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Computational Heat Transfer and Fluid Flow, Qingdao

南方科技大学

GSIS: A Fast-converging & Asymptotic-preserving Solver for the Boltzmann Equation
--- application to shale gas extraction

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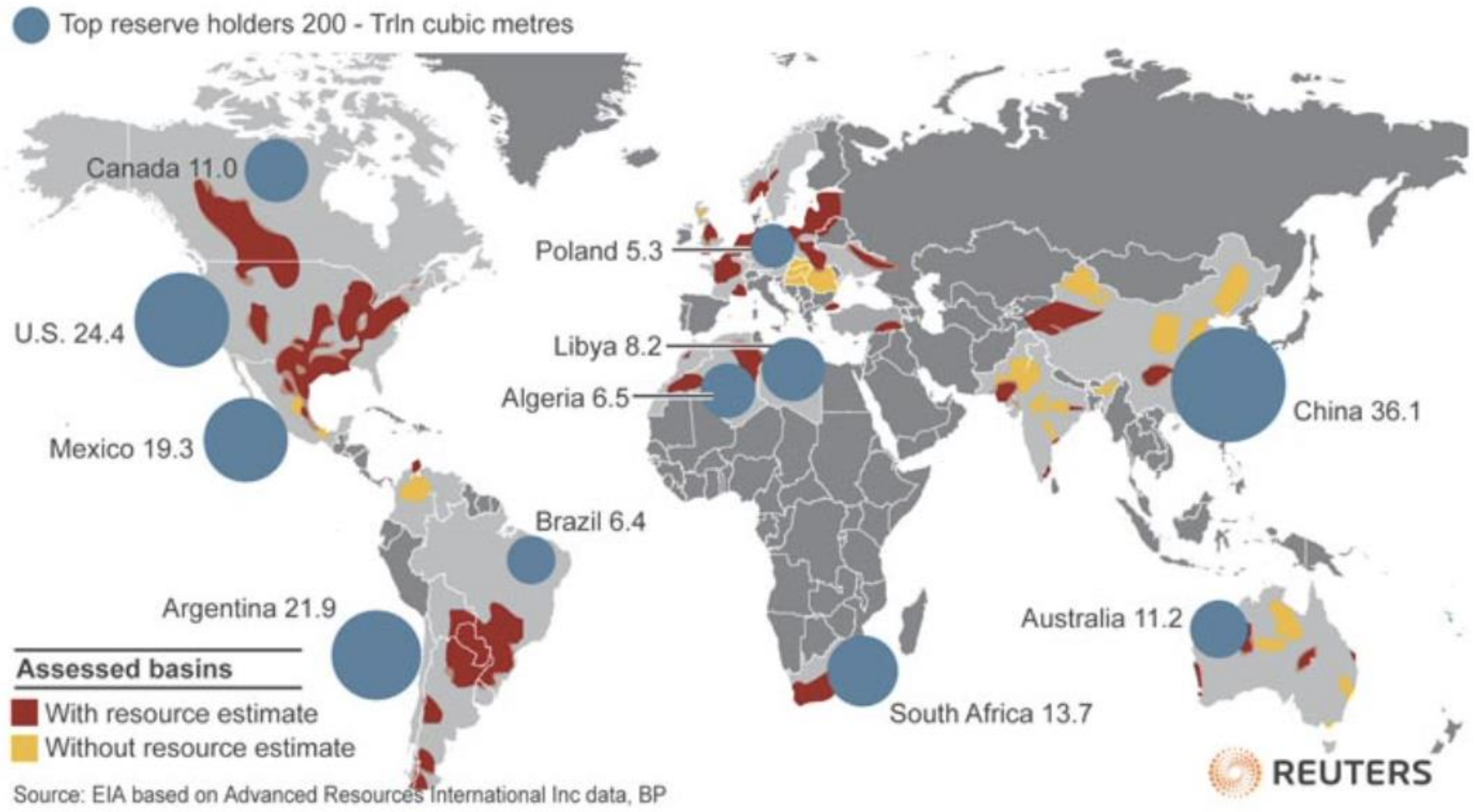
1. Rarefied Gas Flow in Shale Gas Extraction

2. Numerical Method: General Synthetic Iterative Scheme

Global shale gas resources



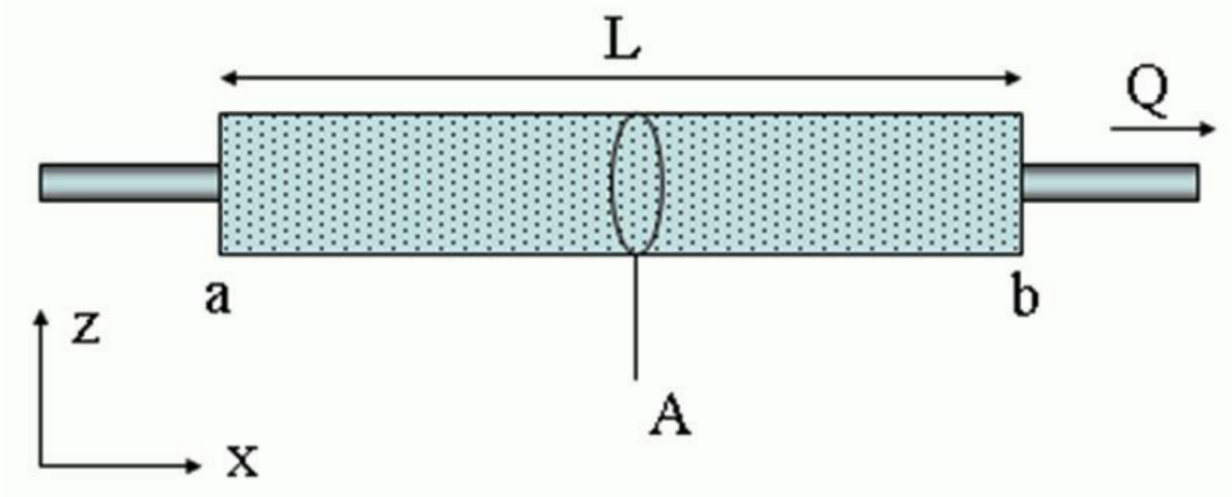
Darcy's law and Klinkenberg's effect

Darcy law: Intrinsic permeability

$$Q = \kappa_\infty \frac{A(p_a - p_b)}{\mu L}$$

Klinkenberg's effect (1941):
Apparent permeability

$$\kappa_a = \kappa_\infty \left(1 + \frac{b}{\bar{p}}\right)$$

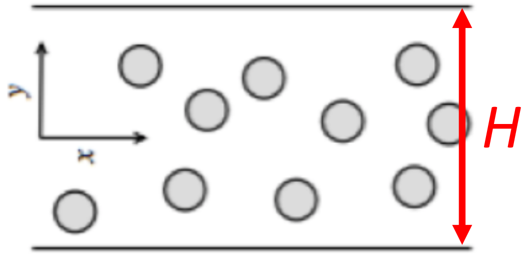


⇐Navier-Stokes eq. with 1st order velocity slip B.C.

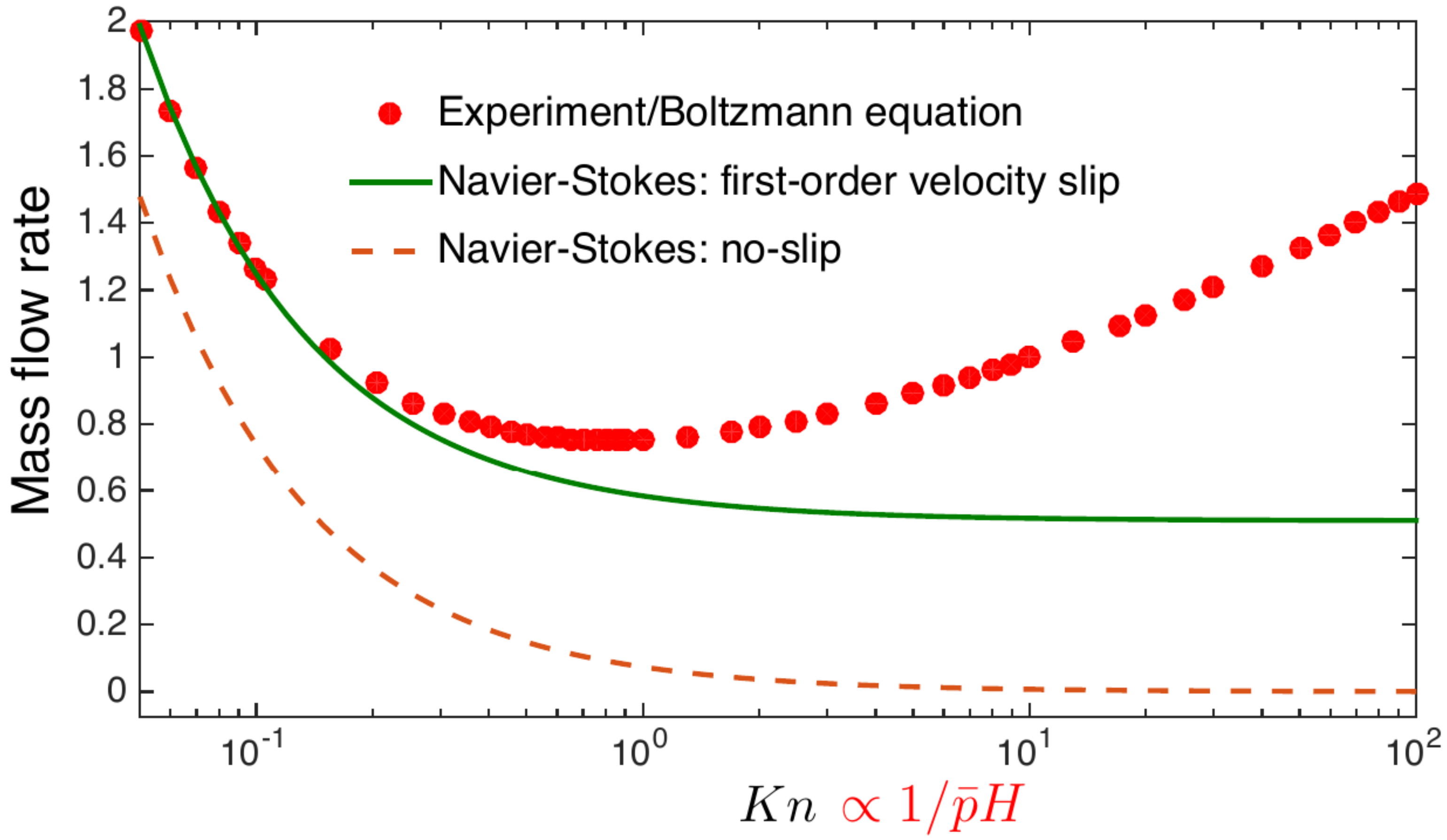
Correction factor $b > 0$, depending on gas, porous medium, gas-surface interaction

