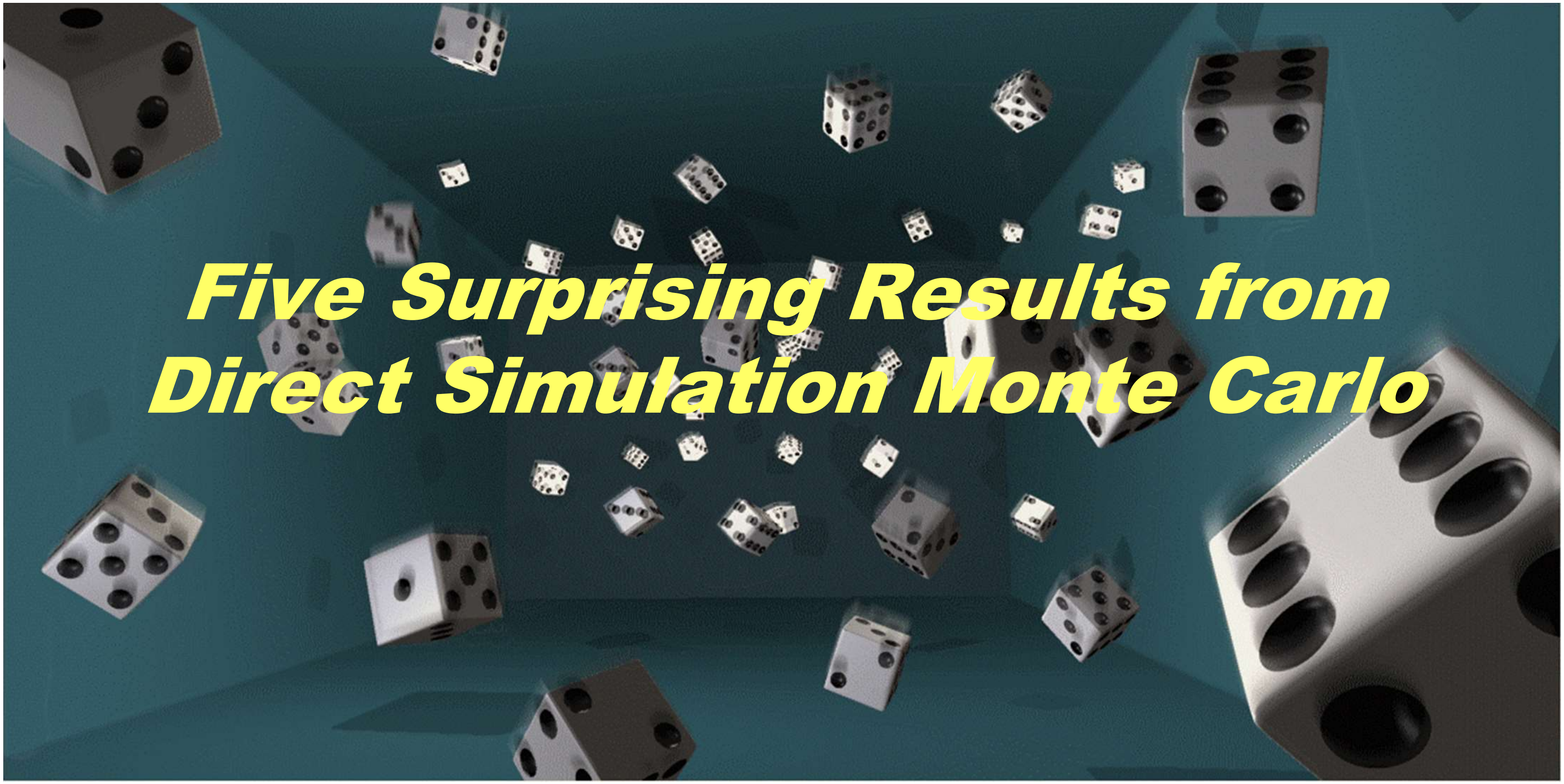


Alejandro L. Garcia

