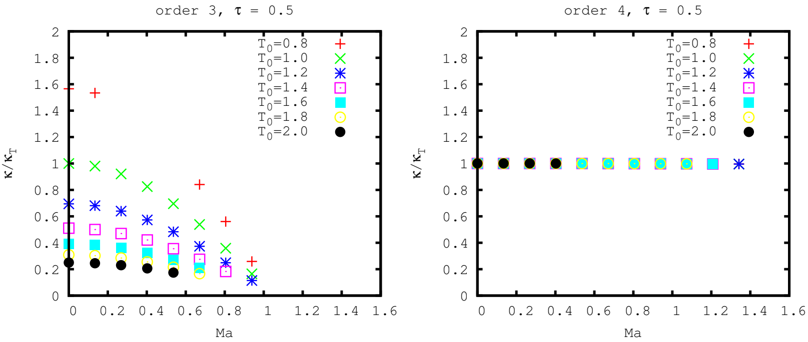
Galilean invariance: Viscosity

Viscosity, measured vs theoretical, in the presence of a homogeneous translational velocity. Left: 19-speed, Right: 39-speed.



Galilean invariance: Thermal diffusivity

Thermal diffusivity, measured vs theoretical, in the presence of a homogeneous translational velocity using 121-speed model.



Outline

The obstacles and solutions

Previous challenges:

- Equilibrium is an iso-thermal small-velocity expansion
- Errors at finite Mach number
- Thermal model constructed *ad hoc*.

In the new approach:

- Moment expansion independent of Mach number
- Clear criteria to fully recover NS energy equations

Flow past a 15° wedge (Static pressure)

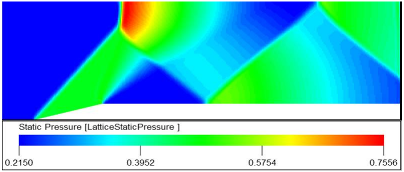


Figure: Ma=1.8. Shock angle: Theory 51°, Simulation 51.5°.

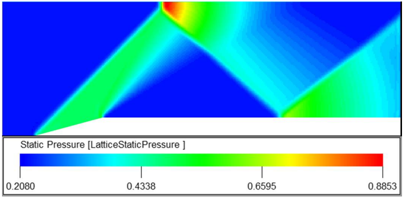


Figure: Ma=2. Shock angle: Theory 45.4°, Simulation 45°.

RAE 2822 transonic airfoil (Ma=0.729, AoA=2.31°.)

LBGK compared with experiment and other codes. [13]

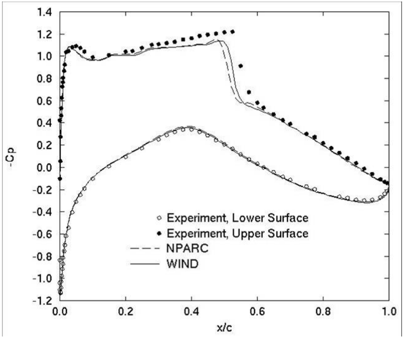


Figure: Other Codes

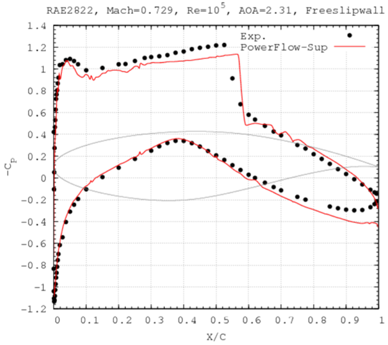


Figure: 39-speed LBGK

[13] http://www.grc.nasa.gov/WWW/wind/valid/raetaf/raetaf01/raetaf01.html

RAE 2822 transonic airfoil (Pressure contours)