Here we focus on how does b vary with $\bar{p}$

Poiseuille flow of rarefied gas



Permeability ∝ normalized mass flow × Kn



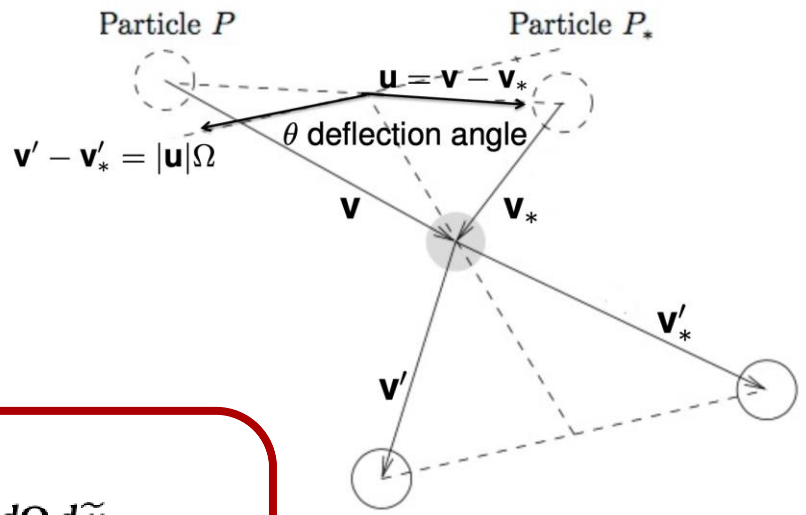
Rarefaction effects: (1) cause velocity slip, and (2) modify the constitutive relation between shear stress and strain rate

Boltzmann equation

Boltzmann equation: $\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \mathbf{a} \cdot \frac{\partial f}{\partial \mathbf{v}} = Q(f, f_*)$

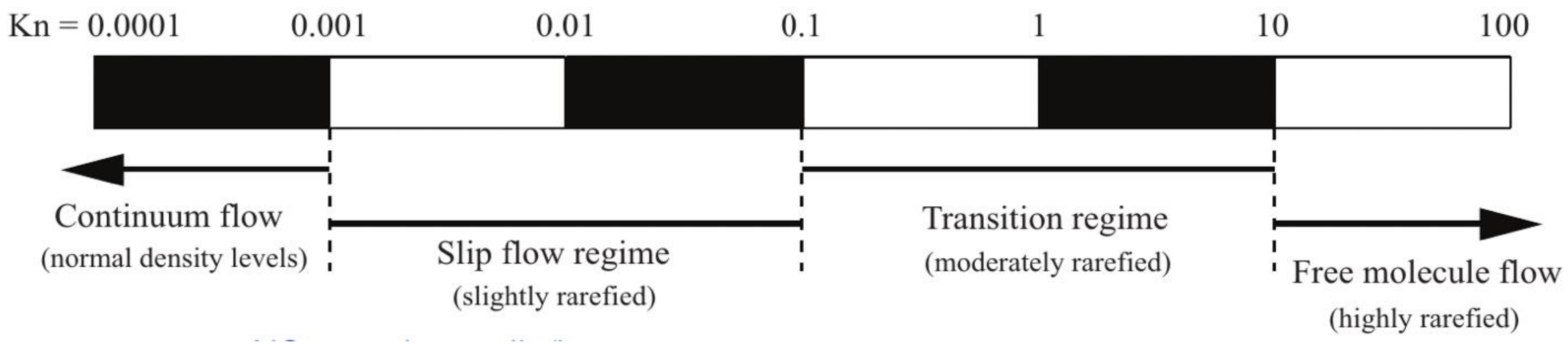
Collision: $Q(f, f_*) = \int\int B(\cos\theta, |\mathbf{u}|)|\mathbf{u}|[f(\mathbf{v}'_*)f(\mathbf{v}') - f(\mathbf{v}_*)f(\mathbf{v})]d\Omega d\mathbf{v}_*$

Gain term Loss term



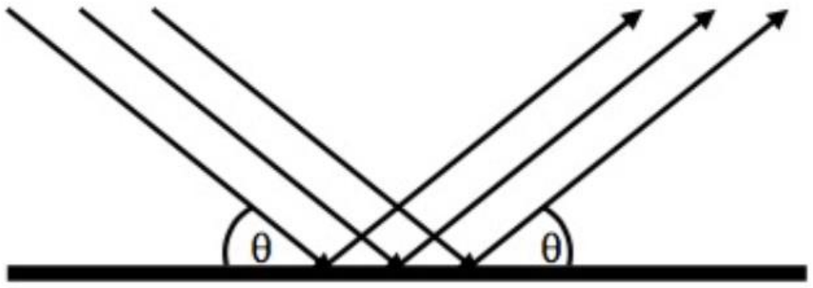
$$\frac{\partial \tilde{f}}{\partial \tilde{t}} + \tilde{v}_2 \frac{\partial \tilde{f}}{\partial \tilde{x}_2} + \tilde{a}_1 \frac{\partial \tilde{f}}{\partial \tilde{v}_1} = \frac{1}{Kn'} \iint \sin^{\alpha+\gamma-1}\left(\frac{\theta}{2}\right) \cos^{-\gamma}\left(\frac{\theta}{2}\right) |\tilde{u}|^{\alpha} [\tilde{f}(\tilde{v}'_*)\tilde{f}(\tilde{v}') - \tilde{f}(\tilde{v}_*)\tilde{f}(\tilde{v})] d\Omega d\tilde{v}_*,$$

Knudsen number: $\mathrm{Kn} = \frac{\lambda}{L}$ λ: mean free path; L: flow length

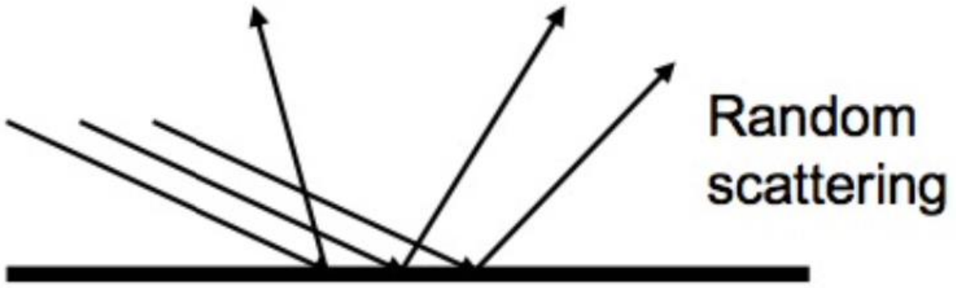


Gas-surface interaction

- The TMAC, σ, defines the proportion of gas molecules reflected diffusively
- For smooth walls: $\sigma \to 0$ and for rough walls: $\sigma = 1$



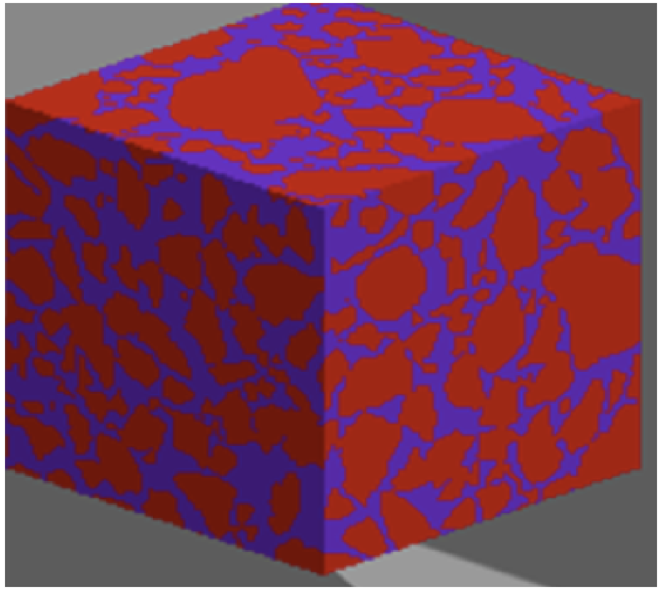
Smooth Wall: Specular Reflection ($\sigma = 0$)

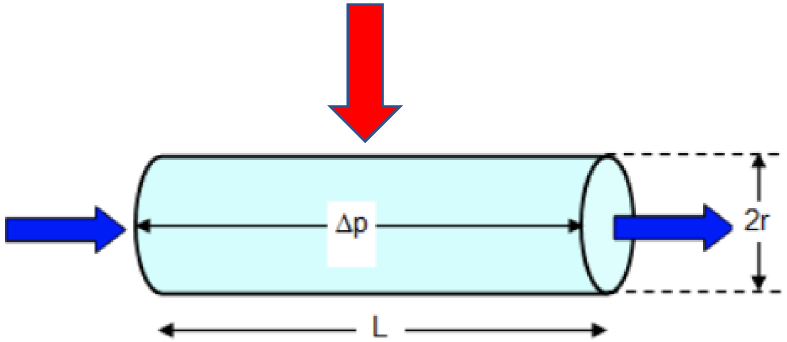


Rough Wall: Diffuse Reflection ($\sigma = 1$)

- Silicon micro-machined components exhibit tangential momentum accommodation coefficients ranging from 0.8 to 1.0 (Arkilic et al., 1997)

Conventional treatment 1: single straight tube

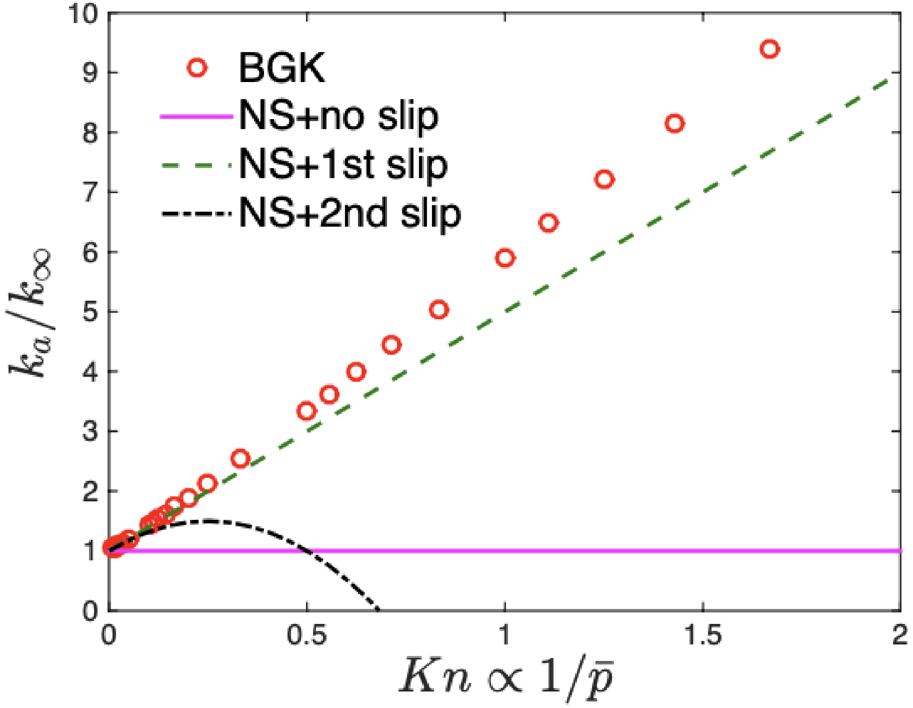




Gas kinetic (e.g. BGK) equation leads to:

$$\frac{k_a}{k_\infty} = \left[1 + \frac{128}{15\pi^2}\tan^{-1}\left(4Kn^{0.4}\right) Kn\right]\left(1 + \frac{4Kn}{1+4Kn}\right)$$

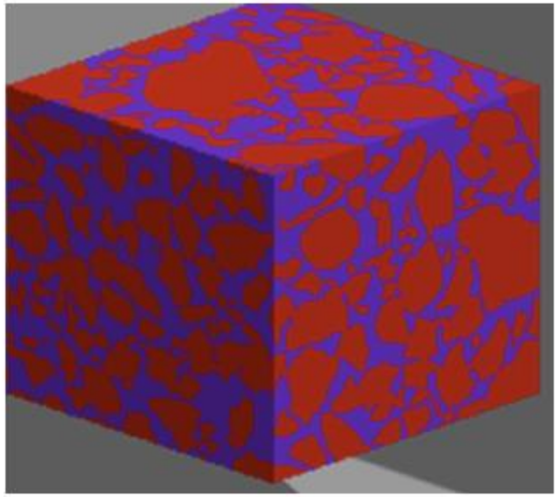
Civan. Transp. Porous. Med. 82 (2010) 375.

