LBM for Rarefied Gas Flows

Seminar: Lattice Boltzmann Methods

Gerasimos Chourdakis

Fakultät für Informatik - Technische Universität München

June 18, 2015

Agenda

1 Introduction

2 Flow regimes

3 Extending LBM to the slip regime

4 LBM in the transition regime

5 A stochastic model for finite Knudsen numbers

6 Conclusion

Motivation

- The Navier-Stokes equations assume continuity.
- The no-slip boundary conditions do not always apply.
- Micro(nano)-electro-mechanical systems (MEMS): far from continuity, slip-velocity observed.

Is everything continuous?

The matter consists of small discrete particles, though it seems to be continuous.

- How to quantify the "continuity"?
- What are the limits of this assumption?
- Can we always apply the Navier-Stokes equations?
- Can we always apply a lattice Boltzmann menthod?
- If not, what can we do about this?

Example: micropumps

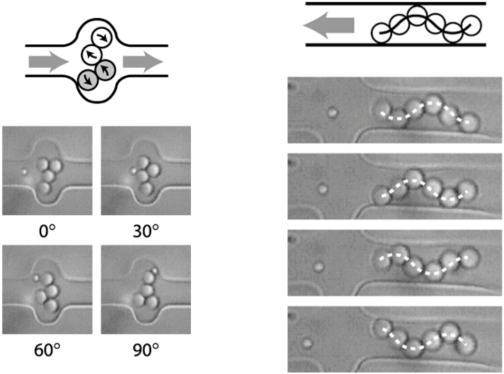

Figure : Colloidal micropumps.[1]

[1] Karniadakis et al. - 2005 [2]

Mean Free Path

Mean Free Path: the average distance that the molecules of a gas are travelling without taking part in collisions.
For hard-sphere gases in thermodynamic equilibrium:

$$\lambda = \frac{1}{\sqrt{2}\pi \cdot n_{\mathrm{g}} \cdot d^2} \tag{1}$$

d: mean molecular diameter, n_{g}: number density
Example (atmospheric conditions):
$\lambda_{\mathrm{air}} = 6.111 \cdot 10^{-8}\,\mathrm{m}$
$\lambda_{\mathrm{He}} = 17.651 \cdot 10^{-8}\,\mathrm{m}$

The Knudsen number

Knudsen number = Mean Free Path / characteristic length

$$\mathrm{Kn} := \frac{\lambda}{L_0} \tag{2}$$

The characteristic length can be, e.g., the width of a channel.

Flow regimes

Empirical Knudsen number ranges:

- **Continuous** $\mathrm{Kn} < 10^{-2}$ (or $\mathrm{Kn} < 10^{-3}$)
- **Slip** $10^{-2} < \mathrm{Kn} < 10^{-1}$ (thermodynamic equilibrium breaks)
- **Transition** $10^{-1} < \mathrm{Kn} < 10$ (continuity assumption breaks)
- **Free molecular** $10 < \mathrm{Kn}$ (almost no intermolecular collisions)

Also, mixed flow regimes for scenarios with very different scales.

Flow regimes (2)

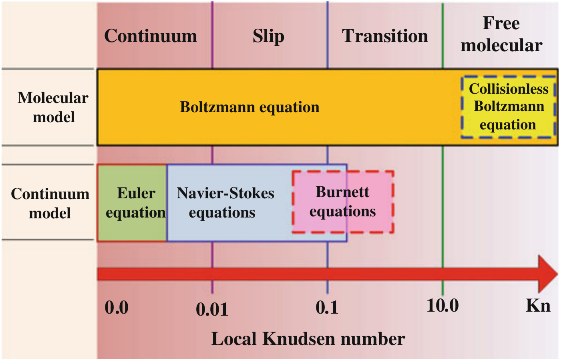

Figure : Gas flow regimes and limits of different CFD approaches. [2]

[2] Zhang et al. - 2012 [7]