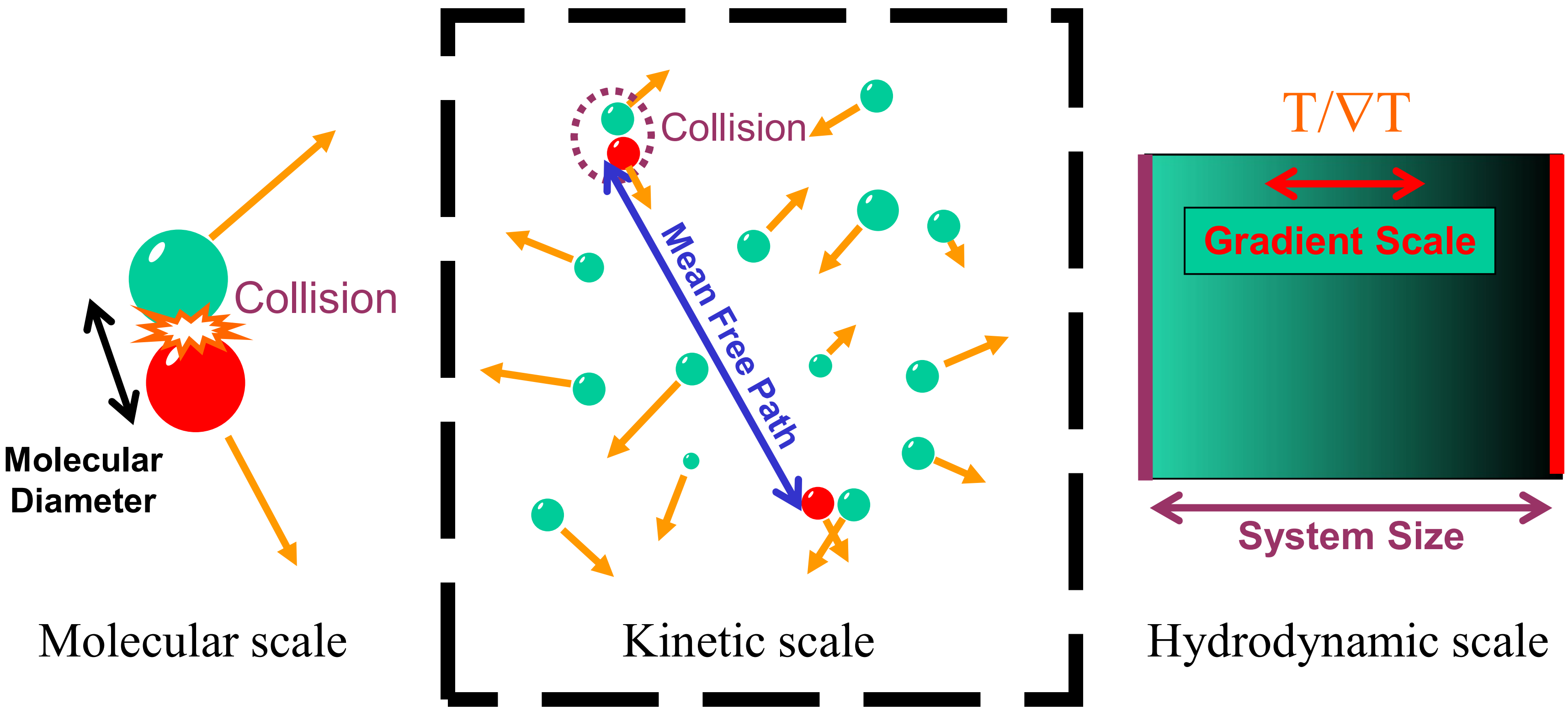
San Jose State University
& Berkeley Lab.