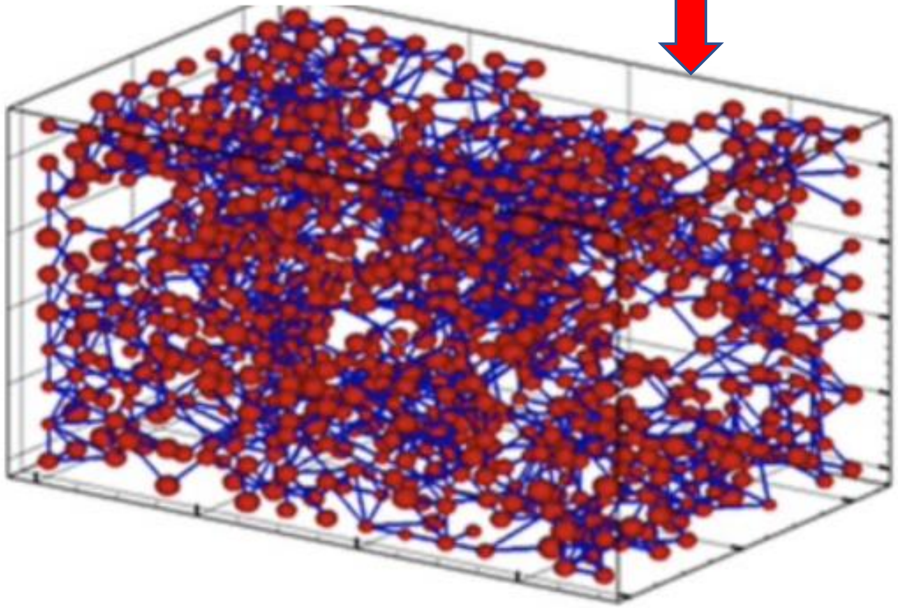


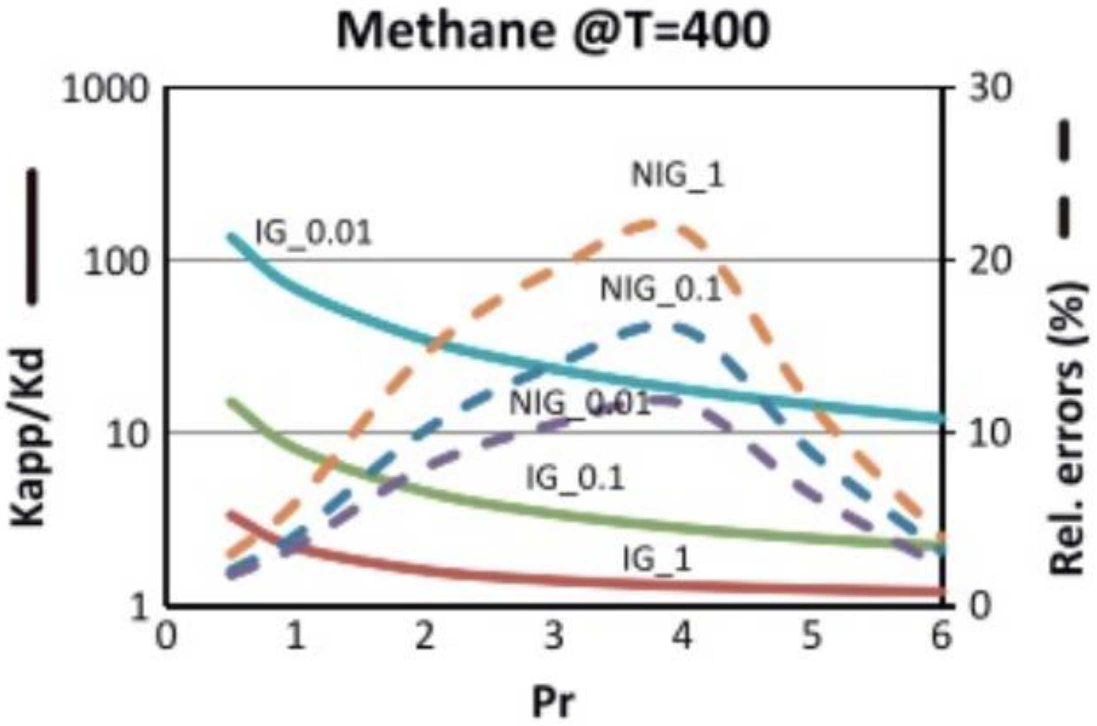
$$\kappa_a = \kappa_\infty\left(1 + \frac{b}{\bar{p}}\right)$$

b increases when $\bar{p}$ decreases

Conventional treatment 2: pore-network model







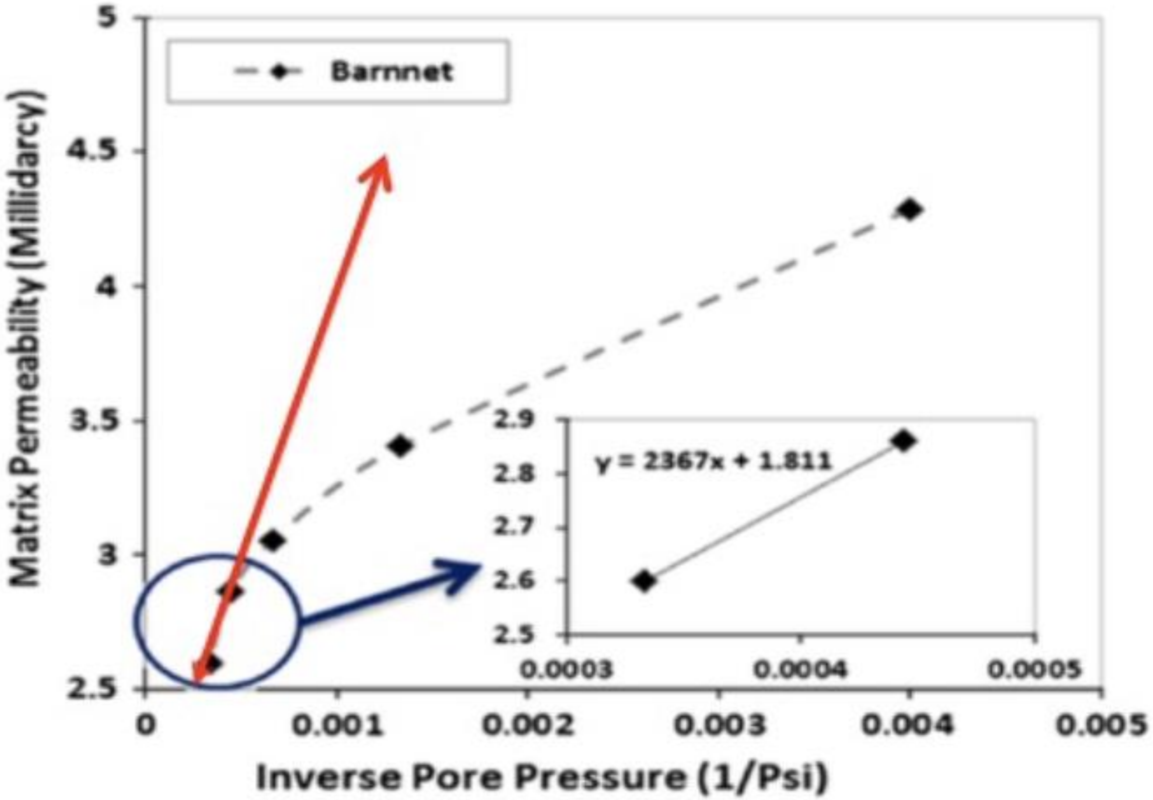
Ma *et al.* Fuel 116 (2014) 498.

The correction factor b is nearly a constant.

Zhang *et al.* Scientific Reports 5 (2015) 13501.

Devil in the details

$\bar{p} = \frac{p_1+p_2}{2}$ (Atmospheres)	$p_1 - p_2$ (Atmospheres)	$\frac{1}{\bar{p}}$ (Atmospheres)$^{-1}$	K_a (Millidarcys)	$\frac{K_a}{K}$	b
0.01665	0.02717	60.1	900	5.29	0.071
0.01779	0.02652	56.2	863	5.07	0.072
0.02130	0.02528	46.96	758	4.44	0.073
0.04890	0.01821	20.46	455	2.67	0.082
0.1738	0.00843	5.75	268	1.58	0.082
1.701	0.02017	0.587	184.9	1.087	0.15
2.659	0.01625	0.3761	180.0	1.058	0.16
3.641	0.01511	0.2748	179.8	1.057	0.21
4.619	0.01412	0.2165	179.1	1.052	0.24
7.04	0.00821	0.1420	176.7	1.038	0.27
12.89	0.00582	0.0776	173.9	1.022	0.29