Extending LBM to the slip regime

The “classical” Bhatnagar-Gross-Krook LBM with bounce-back boundary conditions has some problems:

- The boundary conditions depend on the viscosity
- The observed “slip velocity” is a numerical artifact, it is constant at the wall, without depending on the Knudsen number [3]

Solutions:

- Multiple-Relaxation-Time collision
- Slip-velocity models
- Virtual wall collisions and other ideas

[3] Verhaeghe - 2009 [6]

Multiple-Relaxation-Time

General form of the LB equation:

$$\mathbf{f}(\mathbf{r}_j + \mathbf{c}\delta_{\mathrm{t}}, t + \delta_{\mathrm{t}}) = \mathbf{f}(\mathbf{r}_j, t) + \mathbf{\Omega}[\mathbf{f}(\mathbf{r}_j, t)] + \mathbf{F}(\mathbf{r}_j, t) \tag{3}$$

MRT collision operator:

$$\mathbf{\Omega} = -\mathrm{M}^{-1} \cdot \mathrm{S} \cdot [\mathbf{m} - \mathbf{m}^{(\mathrm{eq})}] \ , \ \ \mathbf{m} = \mathrm{M} \cdot \mathbf{f} \tag{4}$$

where $\mathbf{m}$ is the moment space (and $\mathbf{m}^{(\mathrm{eq})}$ the respective equilibria), S a positive-definite matrix of the relaxation rates and M the matrix that transforms $\mathbf{f}$ to their moments

Slip-velocity models

How does the velocity change near the wall?

A first-order model for the slip regime:

$$u|_{\mathrm{wall}} = \sigma \mathrm{Kn} L_0 \frac{\partial u_{\mathrm{wall}}}{\partial y}, \quad \sigma := (2 - \sigma_\nu)/\sigma_\nu \tag{5}$$

$\sigma_\nu \in (0, 1]$: tangential momentum accommodation coefficient [6].

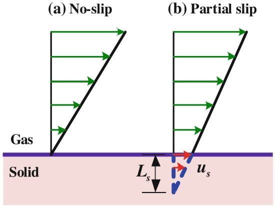

Figure : A linear slip-velocity model [4]

[4] Zhang et al. - 2012 [7]

Boundary conditions

Analytic solution of the lattice Boltzmann equation for the incompressible Poiseuille flow (dimensionless):

$$\tilde{u}(\tilde{y}) = 4\tilde{y}(1 - \tilde{y}) + \tilde{U}_{\mathrm{slip}} \tag{6}$$

where:
$\tilde{u} := (u + G\delta_{\mathrm{t}}/2)/U_{\mathrm{max}}$,
$G := |\nabla p/\rho|$ (acceleration due to a constant pressure gradient),
$\tilde{U}_{\mathrm{slip}} := U_{\mathrm{slip}}/U_{\mathrm{max}}$,
$\tilde{y} := (j - 1/2)/N_{\mathrm{y}}$.

Bounce-Back boundary conditions

For smooth surfaces, the momentum is reversed:

$$f_i(t_{n+1}) = f^*_{inv(i)}(t_n) \tag{7}$$

$$U^{\mathrm{B}}_{\mathrm{slip}} = \frac{1}{4}\Big(\frac{8}{\tau_q} - \frac{8-\tau_s}{2-\tau_s}\Big) G\delta_{\mathrm{t}} \tag{8}$$

τ_s, τ_q: relaxation rates for the stresses and the energy fluxes.
No-slip ($U^{\mathrm{B}}_{\mathrm{slip}} = 0$) if:

$$\tau_q = \frac{8(2-\tau_s)}{(8-\tau_s)} \tag{9}$$

Diffusive boundary conditions

For non-smooth surfaces, the molecules are reflected to random directions:

$$f_i = \frac{\sum_{\mathbf{c}_k} |\mathbf{c}_k \cdot \hat{\mathbf{n}}| f_k^*}{\sum_{\mathbf{c}_k} |\mathbf{c}_k \cdot \hat{\mathbf{n}}| f_k^{(\mathrm{eq})}(\rho_{\mathrm{wall}}, \mathbf{u}_{\mathrm{wall}})} f_{inv(i)}^{(\mathrm{eq})}(\rho_{\mathrm{wall}}, \mathbf{u}_{\mathrm{wall}}) := f_i^{\mathrm{D}}, \;\; \mathbf{c}_k \cdot \hat{\mathbf{n}} < 0 \tag{10}$$