Outline

- Direct Simulation Monte Carlo
- Surprising Poiseuille Flow
- Surprising Couette Flow
- Surprising “Phantom” Flow
- Surprising Diffusive Mixing
- Surprising Brownian Motion

Scales for Dilute Gases

DSMC is the dominant numerical algorithm at the kinetic scale

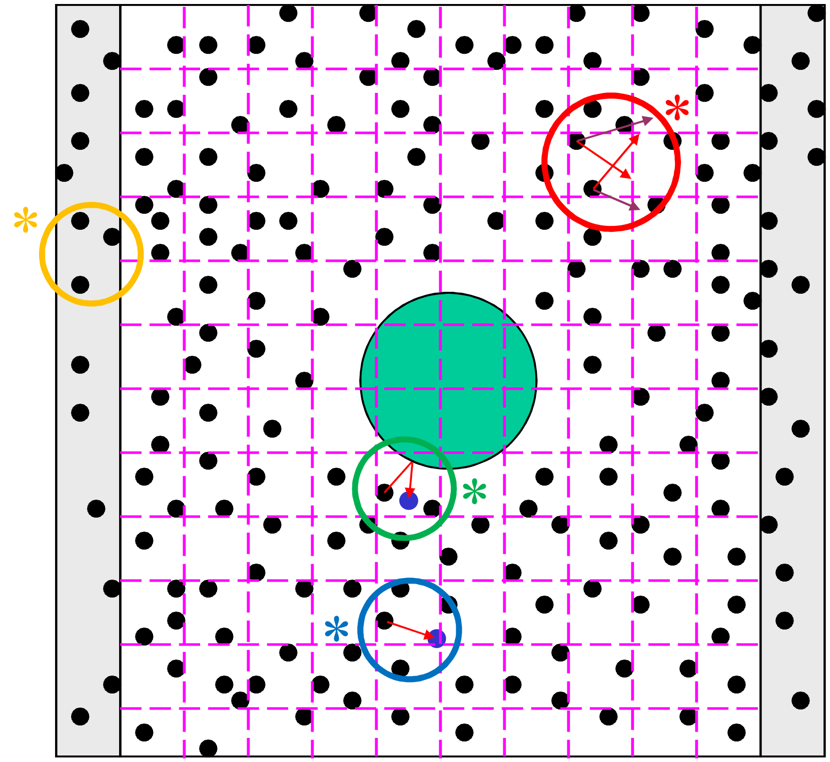


DSMC Algorithm

DSMC resembles MD except in the evaluation of collisions

- Initialize system with particles
- Loop over time steps
  - Create particles at open boundaries *
  - Move *all* the particles *
  - Process any interactions of particle & boundaries *
  - Sort particles into cells
  - Perform random collisions *
  - Sample statistical values

Example: Flow past a sphere

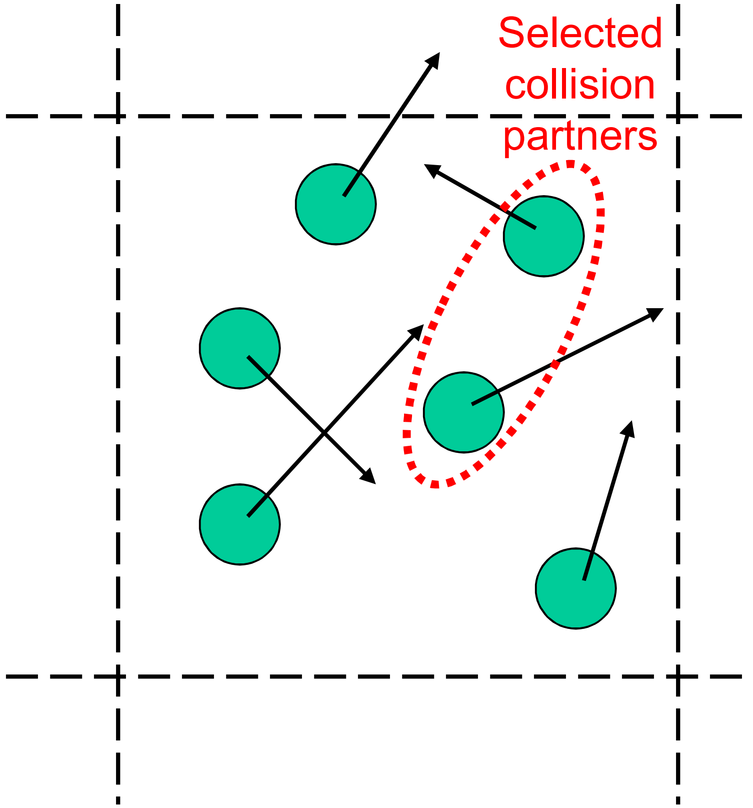


G.A. Bird, *The DSMC Method* (2013)
ALG, *Numerical Methods for Physics* (2015)

