Spring School on the lattice Boltzmann Method,

May 2-6, 2010, Beijing, China

Theory and applications of lattice Boltzmann equation for microscale flows

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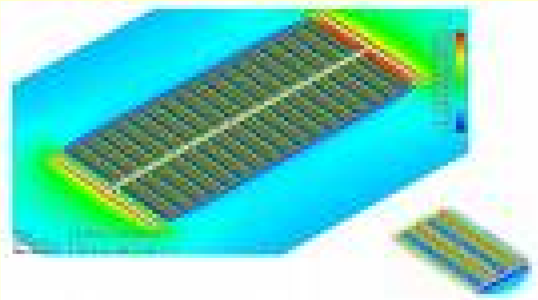
Outline

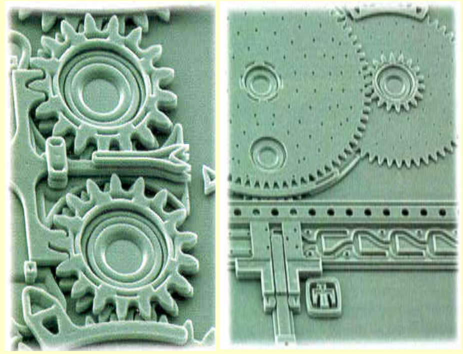
- **Basic Concepts**
- **Extending LBE to micro flows**
  - **Relaxation time and Boundary conditions**
  - **Knudsen Layer**
- **Applications & Extensions**
- **Summary**

1. Basic Concepts

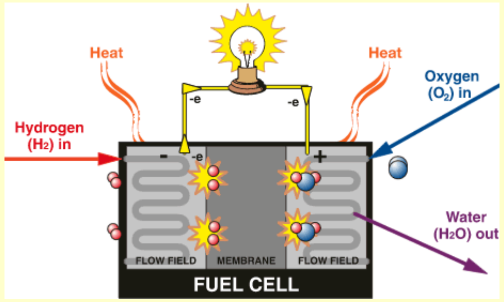
- **Micro Flows**



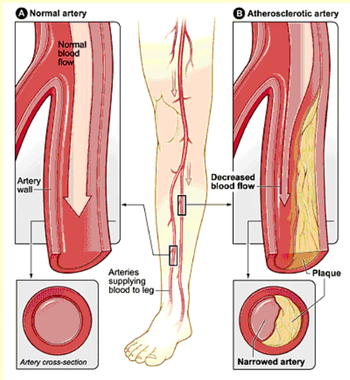
Micro-Chips



MEMS



Fuel Cell



Bio-flow

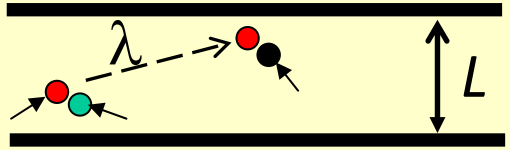
Inhalable particles

- ***Characteristics of Micro flows:***
  - ***Large Knudsen number***

$$\mathrm{Kn} = \frac{\lambda}{L}$$

Mean-free-path $\lambda = \frac{1}{\sqrt{2}\pi n \sigma^2}$

Characteristic length

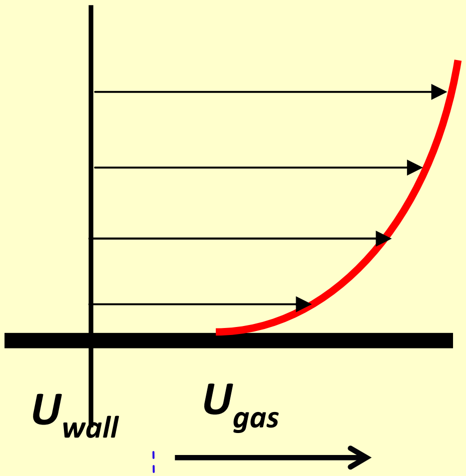


  - ***Discontinuous at solid surface***

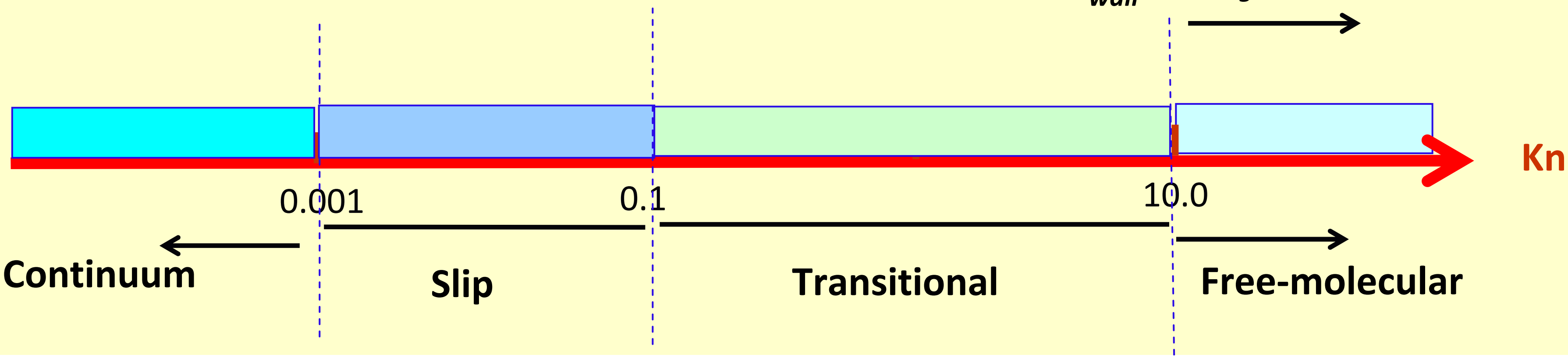
    Velocity slip, temperature jump, …

  - ***Low speed***

    Different from the high-altitude high-speed flows



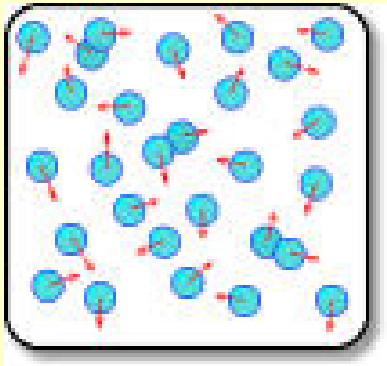
- ***Flow Regimes***



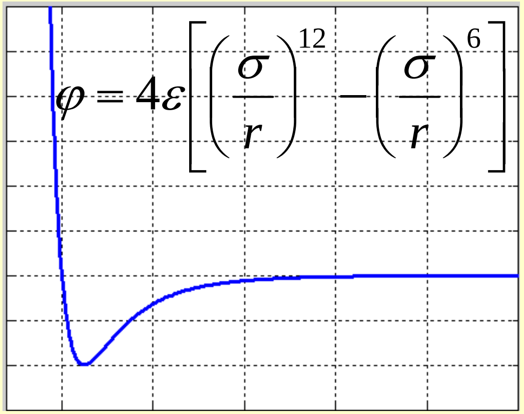
- **Modeling micro gas flows:**
  - **Continuum models**
    - **Navier-Stokes-Fourier equations**
    - **High-order equations: Burnett, Super-Burnett, Argument Burnett, ……**
    - **Moment equations: Grad’s 13, Regularized 13, Gaussian Closure, ……**
  - **Limitations:**
    - **Navier-Stokes is Limited to continuous flows;**
    - **Burnett-type and moment equations are facing some challenging difficulties (boundary conditions, numerical instability,…).**

– Molecular Dynamics (MD)

- Tracking the motion of each molecular (Newton's 2nd-law)



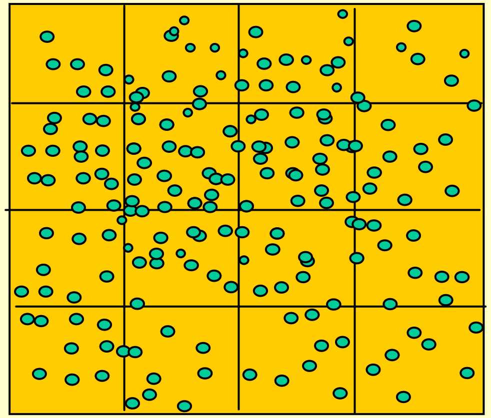
$$\frac{d^2 x_i}{dt^2} = F_i$$



$$\varphi = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

– Advantages and disadvantages

- Detailed microscopic information
- All Kn number
- Expensive computational cost



$$\rho_k \Phi_k = \frac{1}{V_k}\sum_{i\in V_k} m_i \phi_i$$

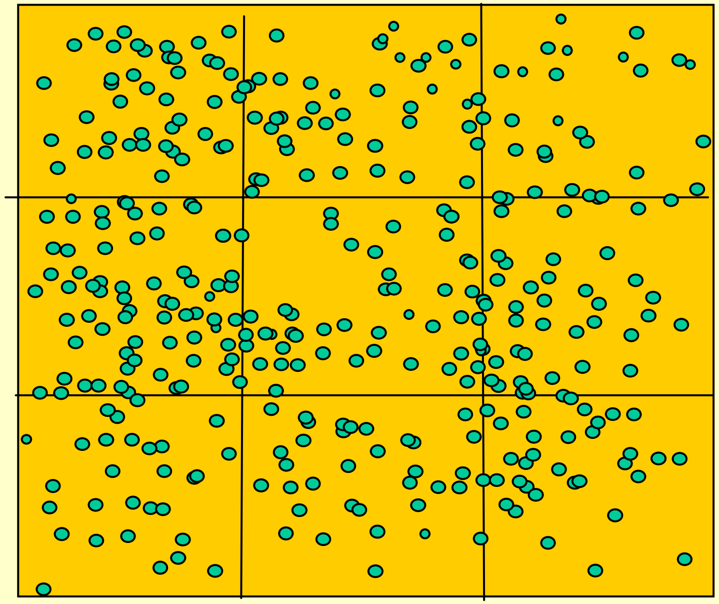
– Direct simulation Monte Carlo (DSMC)

- **Tracking the motion of simulated particles**
- **The motion of the particles are decoupled: collision and free-flight**

$$\frac{d\mathbf{v}_i}{dt} = \Omega_i(p_i, p_j)$$

$$\frac{dx_i}{dt} = v_i$$

$$\Delta t < \tau$$



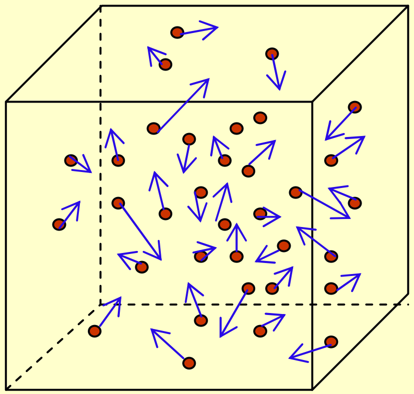
– limitations

- **Large statistical noise for low speed micro flows,**
- **High-computational costs**

– Boltzmann Equation (BE)

- Tracking the evolution of the probability distribution function rather than the individual molecules of the gas.

Ludwig Boltzmann (1844-1906)

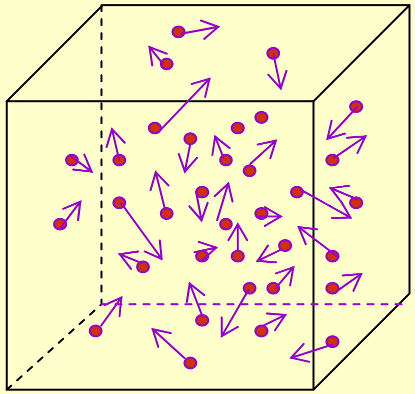


$$\xrightarrow{dt}$$

$$\boldsymbol{x} \to \boldsymbol{x} + \boldsymbol{v}dt$$

$$\boldsymbol{v} \to \boldsymbol{v} + \boldsymbol{a}dt$$

$$t \to t + dt$$



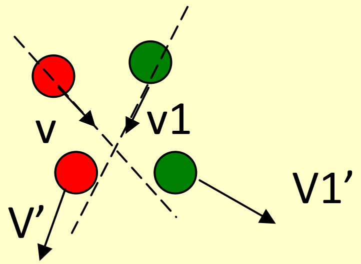
$$dN = f(\mathbf{x}, \mathbf{v}, t)d\mathbf{x}d\mathbf{v} \qquad dN = f(\mathbf{x} + \mathbf{v}dt, \mathbf{v} + \mathbf{a}dt, t + dt)d\mathbf{x}d\mathbf{v}$$

$$f(\boldsymbol{x} + \boldsymbol{v}dt, \boldsymbol{v} + \boldsymbol{a}dt, t + dt)d\boldsymbol{x}d\boldsymbol{v} = f(\boldsymbol{x}, \boldsymbol{v}, t)d\boldsymbol{x}d\boldsymbol{v} + \Omega_B(f, f)d\boldsymbol{x}d\boldsymbol{v}dt$$

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla f + \boldsymbol{a} \cdot \nabla_v f = \Omega_B(f, f)$$

Some properties of the Boltzmann equation

– **Collision operator**



$$\Omega_B(f,f)=\int\left[f(\boldsymbol{x},\boldsymbol{v}_1',t)\,f(\boldsymbol{x},\boldsymbol{v}',t)-f(\boldsymbol{x},\boldsymbol{v}_1,t)\,f(\boldsymbol{x},\boldsymbol{v},t)\right]B(\theta,V)\,d\varepsilon\,d\theta\,d\boldsymbol{v}_1$$

Post-collision

Pre-collision

Depending on
molecular interactions

– **Properties of the collision operator**

Symmetry

$$\int\Omega_B\,\phi(\boldsymbol{v}_1)d\boldsymbol{v}_1=\frac{1}{4}\int\Omega_B\left[\phi(\boldsymbol{v}_1)+\phi(\boldsymbol{v})-\phi(\boldsymbol{v}_1')-\phi(\boldsymbol{v}')\right]d\boldsymbol{v}_1$$

Conservation

$$\int\Omega_B d\boldsymbol{v}=0,\qquad\int\boldsymbol{v}\,\Omega_B d\boldsymbol{v}=0,\qquad\frac{1}{2}\int(\boldsymbol{v}-\boldsymbol{u})^2\,\Omega_B d\boldsymbol{v}=0$$

– **BGK model**

H-theorem $H = \int f \ln f d\mathbf{v}$

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \mathbf{a} \cdot \nabla_{\mathbf{v}} f = \Omega_B(f) \Longrightarrow \frac{dH}{dt} \leq 0$$

$$\frac{dH}{dt} = 0 \quad \overset{\text{(if and only if)}}{\Longleftrightarrow} \quad f^{eq} = \frac{\rho}{(2\pi RT)^{D/2}} \exp\left[-\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{2RT} \right]$$

$$\Omega(f^{(eq)}) = 0 \quad \text{(at equilibrium)}$$

The role of collision is to make the distribution function to approach its equilibrium !!!

BGK model: $\Omega_{BGK} = \frac{\mathbf{1}}{\tau_c}\left[f - f^{(eq)} \right]$

Satisfying the symmetry and conservation properties

- **Hydrodynamics equations from BE**

$$\int \varphi \left[\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla f + \boldsymbol{a} \cdot \nabla_{\boldsymbol{v}} f \right] d\boldsymbol{v} = \int \varphi\, \Omega_B(f) d\boldsymbol{v} \qquad \varphi = 1,\ m\boldsymbol{v}, m v^2/2$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial(\rho\, \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) + \nabla \cdot \boldsymbol{P} = \rho \boldsymbol{a}$$

$$\frac{\partial(\rho\, e)}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\, e) + \nabla \cdot \boldsymbol{q} = 0$$

$$\boldsymbol{P} = \int \boldsymbol{C}\boldsymbol{C} f d\boldsymbol{v},$$

$$\boldsymbol{q} = \int \frac{1}{2} C^2 \boldsymbol{C} f d\boldsymbol{v},$$

$$\boldsymbol{C} = (\boldsymbol{v} - \boldsymbol{u})$$

- **Chapman-Enskog Expansion**

$$f = f^{(0)} + \varepsilon f^{(1)} + \varepsilon^2 f^{(2)} + \cdots \qquad \partial_t = \partial_{t0} + \varepsilon \partial_{t1} + \varepsilon^2 \partial_{t2} + \cdots$$

$$\mathbf{P}^{(0)} = p\mathbf{I}, \quad \mathbf{q}^{(0)} = 0 \longrightarrow \text{Euler}$$

$$\mathbf{P}^{(1)} = \mu \mathbf{S} + \mu'(\nabla \cdot \mathbf{u})\mathbf{I}, \quad \mathbf{q}^{(1)} = -k\nabla T \longrightarrow \text{Navier-Stokes}$$

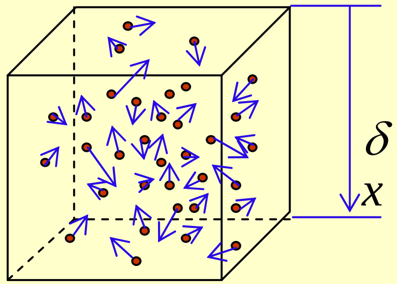
$$\mathbf{P}^{(2)} = \ldots, \quad \mathbf{q}^{(2)} = \ldots \longrightarrow \text{Burnett}$$

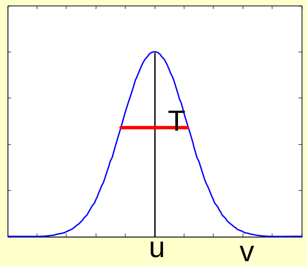
$$\ldots\ldots$$

– Advantages of Boltzmann Equation (for micro-flows)

