Kinetic simulations by the DSBGK method with noise reduction

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CREATING GROWTH, ENHANCING LIVES

Contents:

- Kinetic theory
- Different simulation methods
- DSBGK and its noise reduction technique
- Validation by and comparison with other methods
- Evolution demonstration of some transient solutions

Regime division of gas flows

$$Kn = \frac{\lambda}{L}, \lambda = \frac{16\mu}{5n\sqrt{2\pi m k_{\mathrm{B}} T}}, n = \frac{p}{k_{\mathrm{B}} T}, \lambda_{\mathrm{STP}} \approx 70\ \mathrm{nm}$$

$0.1 < Kn < 1$
Could be Burnett Eq.
+ high-order-slip B.C.

$Kn < 0.01$	$0.01 < Kn < 0.1$	$0.1 < Kn < 10$	$10 < Kn$
N-S Eq. + non-slip B.C.	N-S Eq. + slip B.C.		Simplified Boltzmann Eq.
Continuum regime	**Slip regime**	**Transitional regime**	**Free molecular**

Boltzmann Eq. +molecular refelection B. C.

- MEMS/NEMS (e.g., microchip)
- Vacuum system (e.g., lithography, film coating)
- Knudsen pump (without rotor)
- Shale gas ($D_{\mathrm{pore}} \approx 10$ nm)
- Gas diffusion through membranes, nanotubes
- Mars exploration ($p \approx 610$ Pa, about p_{Earth} at $H \approx 35$ km)
- Spacecraft ($\lambda \approx 1$ cm at $H = 85$ km, space station at $H \approx 400$ km)
- Supersonic flow (shockwave thickness ≈ 200 nm)

Boltzmann equation and Bhatnagar-Gross-Krook model

$$\frac{\partial f}{\partial t} + \underbrace{c_j \frac{\partial f}{\partial x_j}}_{\text{movements}} = \underbrace{\int_{-\infty}^{\infty} \int_{0}^{4\pi} (f' f_1' - f f_1) c_{\mathrm{r}} \sigma \mathrm{d}\Omega \mathrm{d}\vec{c}_1}_{\text{intermolecular collisions}}$$

$f(t, \vec{x}, \vec{c}) \mathrm{d}\vec{x} \mathrm{d}\vec{c}$ is the molecular number inside element $\mathrm{d}\vec{x} \mathrm{d}\vec{c}$

Hard sphere molecular model: $\sigma = \frac{D^2(\mu)}{4}$

$n(t, \vec{x}) = \int_{-\infty}^{\infty} f \mathrm{d}\vec{c}$, and $p = n k_{\mathrm{B}} T$

$\vec{u}(t, \vec{x}) = \frac{1}{n} \int_{-\infty}^{\infty} \vec{c} f \mathrm{d}\vec{c}$

$T(t, \vec{x}) = \frac{2}{3 k_{\mathrm{B}} n} \int_{-\infty}^{\infty} \frac{m(\vec{c} - \vec{u})^2}{2} f \mathrm{d}\vec{c}$

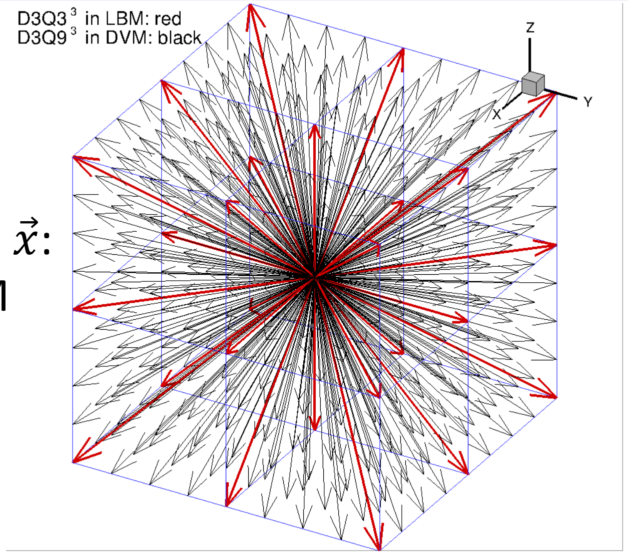
BGK collision model: $\mathrm{RHS} = \upsilon(f^{\mathrm{eq}} - f)$ with $\upsilon = \frac{n k_{\mathrm{B}} T}{\mu}$ or $\upsilon = \frac{5 k_{\mathrm{B}}}{2m} \frac{n k_{\mathrm{B}} T}{\eta}$, or $\upsilon(\vec{c})$

Simulation methods from different communities

Direct Simulation Monte Carlo Method (DSMC): Lagrangian particles (at 2nd RGD, 1960)	Discrete Velocity Method (DVM): Eulerian grids (1964)	Lattice Boltzmann Method (LBM): Eulerian grids (1992~1997)	Direct Simulation BGK Method (DSBGK): Lagrangian particles (at 2nd FCMC, 2009)
• Converge to Boltzmann equation • Standard at arbitrary *Kn* • Costly at low speed due to noise	• Solve kinetic equations • Accurate by FINE grids • Efficient in 2D • Costly in 3D	• Solve BGK-type equation • Use VERY coarse velocity grids • Converge to the N-S equation • Valid at low *Kn* • Efficient	• Converge to the BGK equation • Accurate at low speed (*Ma*<1) • Significant noise reduction • Efficient particularly in large-scale 3D problems at low speed
• PIC-DSMC with the cell mean value method to deposit from particle to grid		• Easy extension to two-phase flows, Darcy flows, boiling, and MHD, etc	

For $\vec{c}$ at each $\vec{x}$:

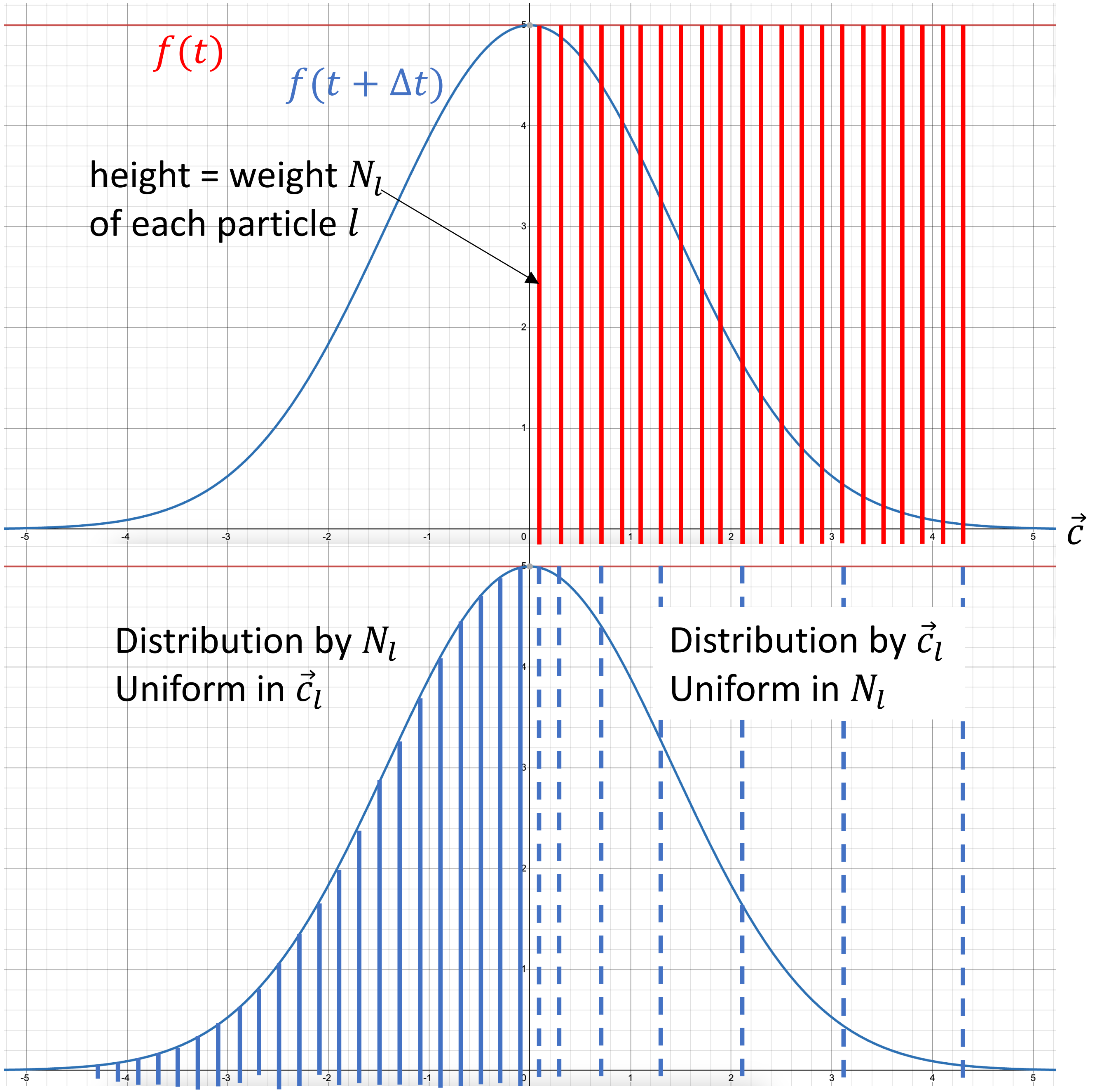
LBM vs. DVM



[1] J Li, *Multiscale and Multiphysics Flow Simulations of Using the Boltzmann Equation*, Springer, 2020.