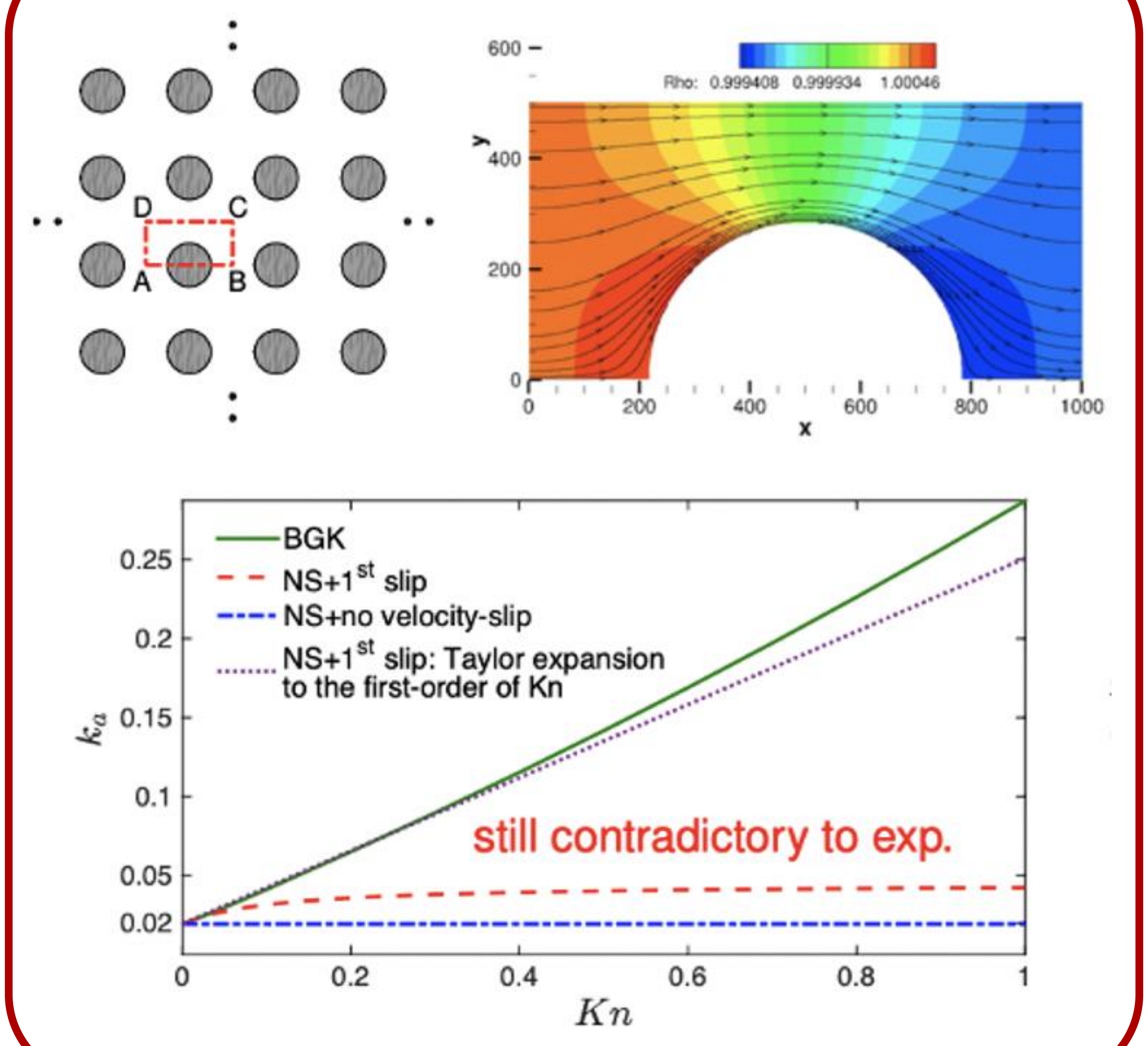


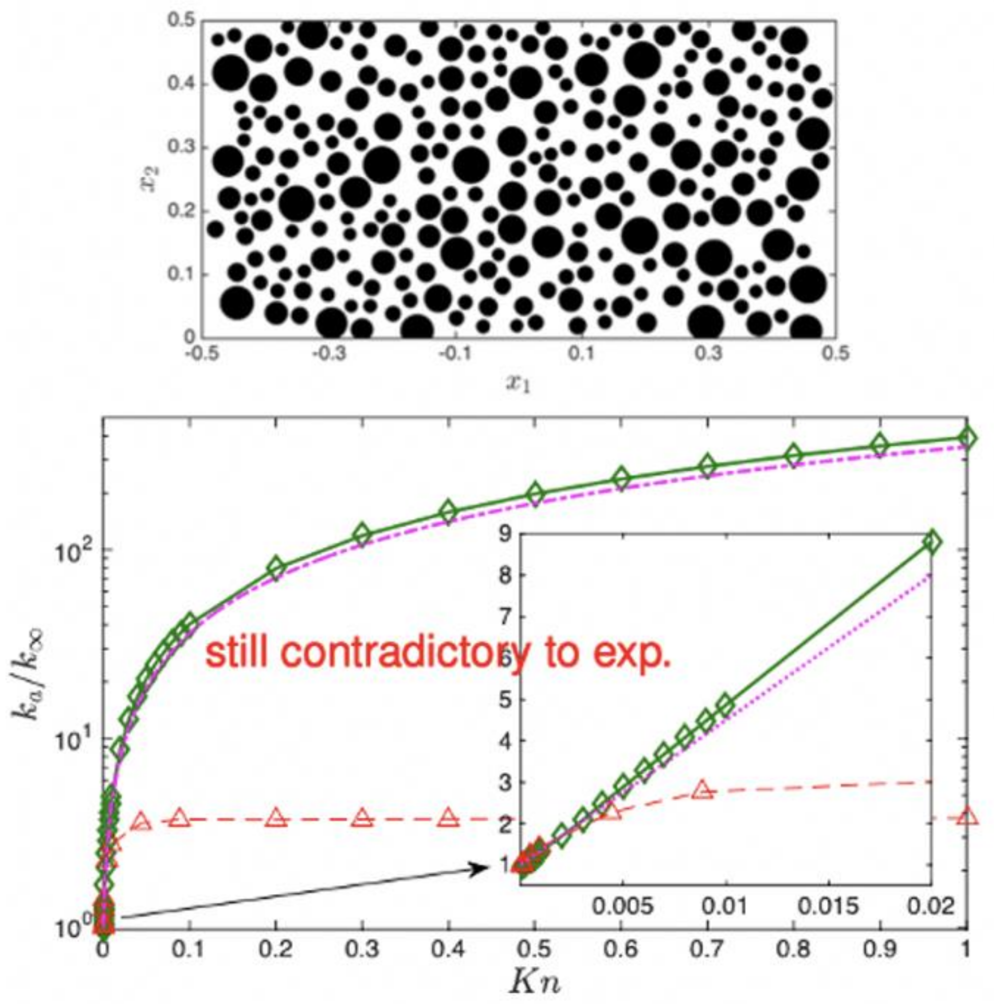
Klinkenberg (1941)
has been long overlooked!

Moghaddam & Jamiolahmady
Fuel 173 (2016) 298.

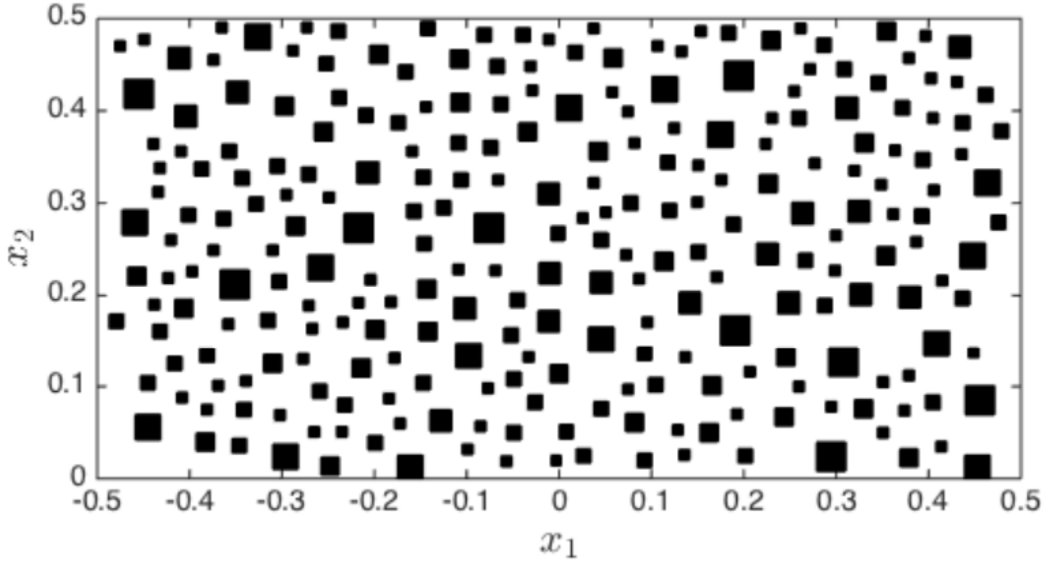
Correction factor b decreases with pressure, contradictory to theory!

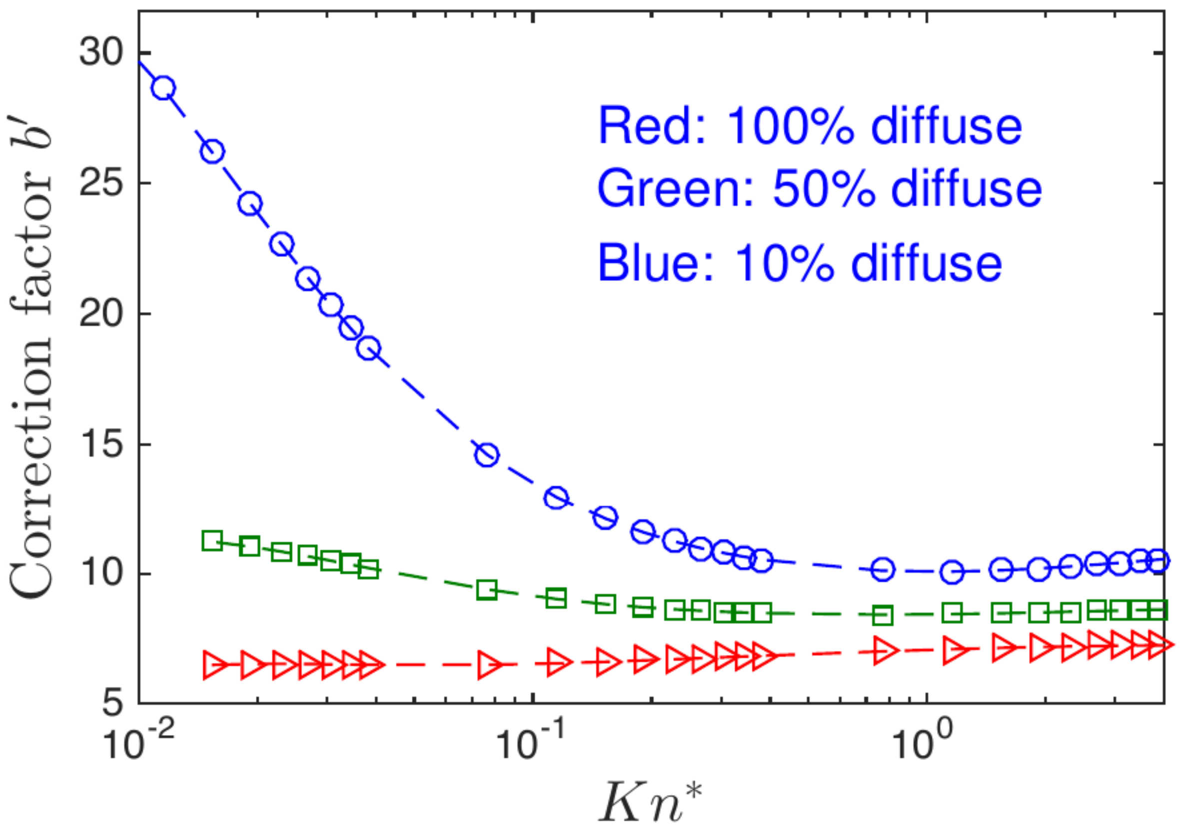
Random circles (diffuse boundary condition)





Importance of gas-surface interaction



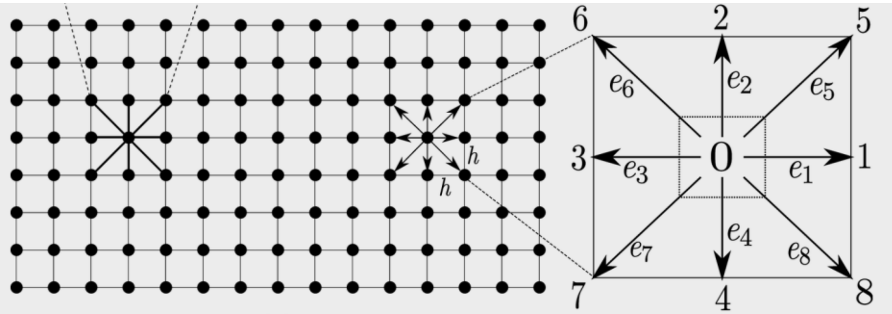


Klinkenberg's exp. can be explained when
(1) the flow path is tortuous
(2) the TMAC is less than 1

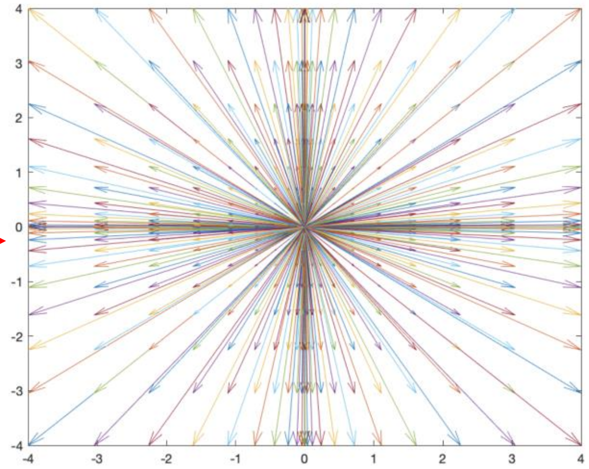
Lei Wu, *et al.* On the apparent permeability of porous media in rarefied gas flows. *J. Fluid Mech*. 822 (2017) 398.

