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Low-variance Deviational Monte Carlo Simulation for Applications in Nanotechnology

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DSMC11, Santa Fe

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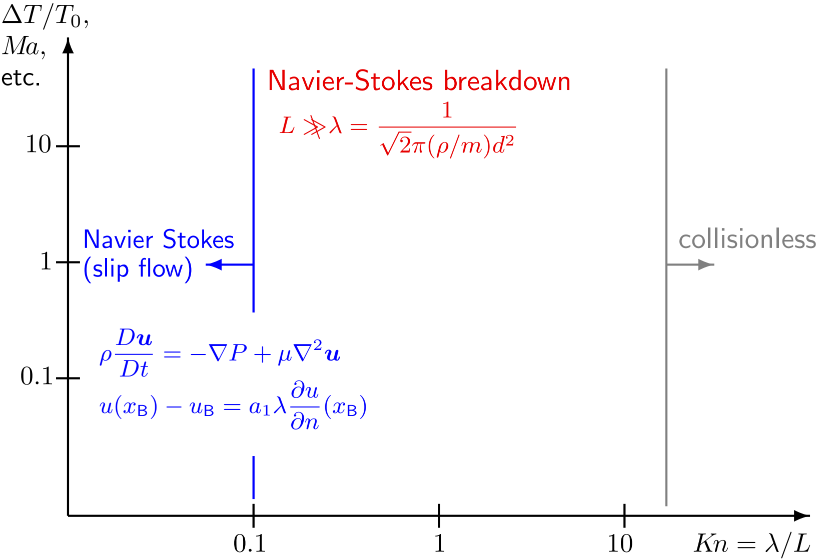
Motivation:

Efficient simulation of molecular gas transport



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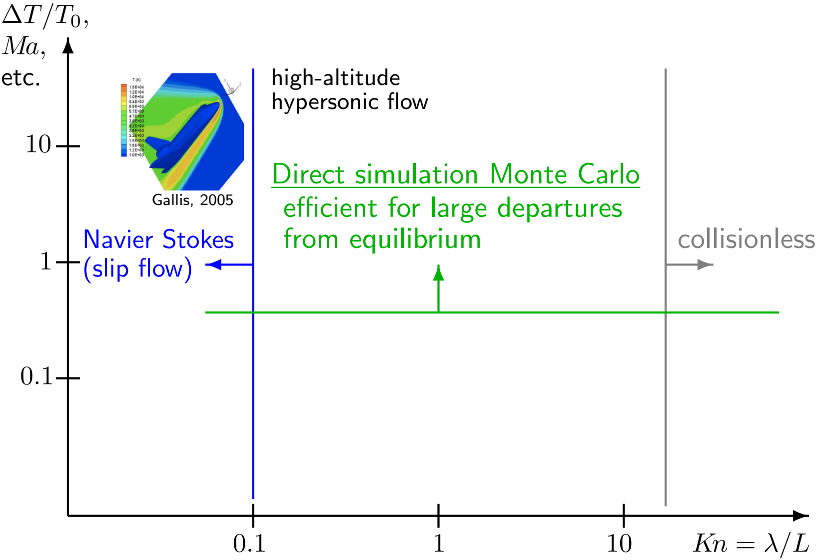

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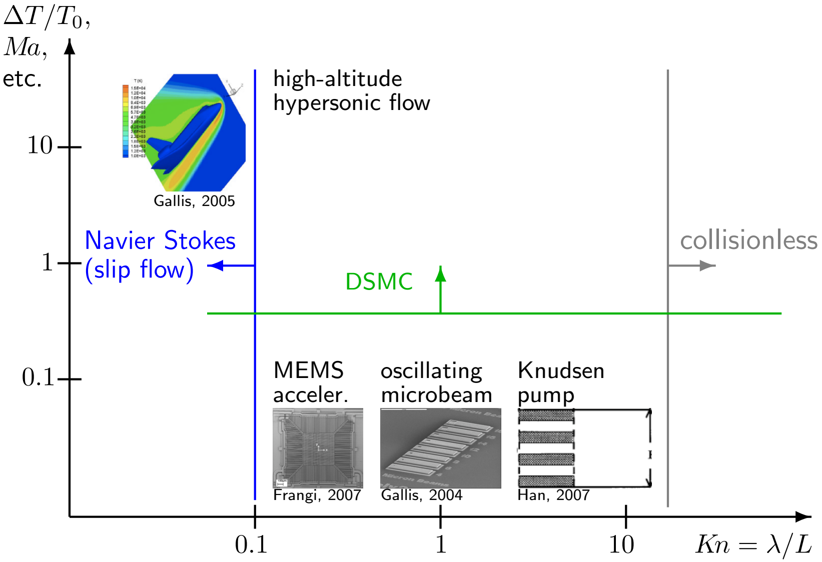