$\hat{\mathbf{n}}$: the normal to the wall unit vector,
$\mathbf{c}_k$: incidental velocities defined by $\mathbf{c}_k \cdot \hat{\mathbf{n}} < 0$ and ρ_{wall},
$\mathbf{u}_{\mathrm{wall}}$: density and velocity at the wall

$$U_{\mathrm{slip}}^{\mathrm{D}} = U_{\mathrm{slip}}^{\mathrm{B}} + \frac{3}{2} N_{\mathrm{y}} G \delta_{\mathrm{t}} = U_{\mathrm{slip}}^{\mathrm{B}} + \frac{3}{2} \frac{L_0 G}{c}, \;\; c := \delta_{\mathrm{x}}/\delta_{\mathrm{t}} \tag{11}$$

Diffusive bounce-back boundary conditions

Combining the BB and the Diffusive boundary conditions:

$$f_i(t_{n+1}) = \beta f^*_{inv(i)}(t_n) + (1-\beta) f_i^{\mathrm{D}}(t_n), \quad \beta \in [0,1] \tag{12}$$

$$U_{\mathrm{slip}}^{\mathrm{BD}} = U_{\mathrm{slip}}^{\mathrm{B}} + \frac{3}{2}\frac{(1-\beta)}{(1+\beta)} N_{\mathrm{y}} G \delta_{\mathrm{t}} = U_{\mathrm{slip}}^{\mathrm{B}} + \frac{3}{2}\frac{(1-\beta)}{(1+\beta)}\frac{L_0 G}{c} \tag{13}$$

Verhaeghe et al. [6]:

$$\beta = \frac{3\mu - \mathrm{Kn} L_0 c \bar{\rho}_{\mathrm{out}}}{3\mu + \mathrm{Kn} L_0 c \bar{\rho}_{\mathrm{out}}} \tag{14}$$

Specular reflective bounce-back boundary conditions

Combining the Specular reflective ("free-slip") and the bounce-back boundary conditions:

$$U_{\mathrm{slip}}^{\mathrm{BR}} = U_{\mathrm{slip}}^{\mathrm{B}} + \frac{3}{2}\frac{(1-\beta)}{\beta} N_{\mathrm{y}} G \delta_{\mathrm{t}} = U_{\mathrm{slip}}^{\mathrm{B}} + \frac{3}{2}\frac{(1-\beta)}{\beta}\frac{L_0 G}{c} \tag{15}$$

Some results (slip regime)

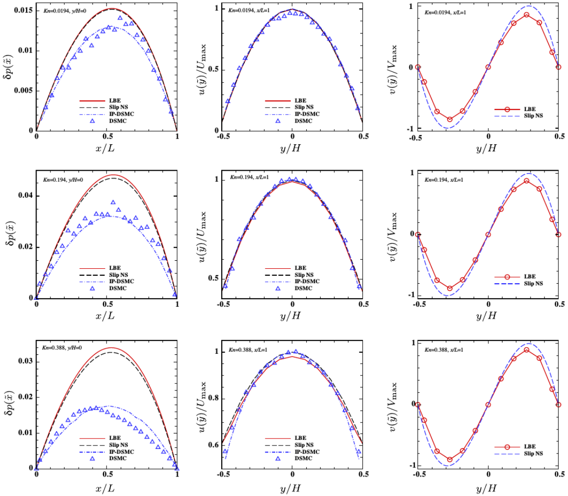

Figure : Results of Verhaeghe et al. [6] for the slip regime, compared to the slip Navier-Stokes, IP-DSMC and DSMC.