Contents

Lattice Boltzmann method vs. Discrete velocity method



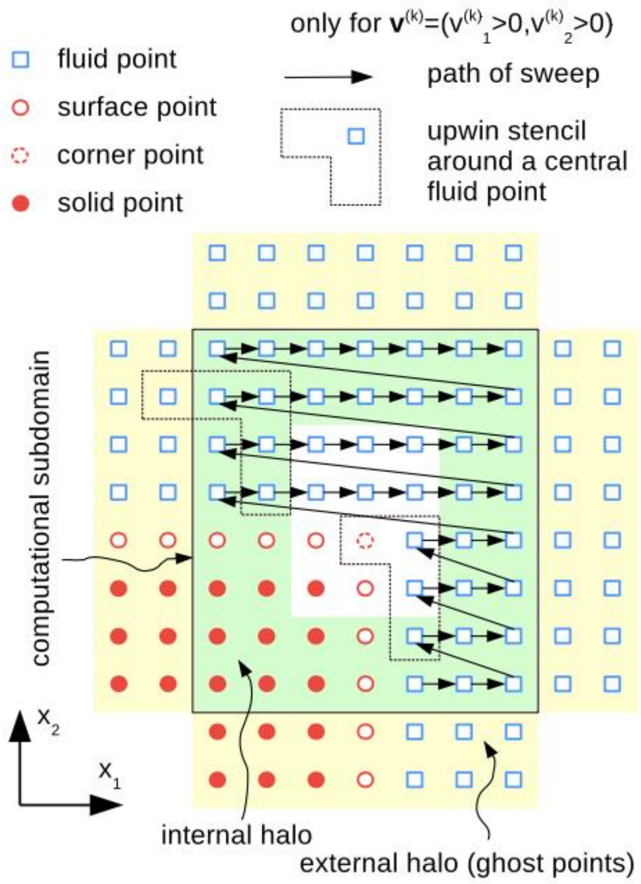
Discrete
velocities

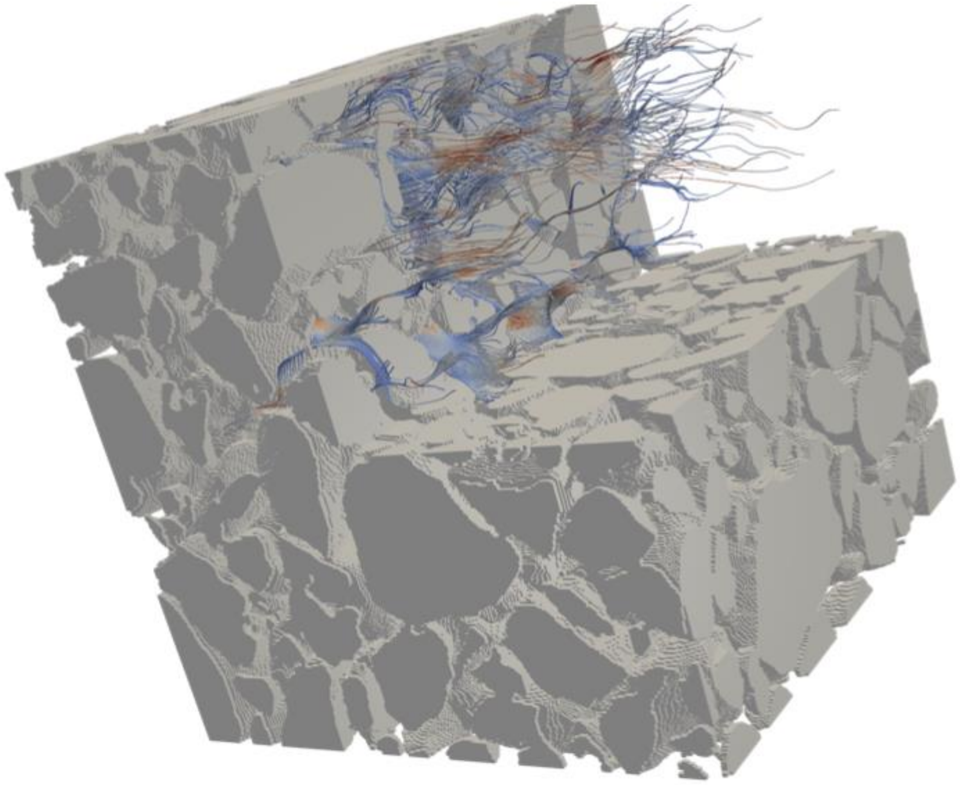


LBM	DVM
Few discrete velocities	Many discrete velocities
Each step computational cost little	Each time step computational cost large
Many time steps	Few time steps
Many spatial grids	Few spatial grids

Numerical method & HPC parallelization

Conventional Iterative Scheme (CIS): $v_1 \frac{\partial f^{k+1}}{\partial x_1} = \underbrace{Q^+(f^k, f^k)}_{\text{gain part}} - \underbrace{\nu(\mathbf{v})}_{\text{collision frequency}} \times f^{k+1}$

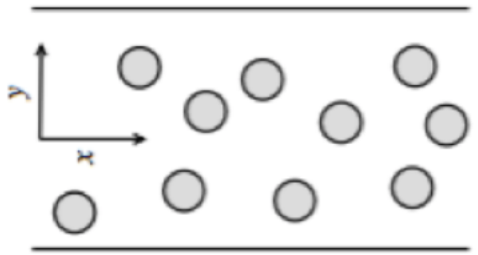




300^3 voxels, 5 min on 12288 CPU cores

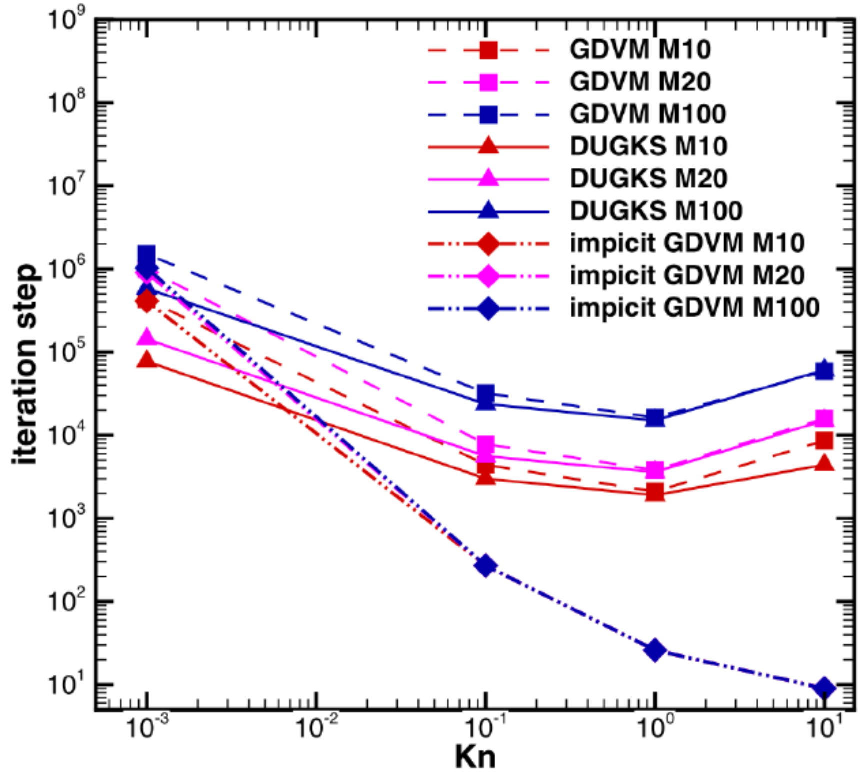
M. T. Ho, *et al*. A multi-level parallel solver for rarefied gas flows in porous media. Computer Physics Communications 234 (2019) 14-25.
M. T. Ho, *et al*. Pore-scale simulations of rarefied gas flows in ultra-tight porous media. Fuel 249 (2019) 341.