DSBGK and its noise reduction technique

Extrapolation of the acceptance-rejection scheme



Model the change of f in the $\vec{c}$ space:

- Acceptance-rejection scheme: solid-red → dashed-blue
- Extrapolation of the scheme: solid-red → solid-blue

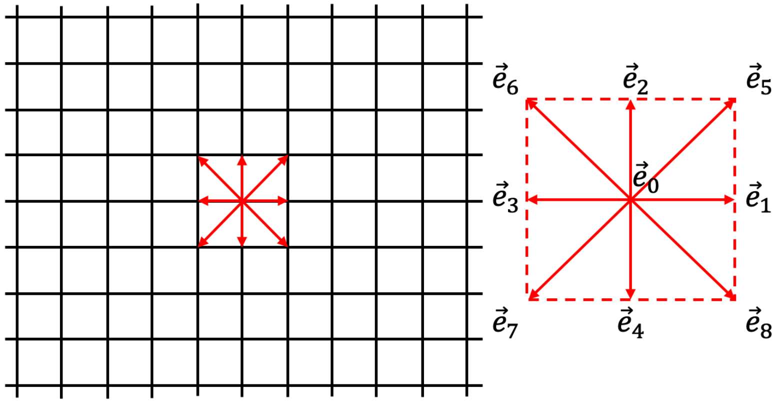
- Generally valid for changing a representative sample $(\vec{x}_l, \vec{c}_l, N_l)$ of arbitrary $f(t)$ to $(\vec{x}_l, \vec{c}_l, N_l \frac{f(t+\Delta t)}{f(t)})$ for $f(t+\Delta t)$
- Statistically valid if $(\vec{x}_l, \vec{c}_l, N_l)$ has noise but its ensemble-average is representative of $f(t)$

DSBGK with a duality of DSMC-LBM

- Start with $(\vec{x}_l, \vec{c}_l, N_l \equiv N_0)$ and $F_l = f(\vec{c}_l) = f^{\mathrm{eq}}(\vec{c}_l)$, and $n_k = n_0, \vec{u}_k = \vec{u}_0, T_k = T_0$ as in DSMC

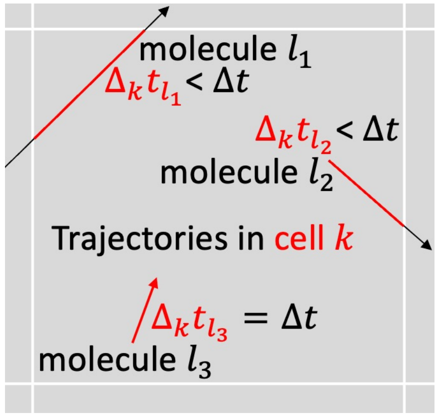
- Adopt idea from lattice-based LBM: $f_\alpha(\vec{x} + \vec{e}_\alpha \Delta t, t + \Delta t) = f_\alpha(\vec{x}, t) + \left[f_\alpha^{\mathrm{eq}}(\vec{x}, t) - f_\alpha(\vec{x}, t)\right]/\tau$

Lattice in $\vec{x}$ space



D2Q9 lattice in $\vec{c}$ space

$\vec{x}_l, \vec{c}_l$ of DSBGK/DSMC are discrete but not limited to lattice points



- Update $\vec{x}_l$ by $\vec{x}_l^{\mathrm{new}} = \vec{x}_l + \vec{c}_l \Delta_k t_l$, as in DSMC but by segmented steps
- Update F_l by $F_l^{\mathrm{new}} = f_k^{\mathrm{eq}} + \left(F_l - f_k^{\mathrm{eq}}\right)\exp(-\upsilon \Delta_k t_l)$, similar to LBM
- Update N_l by $N_l^{\mathrm{new}} = N_l F_l^{\mathrm{new}} / F_l$, according to extrapolation of the acceptance-rejection scheme
- No change of $\vec{c}_l$ because the evolution of f due to collisions has been reflected by changing N_l (extrapolation idea)
- Regulate $n_k, \vec{u}_k, T_k$ of f_k^{eq} using $\sum_{\in k} \Delta_k N_l$, $\sum_{\in k}(\Delta_k N_l m_l \vec{c}_l)$, $\sum_{\in k}(\Delta_k N_l m_l \vec{c}_l^2/2)$ with $\Delta_k N_l = N_l^{\mathrm{new}} - N_l$, for conservations

- Update $\vec{c}_l$, as in DSMC, only after reflecting at walls and then $F_l^{\mathrm{new}} = f_{\mathrm{wall}}(\vec{c}_l^{\mathrm{new}})$, but keep N_l for conservation
- Delete/generate outgoing/incoming particles at open boundaries, as in DSMC, additionally assign $F_l = f_{\mathrm{BC}}^{\mathrm{eq}}(\vec{c}_l)$, $N_l \equiv N_0$

Noise reduction technique

- Update number density: $n_k^{\text{new}} = n_k - \frac{1}{V_k}\sum_{\in k} \Delta_k N_l$, similar for $\vec{u}_k^{\text{new}}$ and T_k^{new}

anchored term

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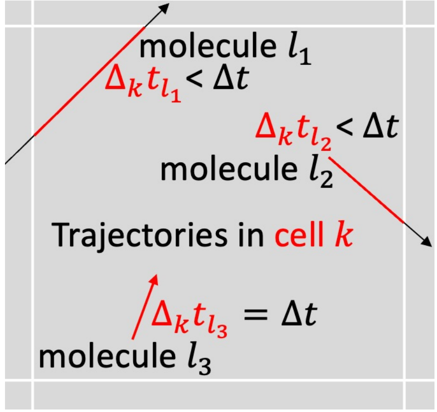
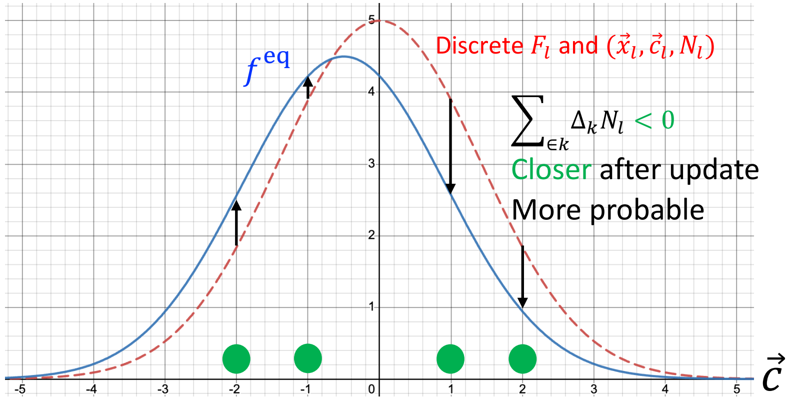
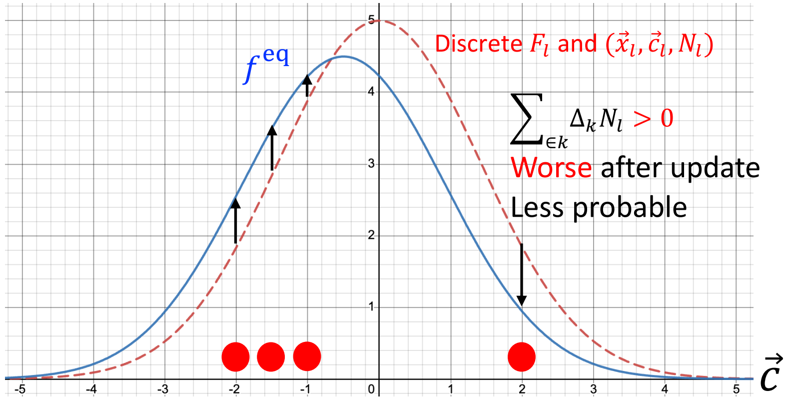


increment due to physics (left-bottom) and noise (right-bottom)