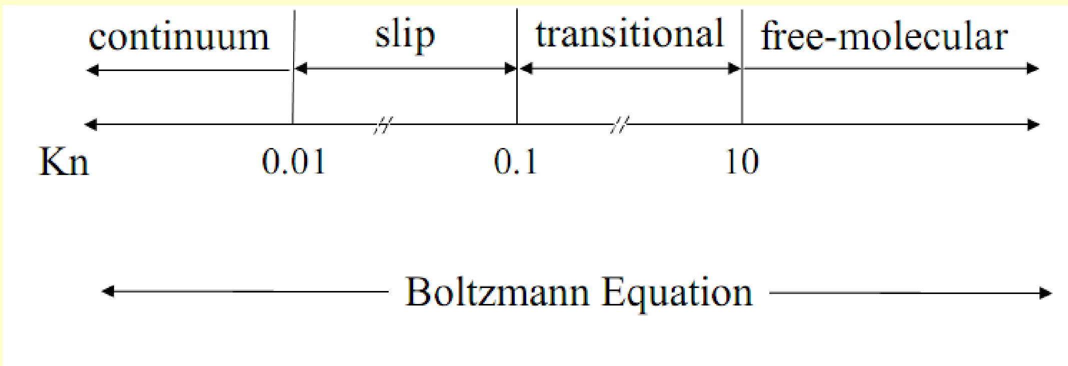
- **No continuum assumption**

$$dN = f(\mathrm{x}, \mathrm{v}, t)\delta V d\mathrm{v}$$





- **Arbitrary Kn number**



The Boltzmann equation can serve as a good base for modeling and simulating micro (gas) flows

- **Solving the Boltzmann Equation**
  - **Linearized Boltzmann Equation (LBE) method**
    - **Finite-difference method (e.g., C. Cercignani)**
    - **Variational approach (e.g., C. Cercignani);**
    - **Discrete velocity method (e.g., T. Ohwada);**

  (Difficult to solve even for simple geometries)

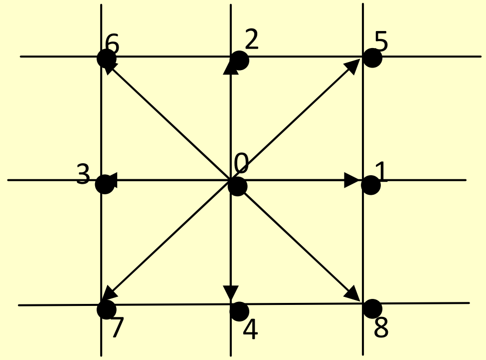
  - **DSMC method– converges to Boltzmann Equation**
  - **Lattice Boltzmann equation (LBE) method**
    - **Efficient discrete kinetic model with simple structure;**
    - **Based on Boltzmann equation, No continuum assumption (in principle)**

  (A potential tool for micro gas flows)

- **Structure of Latice Boltzmann Equation (LBE)**

  – **Evolution of LBE**

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta_t, t+\delta_t) - f_i(\boldsymbol{x}, t) = \Omega_i(f)$$



  – **Collision models**

BGK or Single-Relaxation-Time model (1992, Qian et al., Chen et al.)

$$\Omega_i = -\frac{1}{\tau}\left[f_i - f_i^{(eq)}\right]$$

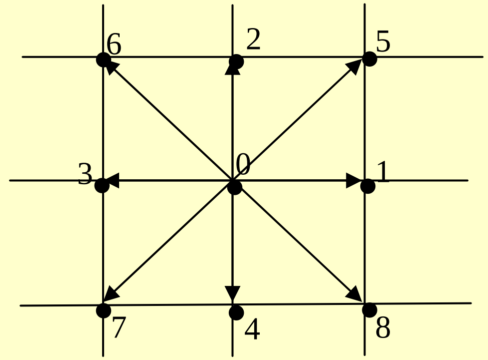
Multiple-Relaxation-Time model (1992, d'Humieres)

$$\Omega_i = -\sum_j M_{ij}^{-1}\tau_j^{-1}(\hat{f}_j - \hat{f}_j^{(eq)}) \qquad \hat{f} = Mf \qquad \hat{f}^{(eq)} = Mf^{(eq)}$$

Received increasing interests due to some important features.

– Example: D2Q9 model

$$\boxed{f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta_t, t+\delta_t) - f_i(\boldsymbol{x},t) = -\sum_j M_{ij}^{-1}\tau_j^{-1}(\hat{f}_j - \hat{f}_j^{(eq)})}$$



$$\hat{f} = Mf = \left(\rho, e, \varepsilon, j_x, q_x, j_y, q_y, p_{xx}, p_{xy}\right)^T$$

$$\boldsymbol{\tau} = \left(0, \tau_e, \tau_\varepsilon, 0, \tau_q, 0, \tau_q, \tau_s, \tau_s\right)^T$$

$$f^{(eq)} = w_i\rho\left[1 + \frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u}\cdot\boldsymbol{u}}{2c_s^2}\right]$$

$$c_s = \sqrt{RT} = \frac{c^2}{3} = \frac{1}{3}\left(\frac{\delta_x}{\delta_t}\right)^2$$

$$\boxed{\rho = \sum_i f_i \qquad \rho\boldsymbol{u} = \sum_i \boldsymbol{c}_i f_i}$$

Theoretical analysis gives the Navier-Stokes equations with

$$\mu = \rho c_s^2\left(\tau_s - \frac{1}{2}\right)\delta_t = p\left(\tau_s - \frac{1}{2}\right)\delta_t \qquad \eta = \rho c_s^2\left(\tau_e - \frac{1}{2}\right)\delta_t$$

$$
\mathsf{M} = \begin{array}{cl}
\left(\begin{array}{rrrrrrrrr}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\
4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\
0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\
0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\
0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\
0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\
0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1
\end{array}\right)
&
\begin{array}{l}
\\ \\ \\ \\ \boldsymbol{c_{ix}} \\ \boldsymbol{c_{iy}} \\ \\ \\ \\
\end{array}
\end{array}
$$

$$
\mathsf{MM}^T = \mathsf{D} \equiv diag[9, 36, 36, 6, 12, 6, 12, 4, 4]
$$

$$\mathsf{M}^{-1} = \mathsf{M}^T\mathsf{D}^{-1}$$

$$= \begin{pmatrix} 1/9 & -1/9 & 1/9 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1/9 & -1/36 & -1/18 & 1/6 & -1/6 & 0 & 0 & 1/4 & 0 \\ 1/9 & -1/36 & -1/18 & 0 & 0 & 1/6 & -1/6 & -1/4 & 0 \\ 1/9 & -1/36 & -1/18 & -1/6 & 1/6 & 0 & 0 & 1/4 & 0 \\ 1/9 & -1/36 & -1/18 & 0 & 0 & -1/6 & 1/6 & -1/4 & 0 \\ 1/9 & 1/18 & 1/36 & 1/6 & 1/12 & 1/6 & 1/12 & 0 & 1/4 \\ 1/9 & 1/18 & 1/36 & -1/6 & -1/12 & 1/6 & 1/12 & 0 & -1/4 \\ 1/9 & 1/18 & 1/36 & -1/6 & -1/12 & -1/6 & -1/12 & 0 & 1/4 \\ 1/9 & 1/18 & 1/36 & 1/6 & 1/12 & -1/6 & -1/12 & 0 & -1/4 \end{pmatrix}$$

Outline

- Basic Concepts
- Extending LBE to micro flows
  - Relaxation time and Boundary conditions
  - Knudsen Layer
- Applications & Extensions
- Summary

2. Extending LBE to micro flows

- **Key problems of LBE for micro-flows**

Standard LBE is designed for continuum flows

Continuum flow	Micro-scale flow
• Characterized by the Reynolds number (Re)	• Characterized by the Knudsen number (Kn)
• No-slip on a wall	• Slip on a wall

Two key problems to simulate micro flows using LBE:

- How to incorporate the Knudsen number into LBE
- How to realize slip boundary conditions

2.1 Incorporating Kn into LBE

Basic idea:

Physically, the mean-free-path λ is related to the relaxation time τ_c:

$$\tau_c = \frac{\lambda}{\bar{c}} = \frac{Kn \cdot L}{\bar{c}}$$

Certain mean particle velocity

The choice is rather diverse in the literature:

- **lattice speed:** $\bar{c} = \delta x / \delta t$
- **mean molecular velocity:** $\bar{c} = \sqrt{8RT/\pi}$
- **root-mean-square velocity** $\bar{c} = \sqrt{3RT}$

Which mean velocity ?

– **Consistency requirement:** in the continuum limit (Kn→0),

$$\tau_c = \frac{\mu}{p}$$

– From kinetic theory (C. Cercignani 1988):

$$\lambda = \frac{\mu}{p}\sqrt{\frac{\pi RT}{2}} \quad \Longrightarrow \quad \boxed{\bar{c} = \sqrt{\frac{\pi RT}{2}} \qquad (\mathrm{Kn} \to 0)}$$

Application to D2Q9 LBE:

$$\mu = \rho c_s^2\left(\tau_s - \frac{1}{2}\right)\delta_t = p\left(\tau_s - \frac{1}{2}\right)\delta_t \qquad \eta = \rho c_s^2\left(\tau_e - \frac{1}{2}\right)\delta_t$$

Kinetic theory gives

$$\lambda = \frac{\mu}{p}\sqrt{\frac{\pi RT}{2}} \longrightarrow \lambda = \left(\tau_s - \frac{1}{2}\right)\delta_t\sqrt{\frac{\pi RT}{2}} = \sqrt{\frac{\pi}{6}}\left(\tau_s - \frac{1}{2}\right)\delta_x$$

$$\boxed{\tau_s = \frac{1}{2} + \sqrt{\frac{6}{\pi}}\,Kn\ N} \qquad Kn = \frac{\lambda}{L} \qquad N = \frac{L}{\delta_x}$$

Remark: Different τ - Kn relationships adopted in previous work

S. Ansumali et al. Physica A 2006 $\tau = \sqrt{2.5}\,Kn\,N$ Sbragaglia & Succi, Phys. Fluids, 2005 $\tau = 0.5 + \sqrt{3}\,Kn\,N$

Nie et al. J. Stat. Phys. 2002 $\tau = 0.5 + \rho Kn\,N/\alpha, \quad \alpha = 0.388$

Lim et al. J. Stat. Phys. 2002; Lee & Lin PRE 2005; Niu et al, Europhys Lett. 2004; Shu et al, J. Stat. Phys 2004; Sofonea et al. J. Comput Phys 2005

$$\tau = 0.5 + Kn\,N \qquad (\lambda = \delta_x)$$

Cannot give correct Knudsen number !

2.2 Kinetic boundary conditions in LBE

Kinetic theory:

$$|\xi \cdot \boldsymbol{n}|\, f(\xi) = \int_{\xi' \cdot \boldsymbol{n} < 0} R(\xi' \to \xi)\, f(\xi')\, |\xi' \cdot \boldsymbol{n}|\, d\xi' \qquad \xi \cdot \boldsymbol{n} > 0$$

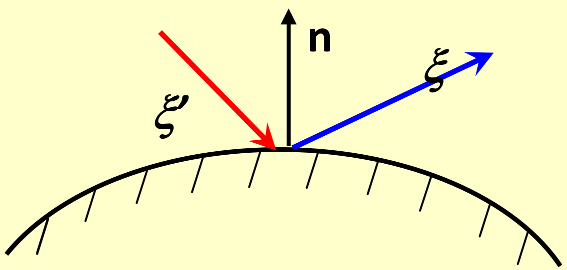
Interaction Kernel

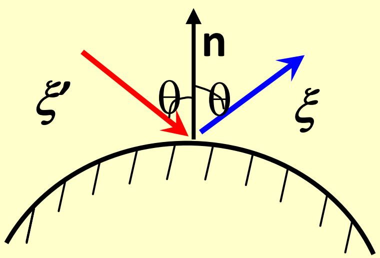
$$\int_{\xi \cdot \boldsymbol{n} > 0} R(\xi' \to \xi)\, d\xi = 1$$

Maxwell's diffuse Kernel

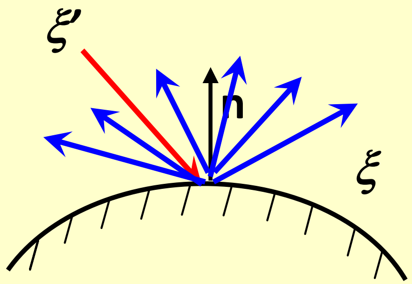
Accommodation coefficient

$$R(\xi' \to \xi) = \sigma_{phy} f^{(eq)}(\boldsymbol{u}_w, T_w, \xi)\, |\xi \cdot \boldsymbol{n}| + (1 - \sigma_{phy})\,\delta(\xi' - \xi + 2\boldsymbol{n}\,\xi \cdot \boldsymbol{n})$$





Specular-reflection

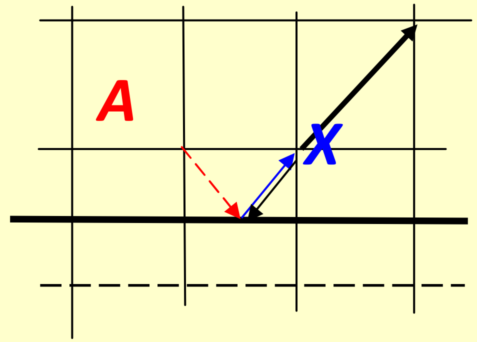


Fully diffusive

Three kinetic boundary conditions for LBE for micro-scale flows

- **Bounce-back / Specular-reflection scheme (BS, S. Succi, PRL, 2002)**

$$f_i(X,t+\delta) = r\left[f_{\bar{i}}^{+} + w_i \rho \frac{2\boldsymbol{c}_i \cdot \boldsymbol{u}_w}{c_s^2} \right]_{(X,t)} + (1-r) f_{i'}^{+}(A,t)$$



Post-collision

$$f_i^{+} = f_i(\boldsymbol{x},t) + \sum_j \Omega_{ij}\left[f_j(\boldsymbol{x},t) - f_j^{(eq)}(\boldsymbol{x},t)\right] + \delta t F_i(\boldsymbol{x},t)$$

- **Discrete Diffuse Scatting scheme (DS, Karlin, PRE, 2002)**

Numerical accommodation coefficient

$$f_i(X,t+\delta t) = \sigma K f_i^{(eq)}(\boldsymbol{u}_w) + (1-\sigma) f_{i'}^{+}(A,t)$$

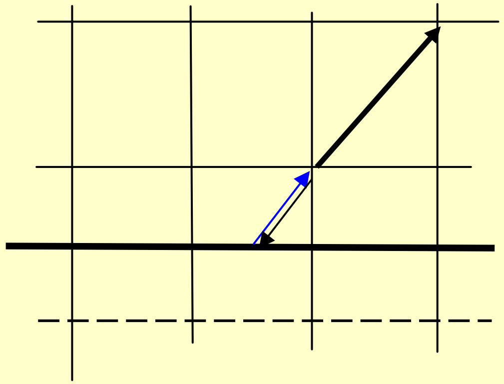
K is a parameter such that

$$\sum_{\boldsymbol{c}_i\cdot\boldsymbol{n}>0} \boldsymbol{c}_i f_i = \sum_{\boldsymbol{c}_j\cdot\boldsymbol{n}<0} \boldsymbol{c}_j f_j$$

- **Diffuse / bounce-back Scheme (DB)**

(first proposed by Luo et al for first-order slip boundary condition of fully diffusive wall, JCP 2009)

$$f_i(X,t+\delta t)=\alpha\left[f_{\bar{i}}^{+}+w_i\rho\frac{2\boldsymbol{c}_i\cdot\boldsymbol{u}_w}{c_s^2}\right]_{(X,t)}+(1-\alpha)\,f_i^{(eq)}(\boldsymbol{u}_w)$$



- **Comments:**
  - **The BS and DS schemes are**
    - **non-local because of the reflection parts**
    - **not easy for curved walls**
  - **The DB scheme is local** and thus can be easily applied to curved walls

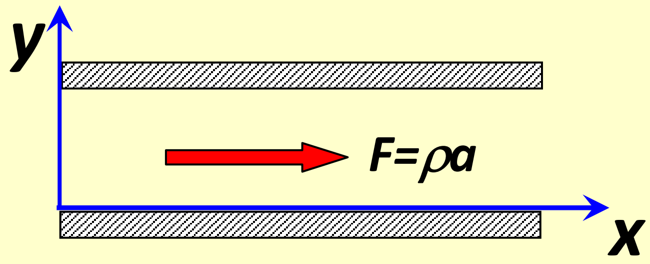
Key points in the 3 schemes:

How to determine the parameters (r, α, σ) ?