Popular public domain codes: dsmcFoam and Sparta

DSMC Collisions

- Sort particles into spatial collision cells
- Loop over collision cells
  - Compute collision frequency in a cell
  - Select random collision partners within cell
  - Process each collision

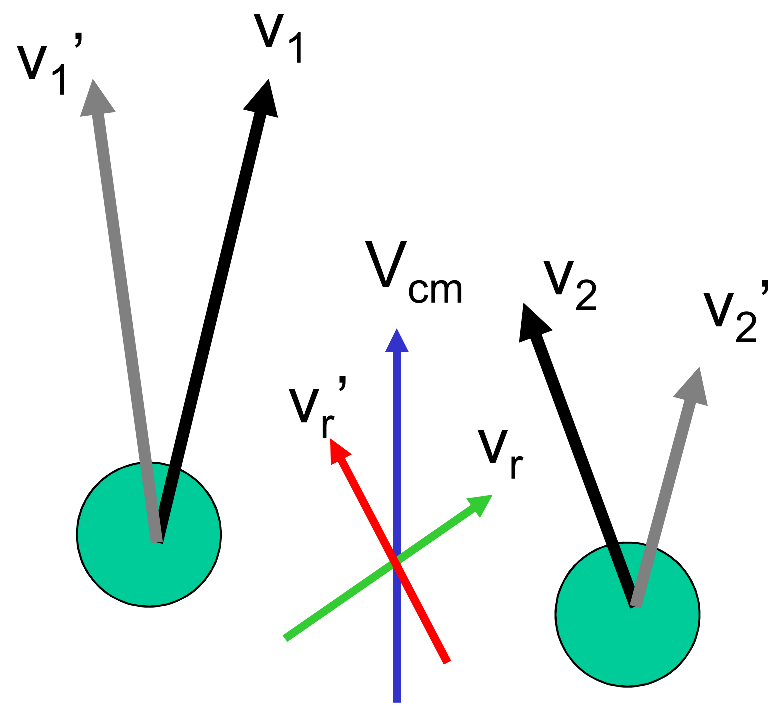


Collision pairs with large relative velocity are more likely to collide but they do *not* have to be on a collision trajectory

Collisions (cont.)

Post-collision velocities (6 variables) given by:

- Conservation of momentum (3 constraints)
- Conservation of energy (1 constraint)
- Random collision solid angle (2 choices)

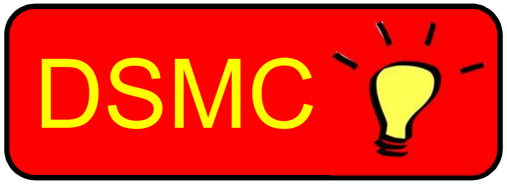


Direction of v_r' is random

Can also model internal molecular energy (e.g., vibrational) as well as chemical reactions (e.g., disassociation)

Discoveries and Confirmations

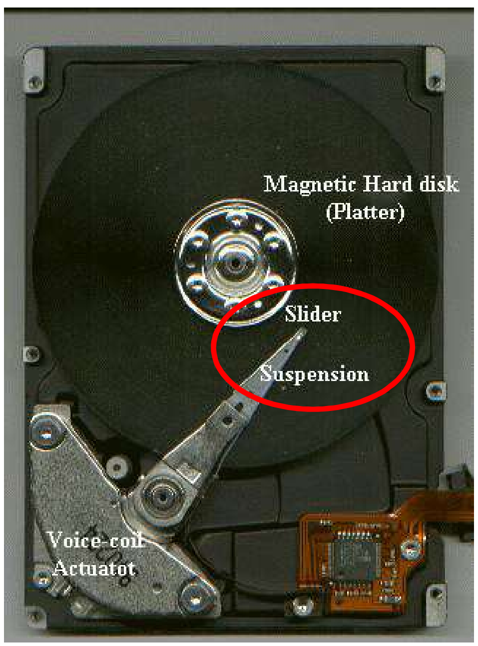
Fluid dynamic effect first discovered by DSMC and later confirmed by theory