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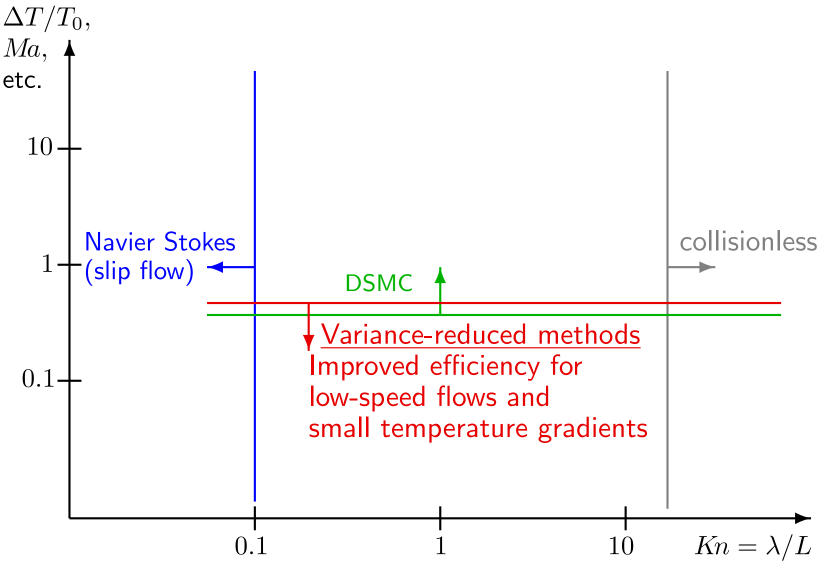
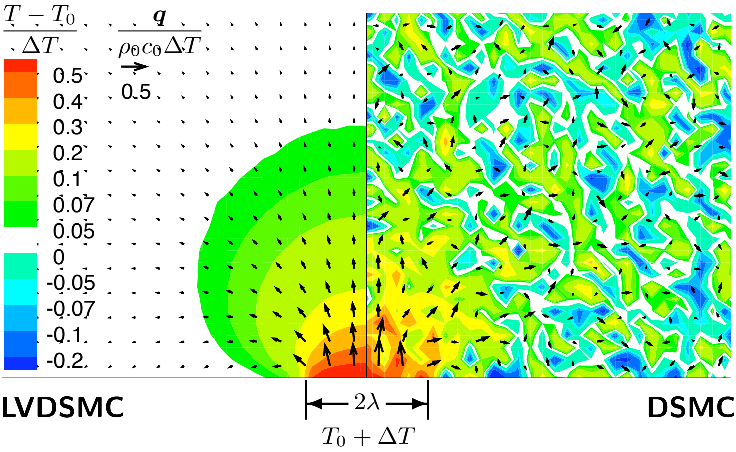


Inefficiency of the DSMC method

Example: transient temperature response of argon gas



$$\boxed{\frac{\Delta T}{T_0} = 0.01 \qquad \frac{c_0 t}{\lambda} = 10}$$

Outline

Relative statistical uncertainty in the hydrodynamic variables[2]

$$\frac{\sigma_{u_x}}{|u_{x,0}|} = \frac{1}{\sqrt{N_\mathsf{C} N_\mathsf{ens}}} \frac{1}{Ma\sqrt{\gamma}}, \quad \frac{\sigma_T}{\Delta T} = \frac{1}{\sqrt{N_\mathsf{C} N_\mathsf{ens}}} \frac{\sqrt{k_\mathsf{B}/c_\mathsf{V}}}{\Delta T/T_0}, \quad \text{etc.}$$

- Small departure from equilibrium ($Ma \ll 1$, $\Delta T/T_0 \ll 1$, etc.) leads to high levels of statistical noise.