Problems of CIS

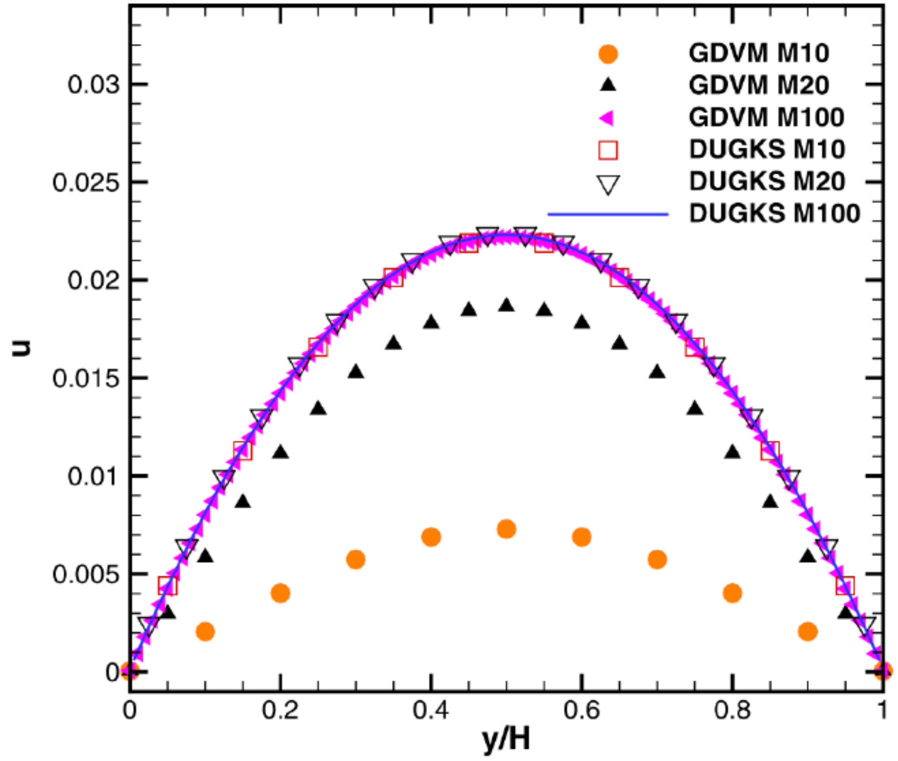


At small Knudsen numbers

Iteration step is huge

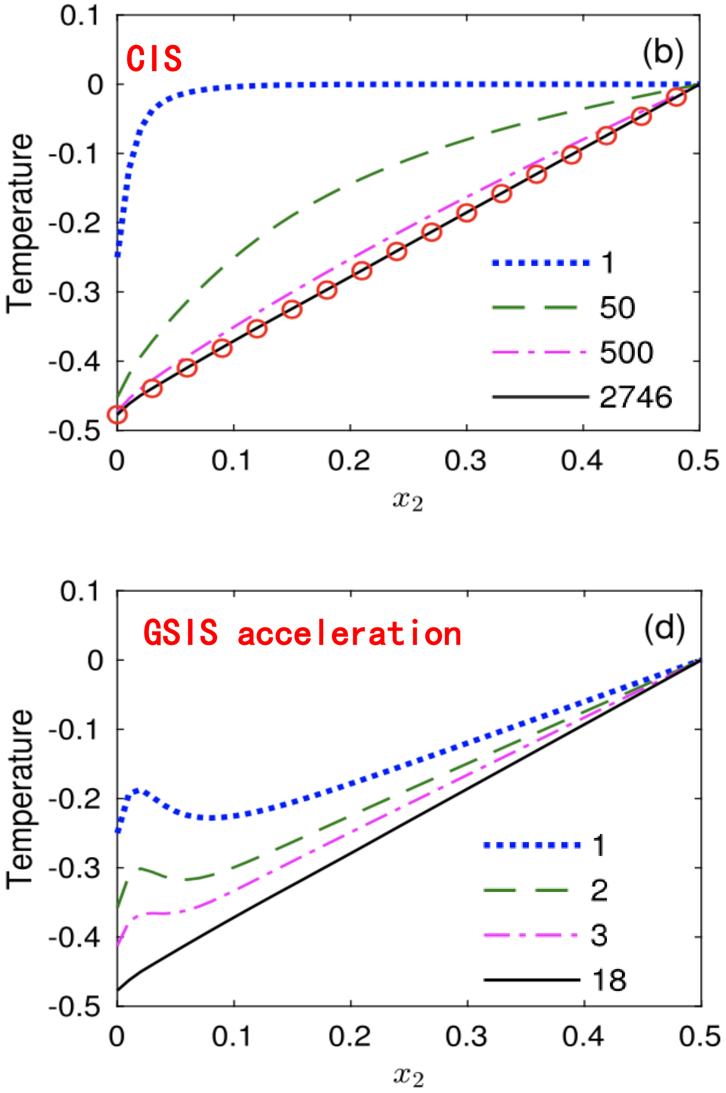


Large numerical dissipations



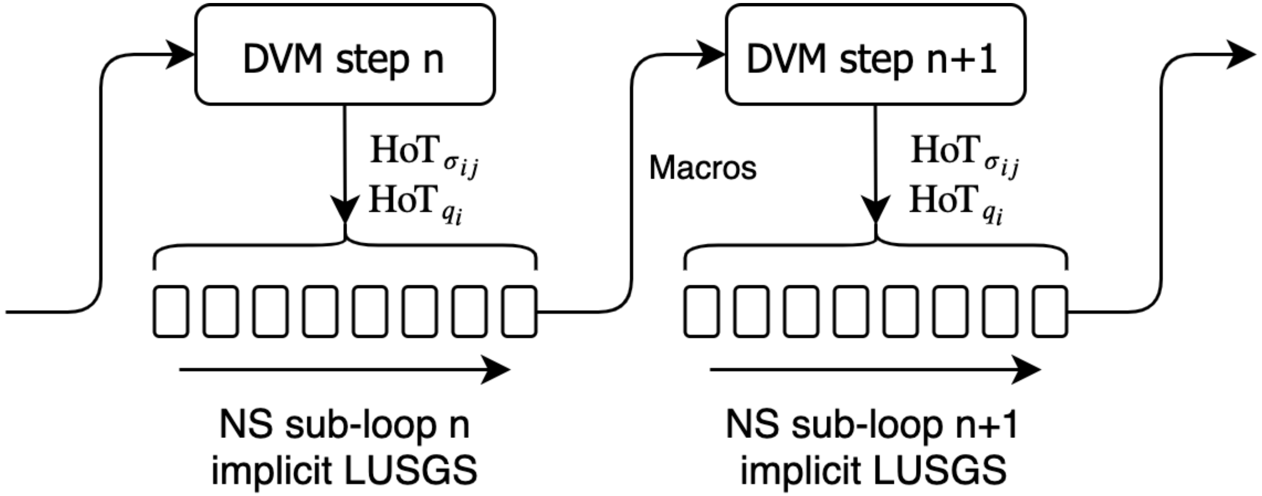
P. Wang *et al*. A comparative study of discrete velocity methods for rarefied gas flows. *Computers & Fluids* 161 (2018) 33.

GSIS: General Synthetic Iterative Scheme



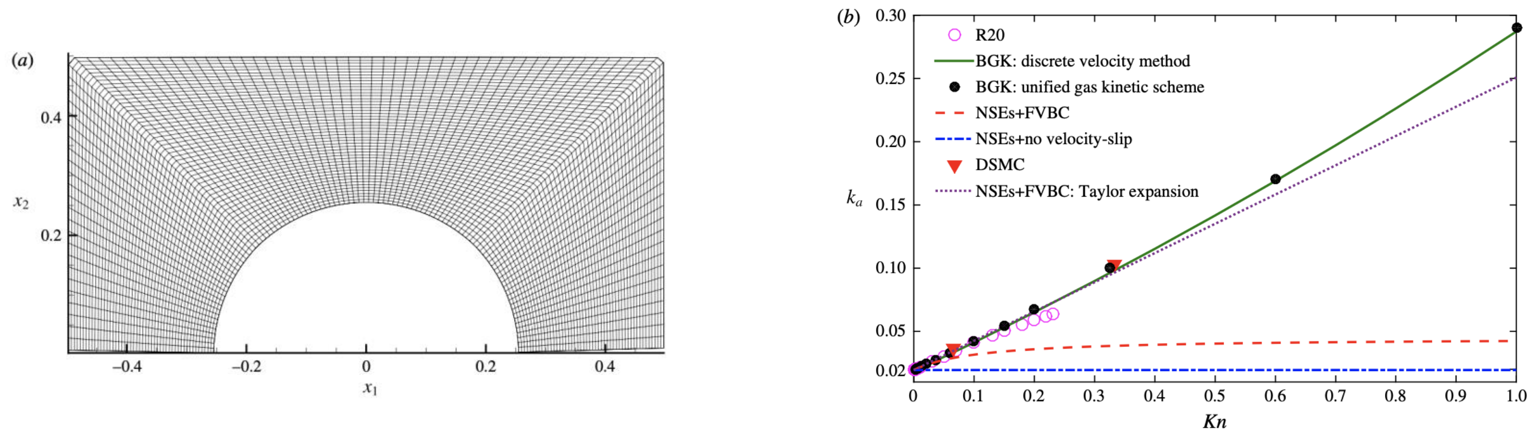
$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial U_i}{\partial x_i} &= 0, \\
2\frac{\partial U_i}{\partial t} + \frac{\partial \rho}{\partial x_i} + \frac{\partial T}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} &= 0, \\
\frac{3}{2}\frac{\partial T}{\partial t} + \frac{\partial q_j}{\partial x_j} + \frac{\partial U_j}{\partial x_j} &= 0,
\end{aligned}
$$

$$
\begin{aligned}
\bar{\sigma}_{ij} &= -2K\frac{\partial \bar{u}_{<i}}{\partial x_{j>}} + \mathrm{HoT}_{\sigma_{ij}}, \\
\bar{q}_i &= -\frac{5K}{4\mathrm{Pr}}\frac{\partial \bar{\tau}}{\partial x_i} + \mathrm{HoT}_{q_i},
\end{aligned}
$$

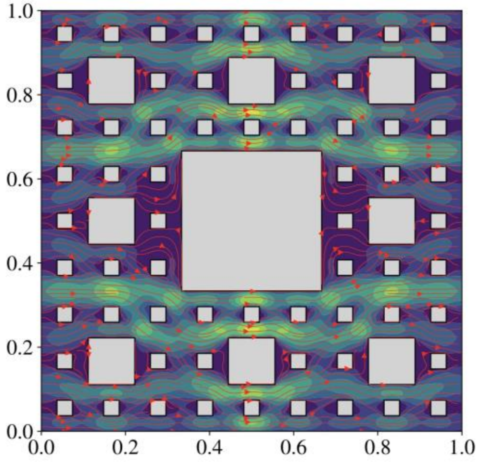


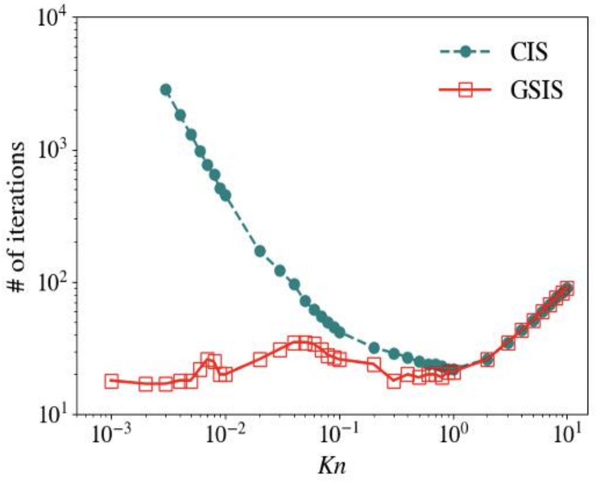
Wei Su, *et al*. Can we find steady-state solutions to multiscale rarefied gas flows within dozens of iterations? *J. Comput. Phys.* 407 (2020) 109245.
Wei Su, Yonghao Zhang, Lei Wu. Multiscale simulation of molecular gas flows by the general synthetic iterative scheme. *Comput. Methods Appl. Mech. Engrg*. 373 (2021) 113548.

Porous media flow



Lei Wu *et al.* On the apparent permeability of porous media in rarefied gas flows. *J. Fluid Mech*. 822 (2017) 398.





Kn=0.003, single CPU
6384 triangles
GSIS: 17 steps; 0.37h
CIS: 2850 steps; 56.6h

Wei Su *et al.* GSIS: An efficient and accurate numerical method to obtain the apparent gas permeability of porous media. *Computers & Fluids* 206 (2020) 104576.