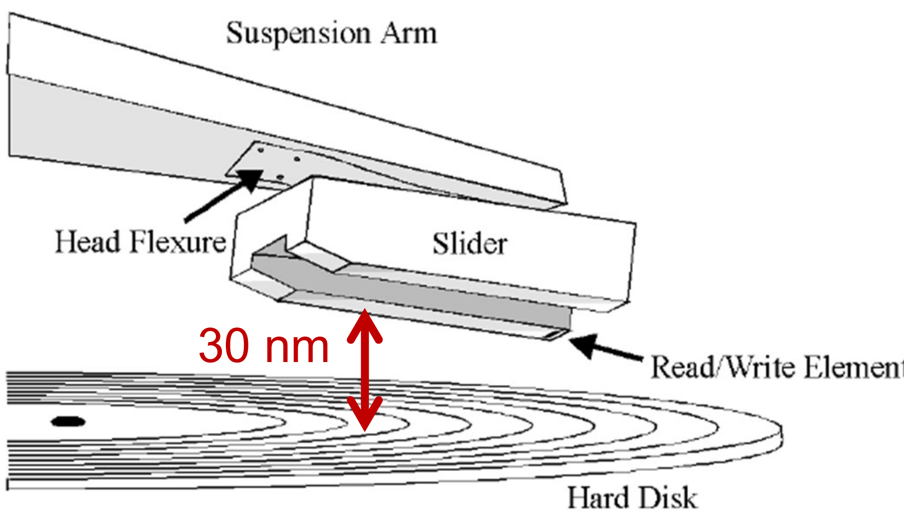


Fluid dynamic effect first predicted by theory and later confirmed by DSMC

Nano-fluidics in Disk Drives

Collision mean free path in air is about 60 nm
Slider (1 mm long) flies about 30 nm above platter



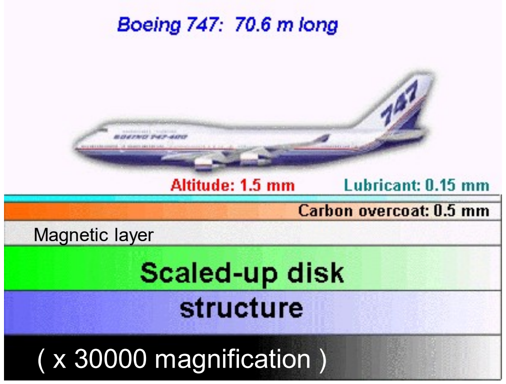


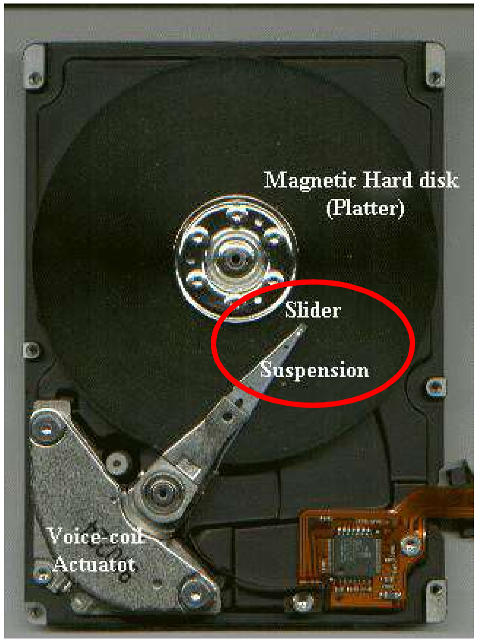
Sensitivity decreases exponentially with height