Low variance deviational simulation Monte Carlo

- Deviational particle approach: simulate $f^\mathrm{d} = f - f^\mathsf{eq}$
- Leads to constant relative uncertainty in the limit of small departure from equilibrium

[2] Hadjiconstantinou et al., *J. Comp. Phys.*, 2003

Variance reduced particle methods:

A brief history

Deviational particle approach

- Unstable, requires particle cancellation

  Baker & Hadjiconstantinou (2005)

  Baker & Hadjiconstantinou (2006)

Low-variance deviational simulation Monte Carlo (LVDSMC)

- Exploits structure of the collision operator to achieve stability
- Hard sphere:
  Homolle & Hadjiconstantinou (2007)
- BGK model:
  Radtke & Hadjiconstantinou (2009)
  Hadjiconstantinou, et al. (2009)
- VHS model:
  Wagner (2007)
  Radtke, et al. (2010, 2011)

Alternative approaches:

Linearized distribution using weights

- Unstable for hard sphere, requiring particle cancellation

  Chun & Koch (2005)

Direct variance reduction of DSMC (VRDSMC)

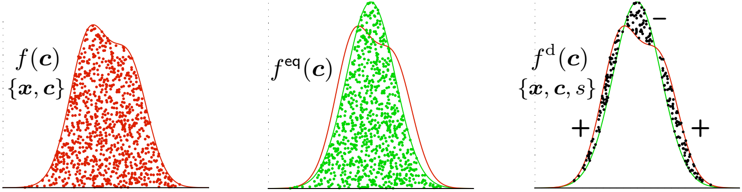
- Kernel density estimation required for stability, resulting in bias error

  Al-Mohssen & Hadjiconstantinou (2010)

LVDSMC simulation method:

Deviational particle approach

Deviational particle approach: $f^{\mathrm{d}} = f - f^{\mathrm{eq}}$



DSMC simulation — equilibrium distribution — deviational simulation

(*differences are exaggerated*)

Fixed equilibrium

$$f^0 = \frac{\rho_0}{\pi^{3/2} c_0^3} \exp\left[-\frac{||\boldsymbol{c} - \boldsymbol{u}_0||^2}{c_0^2}\right]$$

$$c_0 = \sqrt{2RT_0}$$

constant properties:

ρ_0, $\boldsymbol{u}_0$, T_0

Spatially-variable equilibrium

$$f^{\mathrm{MB}} = \frac{\rho_{\mathrm{MB}}}{\pi^{3/2} c_{\mathrm{MB}}^3} \exp\left[-\frac{||\boldsymbol{c} - \boldsymbol{u}_{\mathrm{MB}}||^2}{c_{\mathrm{MB}}^2}\right]$$

$$c_{\mathrm{MB}} = \sqrt{2RT_{\mathrm{MB}}}$$

spatially-variable properties:

$\rho_{\mathrm{MB}}(\boldsymbol{x})$, $\boldsymbol{u}_{\mathrm{MB}}(\boldsymbol{x})$, $T_{\mathrm{MB}}(\boldsymbol{x})$

LVDSMC simulation method:

Advection step

Boltzmann equation

$$\underbrace{\frac{\partial f}{\partial t} + \boldsymbol{c} \cdot \frac{\partial f}{\partial \boldsymbol{x}}}_{\text{advection}} = \underbrace{\frac{1}{m} \int_{\mathcal{S}^2} \mathrm{d}^2\boldsymbol{\Omega} \int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{c}_* \, \sigma \, c_\mathrm{r} \left(f' f'_* - f f_* \right)}_{\text{collision}}$$

Advection step for deviational particles

Fixed equilibrium $f^{eq} = f^0$

$$\frac{\partial f^\mathrm{d}}{\partial t} + \boldsymbol{c} \cdot \frac{\partial f^\mathrm{d}}{\partial \boldsymbol{x}} = 0$$