Rigorous proof of fast convergence

2D BGK for an example: $$\boldsymbol{v}\cdot\frac{\partial h(\boldsymbol{x},\boldsymbol{v})}{\partial \boldsymbol{x}}=\frac{h_{eq}(\boldsymbol{x},\boldsymbol{v})-h(\boldsymbol{x},\boldsymbol{v})}{K},$$

$$h_{eq}(\boldsymbol{x},\boldsymbol{v})=\varrho(\boldsymbol{x})+2\boldsymbol{u}(\boldsymbol{x})\cdot\boldsymbol{v}+\tau(\boldsymbol{x})\left(v^2-1\right),\qquad M(\boldsymbol{x})=(\varrho,u_1,u_2,\tau)=\int mh(\boldsymbol{x},\boldsymbol{v})E(\boldsymbol{v})d\boldsymbol{v},$$

Error functions: $$Y^{(k+1)}(\boldsymbol{x},\boldsymbol{v})=h^{(k+1)}(\boldsymbol{x},\boldsymbol{v})-h^{(k)}(\boldsymbol{x},\boldsymbol{v}),$$

CIS: $$\Phi_M^{(k+1)}(\boldsymbol{x})=M^{(k+1)}(\boldsymbol{x})-M^{(k)}(\boldsymbol{x})=\int mY^{(k+1)}(\boldsymbol{x},\boldsymbol{v})E(\boldsymbol{v})d\boldsymbol{v},$$

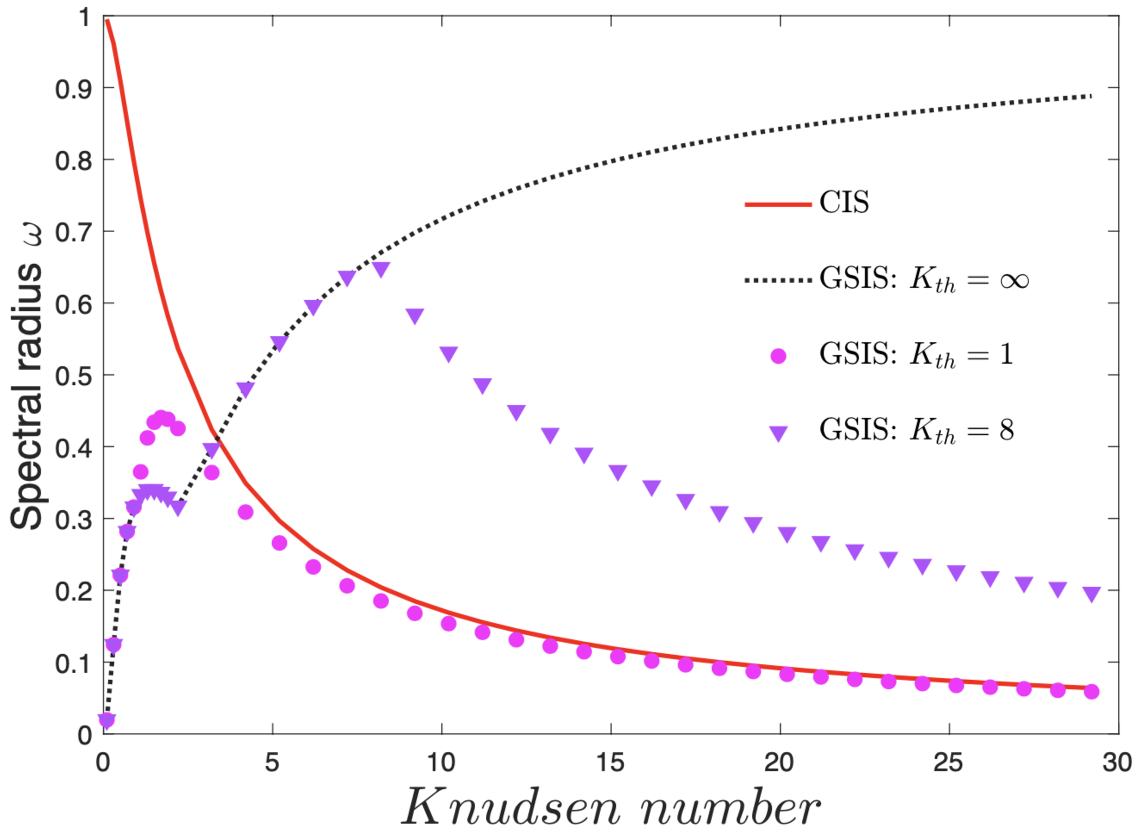
GSIS: $$\boxed{\Phi_M^{(k+1)}(\boldsymbol{x})=M^{(k+1)}(\boldsymbol{x})-M^{(k)}(\boldsymbol{x})=\cancel{\int mY^{(k+1)}(\boldsymbol{x},\boldsymbol{v})E(\boldsymbol{v})d\boldsymbol{v}},}$$

Fourier stability analysis:

$$Y^{(k+1)}(\boldsymbol{x},\boldsymbol{v})=\omega^k y(\boldsymbol{v})\exp(i\boldsymbol{\theta}\cdot\boldsymbol{x}),$$
$$\Phi_M^{(k+1)}(\boldsymbol{x})=\omega^{k+1}\alpha_M\exp(i\boldsymbol{\theta}\cdot\boldsymbol{x}),$$

$\omega \rightarrow 0$, fast convergence
$\omega \rightarrow 1$, slow convergence
$\omega > 1$, blow up

Convergence rate



False convergence

$$|\Phi_M^{(k+1)} - \Phi_M^{(k)}| < \epsilon$$

$$\text{CIS:} \quad |\Phi_M^{(k+1)} - \Phi_M| < \frac{\omega_{CIS}}{1-\omega_{CIS}}\epsilon \to \frac{\epsilon}{Kn^2}, \quad \text{when } Kn \to 0.$$

$$\text{GSIS:} \quad |\Phi_M^{(k+1)} - \Phi_M| < \frac{\omega_{GSIS}}{1-\omega_{GSIS}}\epsilon \to Kn^2\epsilon, \quad \text{when } Kn \to 0.$$

Super convergence

AP: Asymptotic Preserving

After spatial discretization: $$\boldsymbol{v}\cdot\frac{\partial h}{\partial \boldsymbol{x}}+O(\Delta x^n)\delta(h)=\frac{h_{eq}-h}{K},$$

Chapman-Enskog expansion: $$h=h_0+Kh_1+K^2h_2+\cdots,$$

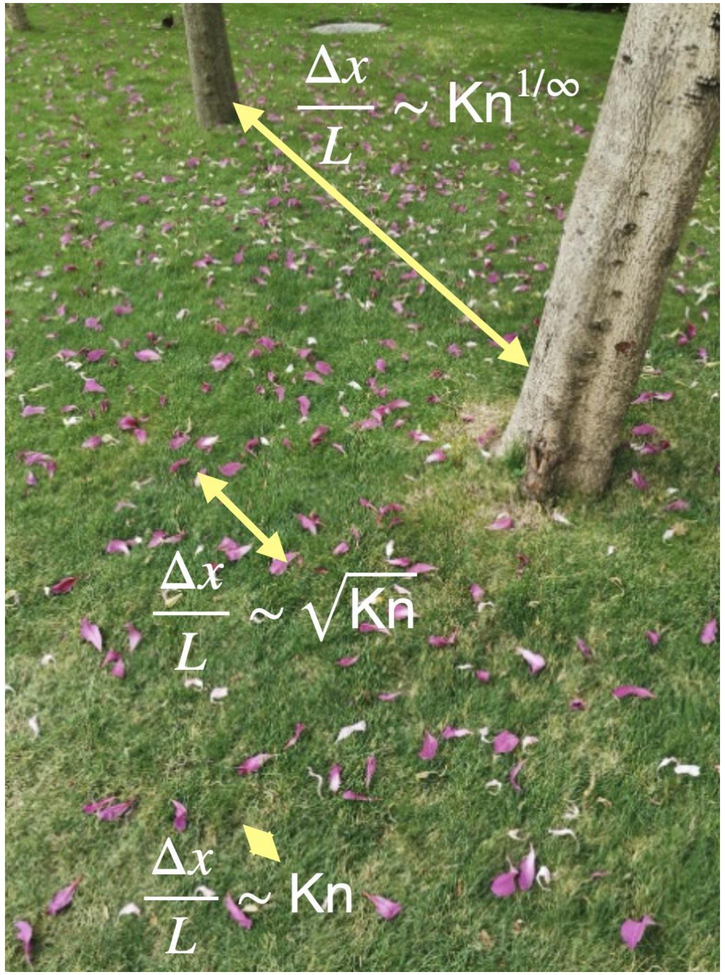
$$\boxed{\Delta x=O(1),}\quad h_0=h_{eq},\quad h_1=-\boldsymbol{v}\cdot\frac{\partial h_{eq}}{\partial \boldsymbol{x}}-\delta(h_{eq}).$$

$$\boxed{\Delta x\sim O(K^{1/2}),}\quad h_0=h_{eq},\quad h_1=-\boldsymbol{v}\cdot\frac{\partial h_{eq}}{\partial \boldsymbol{x}},$$

In GSIS, h_0 is adequate to recover the NS constitutive relations!

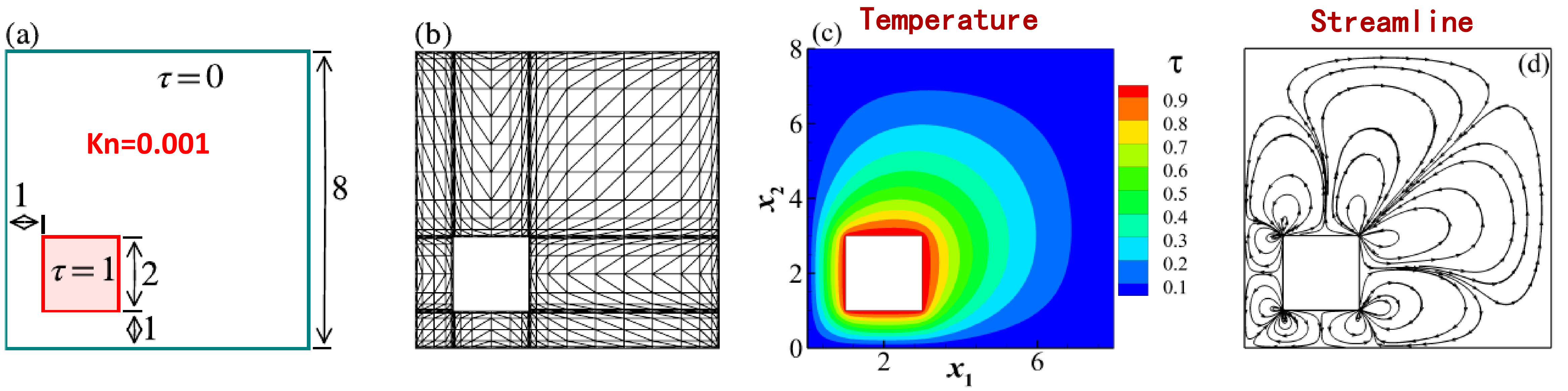
$$\bar{\sigma}_{ij}=-2K\frac{\partial \bar{u}_{<i}}{\partial x_{j>}}+\mathrm{HoT}_{\sigma_{ij}},\qquad \mathrm{HoT}_{\sigma_{ij}}=2K\frac{\partial u_{<i}^{(k+1/2)}}{\partial x_{j>}}-2K\int\left(v_iv_j-\frac{v^2}{2}\delta_{ij}\right)\boldsymbol{v}\cdot\frac{\partial h^{(k+1/2)}}{\partial \boldsymbol{x}}d\boldsymbol{v},$$