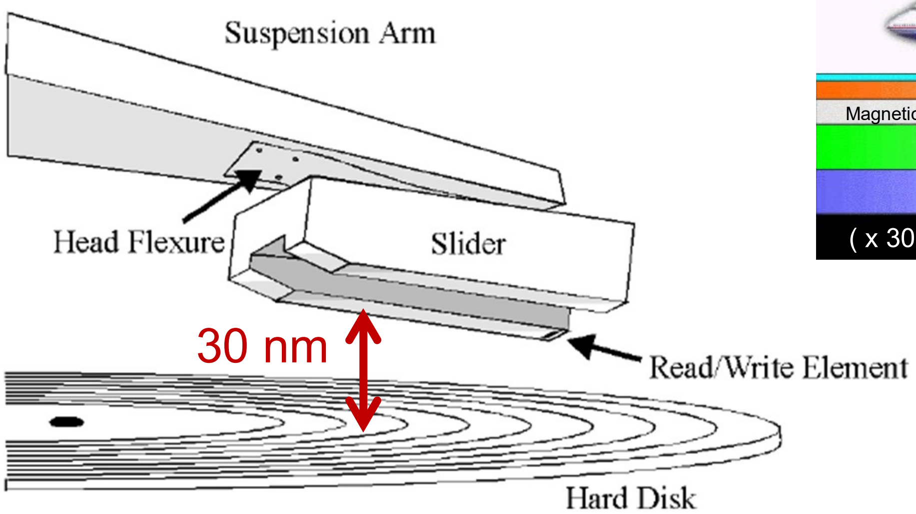
Nano-fluidics in Disk Drives

Collision mean free path in air is about 60 nm
Slider (1 mm long) flies about 30 nm above platter

This is like a 747 flying 1.5 mm above ground.