- Deviational particles advect like DSMC particles

  $\boldsymbol{x}_i \rightarrow \boldsymbol{x}_i + \boldsymbol{c}_i \Delta t$

Variable equilibrium $f^{eq} = f^{MB}$

$$\frac{\partial f^\mathrm{d}}{\partial t} + \boldsymbol{c} \cdot \frac{\partial f^\mathrm{d}}{\partial \boldsymbol{x}} = -\boldsymbol{c} \cdot \frac{\partial f^\mathrm{MB}}{\partial \boldsymbol{x}}$$

- Additional particles generated at cell interfaces

  $$\left[\frac{\partial f^\mathrm{d}}{\partial t} \right]_\mathrm{int} \propto c_n \left[f_-^\mathrm{MB} - f_+^\mathrm{MB} \right]$$

  Inefficient for simulating multiple spatial dimensions

LVDSMC simulation method:

Collision step for the BGK collision model

Bhatnagar-Gross-Krook (BGK) collision model

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} \approx -\frac{f - f^{\text{loc}}}{\tau}; \quad f^{\text{loc}} = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left[-\frac{||\boldsymbol{c}-\boldsymbol{u}||^2}{2RT}\right]$$

Fixed equilibrium distribution[3]

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} \Delta t = \underbrace{\frac{\Delta t}{\tau}(f^{\text{loc}} - f^0)}_{\text{particle generation}} \underbrace{-\frac{\Delta t}{\tau} f^{\text{d}}}_{\text{particle deletion}}$$

- Simple, easy to implement
- Particle sink term provides stability

[3] Hadjiconstantinou, Radtke, and Baker, *J. Heat Trans.*, 2010

Bhatnagar-Gross-Krook (BGK) collision model

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} \approx -\frac{f - f^{\text{loc}}}{\tau}; \quad f^{\text{loc}} = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left[-\frac{||\boldsymbol{c} - \boldsymbol{u}||^2}{2RT}\right]$$

Spatially-variable equilibrium distribution

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} \Delta t = \underbrace{\frac{\Delta t}{\tau}(f^{\text{loc}} - f^{\text{MB}}) - \Delta f^{\text{MB}}}_{\text{particle generation}} \underbrace{+\Delta f^{\text{MB}}}_{\text{change in equilibrium}} \underbrace{-\frac{\Delta t}{\tau} f^{\text{d}}}_{\text{particle deletion}}$$

- Δf^{MB} chosen to eliminate the lower order moments of particle generation distribution

$$\begin{bmatrix} \Delta\rho_{\text{MB}} \\ \Delta\boldsymbol{u}_{\text{MB}} \\ \Delta T_{\text{MB}} \end{bmatrix} = \frac{\Delta t}{\tau} \begin{bmatrix} \rho - \rho_{\text{MB}} \\ \boldsymbol{u} - \boldsymbol{u}_{\text{MB}} \\ T - T_{\text{MB}} \end{bmatrix}$$

- f^{MB} approaches local equilibrium state: consistent with physics inherent in BGK (relaxation-time) model
- Highly efficient for continuum limit ($Kn \to 0$)

LVDSMC simulation method:

Collision step for the BGK collision model

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Spatially-variable equilibrium distribution: linearized version[4]

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} \Delta t = \underbrace{\frac{\Delta t}{\tau}\left(f^{\text{loc}} - f^{\text{MB}}\right) - \Delta f^{\text{MB}}}_{\text{particle generation } \to 0} \underbrace{+\Delta f^{\text{MB}}}_{\text{change in equilibrium}} \underbrace{-\frac{\Delta t}{\tau} f^{\text{d}}}_{\text{particle deletion}}$$

- In the linearized regime ($Ma \ll 1$, $\Delta T \ll T_0$, etc.), no particle generation required
- Simplified collision step
- Highly-efficient overall method for 1D transport

[4] Radtke and Hadjiconstantinou, *Phys. Rev. E*, 2009

Simulation example:

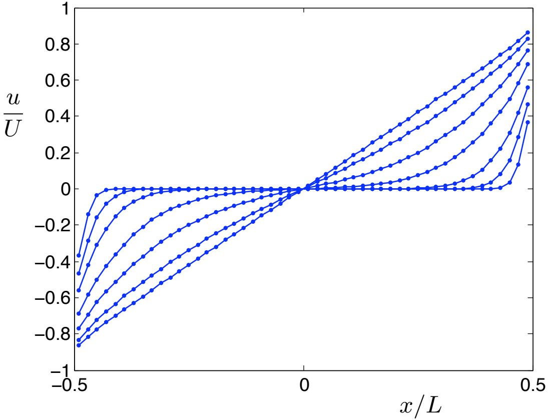
- BGK, spatially-variable equilibrium distribution
- Transient shear problem

Details

- $Kn = 0.1$
- $u\left(\pm\frac{L}{2}\right) = \mp U$

  $U \ll c_0$

CPU time:
70 sec. (3.0 GHz)



DSMC11

G. Radtke

Motivation

Outline

Introduction

Stat. error

VR Methods

LVDSMC

Advection

BGK Coll.

VHS Coll.

Applications

Temp. jump

Kn pumps

Conclusion

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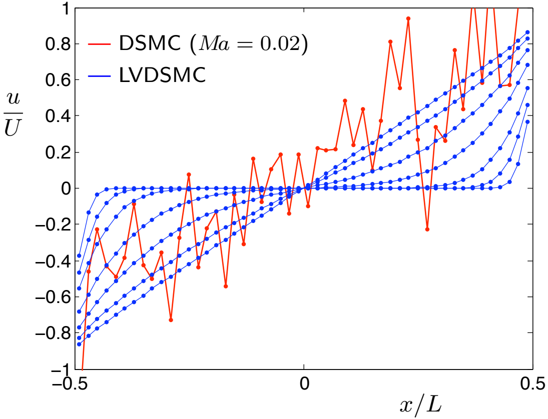
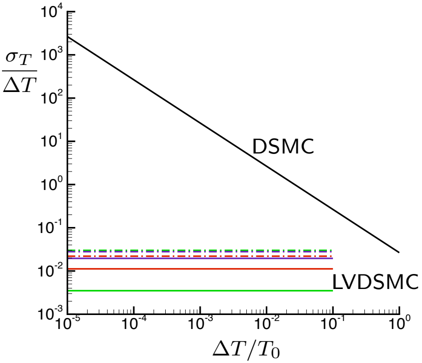


Numerical efficiency:

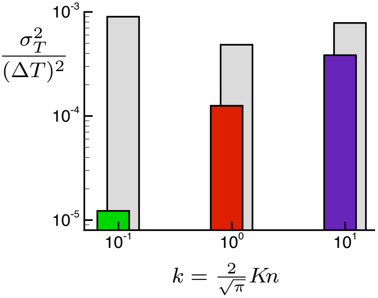
BGK LVDSMC methods

Statistical error in temperature LVDSMC vs. DSMC



- For a single cell in the center of the simulation containing ≈ 950 particles (all methods)

LVDSMC: fixed vs. spatially-variable equilibrium



- Gray: fixed equilibrium
- Colors: spatially-variable equilibrium

VHS collision model

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} = C_\beta \int_{\mathcal{S}^2} \mathrm{d}^2\boldsymbol{\Omega} \int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{c}_* \, c_\mathrm{r}^\beta \left(f' f'_* - f f_*\right)$$

Deviational collision step ($f^\mathrm{d} = f - f^0$)

$$\left[\frac{\partial f}{\partial t}\right]_{\text{coll}} = \underbrace{\mathcal{L}[f^\mathrm{d}]}_{\text{linear part}} + \underbrace{\mathcal{Q}[f^\mathrm{d}, f^\mathrm{d}]}_{\text{nonlinear part}}$$