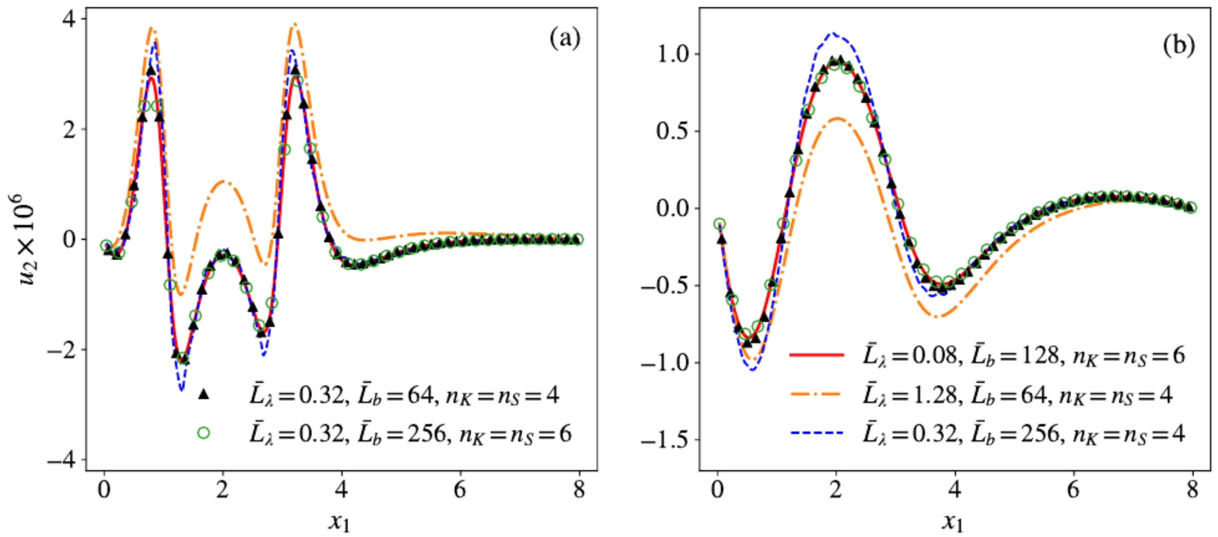
$$\bar{q}_i=-K\frac{\partial\bar{\tau}}{\partial x_i}+\mathrm{HoT}_{q_i},\qquad \mathrm{HoT}_{q_i}=K\frac{\partial \tau^{(k+1/2)}}{\partial x_i}-K\int v_i(v^2-2)\boldsymbol{v}\cdot\frac{\partial h^{(k+1/2)}}{\partial \boldsymbol{x}}d\boldsymbol{v}.$$



Conclusion: if macroscopic equations can be solved exactly, then GSIS is equivalent to Navier-Stokes even when *Δx=O(1)*.

A challenging test: Thermal edge flow



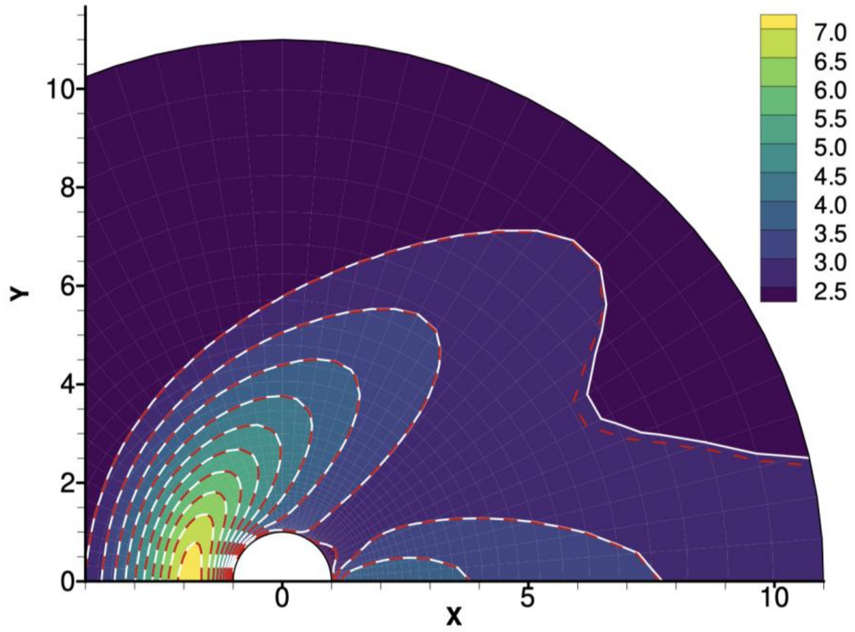


Iteration number: 50
5 minutes

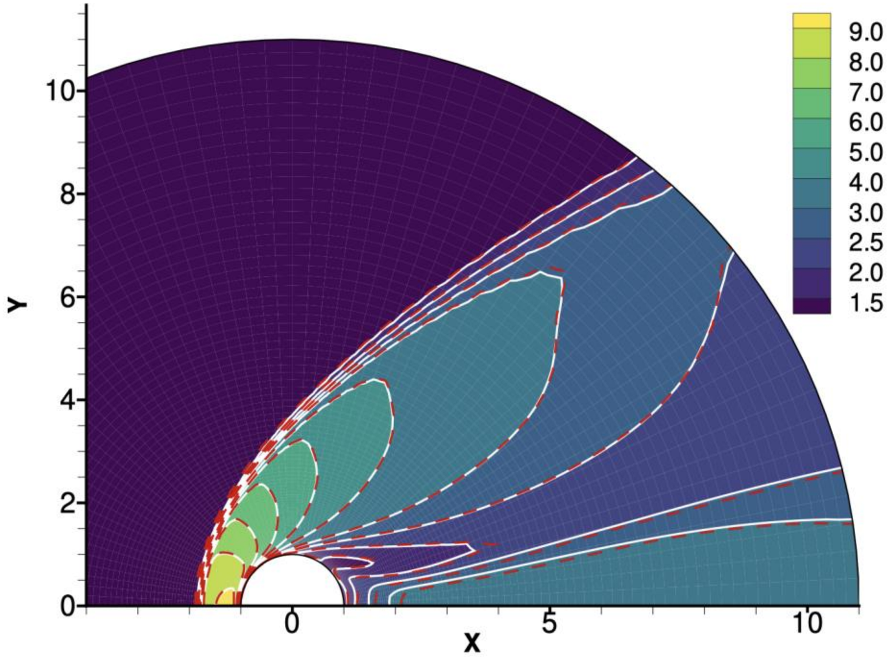
Wei Su, Lianhua Zhu, Lei Wu. Fast convergence and asymptotic preserving of the general synthetic iterative scheme, *SIAM Journal on Scientific Computing* 42 (2020) B1517.

Hypersonic flow: Ma=5

Kn = 1, temperature



Kn = 0.01, temperature

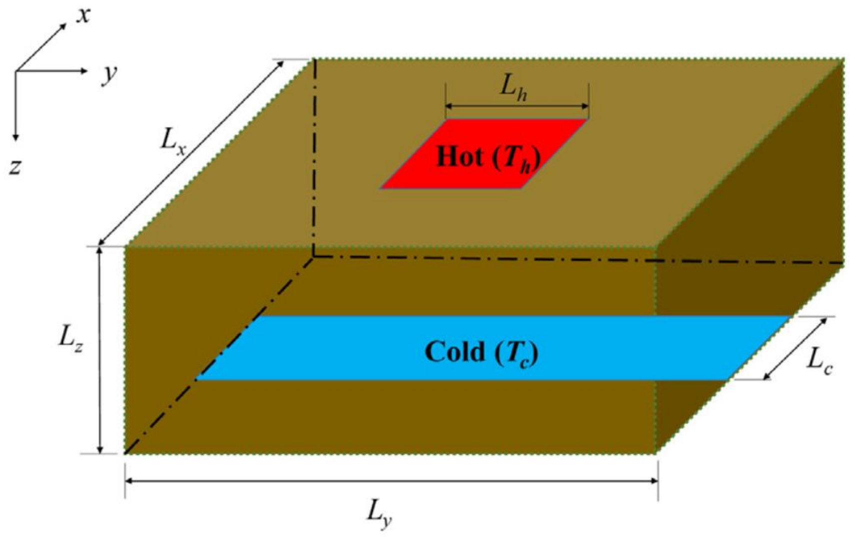


Lianhua Zhu, Xingcai Pi, Wei Su, Zhihui Li, Yonghao Zhang, Lei Wu. General synthetic iteration scheme for nonlinear gas kinetic simulation of multi-scale rarefied gas flows. *J. Comput. Phys.* 430 (2021) 110091.

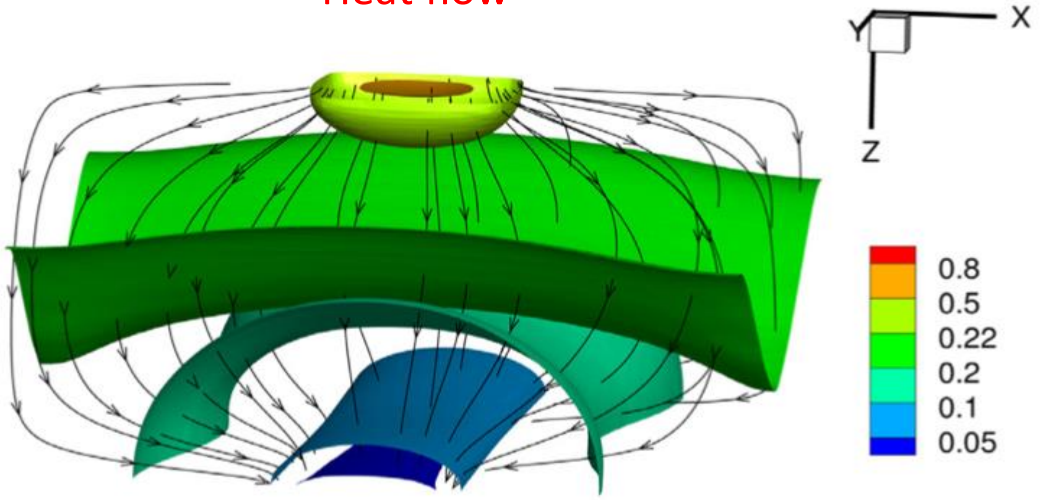
Phonon transport

Singe relaxation-time model: $\boldsymbol{v}\boldsymbol{s} \cdot \nabla e = \frac{e^{eq} - e}{\tau}$

$$T = T_{\mathrm{ref}} + \left(\sum_p \int_{\omega_{\min,p}}^{\omega_{\max,p}} \frac{\int_{4\pi} e d\Omega}{\tau} d\omega \right) \times \left(\sum_p \int_{\omega_{\min,p}}^{\omega_{\max,p}} \frac{C}{\tau} d\omega \right)^{-1}.$$



Heat flow



Dual relaxation-time model: $\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = \frac{f_R^{eq} - f}{\tau_R} + \frac{f_N^{eq} - f}{\tau_N}$

Chuang Zhang, Songze Chen, Zhaoli Guo, Lei Wu. A fast synthetic iterative scheme for the stationary phonon Boltzmann transport equation. *International Journal of Heat and Mass Transfer* 174 (2021) 121308.
Jia Liu, Lei Wu. A fast-converging scheme for the phonon Boltzmann equation with dual relaxation times. *arxiv:2107.06688.*

Conclusions

General Synthetic Iterative Scheme

- Super convergence
- Asymptotic preserving to Navier-Stokes
- Compatible to traditional CFD
- Universality: does not rely on the specific form of Boltzmann collision operator

To me, GSIS is Jesus!