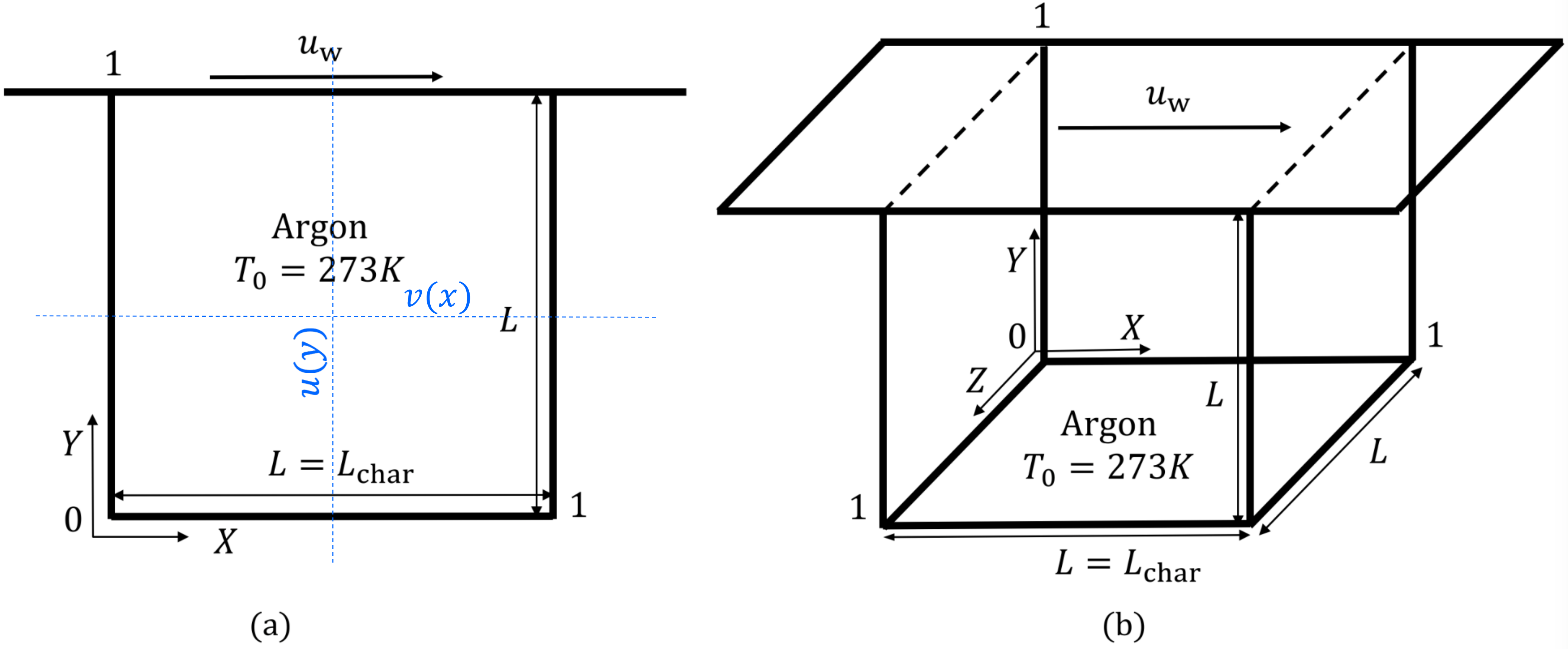
- Special case with $(\vec{x}_l, \vec{c}_l, N_l)$ and F_l of $f(\forall t, \forall \vec{x}) \equiv f^{\text{eq}}$, $\rightarrow \Delta_k N_l \equiv 0$ and $n_k \equiv n_0$ as expected, → zero noise
- General case with $(\vec{x}_l, \vec{c}_l, N_l)$ and F_l of $f \neq f^{\text{eq}}$
  - Avoid noise from number randomness (e.g., $4 < nV = 10$ moving symmetrically, bottom-left figure)
  - Bring noise by asymmetric/random distribution of moving particles, bottom-right figure
  - In general, have noise reduction due to $\sum_{\in k} \Delta_k N_l \ll \sum_{\in k} N_l$, as $\Delta_k N_l \propto \left(f - f^{\text{eq}}\right)$, $\propto \Delta t$, $\propto \Delta x$, and $\sum_{\in k} \Delta \pm$





Validations, comparisons and demonstrations

Lid-driven cavity flow

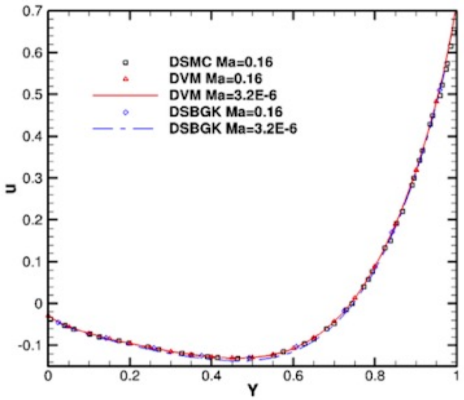


Minimum velocity grids by DVM in 3D
4×24×12 at $Kn = 0.1$
4×40×12 at $Kn = 1.0$
4×48×12 at $Kn = 8.0$

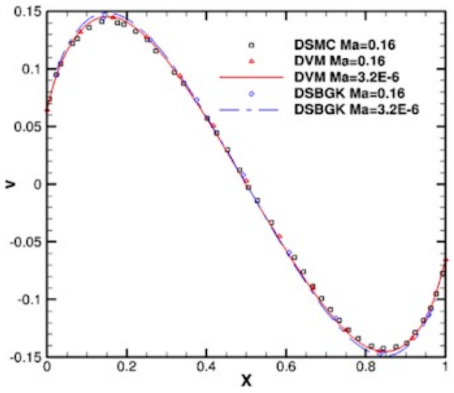
Minimum simulated molecules by DSBGK
10 at $Kn = 0.1$
10 at $Kn = 1.0$
10 at $Kn = 8.0$

[1] MT Ho, J Li, L Wu, JM Reese, YH Zhang, *Computers & Fluids*, **181**: 143-159, 2019.

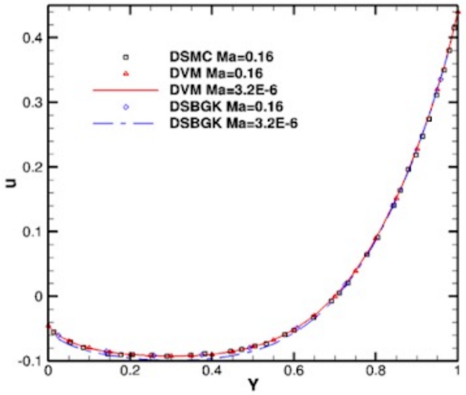
2D cases:
$Kn = 0.1, 1, 8$
$Ma = 0.16, 3.2\times10^{-6}$



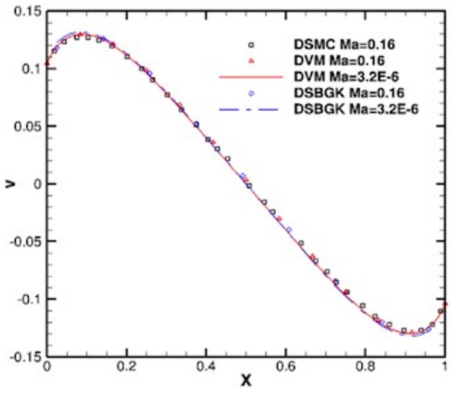
(a) u at Kn= 0.1



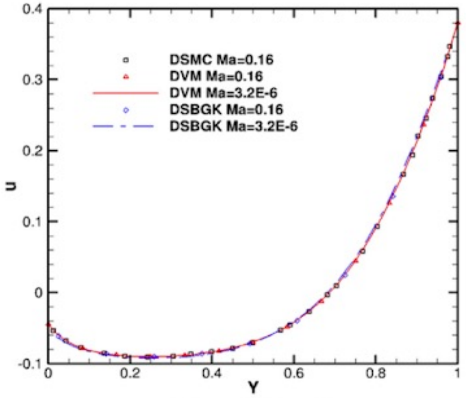
(b) v at Kn= 0.1



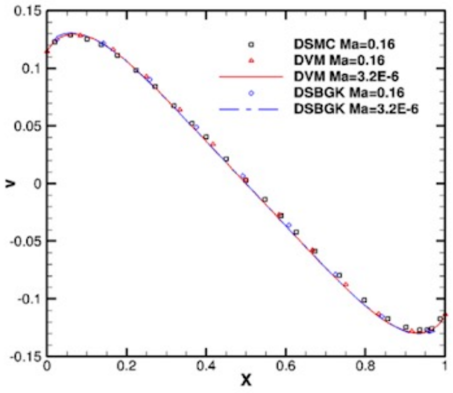
(c) u at Kn= 1



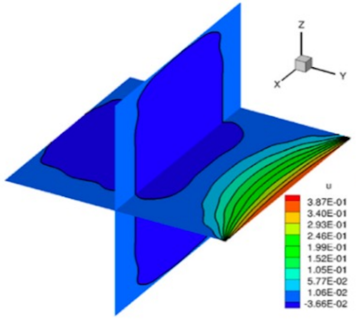
(d) v at Kn= 1



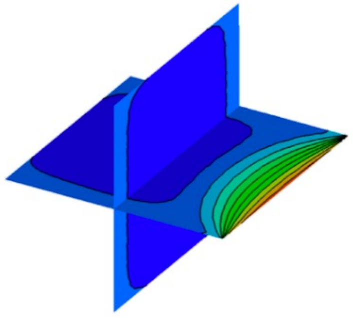
(e) u at Kn= 8

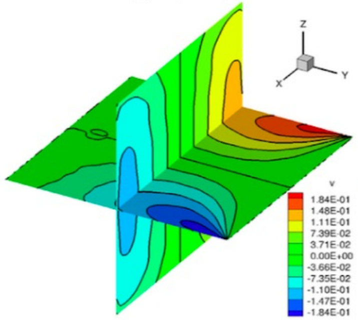


(f) v at Kn= 8

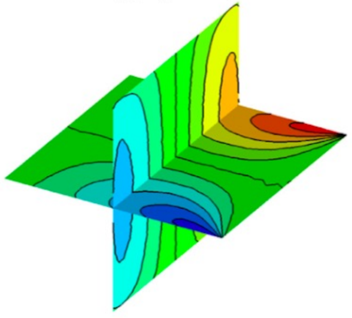


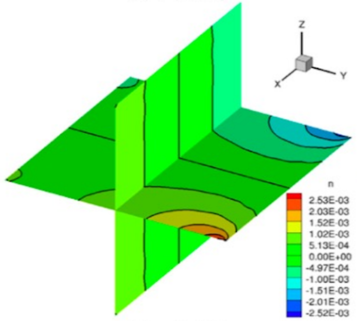
(a) u (DVM)


(b) u (DSBGK)

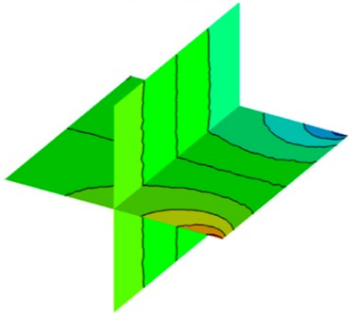


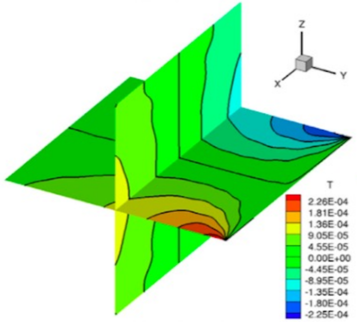
(c) v (DVM)