Analysis of kinetic boundary conditions: the plane Poiseuille flow case

- **Assumptions (unidirectional flow)**

$$\rho = \rho_0 \qquad v = 0 \qquad \frac{\partial \phi}{\partial x} = 0$$

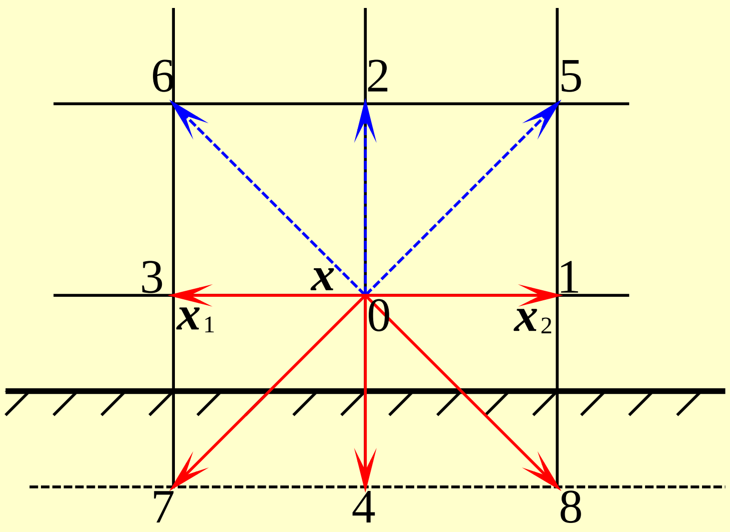


- **BS scheme** (Bounce-back/specular-reflection)

$$f_2(\boldsymbol{x}, t+\delta t) = f_4^+(\boldsymbol{x}, t)$$

$$f_5(\boldsymbol{x}, t+\delta t) = r\left[f_7^+ + w_5 \rho \frac{2\boldsymbol{c}_5 \cdot \boldsymbol{u}_w}{c_s^2} \right]_{(\boldsymbol{x},t)} + (1-r) f_8^+(\boldsymbol{x}_1, t)$$

$$f_6(\boldsymbol{x}, t+\delta t) = r\left[f_8^+ + w_6 \rho \frac{2\boldsymbol{c}_6 \cdot \boldsymbol{u}_w}{c_s^2} \right]_{(\boldsymbol{x},t)} + (1-r) f_7^+(\boldsymbol{x}_2, t)$$

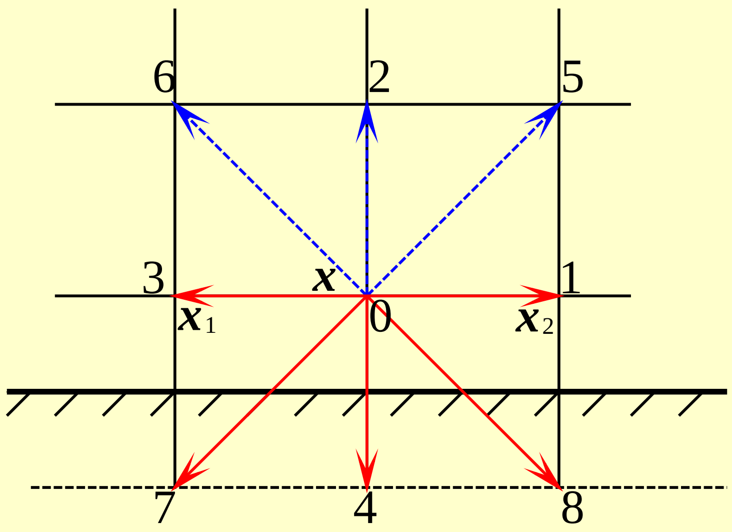


- **DS scheme** (Diffuse-scatting)

$$f_2(\boldsymbol{x}, t+\delta t) = \sigma f_2^{(eq)}(\rho_w, \boldsymbol{u}_w) + (1-\sigma) f_4^+(\boldsymbol{x}, t)$$

$$f_5(\boldsymbol{x}, t+\delta t) = \sigma f_5^{(eq)}(\rho_w, \boldsymbol{u}_w) + (1-\sigma) f_8^+(\boldsymbol{x}_1, t)$$

$$f_6(\boldsymbol{x}, t+\delta t) = \sigma f_6^{(eq)}(\rho_w, \boldsymbol{u}_w) + (1-\sigma) f_7^+(\boldsymbol{x}_2, t)$$



- **DB scheme** (Diffuse / Bounce-back)

$$f_2(\boldsymbol{x}, t+\delta t) = \alpha f_4^+(\boldsymbol{x}, t) + (1-\alpha) f_2^{(eq)}(\rho_w, \boldsymbol{u}_w)$$

$$f_5(\boldsymbol{x}, t+\delta t) = \alpha \left[f_7^+ + w_5 \rho \frac{2\boldsymbol{c}_5 \cdot \boldsymbol{u}_w}{c_s^2} \right]_{(\boldsymbol{x}, t)} + (1-\alpha) f_5^{(eq)}(\rho_w, \boldsymbol{u}_w)$$

$$f_6(\boldsymbol{x}, t+\delta t) = \alpha \left[f_8^+ + w_6 \rho \frac{2\boldsymbol{c}_6 \cdot \boldsymbol{u}_w}{c_s^2} \right]_{(\boldsymbol{x}, t)} + (1-\alpha) f_6^{(eq)}(\rho_w, \boldsymbol{u}_w)$$

- Analysis of the velocity profile

LBE

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\delta_t, t+\delta_t) - f_i(\boldsymbol{x},t) = -\sum_j M_{ij}^{-1}\tau_j^{-1}(\hat{f}_j - \hat{f}_j^{(eq)}) + \delta_t F_i$$

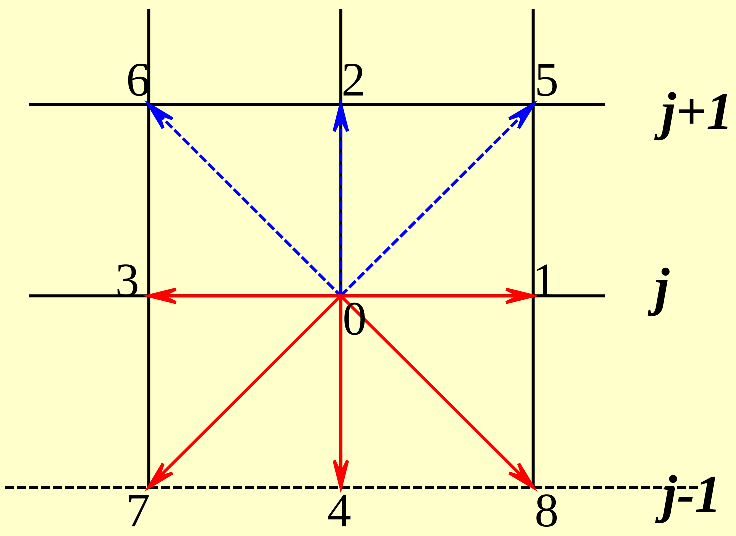
$$\overline{F}_i = w_i\rho\left[\frac{\boldsymbol{c}_i\cdot\boldsymbol{a}}{c_s^2} + \frac{(\boldsymbol{ua}+\boldsymbol{au}):(c_s^2\boldsymbol{I}-\boldsymbol{c}_i\boldsymbol{c}_i)}{c_s^4}\right]$$

With the assumption of unidirectional, at steady state we have the following relation for an inner node *j*

$$f_1(j)-f_3(j)=f_1^+(j)-f_3^+(j)$$

$$f_5(j)-f_6(j)=f_5^+(j-1)-f_6^+(j-1) \qquad f_5(j+1)-f_6(j+1)=f_5^+(j)-f_6^+(j)$$

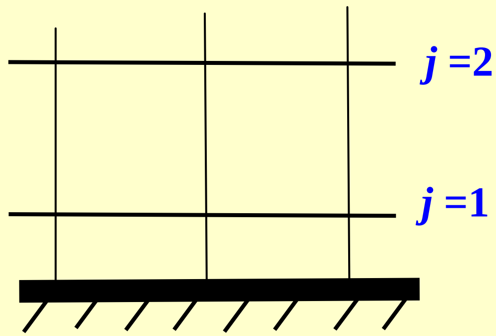
$$f_8(j)-f_7(j)=f_8^+(j+1)-f_7^+(j+1) \qquad f_8(j-1)-f_7(j-1)=f_8^+(j)-f_7^+(j)$$



$$\nu\frac{u_{j+1}-2u_j+u_{j-1}}{\delta x^2} = a$$

$$u_j = U_0\frac{y_j}{H}\left(1-\frac{y_j}{H}\right)+u_s \qquad U_0 = aH^2/2\nu$$

- # Determination of slip velocity



$$\rho u_1 = c\left(f_1^1 - f_3^1\right) + c\left(f_5^1 - f_6^1\right) + c\left(f_8^1 - f_7^1\right) + \frac{\delta t}{2}\rho a$$

Boundary condition

$$u_j = U_0 \frac{y_j}{H}\left(1 - \frac{y_j}{H}\right) + u_s$$

$$\frac{u_s}{U_0} = \begin{cases} \dfrac{1-r}{r}\sqrt{\dfrac{6}{\pi}}Kn + \dfrac{\chi}{2\pi}Kn^2, & \textbf{BS} \\ \dfrac{2-\sigma}{\sigma}\sqrt{\dfrac{6}{\pi}}Kn + \dfrac{\chi}{2\pi}Kn^2, & \textbf{DS} \\ \dfrac{1-\alpha}{1+\alpha}\sqrt{\dfrac{6}{\pi}}Kn + \dfrac{\chi}{2\pi}Kn^2, & \textbf{DB} \end{cases}$$

$$\chi = \frac{16\tau_s\tau_q - 8\tau_s - 8\tau_q + 1}{(\tau_s - 0.5)^2}$$

the slippages at the first order of Kn depend on the kinetic boundary condition, while those at the order of Kn^2 are all identical. This means that the three schemes are equivalent as $\sigma = 1+\alpha = 2r$.

- **Realization of a given 2nd-order slip boundary condition**

Consider the 2nd-order slip boundary condition

$$u_s = L_1 \lambda \partial_y u - L_2 \lambda^2 \partial_y^2 u$$

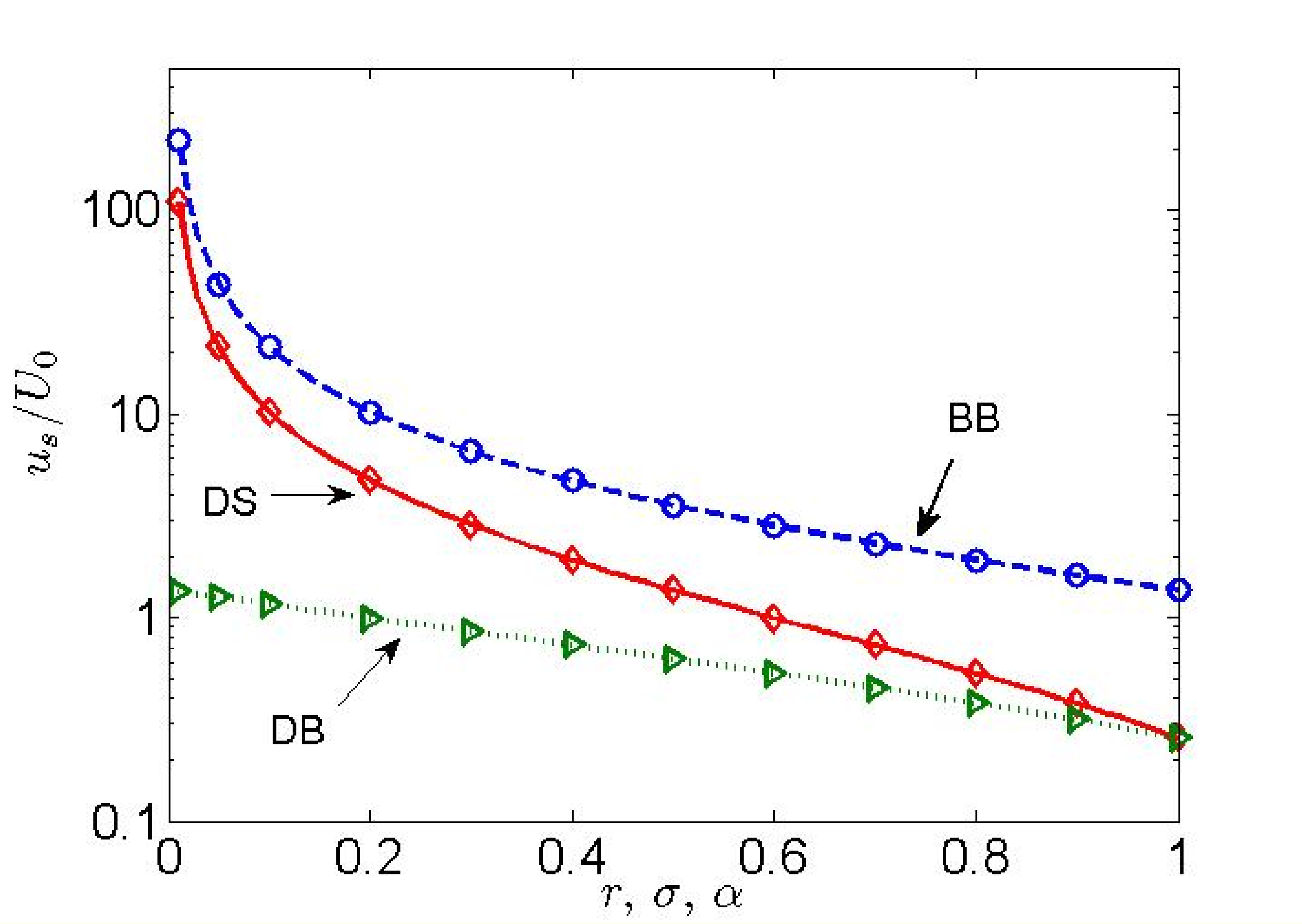
This BC gives

$$\frac{u_s}{U_0} = L_1 Kn + 2L_2 Kn^2$$

In order to realize this BC, we should choose

$$\boxed{r = \frac{\sigma}{2} = \frac{1+\alpha}{2} = \left(1 + \sqrt{\frac{\pi}{6}} L_1\right)^{-1}, \quad \tau_q = 0.5 + \frac{4\pi L_2 (\tau_s - 0.5)^2 + 3}{16(\tau_s - 0.5)}}$$

Numerical results: Slip velocity of the kinetic boundary conditions



2.3 Discrete effects in the kinetic B.C.

Can we take $\sigma = \sigma_{phy}$ in the DS scheme ?

Example: Fully diffusive wall (σ_{phy}= 1)

- **The Boltzmann equation gives (C. Cercignani):**

$$U_s = 4.586\,Kn + 7.804\,Kn^2$$

Discrete Effects !

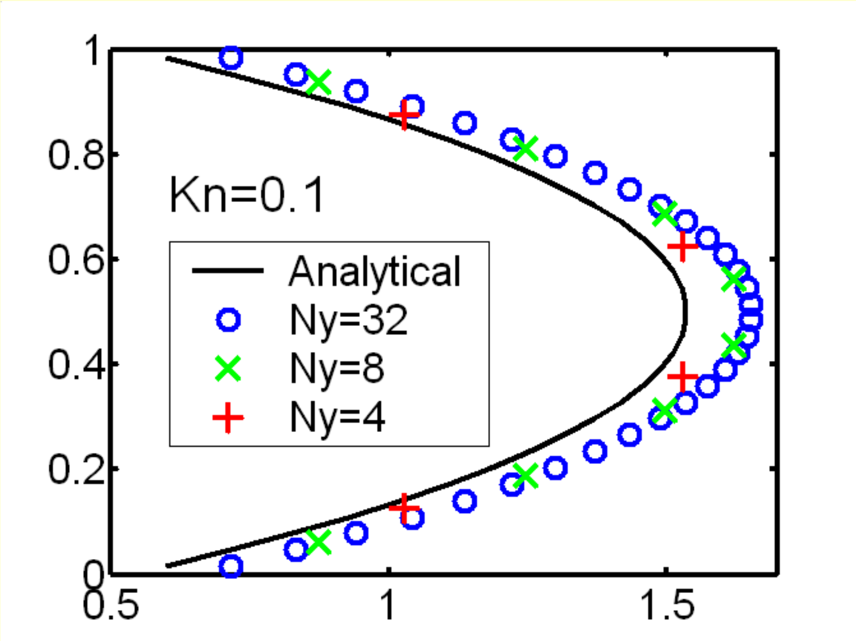
- **The LBE gives**

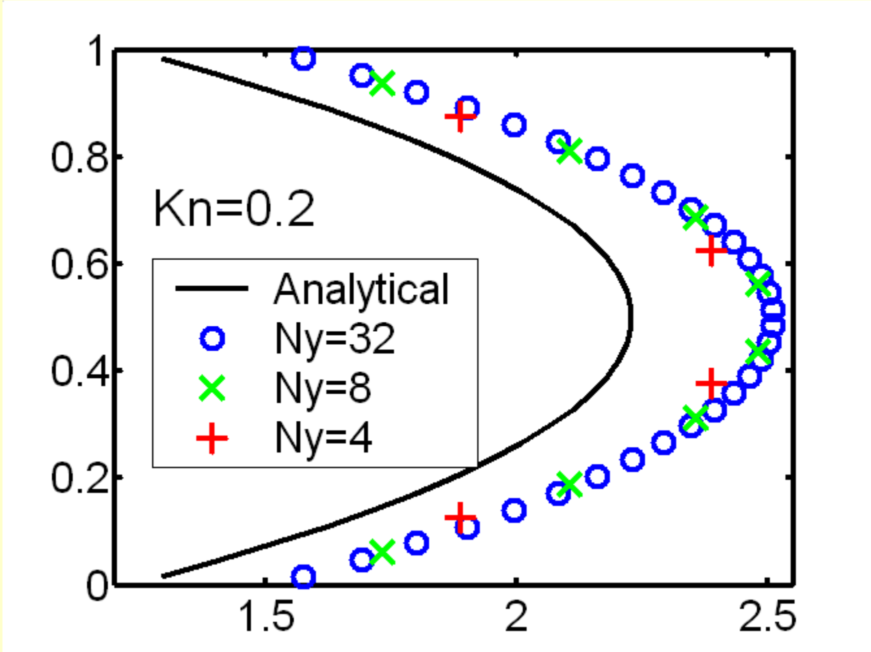
$$U_s = 4\sqrt{\frac{6}{\pi}}Kn + \frac{32}{\pi}Kn^2 - \Delta^2 \approx 5.528\,Kn + 10.186\,Kn^2 - \Delta^2$$

Proper choice:

$$\boxed{\sigma = 2\left(1+\sqrt{\frac{\pi}{6}}L_1\right)^{-1} \approx 1.093, \quad \tau_q = 0.5 + \frac{4\pi L_2(\tau_s - 0.5)^2 + 3}{16(\tau_s - 0.5)}}$$