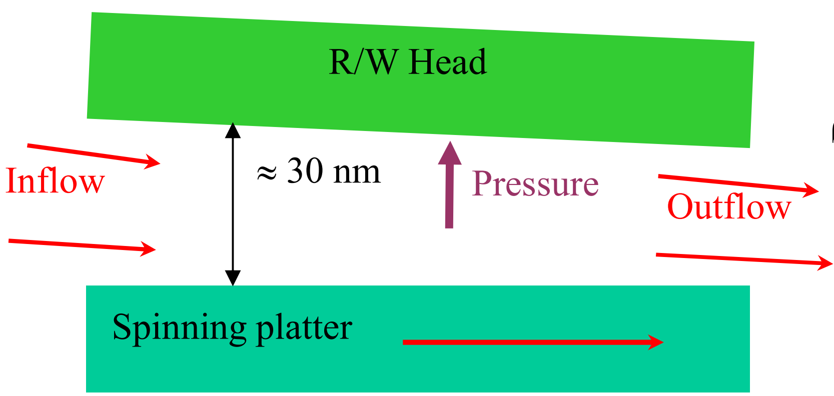


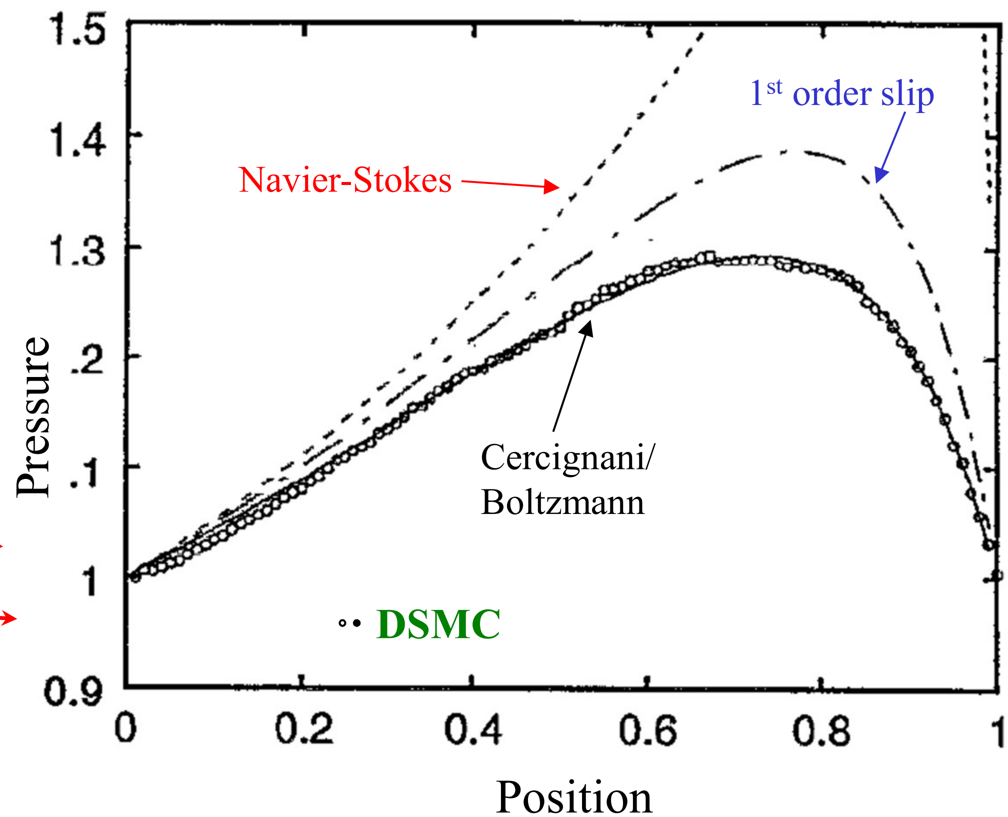


Sensitivity decreases exponentially with height

DSMC Simulation of Air Slider

Flow between platter and read/write head of a disk drive





DSMC✓

F. Alexander, ALG, and B. Alder, *Phys. Fluids* **6** 3854 (1994).

Fluctuations & Measurements

In particle simulations (DSMC, MD, etc.) due to random fluctuations the fractional error in the measured fluid velocity is

$$E_u = \frac{\sigma_u}{|u_x|} = \frac{\sqrt{\langle \delta u_x^2 \rangle} / \sqrt{S}}{|u_x|} \approx \frac{1}{\sqrt{SN}} \frac{1}{\mathrm{Ma}}$$

(from statistical mechanics)

where S is number of samples, Ma is Mach number.

Fluctuations & Measurements

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(from statistical mechanics)

where S is number of samples, Ma is Mach number.

For desired accuracy of E_u = 1% with N = 100 particles per cell

$$S \approx \frac{1}{N\mathrm{Ma}^2 E_u^2} \propto \frac{1}{\mathrm{Ma}^2}$$

$S \approx 10^2$ samples for Ma =1.0 (Aerospace flow)
$S \approx 10^8$ samples for Ma = 0.001 (Microscale flow)