(d) v (DSBGK)

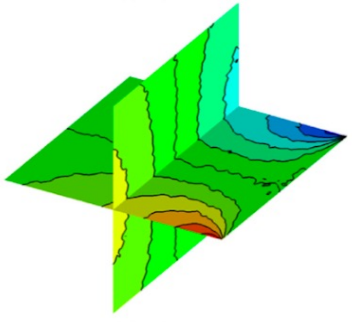


(e) n (DVM)


(f) n (DSBGK)



(g) T (DVM)


(h) T (DSBGK)

3D case:
$Kn = 8$
$Ma = 3.2\times10^{-3}$

Mass flow rate through short channels

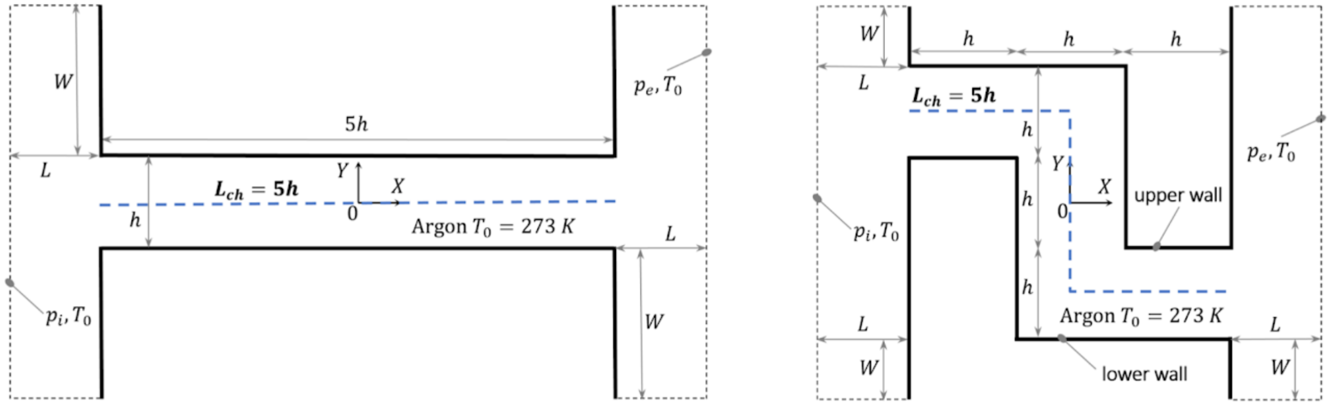
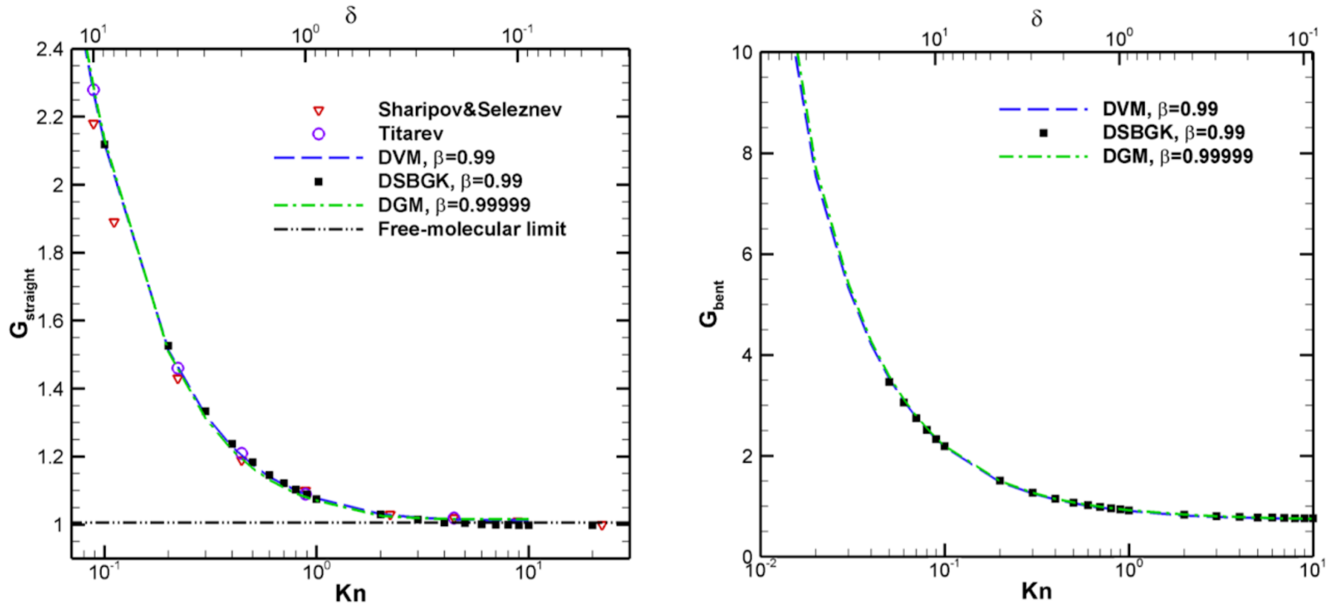


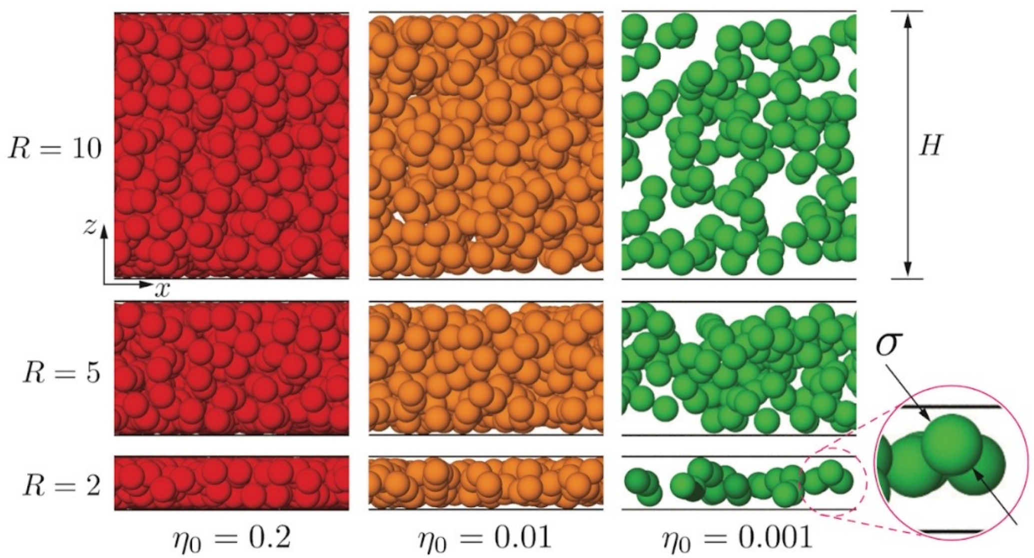
Fig. 1. Pressure-driven gas flows from the left-hand reservoir to the right-hand reservoir through the straight channel (left) and the bent channel (right) of the same height *h* and axis length *L*_ch = 5*h*. Note that only small parts of the reservoirs are illustrated here [12].