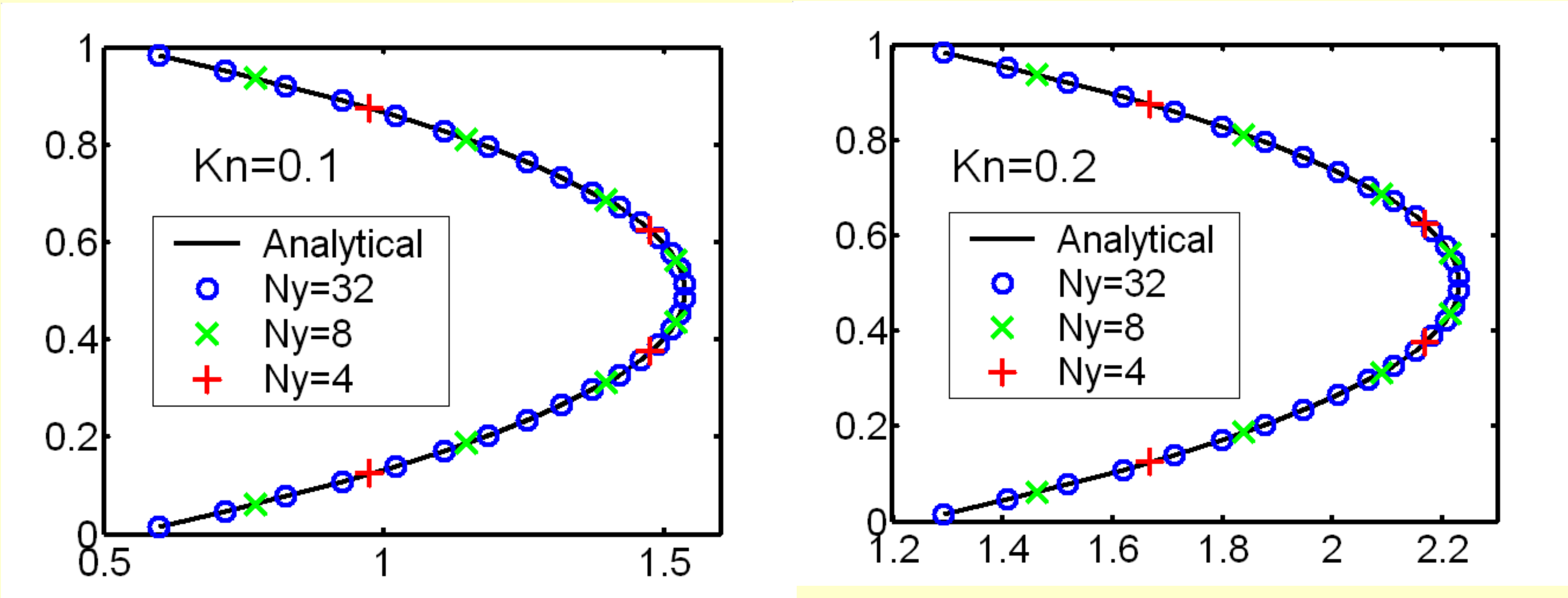
LBE with fixed σ (=1) and $\tau_q = \tau_s$





LBE results Over-predict the slip, and are mesh dependent

MRT-LBE with modified σ (=1.093) and τ_q

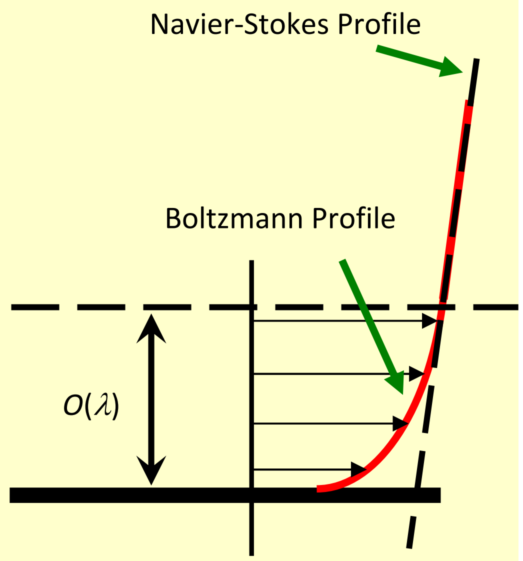


Excellent agreement even with a coarse mesh (+)

Outline

- Basic Concepts
- Extending LBE to micro flows
  - Relaxation time and Boundary conditions
  - Knudsen Layer
- Applications & Extensions
- Summary

- **Knudsen Layer (KL)**
  - **rare inter-molecular collisions**
  - **failure of quasi thermodynamic equilibrium**
  - **inadequate of Navier-Stokes equations**
- **LBE**
  - **most existing models aim to solve Navier-Stokes equation**
  - **insufficient to capture the Knudsen Layer**



Extending LBE to capture the KL

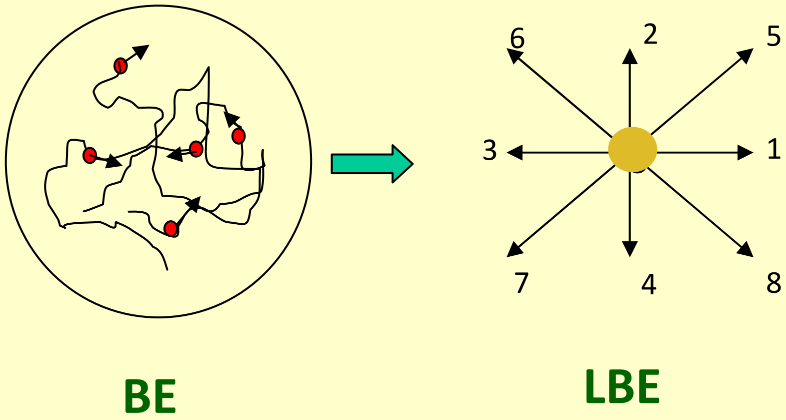
- **Two ways:**
  - **Improve the discretization accuracy of LBE (Shan 2006)**

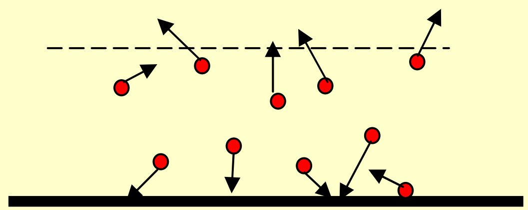
    Key point: increaseing the symmetric of discrete velocitis, so that LBE can match the BE at higher orders than NS level

    Test case: Pressure driven Poiseuille flow

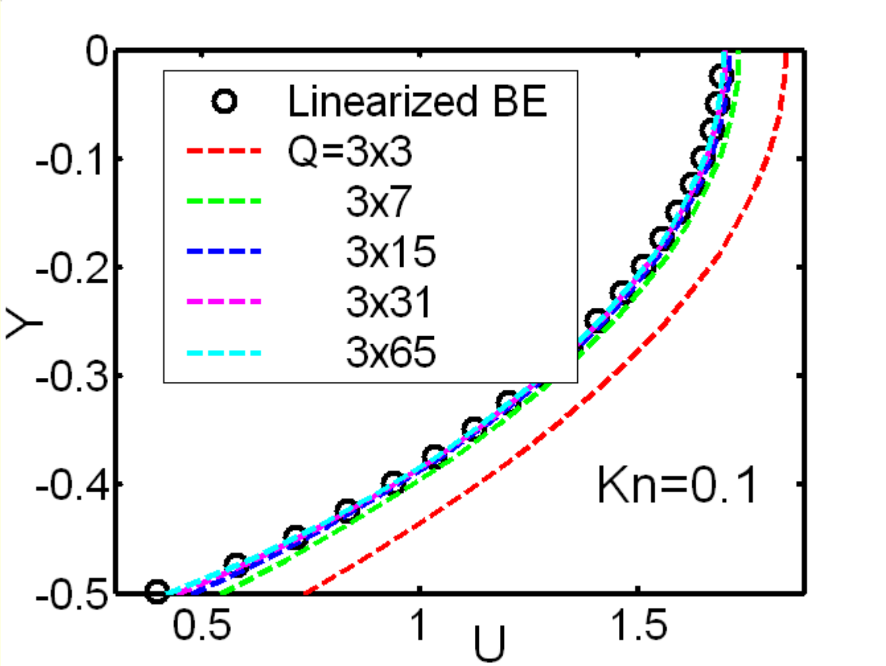
  - **Modeling the Knudsen layer (Guo 2006,2008; Zhang 2006).**

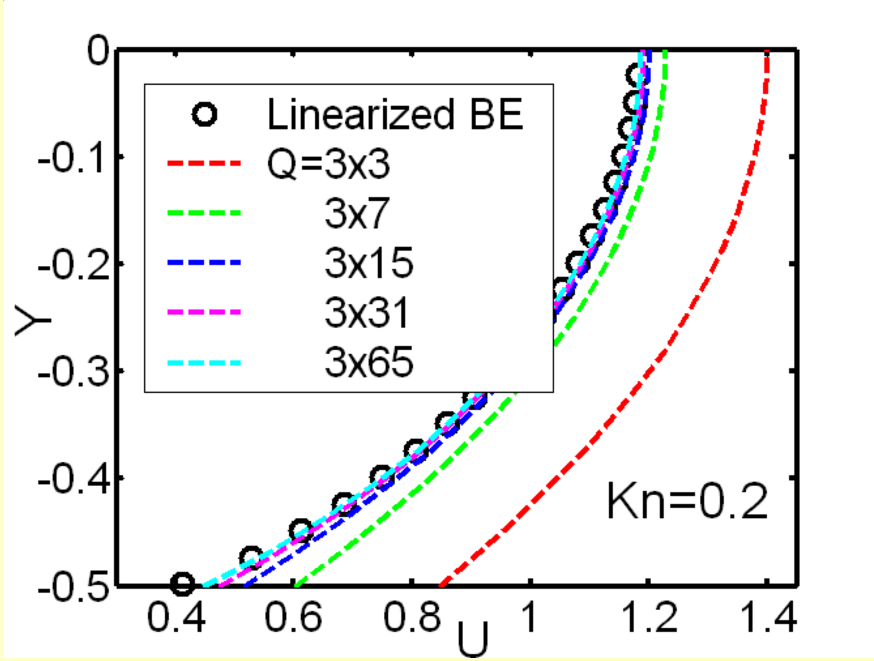
    Key point: incorporating the gas-wall collision effect into the model





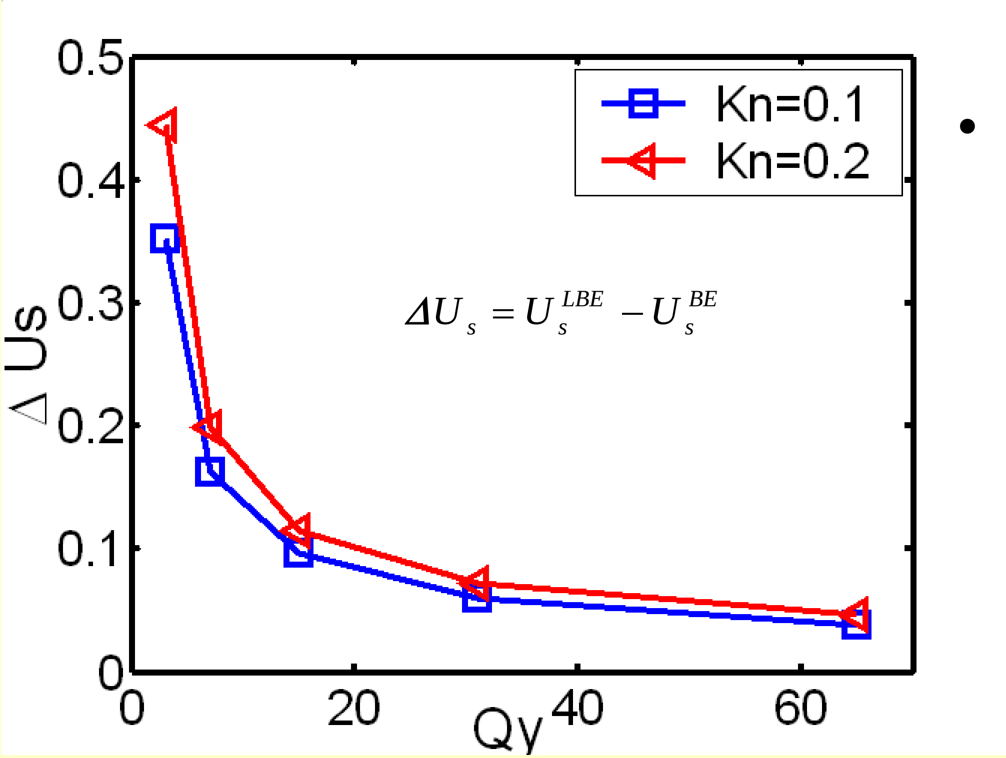
Test case: Pressure driven Poiseuille flow





With increasing number of discrete velocities (c_{iy}), the predicted velocities approach to the analytical solutions of the BE.

Errors in the slip velocity



With increasing number of discrete velocities (c_{iy}), the slip velocity approaches to the analytical solution of the BE.

- **Remark on high-order LBE:**
  - **The Knudsen layer can be captured by LBE given the discretization accuracy is sufficient**
  - **Computational cost will be expensive if the number of discrete velocities is large.**

Modeling the Knudsen layer

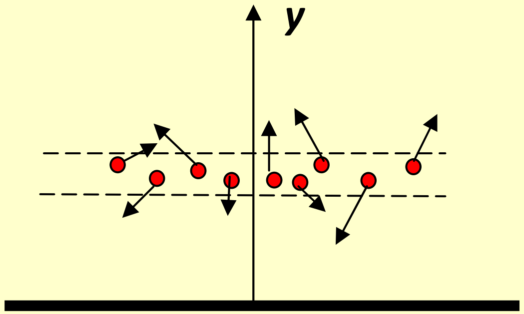
Basic idea:

- The effect of gas-wall collision on the local mean-free-path

$$\lambda_{local} = \lambda_\infty \phi(Kn, y)$$

- The relaxation time can be related to the local mean-free-path

$$\tau_{local} = \lambda_{local} / c^*$$



Key point: the effective function ϕ

Z.L. Guo et al: 2006

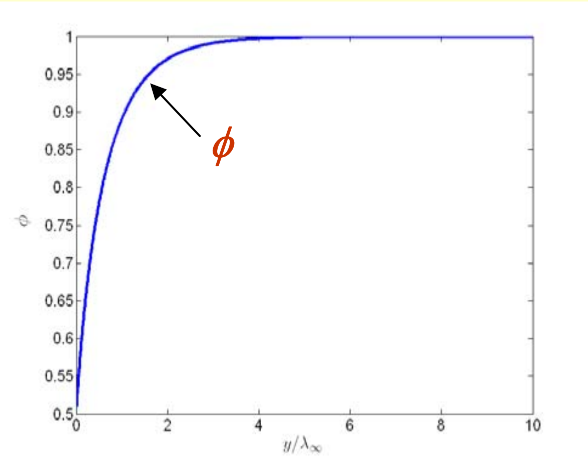
$$\phi = \frac{2}{\pi}\arctan(\sqrt{2}Kn^{-3/4})$$

Y.H. Zhang et al: 2006

$$\phi = [1 + 0.7C\exp(-Cy/\lambda_\infty)]^{-1}$$

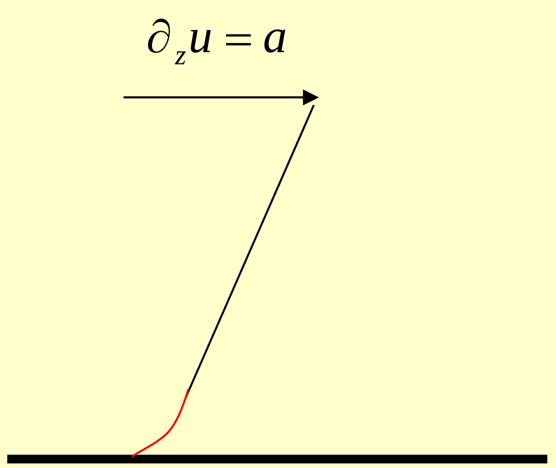
Z.L. Guo et al: 2008

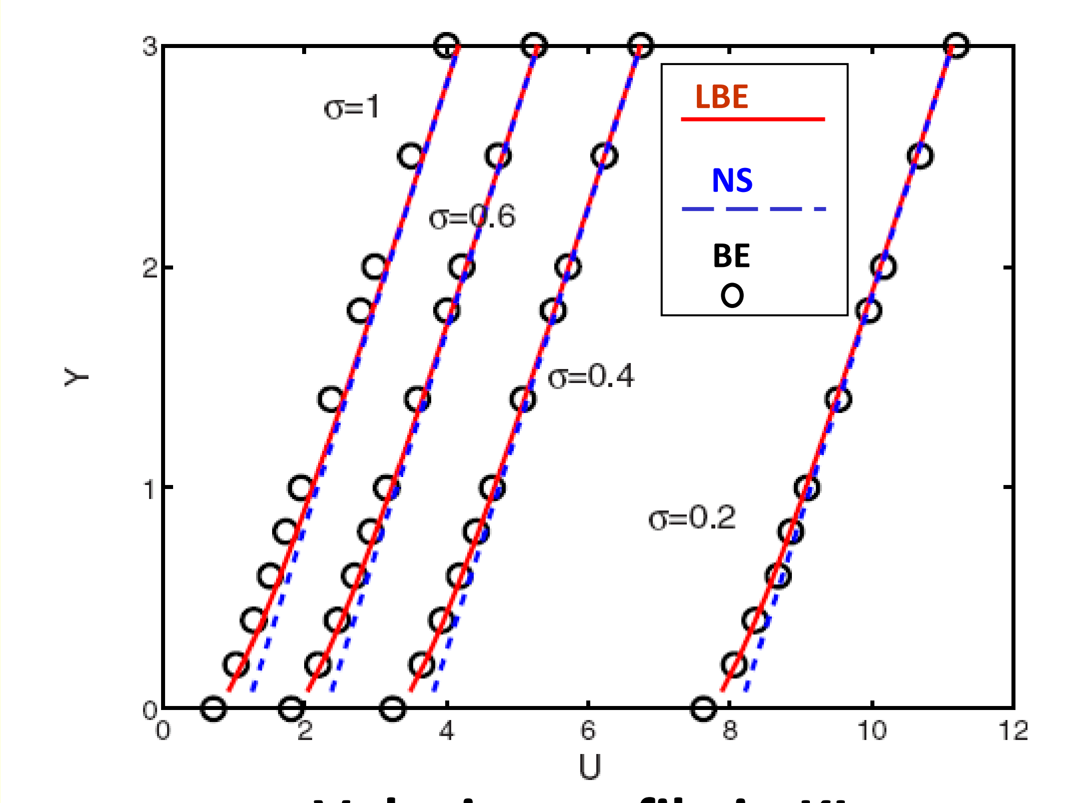
$$\phi(y) = \frac{1}{2}\left[\xi\left(\frac{y}{\lambda_\infty}\right) + \xi\left(\frac{H-y}{\lambda_\infty}\right)\right]$$



$$\xi(\alpha) = 1 + (\alpha - 1)e^{-\alpha} - \alpha^2 E_i(\alpha) \qquad E_i(\alpha) = \int_1^\infty t^{-1} e^{-\alpha t} dt$$