Linear part[5]

$$\mathcal{L}[f^\mathrm{d}] = \int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{c}_* \left[2K^{(1)} - K^{(2)}\right](\boldsymbol{c}, \boldsymbol{c}_*) \, f^\mathrm{d}_* - \nu f^\mathrm{d}$$

$$K^{(1)}(\boldsymbol{c}, \boldsymbol{c}_*) = \frac{4C_\beta}{||\boldsymbol{c} - \boldsymbol{c}_*||} \int_{\Gamma_\perp(\boldsymbol{c} - \boldsymbol{c}_*)} \mathrm{d}^3\boldsymbol{\zeta} \, \frac{f^0(\boldsymbol{c} + \boldsymbol{\zeta})}{||\boldsymbol{c} - \boldsymbol{c}_* - \boldsymbol{\zeta}||^{1-\beta}}$$

$$K^{(2)}(\boldsymbol{c}, \boldsymbol{c}_*) = 4\pi C_\beta ||\boldsymbol{c} - \boldsymbol{c}_*||^\beta f^0$$

$$\nu(\boldsymbol{c}) = 4\pi C_\beta \int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{c}_* ||\boldsymbol{c} - \boldsymbol{c}_*||^\beta f^0_*$$

[5] Cercignani, 1969; Wagner, *Monte Carlo Meth. Appl.*, 2008; etc.

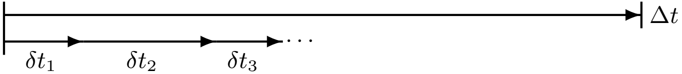
LVDSMC simulation method:

Collision step for the VHS collision model

Linear part of the VHS collision operator

$$\mathcal{L}[f^{\mathrm{d}}] = \underbrace{\int_{\mathcal{R}^3} \mathrm{d}^3\boldsymbol{c}_* \left[2K^{(1)} - K^{(2)}\right](\boldsymbol{c}, \boldsymbol{c}_*)\, f_*^{\mathrm{d}}}_{\text{particle generation}} \qquad \underbrace{-\nu f^{\mathrm{d}}}_{\text{particle deletion}}$$

Markov jump processes[6]



particle generation and deletion events processed during stochastic collision time steps

Initial implementation

Radtke, Hadjiconstantinou, and Wagner, *RGD* 27, 2010

Mass-conservative version

Radtke, Hadjiconstantinou, and Wagner, *Phys. Fluids*, 2011

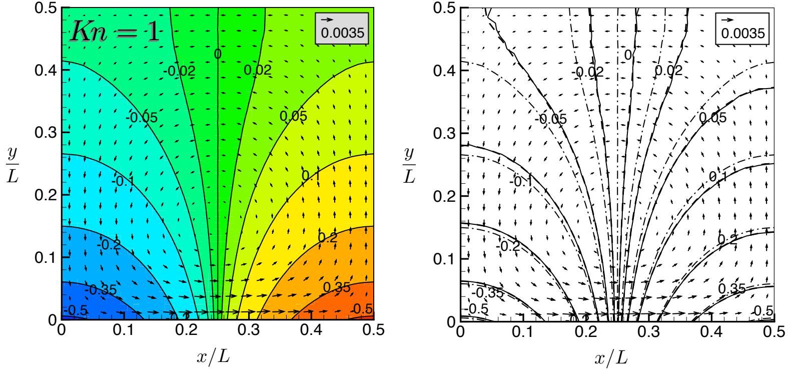
- Simulations with ~ 10 particles per cell, without random walks in the hydrodynamic variables!

[6] Wagner, *Monte Carlo Meth. Appl.*, 2008

Validation: mass-conservative, VHS

Response of argon gas to spatially-varrying boundary temperature

$\Delta T \to 0$ $\quad$ $\Delta T = 0.05T_0$



Contour: $(T - T_0)/\Delta T$

Vector: $\dfrac{\boldsymbol{u}/c_0}{\Delta T/T_0}$

$- \cdot -$ $\Delta T \to 0$

$- - -$ LVDSMC

—— DSMC

Applications:

Second-order temperature jump

Second-order jump boundary condition

$$T\left(x_{\mathrm{B}}\right)-T_{\mathrm{B}}=b_1\lambda\frac{\mathrm{d}T}{\mathrm{d}n}\left(x_{\mathrm{B}}\right)+b_2\lambda^2\frac{\mathrm{d}^2T}{\mathrm{d}n^2}\left(x_{\mathrm{B}}\right)$$