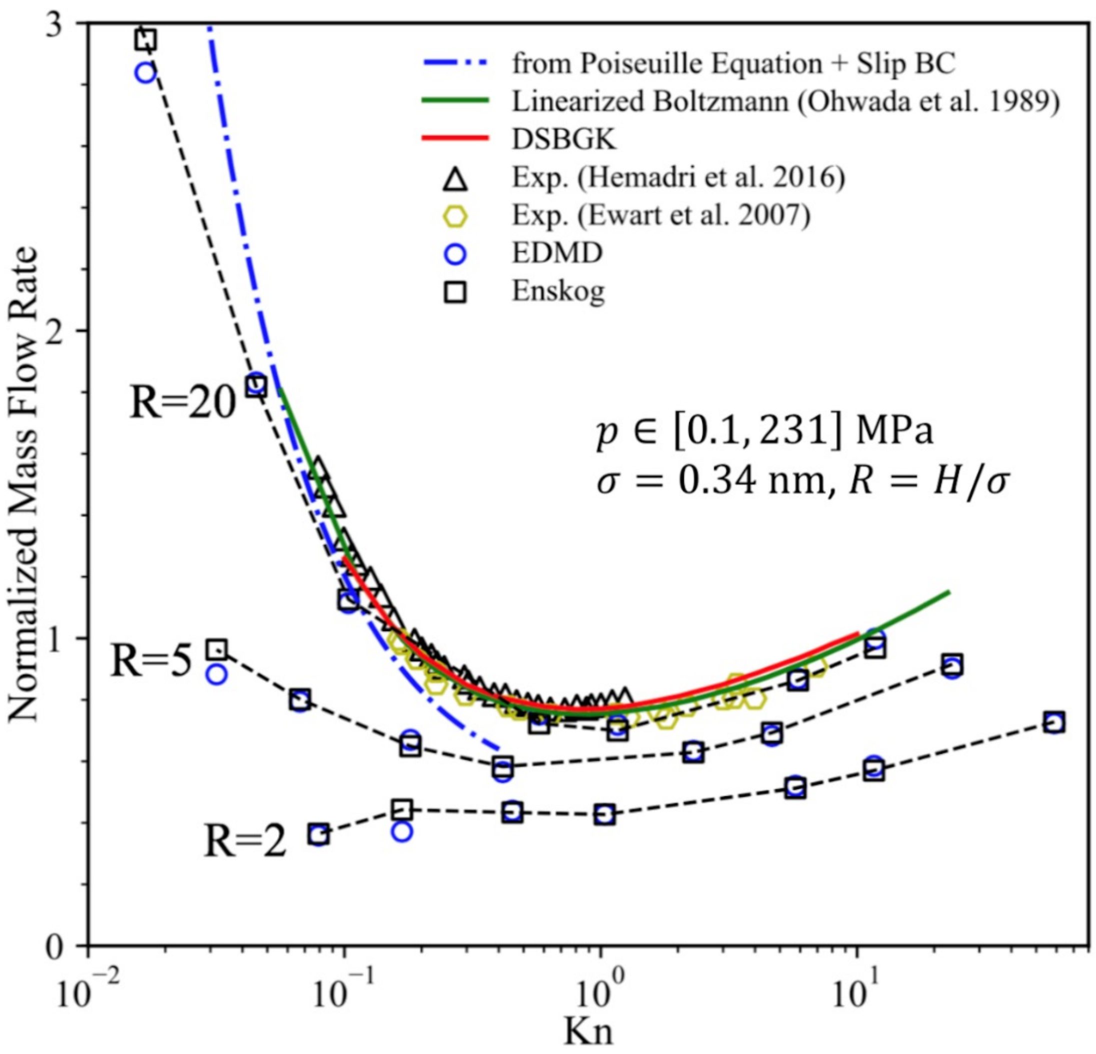


(a) Straight channel (b) Bent channel

[1] MT Ho, J Li, W Su, L Wu, MK Borg, ZH Li, YH Zhang, *Journal of Fluid Mechanics*, **901**: A26, 2020.

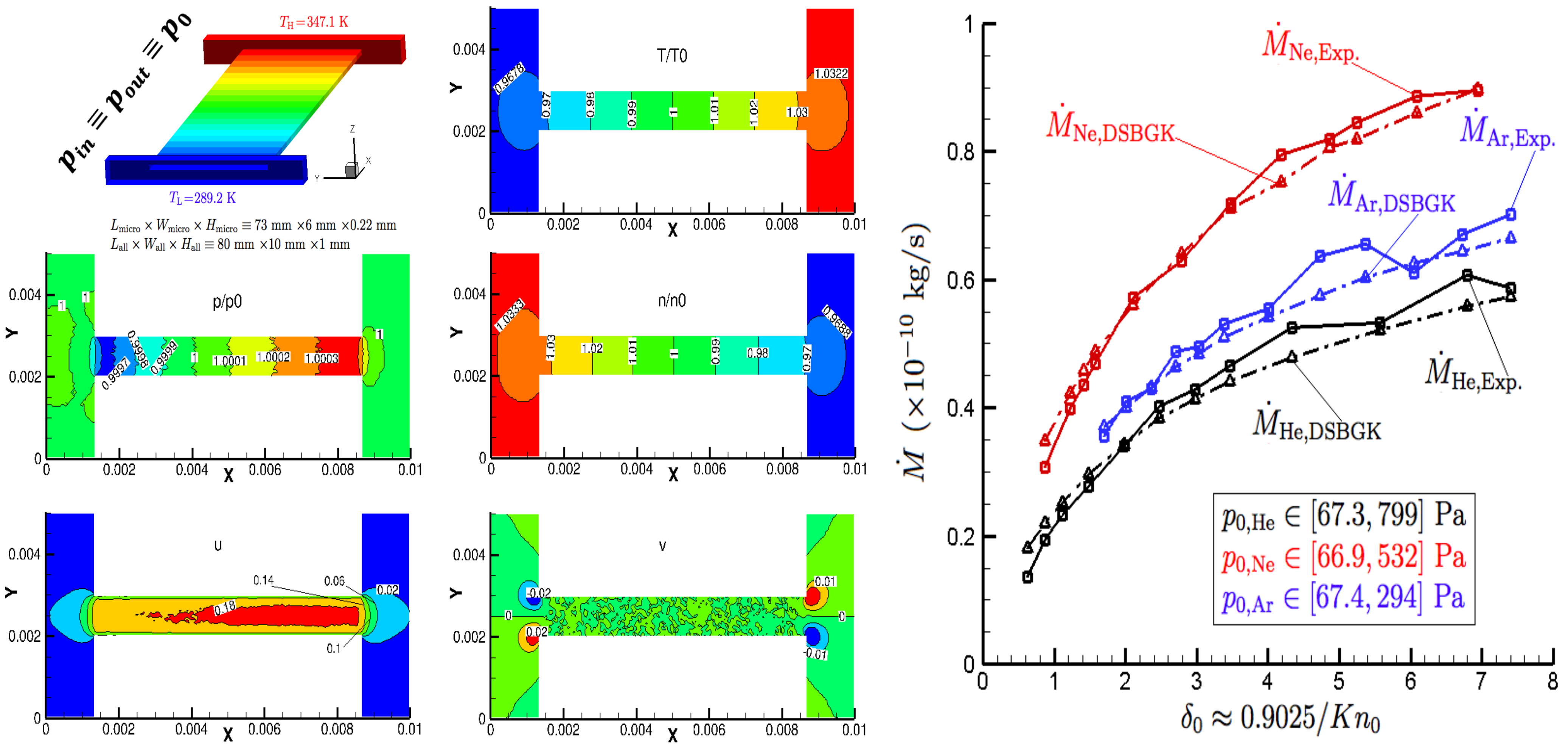
Mass flow rate through nano-channel with confinement





[1] Q Sheng, L Gibelli, J Li, M Borg, YH Zhang, *Physics of Fluids*, **32**: 092003, 2020. (+ more data here)

Thermal transpiration flow

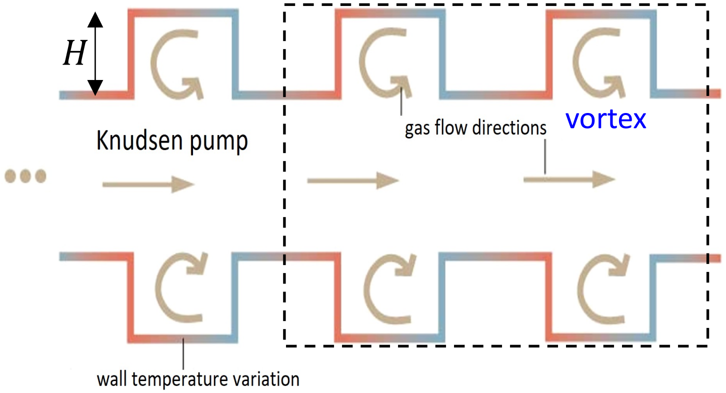


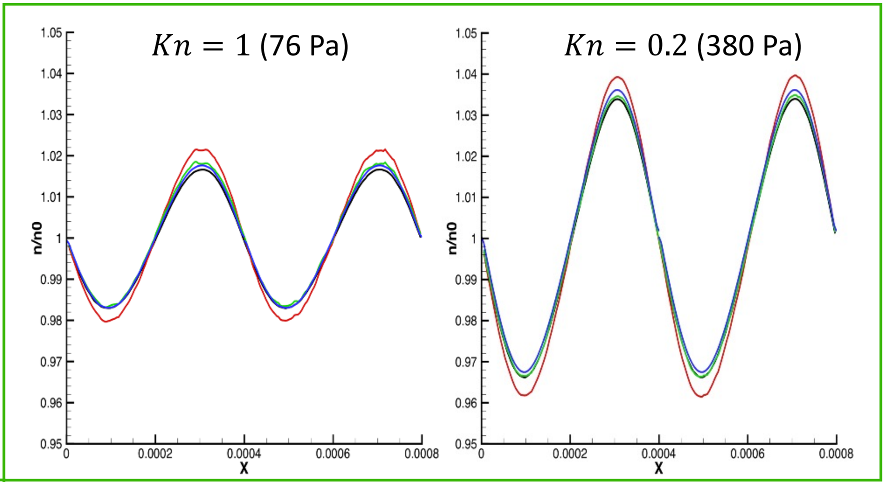
[1] H Yamaguchi, P Perrier, MT Ho, JG Meolans, T Niimi, I Graur, *Journal of Fluid Mechanics*, **795**: 690-707, 2016.

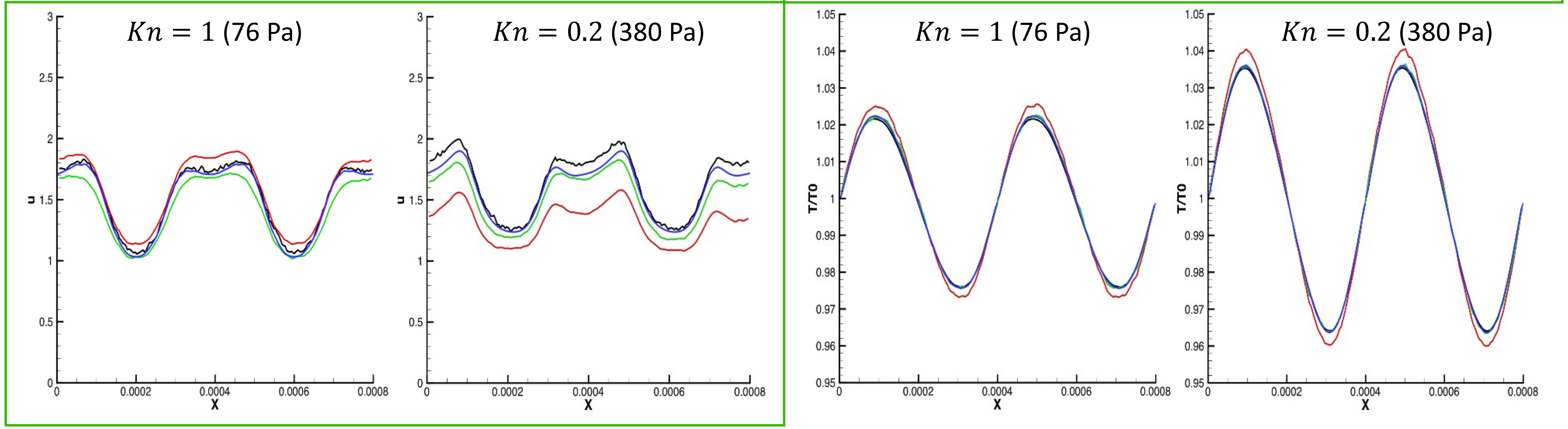
[2] J Li, CP Cai and ZH Li, *International Communications in Heat and Mass Transfer*, **119**: 104924, 2020.