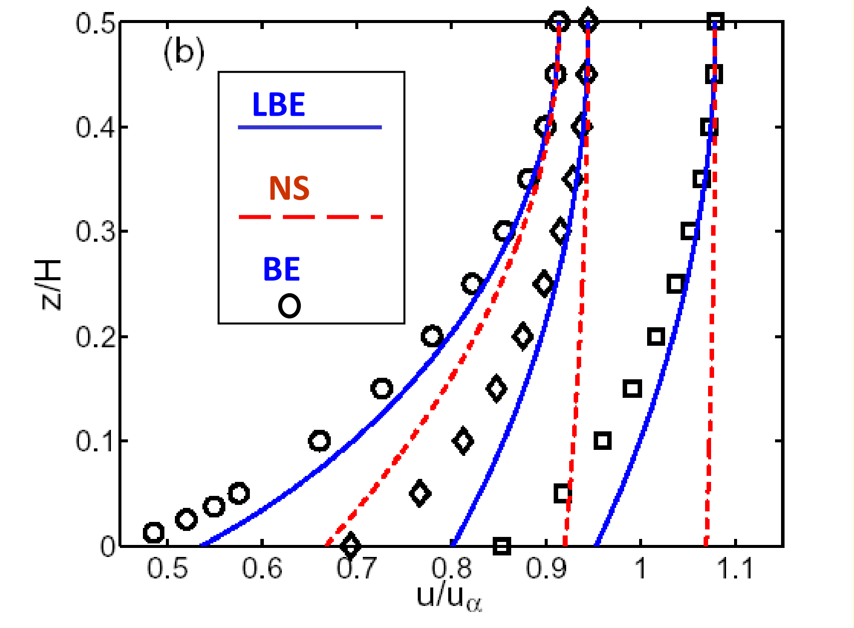
Test case: Kramers problem



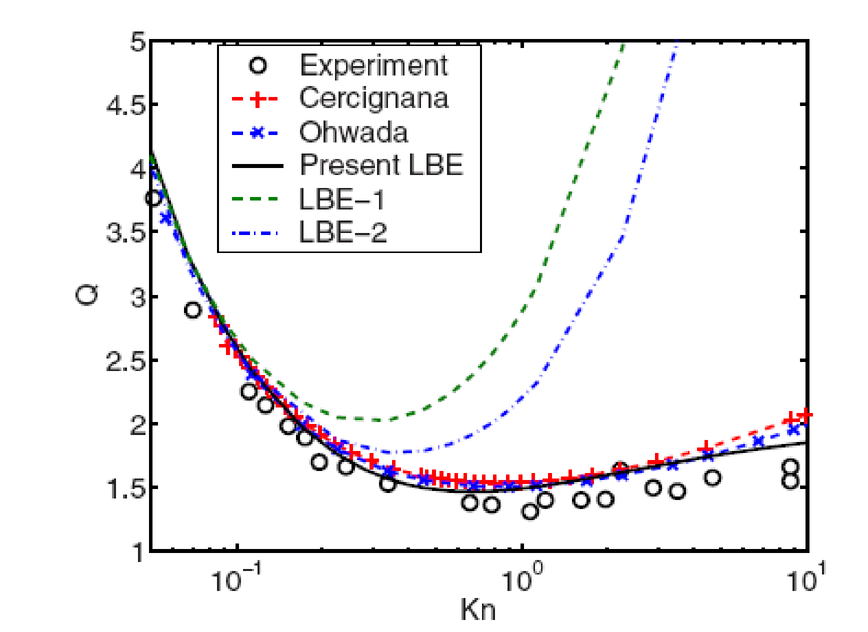


Velocity profile in KL

Test case: Poiseuille flow



Velocity profile



Mass flux

Kn = 0.4512, 4.512, 11.28

Outline

- Basic Concepts
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- Summary

3. Applications & Extensions

3.1 Flows in a rough channel

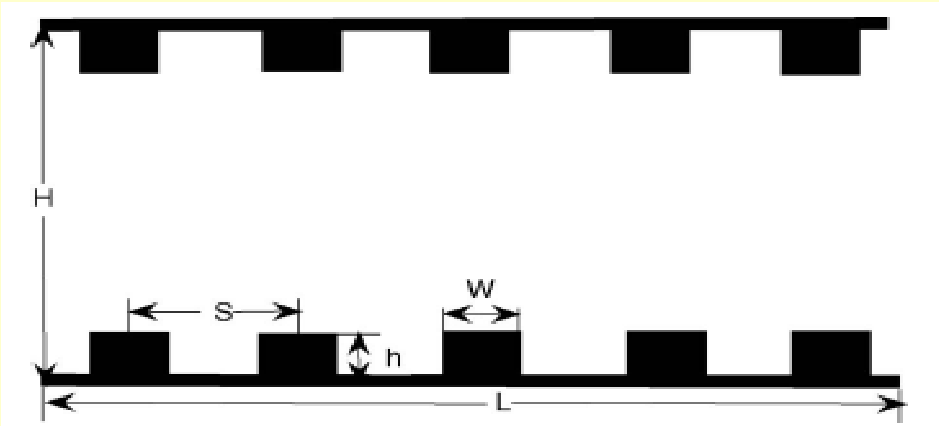
Roughness modeling: array of blocks distributed uniformly and symmetrically

Relative roughness

$e = 2h/H$

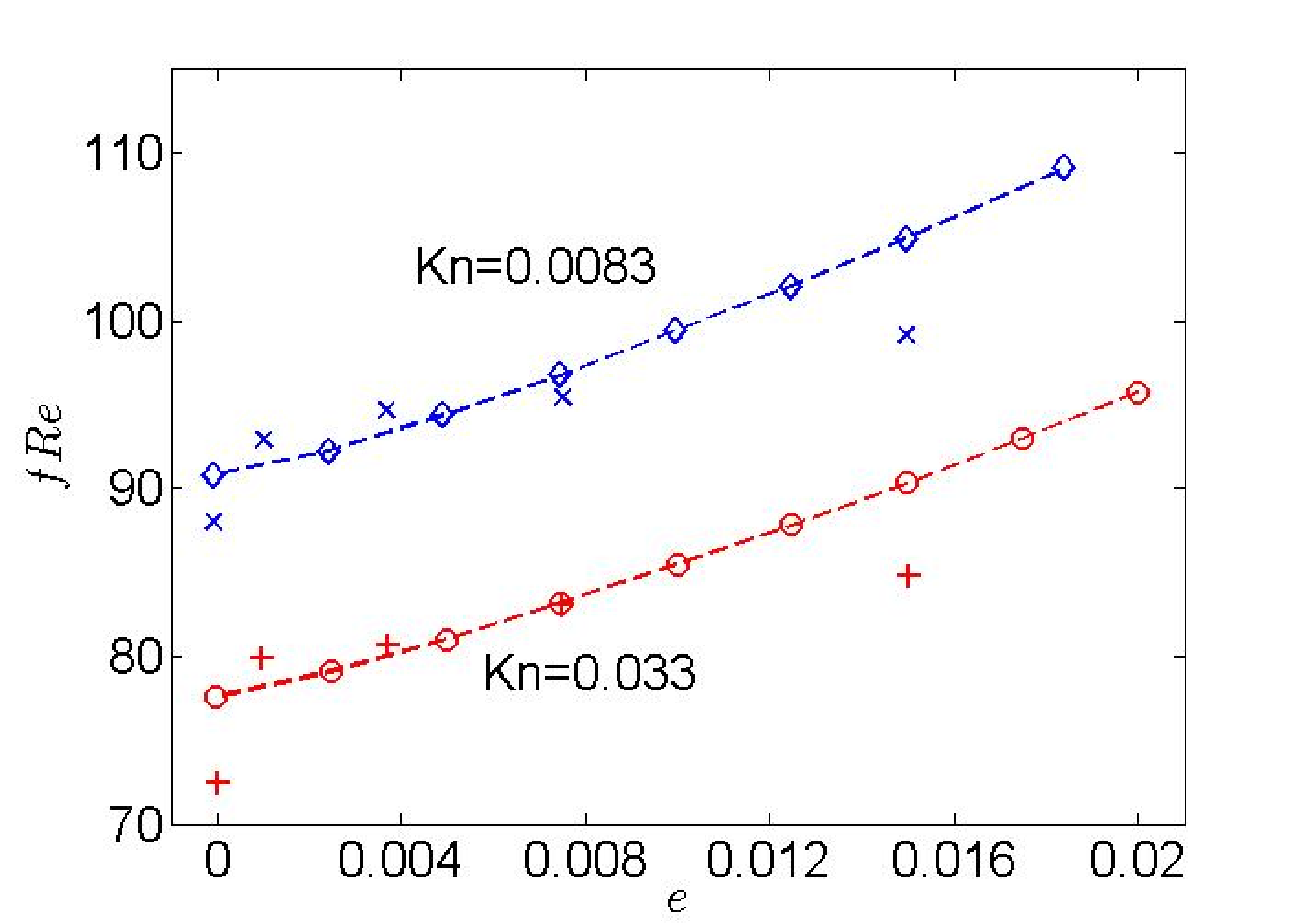
Roughness distribution

$\varepsilon = h/S$

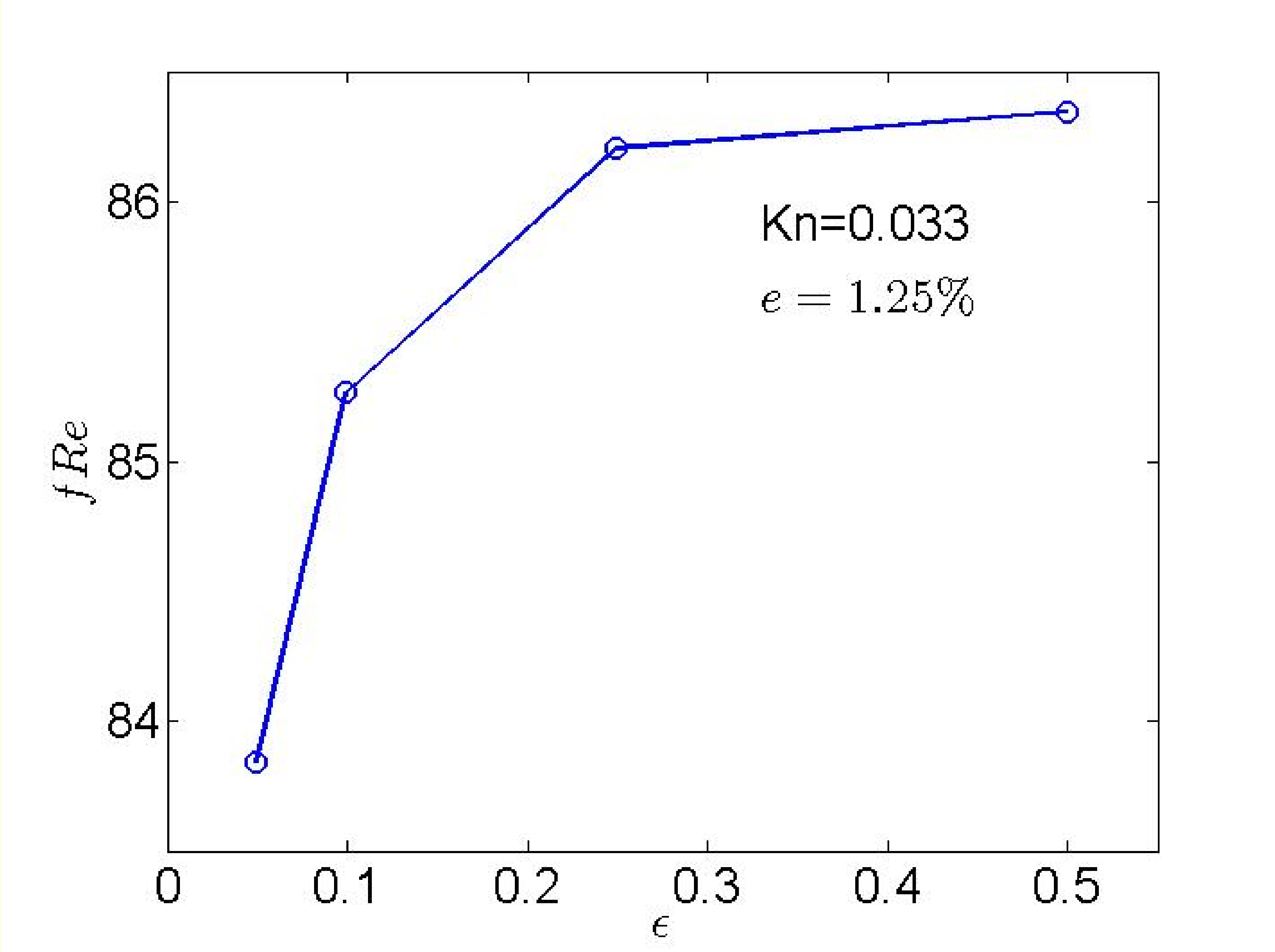


Drag coefficient vs relative roughness

$$f \ \mathrm{Re} = -\frac{8H^2}{\mu \bar{u}} \frac{\partial P}{\partial x}$$



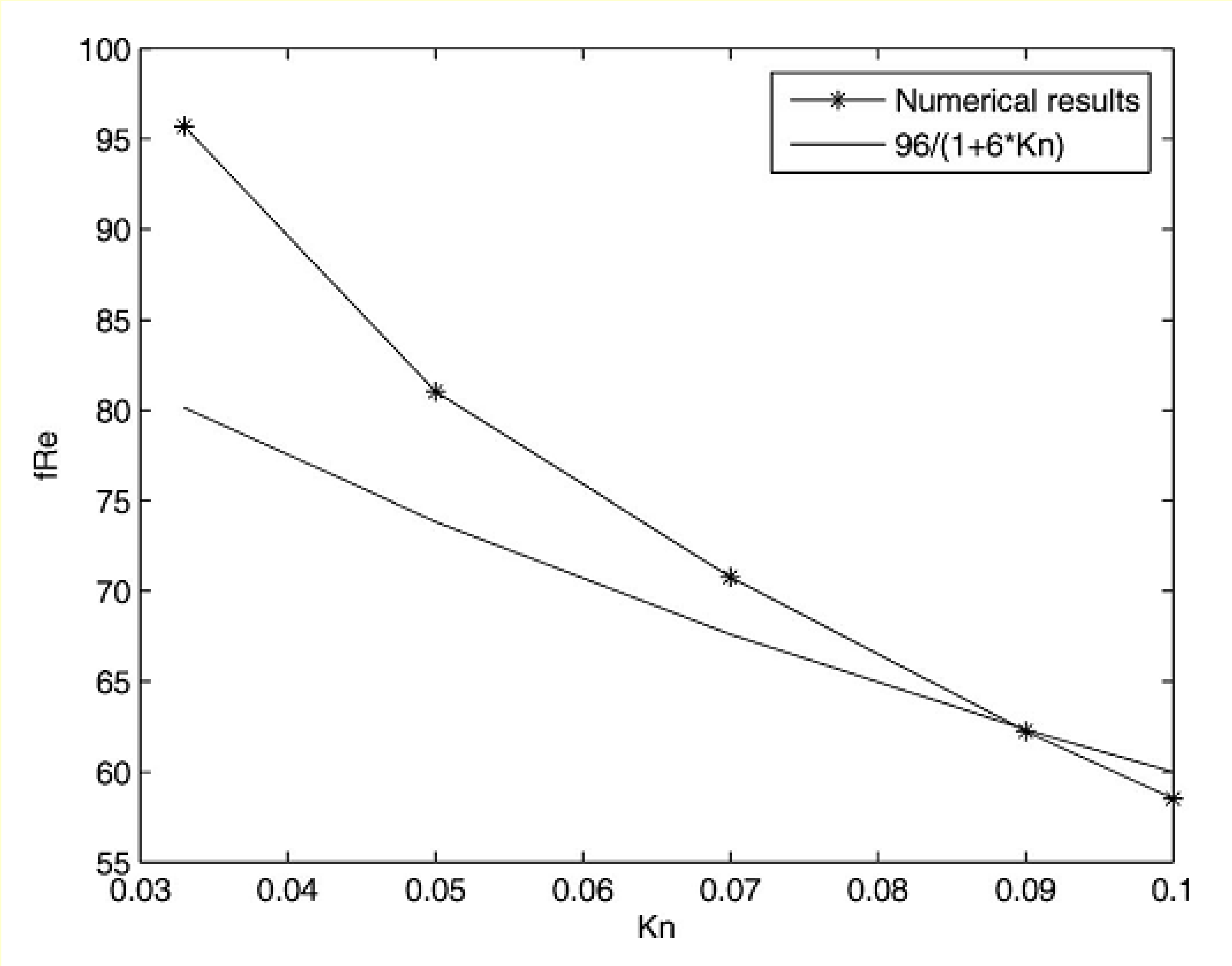
Drag coefficient vs roughness distribution