LBM in the transition regime (1)

Near the walls, the MFP is shorter and the viscosity decreases:

$$\mu_{\mathrm{e}} = \mu_0 \frac{1}{1 + \alpha \mathrm{Kn}}, \quad \alpha \approx 2 \tag{16}$$

Effective MFP:

$$\lambda_{\mathrm{e}} = \frac{\mu_{\mathrm{e}}}{p} \cdot \sqrt{\frac{\pi R T}{2}} \tag{17}$$

Second-order slip-velocity model[5]:

$$U_{\mathrm{slip}} = B_1 \sigma_\nu \lambda_{\mathrm{e}} \frac{\partial u}{\partial y}\bigg|_{\mathrm{wall}} - B_2 \lambda_{\mathrm{e}}^2 \frac{\partial^2 u}{\partial y^2}\bigg|_{\mathrm{wall}}, \quad \sigma_\nu = (2 - \sigma)/\sigma \tag{18}$$

[5] Li et al. - 2011 [3], Zhang et al. - 2012 [7]

LBM in the transition regime (2)

Li et al. [3] use MRT and set:

$$\tau_s = \frac{1}{2} + \sqrt{\frac{6}{\pi}}\frac{N\mathrm{Kn}}{(1+\alpha\mathrm{Kn})}\ , \quad N = H/\delta_\mathrm{x} \tag{19}$$

$$\tau_q = \frac{1}{2} + \frac{3 + 4\pi\tilde{\tau}_s^2 B_2}{16\tilde{\tau}_s}\ , \quad \tilde{\tau}_s = \tau_s - 0.5 \tag{20}$$

For the diffusive bounce-back boundary conditions:

$$\beta = \frac{1}{1 + B_1\sigma_\nu\sqrt{\pi/6}} \tag{21}$$

Some results (transition regime)

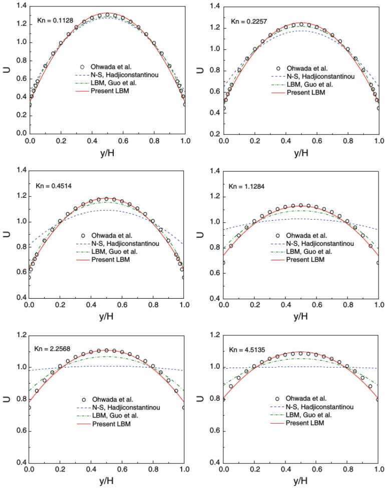

Figure : Results of Li et al. [3] for the transition regime, compared to the Navier-Stokes and other approaches.

Virtual wall collisions (Toschi and Succi) (1)

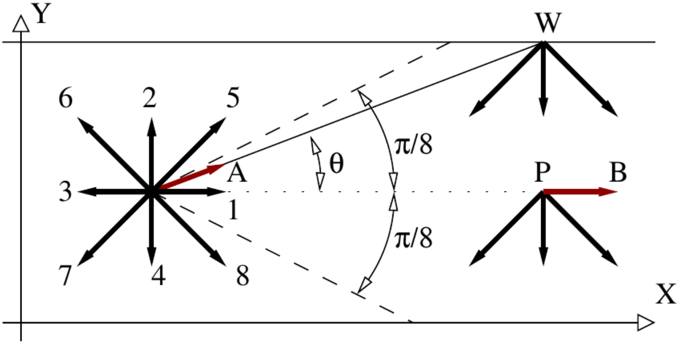

Figure : All the molecules that were going to travel within the $-\pi/8 < \theta < \pi/8$ range are actually mapped to a single direction. Because this direction is parallel to the flow, and because the intermolecular collisions are rare, these molecules will never collide with the walls and they will continue accelerating.