Thermal transpiration flow (cont'd)

Two stages of Knudsen pump with H=100 microns.
Argon: $T_{\min} = 280$ K and $T_{\max} = 340$ K.





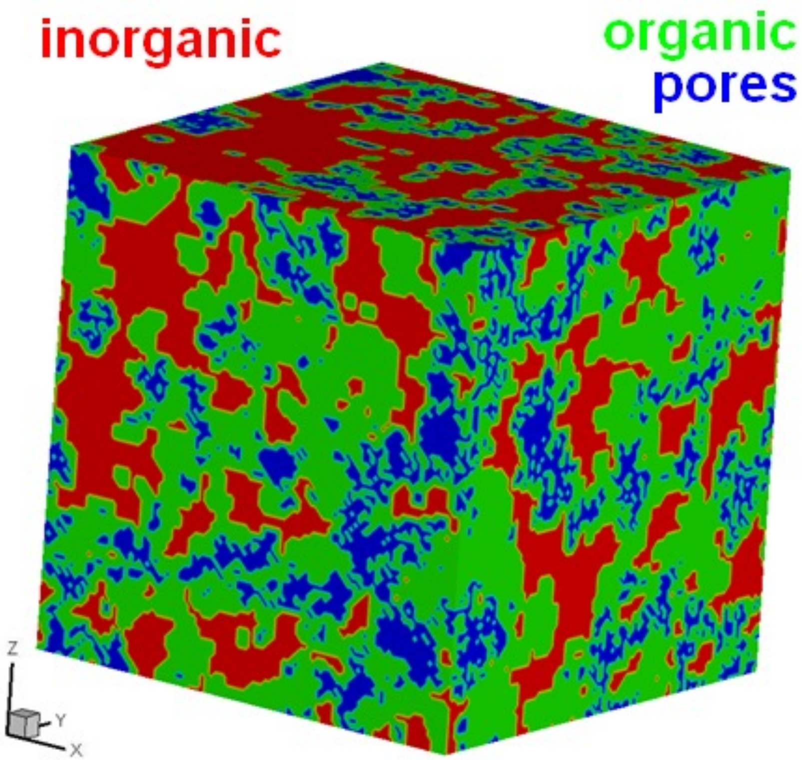


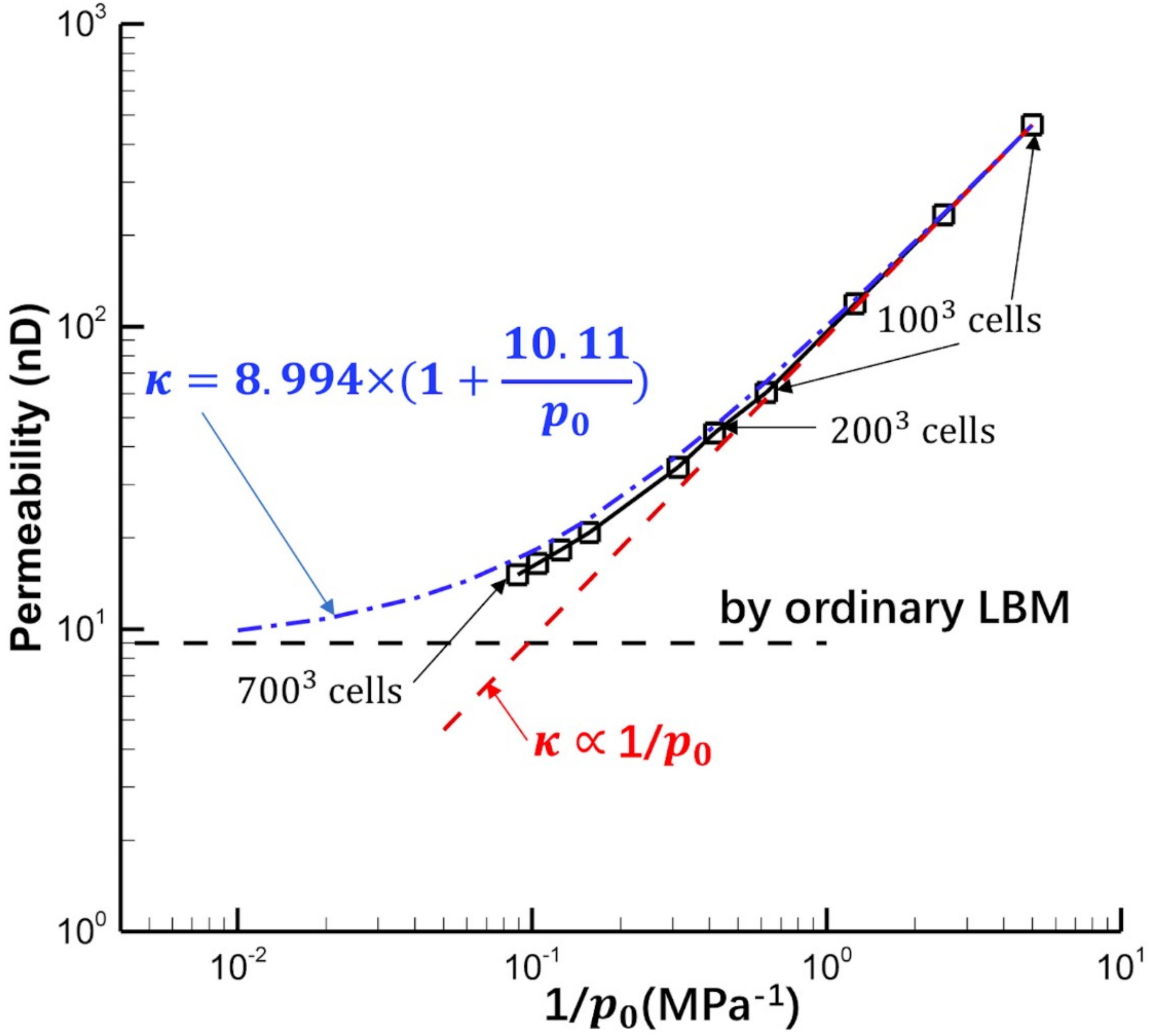
Distributions of n/n_0, T/T_0 and u on the centerline along the x axis obtained by the **DSMC** simulation (black), the **GKUA** simulation based on the Shakhov equation (blue), and the **DSBGK** simulation of using $\tau = \tau(\mu)$ (red) and $\tau = \tau(\eta)$ (green), respectively.

[1] J Li, CP Cai and ZH Li, *International Communications in Heat and Mass Transfer*, **119**: 104924, 2020.

Shale gas permeability of a real digital rock

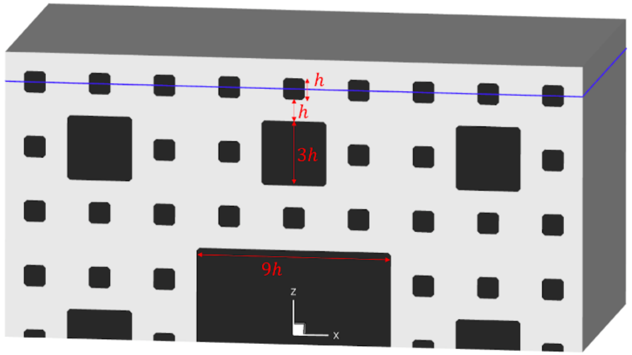
100^3 voxels of size $= 2.82$ nm





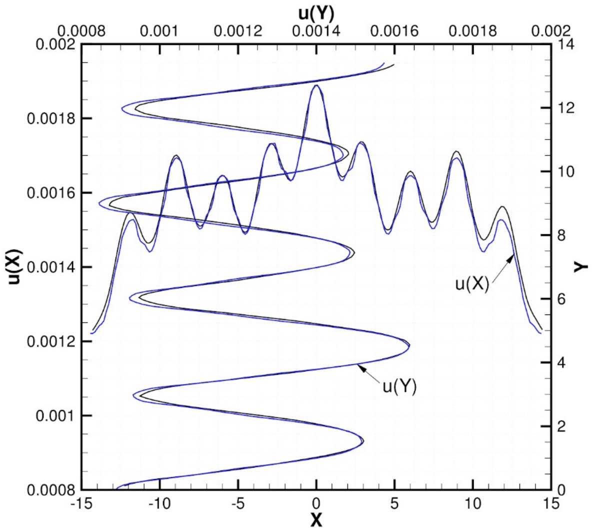
[1] J Li, *Fuel,* **250**: 154-159, 2019.