Drag coefficient vs Kn

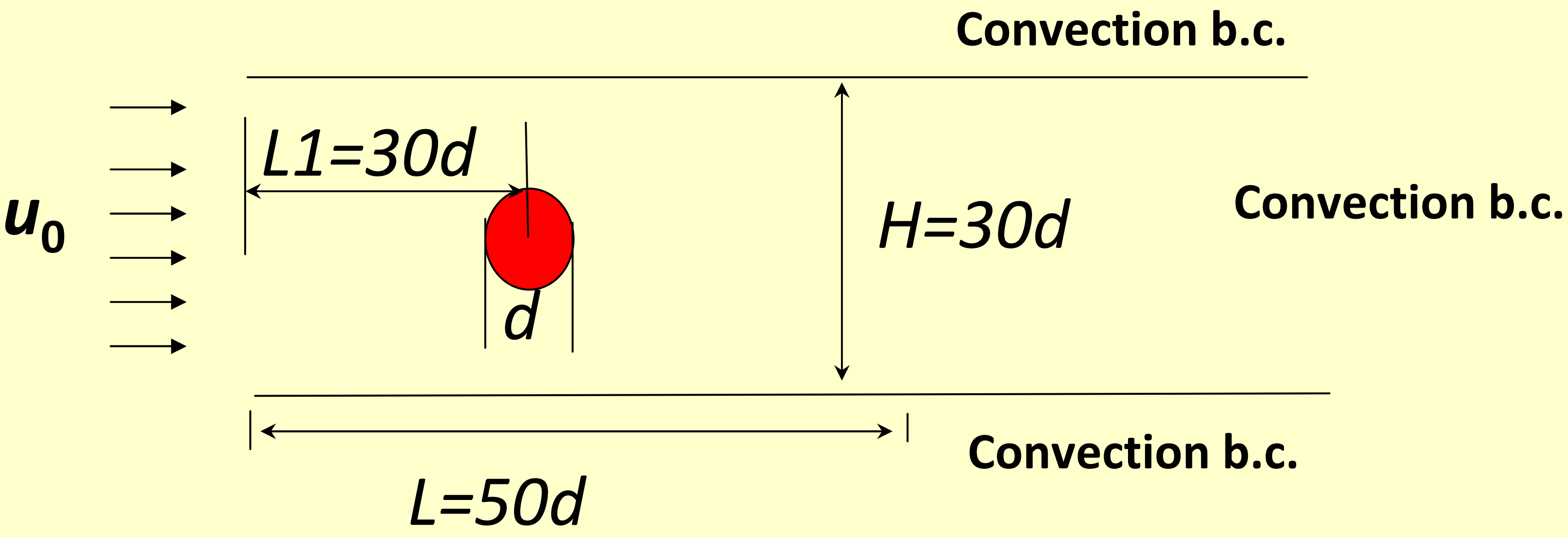
e =2%

ε *=0.08*



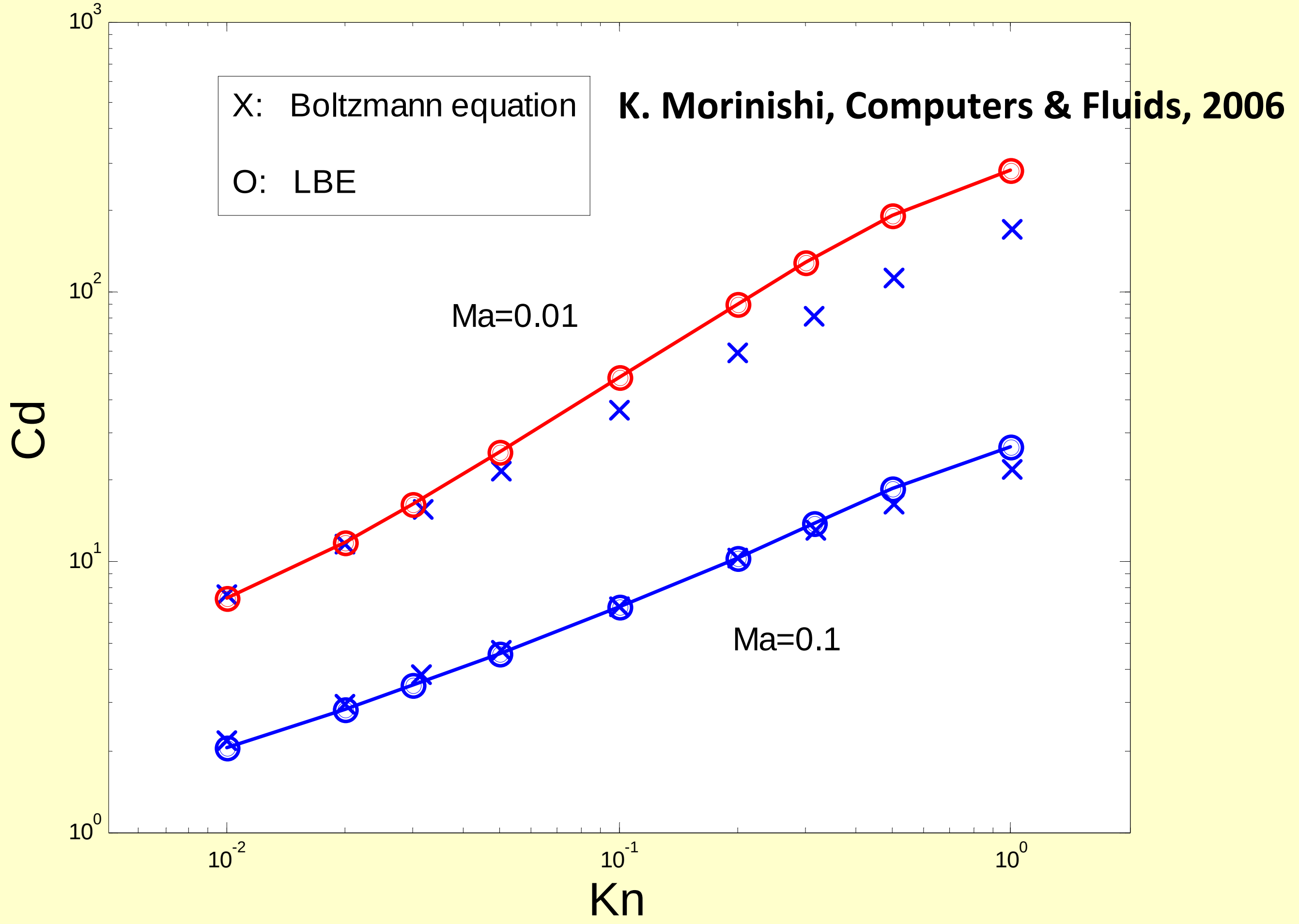
3.2 Flows with curved walls

Flow around a micro-cylinder

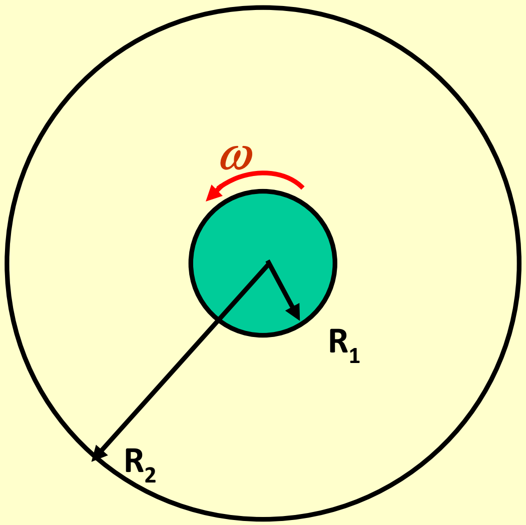


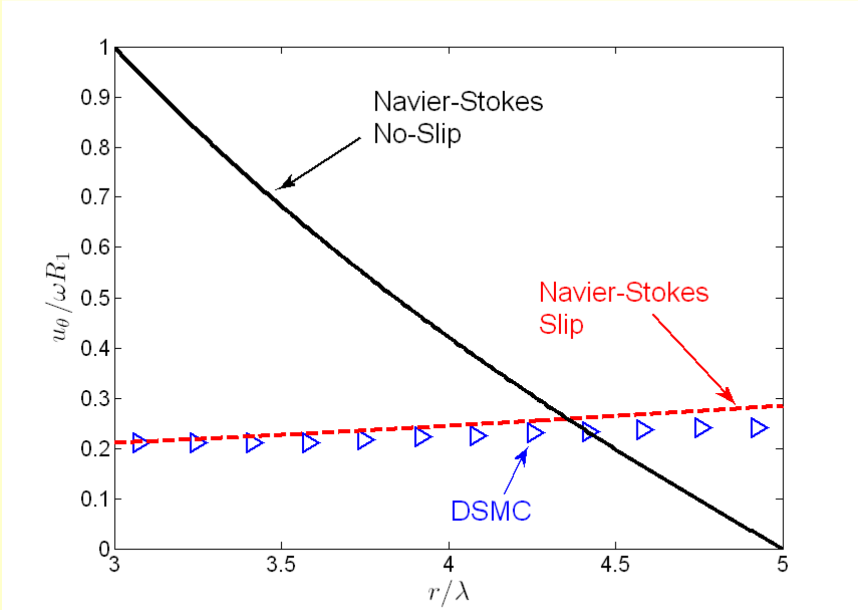
Computational mesh: 300 x 500

Drag coefficients vs Kn



- **Velocity inversion**





- Previous work
  - Navier-Stokes (NS) equation with slip boundary conditions (BC)
    - Slip BC with curvature effect (**Einzel et al. PRL1990, Int. J. Mod. Phys B 1992**)
    - Generalized Maxwell's slip BC (**Lockerby et al, PRE 2004**)
    - Langmuir BC (**Myong et al. POF 2005**)
  - Direct Simulation Monte Carlo (DSMC)

    (Tibbs et al. PRE 1997; Aoki et al. PRE 2003)
  - Molecular Dynamics (MD)

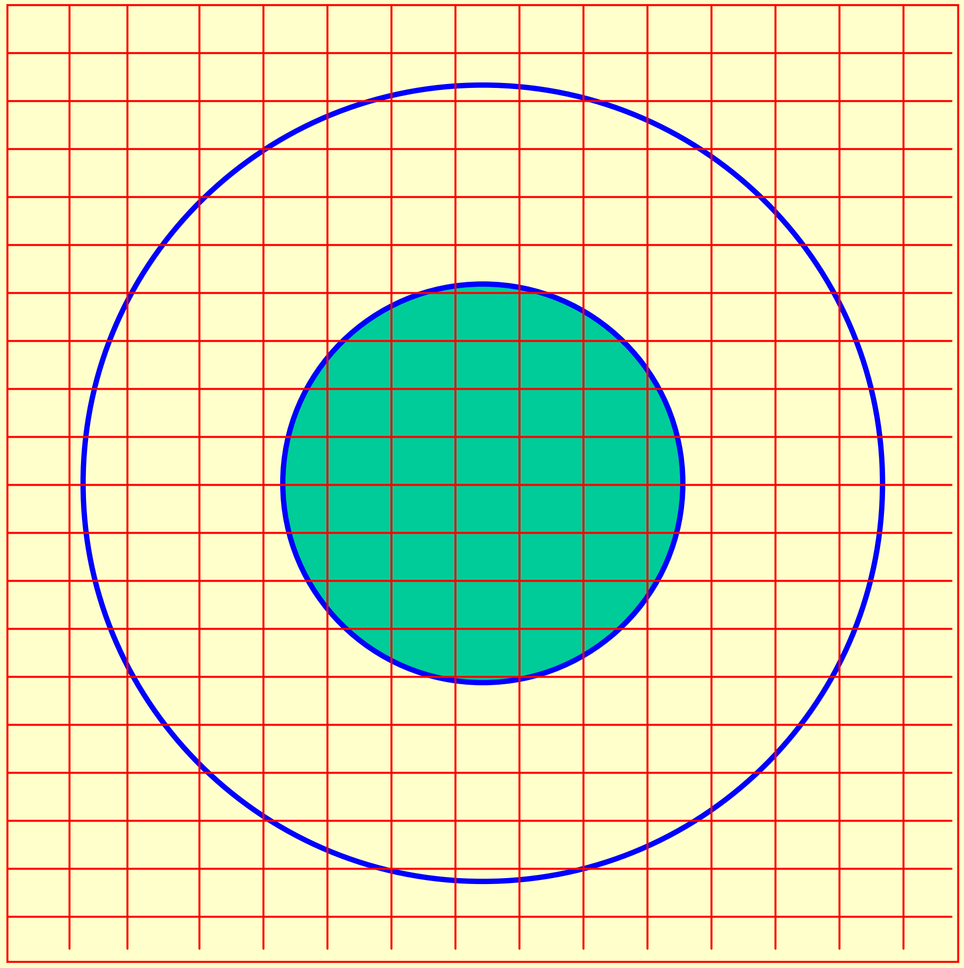
    (**Jung. PRE 2007; Kim PRE 2009**)
  - Boltzmann equation with kinetic boundary condition

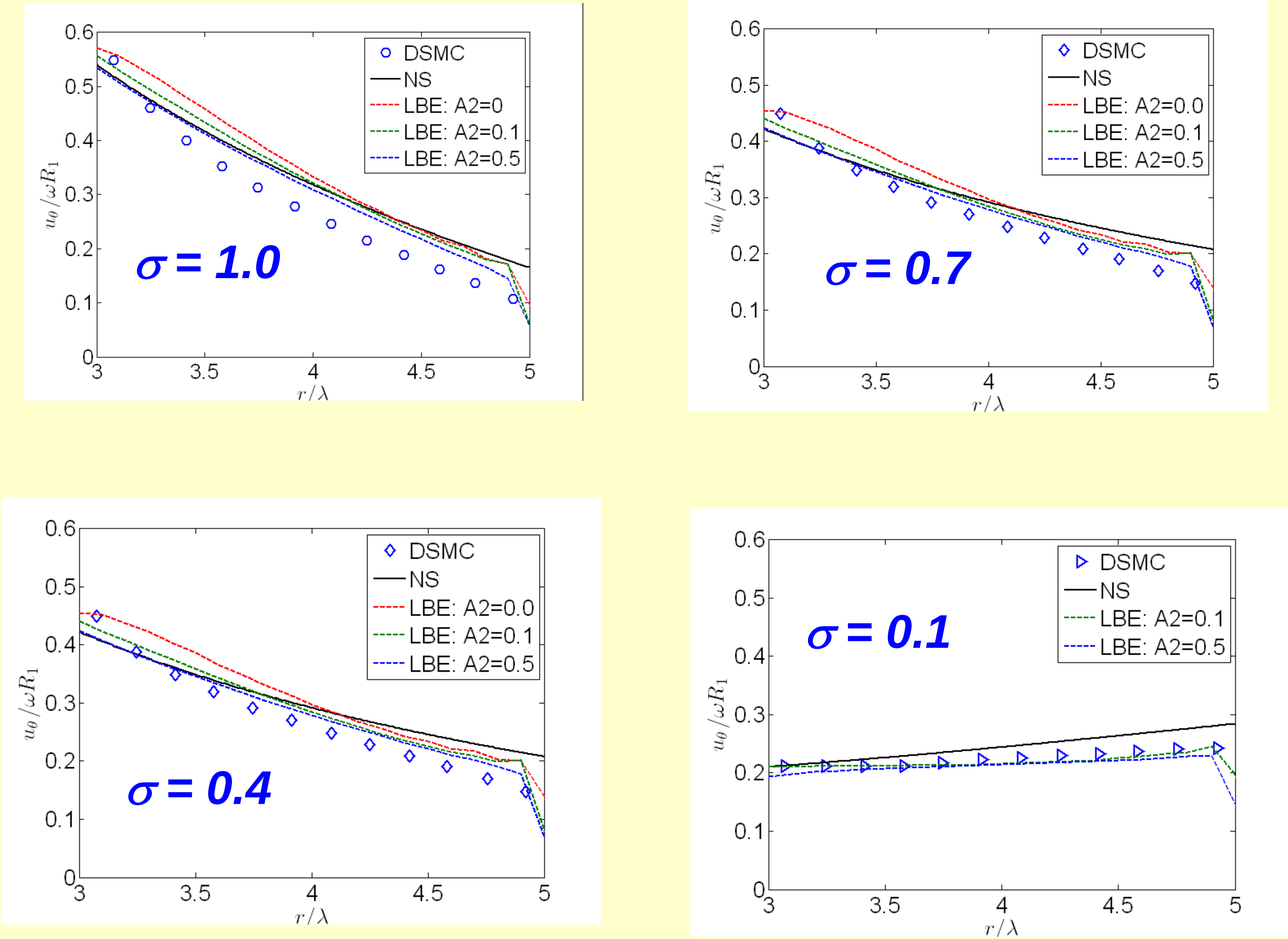
    (Tibbs et al. PRE 1997; Aoki et al. PRE 2003)

- **Computation setup**

$$R_1 = 3\lambda \qquad R_2 = 5\lambda$$

- **Domain: 11$\lambda \times$ 11λ**
  Mesh: 110 $\times$ 110




σ = 1.0
DSMC
NS
LBE: A2=0
LBE: A2=0.1
LBE: A2=0.5
σ = 0.7
LBE: A2=0.0
σ = 0.4
σ = 0.1
$u_\theta/\omega R_1$
r/λ

3.3 Klinkenberg effect in compact porous media

Klinkenberg effect:

The effective permeability of a porous media depends on the average pressure

$$K_g = K_\infty \left(1 + \frac{b_k}{\bar{p}}\right) \qquad b_k$$

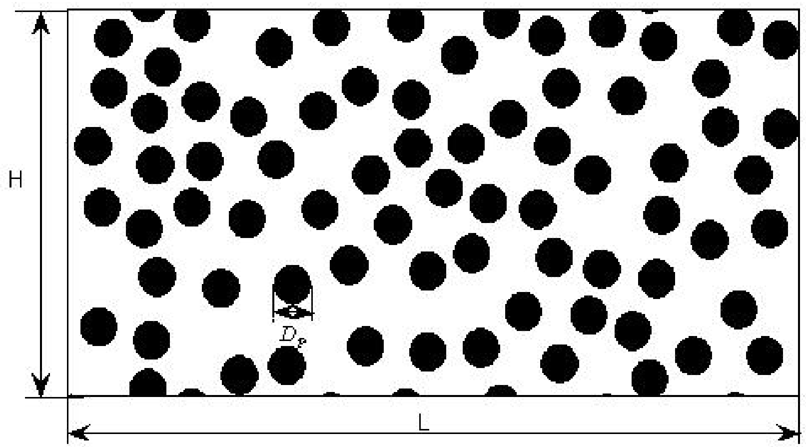
Knudsen number:

$$Kn = \frac{\lambda}{D_{pore}} \qquad D_{pore} = \frac{2\varepsilon}{3(1-\varepsilon)} D_p$$

effective pore size

Periodic B.C.