Virtual wall collisions (Toschi and Succi) (2)

Probability of virtual wall collision:
probability to avoid intermolecular collisions before hitting the wall,
multiplied by the probability to collide with the wall in a time step :

$$p(x, y; t) = \exp(-1/\mathrm{Kn}) \cdot \left(1 - \exp\left(-\frac{c \cdot \mathrm{d}t \cdot \sin(\theta(x, y))}{H}\right)\right) \qquad (22)$$

After colliding with the upper boundary:

$$f_1' = f_1(1-p) \quad , \quad f_{7,8}' = f_{7,8} + pf_1/6 \quad , \quad f_4' = f_4 + 4pf_1/6$$
$$f_3' = f_3(1-p) \quad , \quad f_{5,6}' = f_{5,6} + pf_3/6 \quad , \quad f_2' = f_2 + 4pf_3/6$$

In this way, particles are re-distributed to other directions.

Some results (Virtual wall collisions)

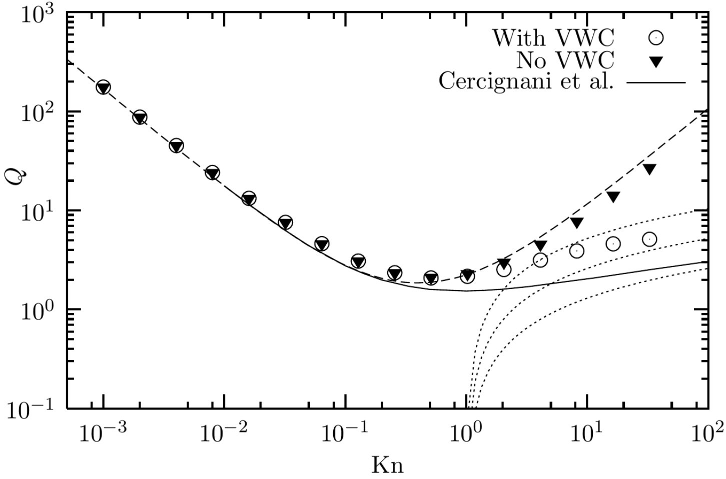

Figure : Results of Toschi and Succi [5] (mass flux) with Ansumali-Karlin BC, with and without virtual-wall-collisions, compared to a prediction.

Conclusions

- The continuous methods are not the correct tool for microfluids!
- LBM can be applied, MRT collision is suggested.
- LBM can work well in the slip and the transition regime, by adjusting the boundary conditions.
- Virtual wall collisions can fix the freely-accelerating beams.
- What happens in the free-molecular regime?

References I

[1] Robert Barber and David Emerson.
Challenges in modeling Gas-Phase flow in microchannels: From slip to transition.
Heat Transfer Engineering, 27(4):3–12, May 2006.

[2] George Karniadakis, Ali Beskok, and Nayaran Aluru.
Microflows and nanoflows: fundamentals and simulation.
Interdisciplinary applied mathematics. Springer, 2005.

[3] Q. Li, Y.L. He, G.H. Tang, and W.Q. Tao.
Lattice Boltzmann modeling of microchannel flows in the transition flow regime.
Microfluidics and Nanofluidics, 10(3):607–618, 2011.

References II

[4] Vasilis K. Michalis, Alexandros N. Kalarakis, Eugene D. Skouras, and Vasilis N. Burganos.
Rarefaction effects on gas viscosity in the Knudsen transition regime.
Microfluidics and Nanofluidics, 9(4-5):847–853, 2010.

[5] F. Toschi and S. Succi.
Lattice Boltzmann method at finite Knudsen numbers.
EPL (Europhysics Letters), 69(4):549, 2005.

[6] Frederik Verhaeghe, Li-Shi Luo, and Bart Blanpain.
Lattice Boltzmann modeling of microchannel flow in slip flow regime.
Journal of Computational Physics, 228(1):147 – 157, 2009.

[7] Wen-Ming Zhang, Guang Meng, and Xueyong Wei.
A review on slip models for gas microflows.
Microfluidics and Nanofluidics, 13(6):845–882, 2012.