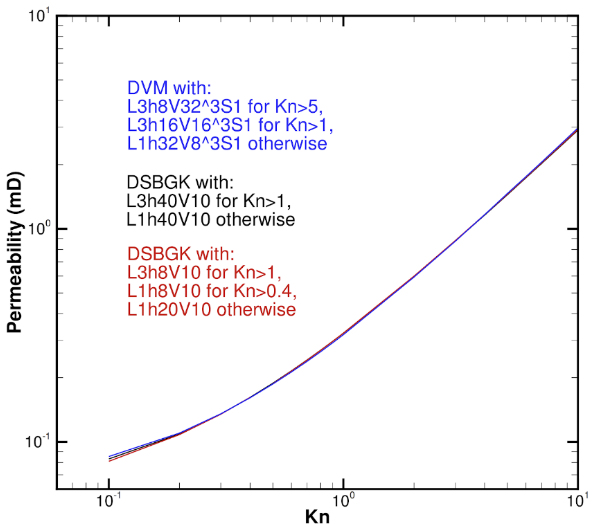
Performance comparison between DSBGK and DVM

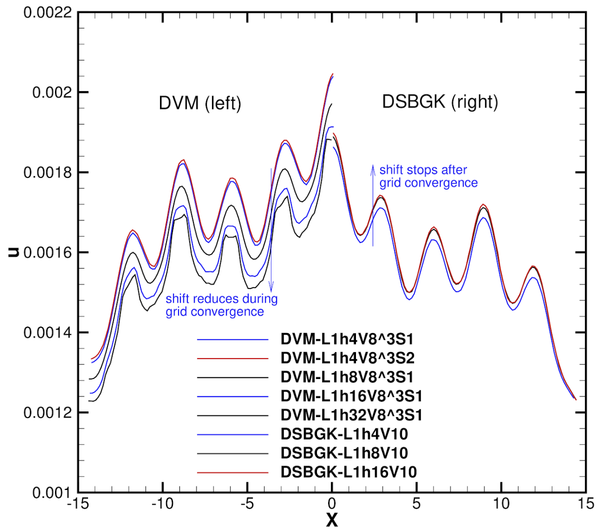


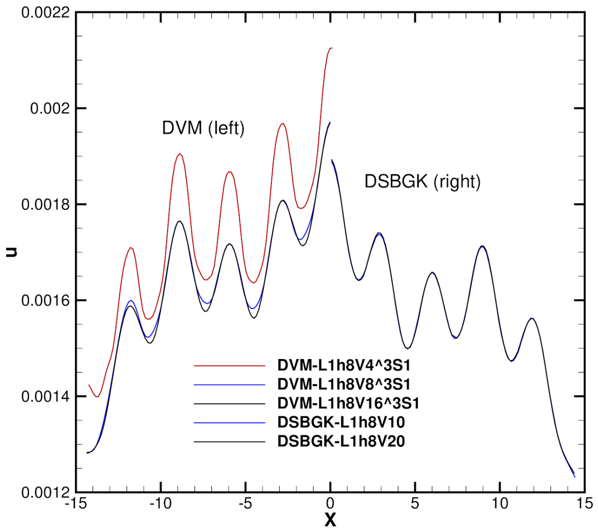
Kn=1 by default

DSBGK	$L0h4V10$	$L3h4V10$	$L1h4V10$	$\boldsymbol{L1h8V10}$	$L1h8V20$
G	0.2125	0.2099	0.2110	0.2126	0.2126
Memory (GB)	0.3060	0.3780	0.3310	2.624	4.570
CPU time (sec)	1729×1	2270×1	1916×1	17518×2	17333×4
DVM	$L1h4V8^3$	$L1h8V8^3$	$L1h8V16^3$	$L1h16V8^3$	$\boldsymbol{L1h32V8^3}$
G	0.2299	0.2204	0.2189	0.2134	0.2090
Memory (GB)	2.304	15.23	110.3	109.6	$\approx 7 \times 109.6$
CPU time (sec)	60.09×8	488.8×8	4759×8	3410×8	4770×64









Minimum cost by **DVM** : 767 GB memory, 2^3×8 CPU cores and 4770×64 seconds of CPU time

Minimum cost by **DSBGK**: 2.6 GB memory, 2 CPU cores and 17518×2 seconds of CPU time

[1] J Li, MT Ho, MK Borg, CP Cai, ZH Li, YH Zhang, *Computers & Fluids*, **226**: 105017, 2021.

Comparison with other kinetic methods

DVM vs. other deterministic methods:

- DVM adopted in our performance comparison is cheaper than its variants for $Kn > 0.01$
- Only for continuum regime of $Kn < 0.01$, UGKS/DUGKS/GSIS can use coarser spatial grids, and GSIS can also use less iteration steps (see [1], [2], [3])

DSBGK vs. other statistical particle methods:

- DSBGK uses much less averaging samples than LVDSMC (see [4] and [5])
- DSBGK uses much, much less averaging samples than DSMC at low speeds (obviously)

Fortran MPI solver based on DSBGK:

- More info @ https://sites.google.com/view/nanogassim/welcome

[1] P Wang, MT Ho, L Wu, ZL Guo, YH Zhang, *Computers & Fluids*, **161**: 33-46, 2018.

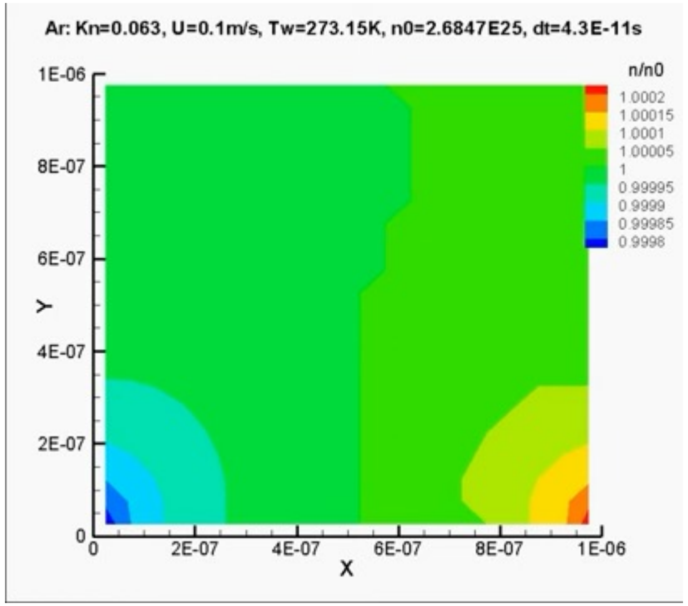
[2] Q Gu, MT Ho, YH Zhang, *Computers & Fluids*, **222**: 104932, 2021.

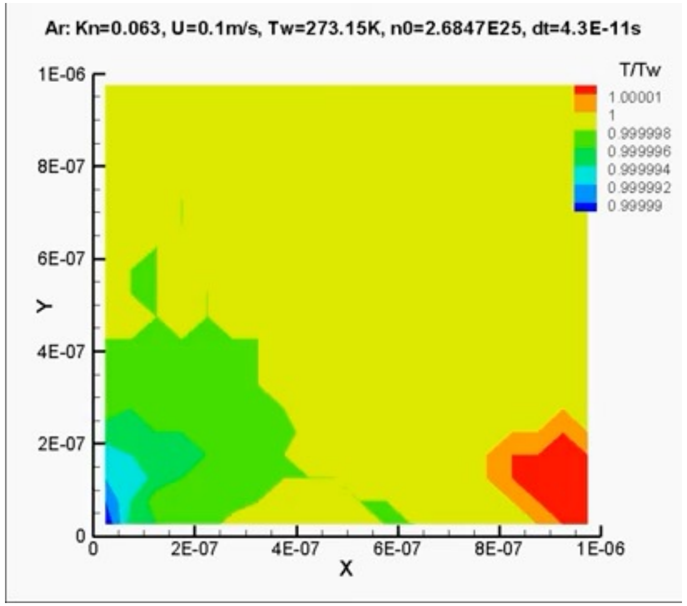
[3] W Su, MT Ho, YH Zhang, L Wu, *Computers & Fluids*, **206**: 104576, 2020.

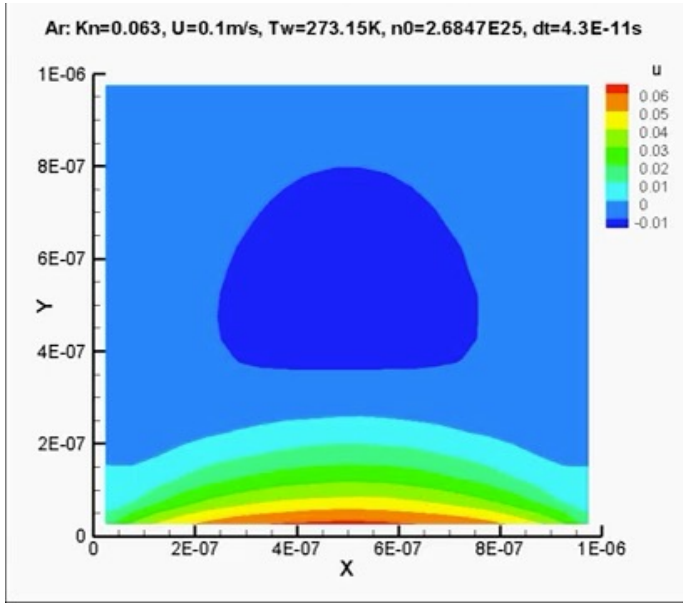
[4] FD Bosco, YH Zhang, *Transport in Porous Media*, **138**: 25-48, 2021.