P_{in}



P_{out}

Periodic B.C.

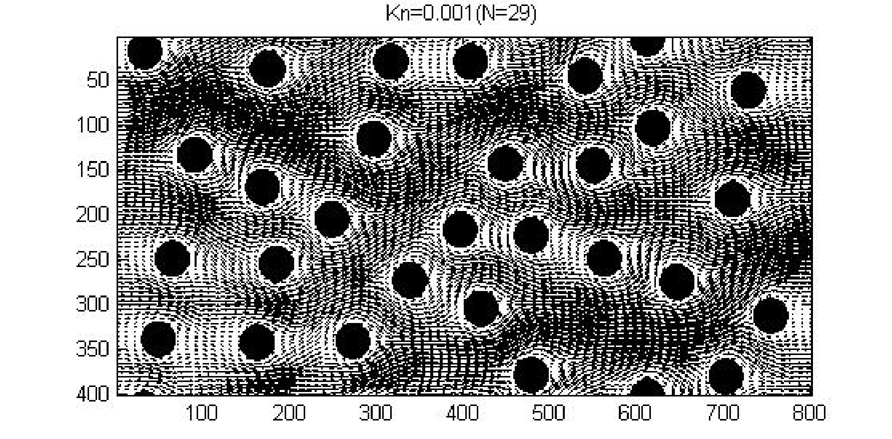
LBE: MRT-D2Q9

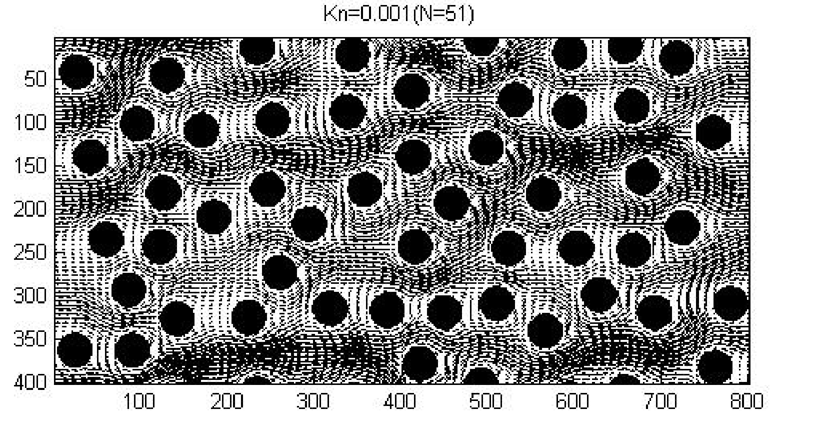
$$\tau_s - \frac{1}{2} = \sqrt{\frac{6}{\pi}} \frac{Kn}{\Delta}$$

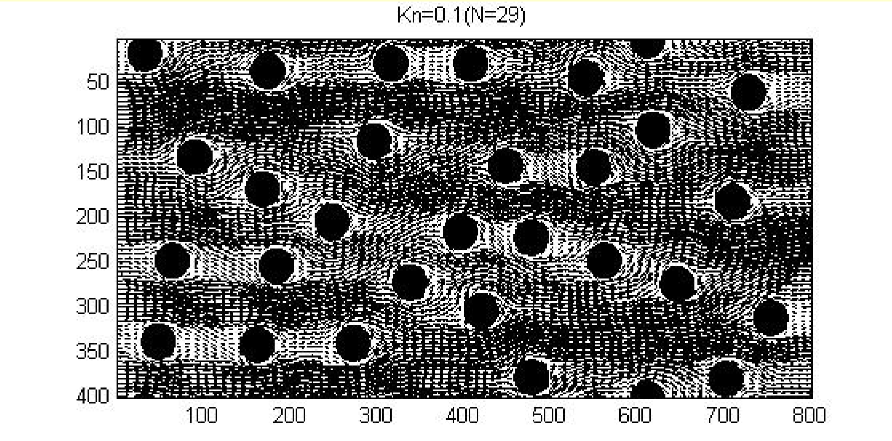
Boundary condition: Maxwell + Bounce-Back

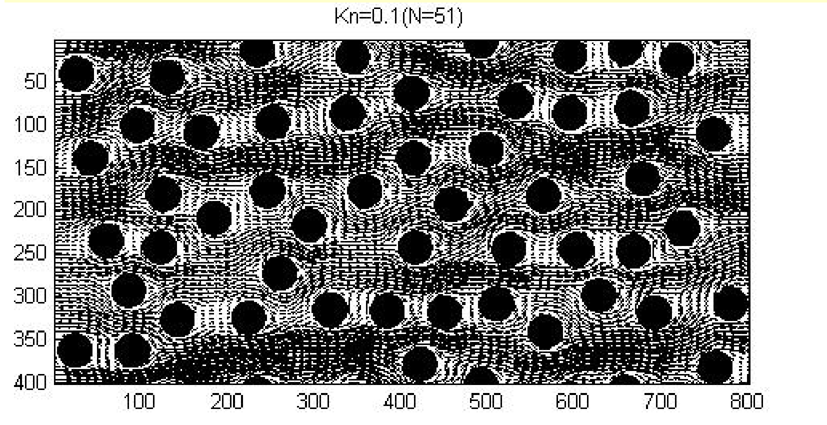
$$f_i = r f_i^{(eq)}(\boldsymbol{u}_w) + (1-r) f_{-i}^*$$

$$r = \frac{2A_1}{A_1 + \sqrt{6/\pi}}, \quad \tau_q = 0.5 + \frac{(\tau_s - 0.5)^2 + 3}{16(\tau_s - 0.5)}$$

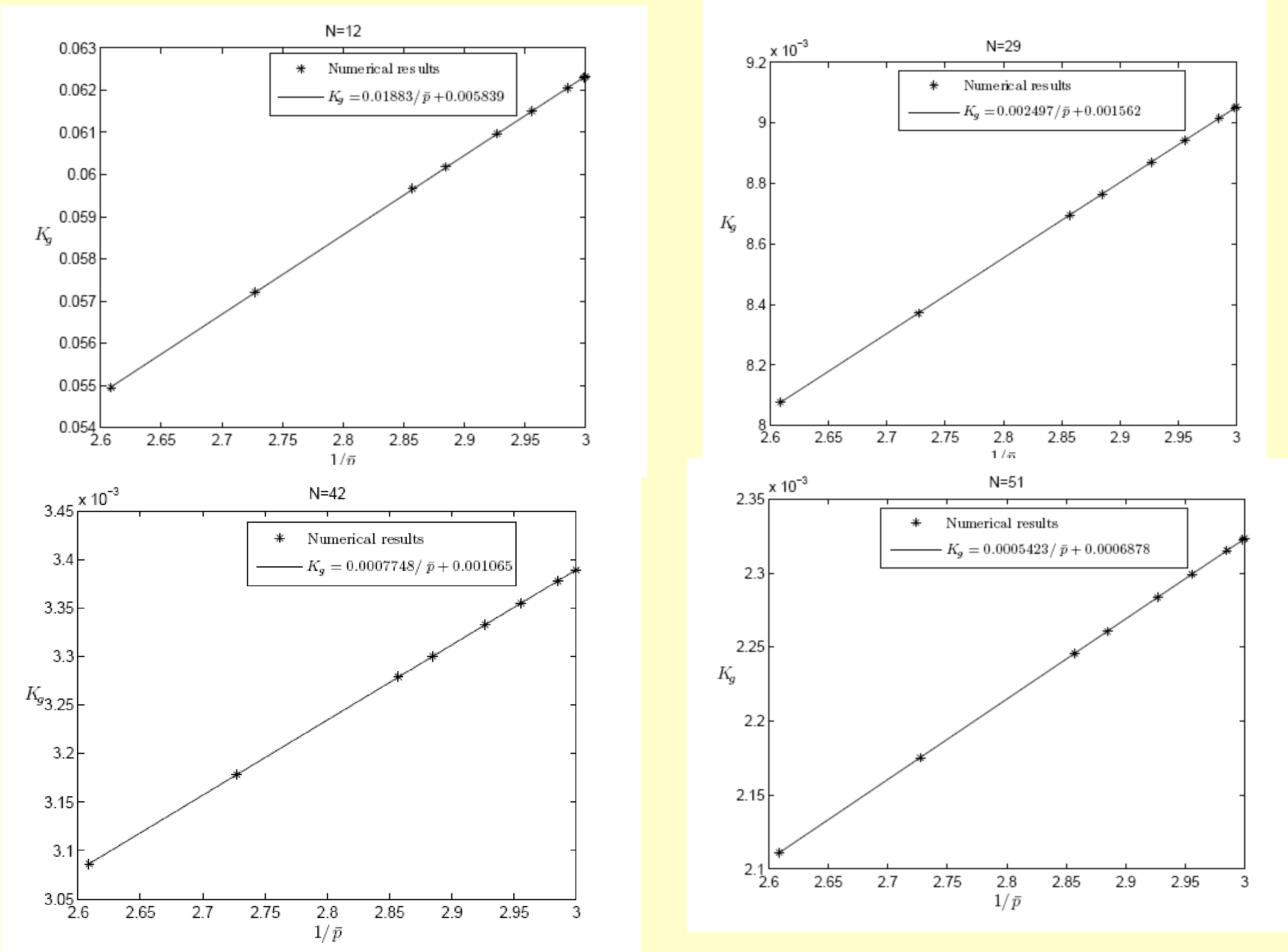

Kn=0.001(N=29)
50 100 150 200 250 300 350 400
100 200 300 400 500 600 700 800


Kn=0.001(N=51)
50 100 150 200 250 300 350 400
100 200 300 400 500 600 700 800


Kn=0.1(N=29)
50 100 150 200 250 300 350 400
100 200 300 400 500 600 700 800


Kn=0.1(N=51)
50 100 150 200 250 300 350 400
100 200 300 400 500 600 700 800

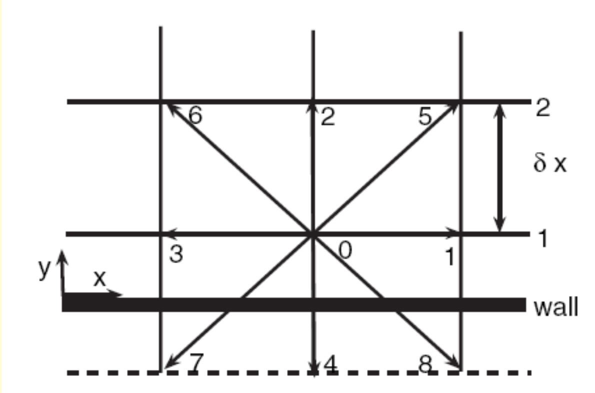
Kn=0.1


N=12
Numerical results
$K_g = 0.01883/\bar{p} + 0.005839$
K_g
$1/\bar{p}$
N=29
x 10^{-3}
Numerical results
$K_g = 0.002497/\bar{p} + 0.001562$
K_g
N=42
x 10^{-3}
Numerical results
$K_g = 0.0007748/\bar{p} + 0.001065$
K_g
$1/\bar{p}$
N=51
x 10^{-3}
Numerical results
$K_g = 0.0005423/\bar{p} + 0.0006878$
K_g
$1/\bar{p}$

3.4 LBE for micro flow with heat transfer

$$f_i(\mathbf{x}+\mathbf{c}_i\delta t, t+\delta t) - f_i(\mathbf{x}, t) = -\frac{(f_i - f_i^{(eq)})}{\tau_f}$$

$$g_i(\mathbf{x}+\mathbf{c}_i\delta t, t+\delta t) - g_i(\mathbf{x}, t) = -\frac{(g_i - g_i^{(eq)})}{\tau_g},$$



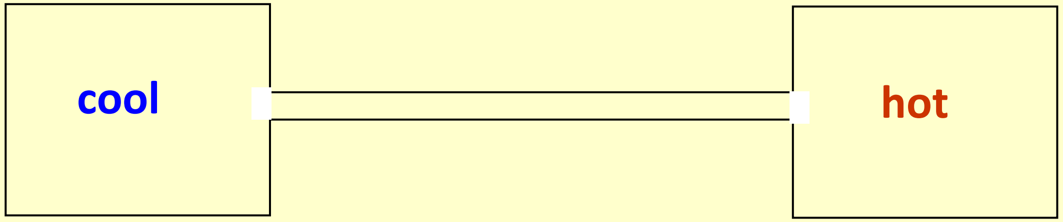
Maxwell + Specular-Reflection

$$f_2 = \sigma f_2^{(eq)}(\mathbf{u}_w) + (1-\sigma) f_4^+,$$
$$f_5 = \sigma f_5^{(eq)}(\mathbf{u}_w) + (1-\sigma) f_8^+,$$
$$f_6 = \sigma f_6^{(eq)}(\mathbf{u}_w) + (1-\sigma) f_7^+,$$
$$g_2 = \sigma' g_2^{(eq)}(\mathbf{u}_w, T_w) + (1-\sigma') g_4^+,$$
$$g_5 = \sigma' g_5^{(eq)}(\mathbf{u}_w, T_w) + (1-\sigma') g_8^+,$$
$$g_6 = \sigma' g_6^{(eq)}(\mathbf{u}_w, T_w) + (1-\sigma') g_7^+,$$

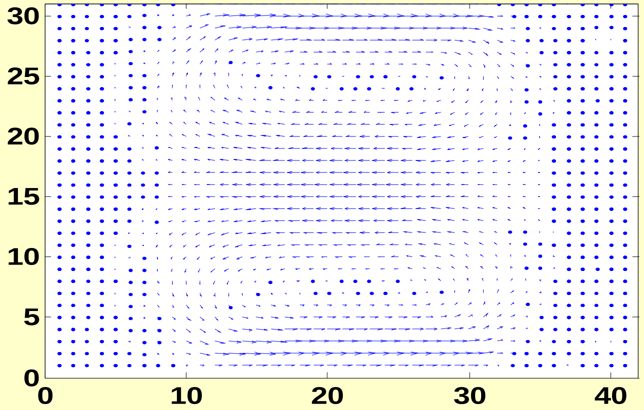
Maxwell + Bounce-Back

$$f_2 = \sigma f_2^{(eq)}(\mathbf{u}_w) + (1-\sigma)(f_4^+ + 2\rho\omega_2 \mathbf{c}_2 \cdot \mathbf{u}_w / RT_0),$$
$$f_5 = \sigma f_5^{(eq)}(\mathbf{u}_w) + (1-\sigma)(f_7^+ + 2\rho\omega_5 \mathbf{c}_5 \cdot \mathbf{u}_w / RT_0),$$
$$f_6 = \sigma f_6^{(eq)}(\mathbf{u}_w) + (1-\sigma)(f_8^+ + 2\rho\omega_6 \mathbf{c}_6 \cdot \mathbf{u}_w / RT_0),$$
$$g_2 = \sigma' g_2^{(eq)}(\mathbf{u}_w, T_w) + (1-\sigma') g_4^+,$$
$$g_5 = \sigma' g_5^{(eq)}(\mathbf{u}_w, T_w) + (1-\sigma') g_7^+,$$
$$g_6 = \sigma' g_6^{(eq)}(\mathbf{u}_w, T_w) + (1-\sigma') g_8^+,$$