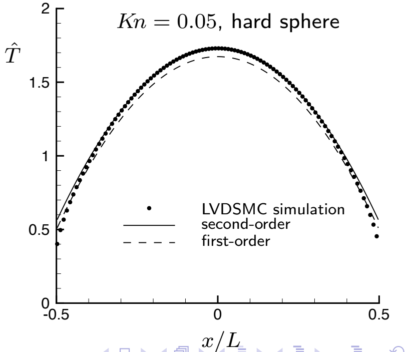
Internal heat generation problem

$$-K\frac{\mathrm{d}^2T}{\mathrm{d}x^2}=\dot{q}'''$$

- b_1 is known (Sone, 2007)
- b_2 can be calculated using LVDSMC

  Radtke, Hadjiconstantinou, Takata, and Aoki, *in preparation*

  Takata, Aoki, Hattori, and Hadjiconstantinou, *in preparation*



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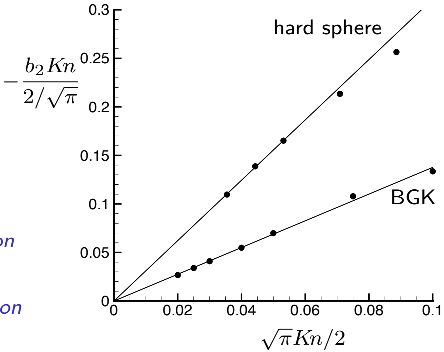
Parameter fit

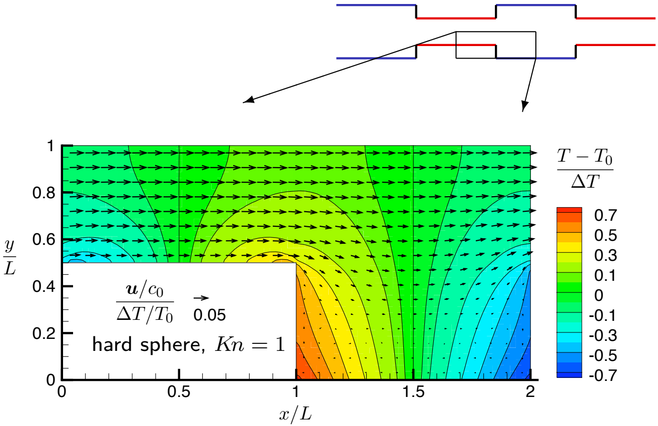


Applications:

Simulation of Knudsen pumps

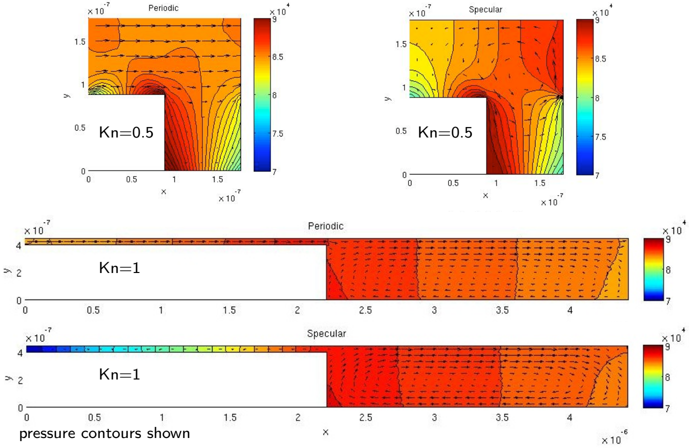
LVDSMC approach:

able to efficiently resolve the $\Delta T/T_0 \to 0$ limit.



Study of Kn pump performance for different configurations

T. A. Klein, MIT SM Thesis, *in progress*.



pressure contours shown

BGK particle simulation methods

- Fixed equilibrium: most efficient for general multi-dimensional geometries
- Spatially-variable equilibrium: highly-efficient for resolving the continuum ($Kn \to 0$) limit

Advanced VHS particle simulation method

- Collisions simulated as Markov jump events without time step error in the collision step
- Extended to include mass conservation, enabling efficient simulation of gas flows with ~ 10 particles per cell

LVDSMC simulation codes available at:

http://web.mit.edu/ngh-group