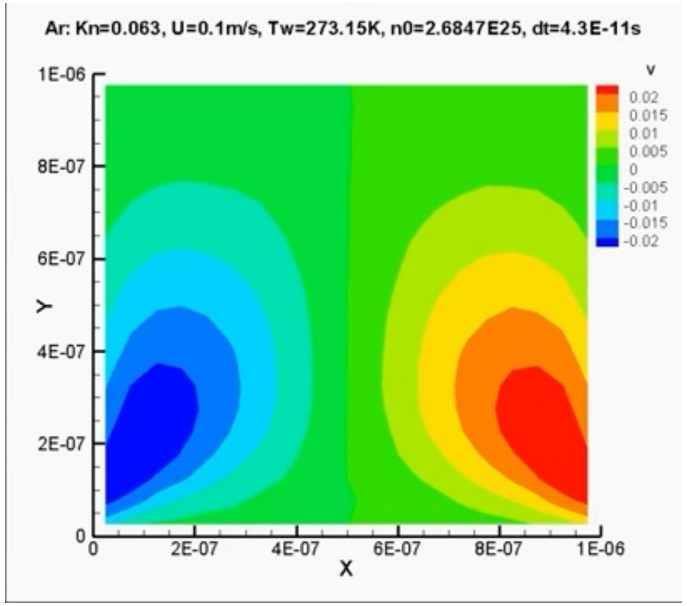
[5] J Li, MT Ho, MK Borg, CP Cai, ZH Li, YH Zhang, *Computers & Fluids*, **226**: 105017, 2021.

Lid-driven cavity flow (video online)

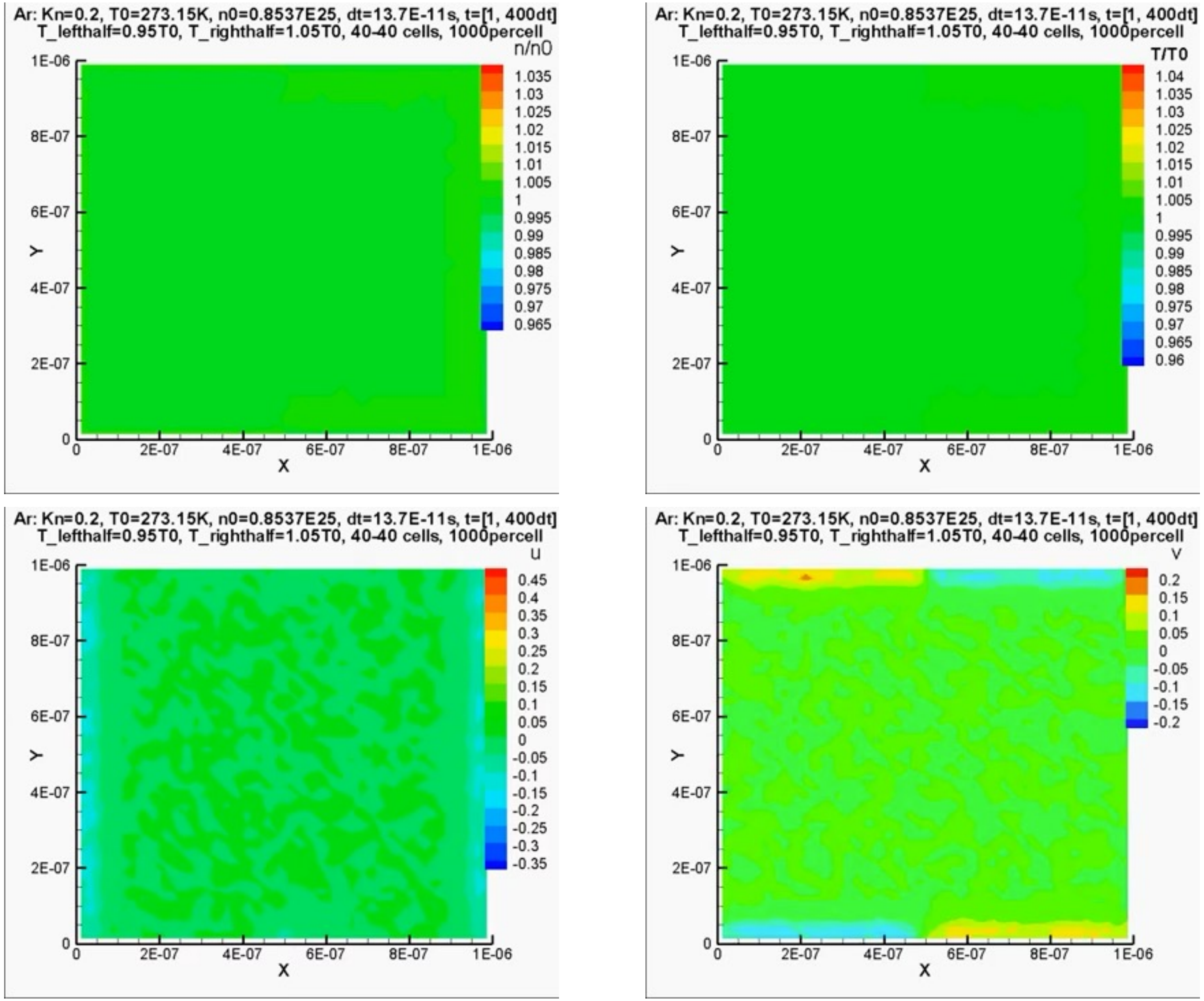




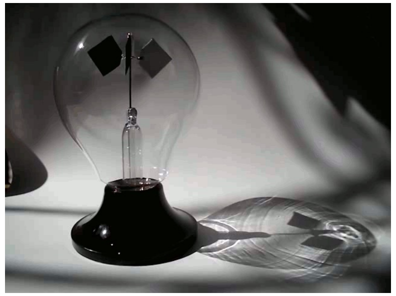




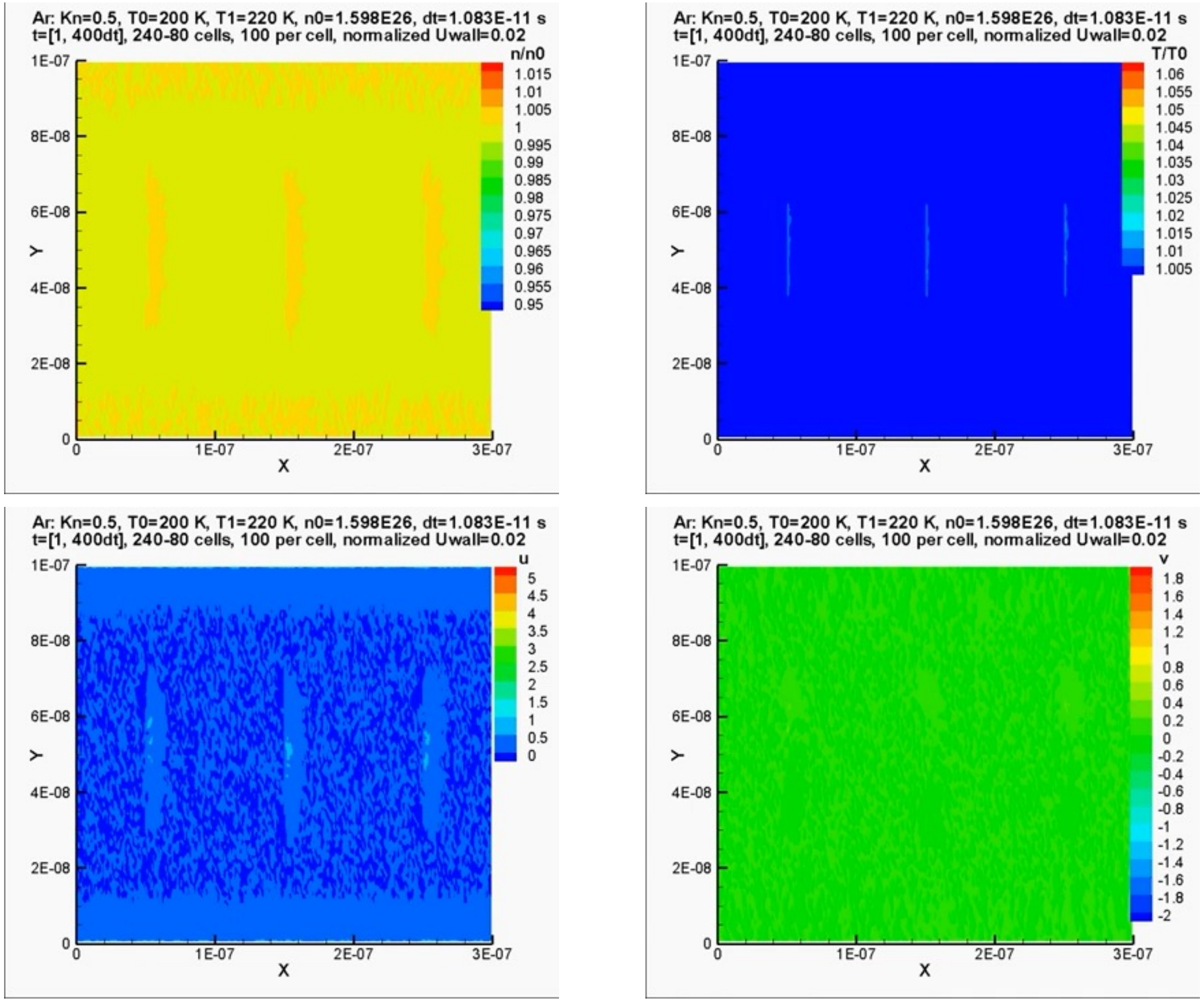
Thermal transpiration flow (video online)



Radiometer flow (video online)



from Wikipedia



Thank you