Thermal creep



Kn=0.01



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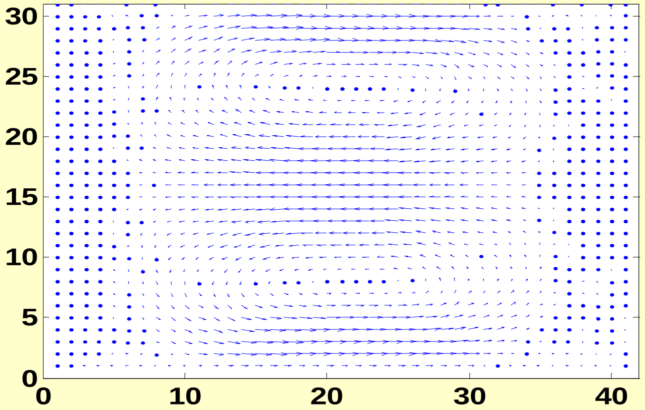
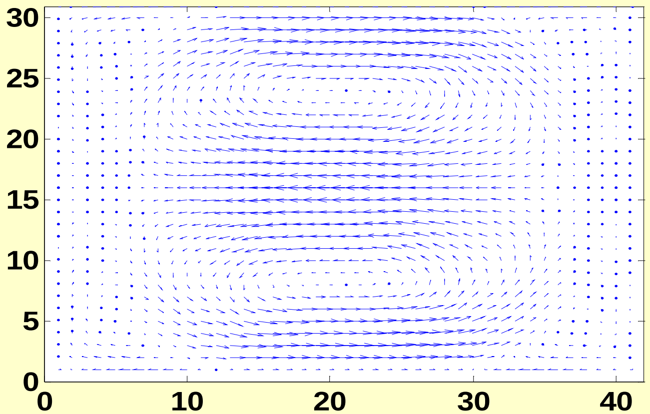
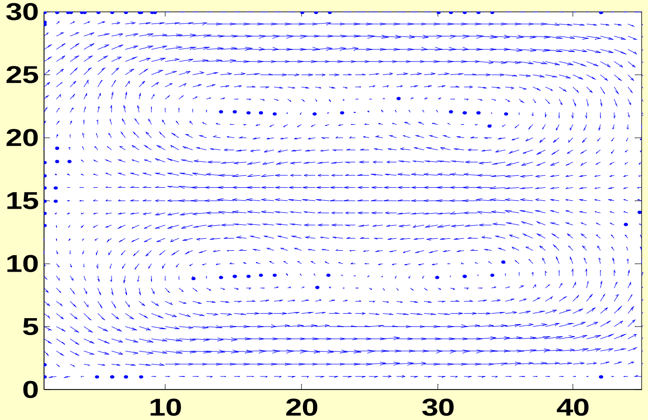


Kn=0.1



Kn=0.3



3.5 LBE for micro flow of binary mixture

Evolution equation

$$\boxed{f_{\sigma i}(\boldsymbol{x}+\boldsymbol{c}_i\delta_t, t+\delta_t) - f_{\sigma i}(\boldsymbol{x},t) = \Omega_{\sigma i}(f) = -\sum_j (M^{-1}SM)_{ij}\left[f_{\sigma j} - f_{\sigma j}^{(eq)}\right]}$$

$$f_{\sigma i}^{(eq)} = \omega_i \rho_\sigma \left[\alpha_\sigma + \frac{\boldsymbol{c}_i\cdot\boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u}\cdot\boldsymbol{u}}{2c_s^2}\right] \qquad S = diag\left[0,\ \tau_e,\ \tau_\varepsilon,\ \tau_d,\ \tau_q,\ \tau_d,\ \tau_q,\ \tau_s,\ \tau_s\right]$$

$$\rho_\sigma = \sum_i f_{\sigma i}, \quad \rho = \rho_\sigma + \rho_\varsigma, \quad \rho\boldsymbol{u} = \sum_\sigma\sum_i \boldsymbol{c}_i f_{\sigma i}, \quad \rho_\sigma \boldsymbol{u}_\sigma = \frac{\tau_d - 0.5}{\tau_d}\sum_i \boldsymbol{c}_i f_{\sigma i} + \frac{\rho_\sigma \boldsymbol{u}}{2\tau_d},$$

Transport coefficients

$$\nu = c_s^2\left(\tau_s - \frac{1}{2}\right)\delta_t, \qquad \zeta_\sigma = c_s^2(2-s_\sigma)\left(\tau_s - \frac{1}{2}\right)\delta_t, \qquad D_{\sigma\varsigma} = \frac{m_r \rho}{m_\sigma m_\varsigma n} c_s^2\left(\tau_d - \frac{1}{2}\right)\delta_t,$$

$$m_r = \min\left(m_\sigma,\ m_\varsigma\right), \qquad s_\sigma = m_r / m_\sigma$$

Boundary condition: Bounce-back + Specular-reflection

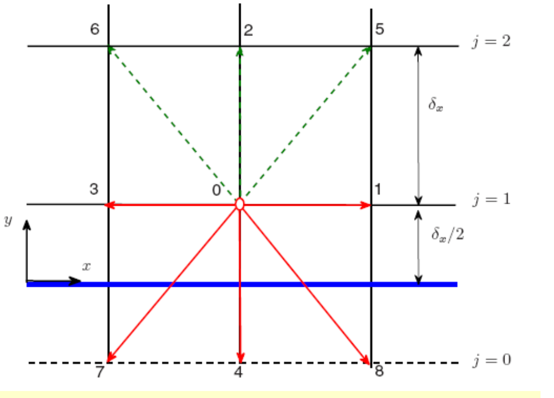
$$f_{\sigma 2}^1 = \tilde{f}_{\sigma 4}^1 + 2r_\sigma \rho_\sigma \boldsymbol{c}_2 \cdot \boldsymbol{u}_w / c_s^2,$$

$$f_{\sigma 5}^1 = r_\sigma \tilde{f}_{\sigma 7}^1 + (1-r_\sigma)\tilde{f}_{\sigma 8}^1 + 2r_\sigma \rho_\sigma \boldsymbol{c}_5 \cdot \boldsymbol{u}_w / c_s^2,$$

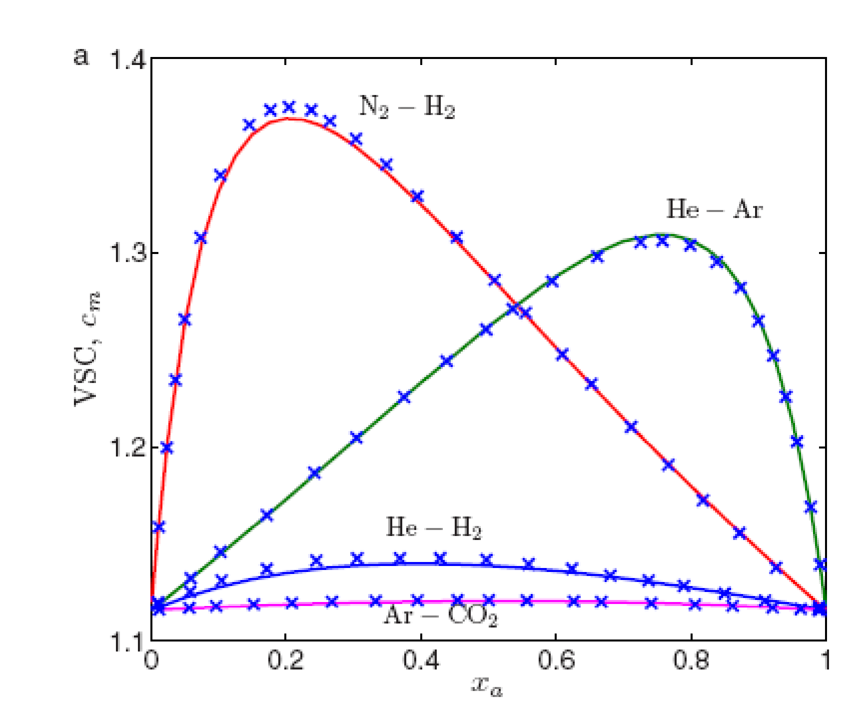
$$f_{\sigma 6}^1 = r_\sigma \tilde{f}_{\sigma 8}^1 + (1-r_\sigma)\tilde{f}_{\sigma 7}^1 + 2r_\sigma \rho_\sigma \boldsymbol{c}_6 \cdot \boldsymbol{u}_w / c_s^2,$$

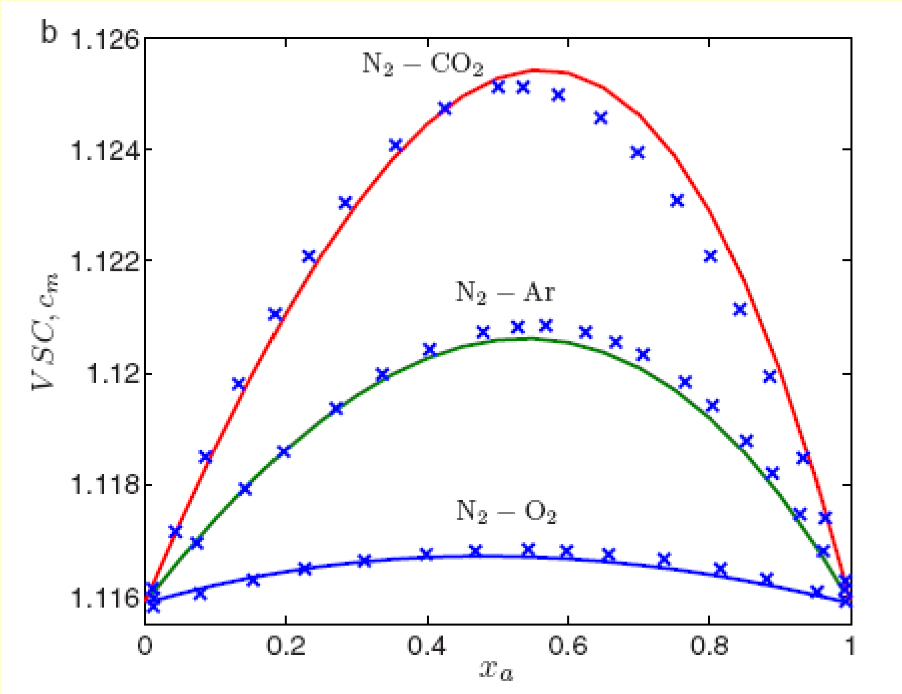
$$r_\sigma = r = \left[1 + c_m\sqrt{\frac{\pi}{6}\frac{m_x}{m_r}}\right]^{-1}$$

$$m_x = \rho / n$$



Velocity slip coefficient of binary gases: Fully diffusive wall





×: Linearized Boltzmann equation (I. N. Ivchenko et al. J. Vac. Sci. Technol. A 1997.)

——: LBE

4. Summary

- **LBE provides a potential way for modeling and simulating micro flows;**
- **Care must be taken when applying LBE to microflows, particularly**
  - **The relaxation time(s) must be properly defined**
  - **Discrete effects in boundary conditions must be considered**
- **Capturing the flows in Knudsen layer efficiently with LBE is still an open problem.**

Acknowledgements

Prof. P. Asinari

Prof. B.C. Shi

Prof. K. Xu

Prof. T.S. Zhao

Prof. C.G. Zheng

Dr. Z.H. Chai

Mr. J.H. Lu

Mr. H.L. Wang

Mr. L. Wang

Mr. L. Zheng

Thank you for your attention!

- Appendix: Analysis of the velocity profile of the LBE for the Poiseuille flow

LBE

$$\boldsymbol{f}(\boldsymbol{x}+\boldsymbol{c}_i\delta_t, t+\delta_t) = \boldsymbol{f}^+(\boldsymbol{x},t) = \boldsymbol{M}^{-1}\left[\hat{\boldsymbol{f}} - \boldsymbol{S}(\hat{\boldsymbol{f}} - \hat{\boldsymbol{f}}^{(eq)}) + \delta_t\left(\boldsymbol{I} - \frac{\boldsymbol{S}}{2}\right)\hat{\boldsymbol{F}}\right] = \boldsymbol{M}^{-1}\hat{\boldsymbol{f}}^+(\boldsymbol{x},t)$$

$$\rho = \sum_i f_i \qquad \rho\boldsymbol{u} = \sum_i \boldsymbol{c}_i f_i + \frac{\delta_t}{2}\boldsymbol{F}$$

$$\hat{\boldsymbol{f}} = \boldsymbol{M}\boldsymbol{f} = \begin{bmatrix} \rho \\ e \\ \varepsilon \\ j_x \\ q_x \\ j_y \\ q_y \\ p_{xx} \\ p_{xy} \end{bmatrix} = \begin{bmatrix} \rho \\ e \\ \varepsilon \\ \rho u - \delta_t \rho a / 2 \\ q_x \\ 0 \\ q_y \\ p_{xx} \\ p_{xy} \end{bmatrix} \qquad \hat{\boldsymbol{f}}^{(eq)} = \boldsymbol{M}\boldsymbol{f}^{(eq)} = \begin{bmatrix} \rho \\ -2\rho + 3\rho u^2 \\ \rho - 3\rho u^2 \\ \rho u \\ -\rho u \\ 0 \\ 0 \\ \rho u^2 \\ 0 \end{bmatrix} \qquad \hat{\boldsymbol{F}} = \begin{bmatrix} 0 \\ 6\rho a u \\ -6\rho a u \\ \rho a \\ -\rho a \\ 0 \\ 0 \\ 2\rho a u \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} f_{13}^{+} \\ f_{56}^{+} \\ f_{87}^{+} \end{bmatrix} = \begin{bmatrix} f_1^{+} - f_3^{+} \\ f_5^{+} - f_6^{+} \\ f_8^{+} - f_7^{+} \end{bmatrix} = \begin{bmatrix} -q_x/3 + \rho u/3 + \rho a\delta_t/2 + s_q(q_x/3 + \rho u/3 - \rho a\delta_t/6) \\ q_x/6 + \rho u/3 + s_q(-q_x/6 - \rho u/6 + \rho a\delta_t/12) + (1 - s_\nu/2)p_{xy} \\ q_x/6 + \rho u/3 + s_q(-q_x/6 - \rho u/6 + \rho a\delta_t/12) - (1 - s_\nu/2)p_{xy} \end{bmatrix}$$

$$\begin{bmatrix} f_{13} \\ f_{56} \\ f_{87} \end{bmatrix} = \begin{bmatrix} f_1 - f_3 \\ f_5 - f_6 \\ f_8 - f_7 \end{bmatrix} = \begin{bmatrix} -q_x/3 + \rho u/3 - \rho a\delta_t/6 \\ q_x/6 + \rho u/3 - \rho a\delta_t/6 + p_{xy}/2 \\ q_x/6 + \rho u/3 - \rho a\delta_t/6 - p_{xy}/2 \end{bmatrix}$$

$$f_{13}^{+} = f_{13} \Rightarrow q_x = -\rho u + \frac{1}{2}\left(1 - 4\tau_q\right)\rho a\delta_t$$

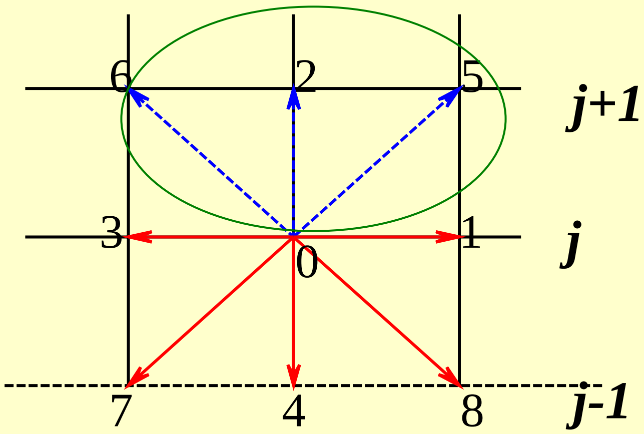
$$f_{56}^{+}(j) = f_{56}(j+1)$$

$$\begin{bmatrix} f_{56}^{+} \\ f_{87}^{+} \\ f_{56} \\ f_{87} \end{bmatrix} = \begin{bmatrix} \frac{1}{6}\rho u + \frac{1}{2}(1-\tau_\nu)p_{xy} + (\frac{1}{12} - \frac{1}{3}\tau_q)\rho a\delta_t \\ \frac{1}{6}\rho u - \frac{1}{2}(1-\tau_\nu)p_{xy} + (\frac{1}{12} - \frac{1}{3}\tau_q)\rho a\delta_t \\ \frac{1}{6}\rho u + \frac{1}{2}p_{xy} - (\frac{1}{12} + \frac{1}{3}\tau_q)\rho a\delta_t \\ \frac{1}{6}\rho u - \frac{1}{2}p_{xy} - (\frac{1}{12} + \frac{1}{3}\tau_q)\rho a\delta_t \end{bmatrix}$$

$$f_{87}(j) = f_{87}^{+}(j+1)$$

$$f_{87}^{+}(j) = f_{87}(j-1)$$

$$f_{56}(j) = f_{56}^{+}(j-1)$$



$$f_{56}^{+}(j)=f_{56}(j+1)$$

$$\tfrac{1}{2}\left[(1-\tau_v)p_{xy}^{j}-p_{xy}^{j+1}\right]+\tfrac{1}{6}\rho a\delta_t$$

$$=\tfrac{1}{6}\rho(u_{j+1}-u_j)$$

$$f_{87}(j)=f_{87}^{+}(j+1)$$

$$\tfrac{1}{2}\left[-p_{xy}^{j}+(1-\tau_v)p_{xy}^{j+1}\right]-\tfrac{1}{6}\rho a\delta_t$$

$$=\tfrac{1}{6}\rho(u_{j+1}-u_j)$$

$$p_{xy}^{j}=-\frac{1}{3\tau_v}\rho(u_{j+1}-u_j)-\frac{1}{3(2-\tau_v)}\rho a\delta_t$$

$$p_{xy}^{j+1}=-\frac{1}{3\tau_v}\rho(u_{j+1}-u_j)+\frac{1}{3(2-\tau_v)}\rho a\delta_t$$

$$p_{xy}^{j}=-\frac{1}{3\tau_v}\rho(u_j-u_{j-1})+\frac{1}{3(2-\tau_v)}\rho a\delta_t$$

$$p_{xy}^{j} = -\tfrac{1}{3\tau_v}\rho(u_{j+1} - u_j) - \tfrac{1}{3(2-\tau_v)}\rho a \delta_t$$

$$p_{xy}^{j} = -\tfrac{1}{3\tau_v}\rho(u_j - u_{j-1}) + \tfrac{1}{3(2-\tau_v)}\rho a \delta_t$$

$$\nu \frac{u_j - 2u_j + u_{j-1}}{\delta_x^2} + a = 0 \qquad \nu = \frac{1}{3}\left(\tau_v - \frac{1}{2}\right)\delta_x$$

$$\left(\quad \nu \frac{\partial^2 u}{\partial y} + a = 0 \quad \right)$$

$$u_j = U_0 \frac{y_j}{H}\left(1 - \frac{y_j}{H}\right) + u_s \qquad U_0 = aH^2 / 2\nu$$