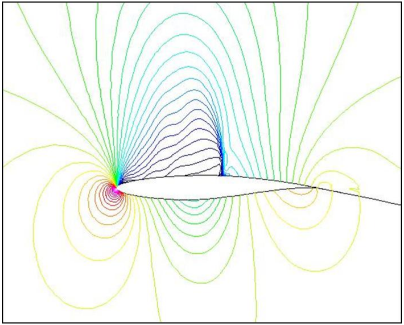


Figure: WIND

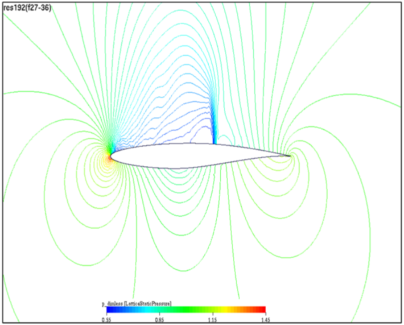


Figure: Lattice Boltzmann

Outline

High Knudsen number flows

- BGK is beyond Navier-Stokes.
- More velocities ⇔ more moments
- High-Kn by using more velocities? [a]

[a] Zhang *et al, Phys Rev E*, **74**, 046703, (2006); Kim *et al, J Comp Phys*, **227**, 8655, (2008); Colosqui *et al, Phys Fluids*, **21**, 013105, (2009)

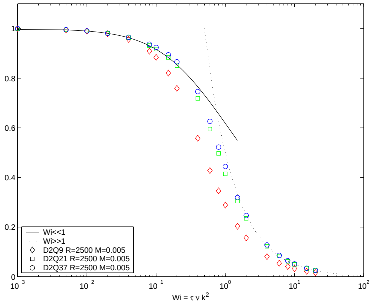


Figure: Shear wave decay rate at different Weissenberg number by LBGK models of different orders.

Non-Ideal gases LBGK model

- Inter-particle interaction ignored in Boltzmann equation. One has to go to the next equation in BBGKY [14]:

$$\frac{\partial f_1}{\partial t} + \boldsymbol{\xi}_1 \cdot \nabla_{\mathbf{r}_1} f_1 = \int \nabla_{\boldsymbol{\xi}_1} f_2 \cdot \nabla_{\mathbf{r}_1} V(|\mathbf{r}_1 - \mathbf{r}_2|) d\boldsymbol{\xi}_2 d\mathbf{r}_2$$

- Leading order effect: a self-consistent mean-field body force:

$$\mathbf{a} \cdot \nabla_{\xi} f \quad \text{where} \quad \mathbf{a} = \int \rho(\mathbf{r}_2) g(\mathbf{r}_1, \mathbf{r}_2) \nabla_{\mathbf{r}_1} V(|\mathbf{r}_1 - \mathbf{r}_2|) d\mathbf{r}_2$$

- Shan-Chen model reinvented
- Link between the "pseudo-potential" and the pair-wise potential [15].

[14] Martys, *Int. J. Mod. Phys. C*, **10**, 1367, (1999); He & Doolen, *J. Stat. Phys.*, **107**, 309, (2002); Martys, *Physica A*, **362**, 57, (2005)
[15] He, Shan & Doolen, *Phys. Rev. E*, **57**, R13, (1998)

A general Multiple Relaxation Time model

- Linear modes have different decay rates[16]. Variable Prandtl number.
- BGK collision term in Hermite spectrum space:

$$-\frac{1}{\tau}\left[f - f^{(0)}\right] = -\frac{1}{\tau}\sum_{n=0}^{\infty}\frac{1}{n!}\left[\mathbf{a}^{(n)} - \mathbf{a}_0^{(n)}\right]\mathcal{H}^{(n)}(\xi)$$

- Mode separation in spectrum space. An direct extension[17]:

$$-\sum_{n=0}^{\infty}\frac{1}{\tau}_n\frac{1}{n!}\left[\mathbf{a}^{(n)} - \mathbf{a}_0^{(n)}\right]\mathcal{H}^{(n)}(\xi)$$

- lattice independent

[16] d'Humières, *et al*, *Phil. Trans. R. Soc. Lond. A*, **360**, 437, (2002)
[17] Shan & Chen, *Int. J. Mod. Phyc. C*, **18**, 635, (2007)

Thank you!