N. Hadjiconstantinou, ALG, M. Bazant, and G. He, *J. Comp. Phys.* **187** 274-297 (2003)

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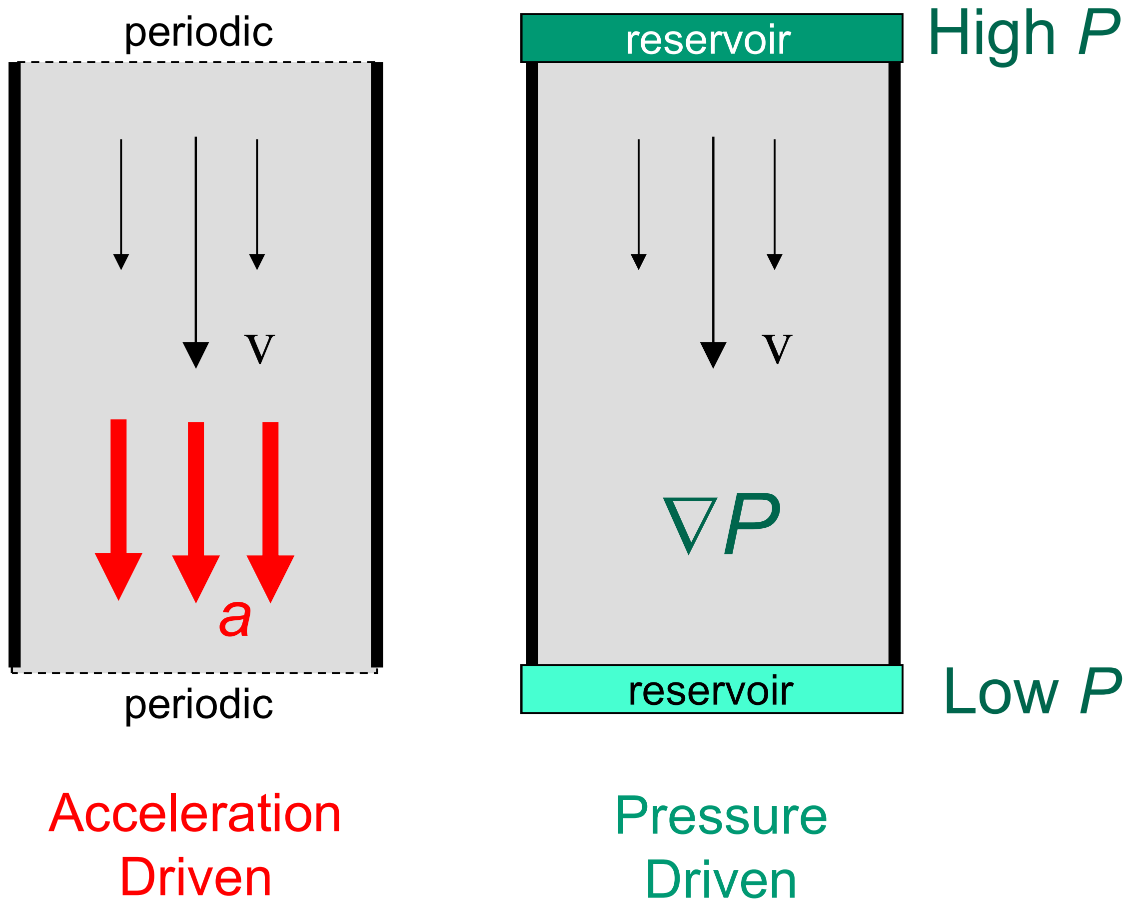
Plane Poiseuille Flow

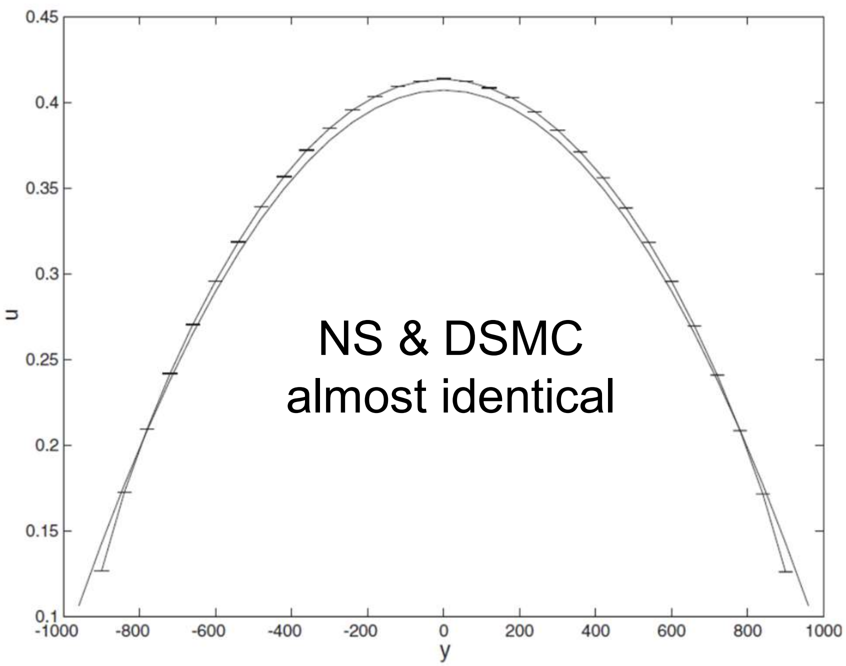
Cause fluid flow as acceleration-driven or as pressure-driven Poiseuille flow



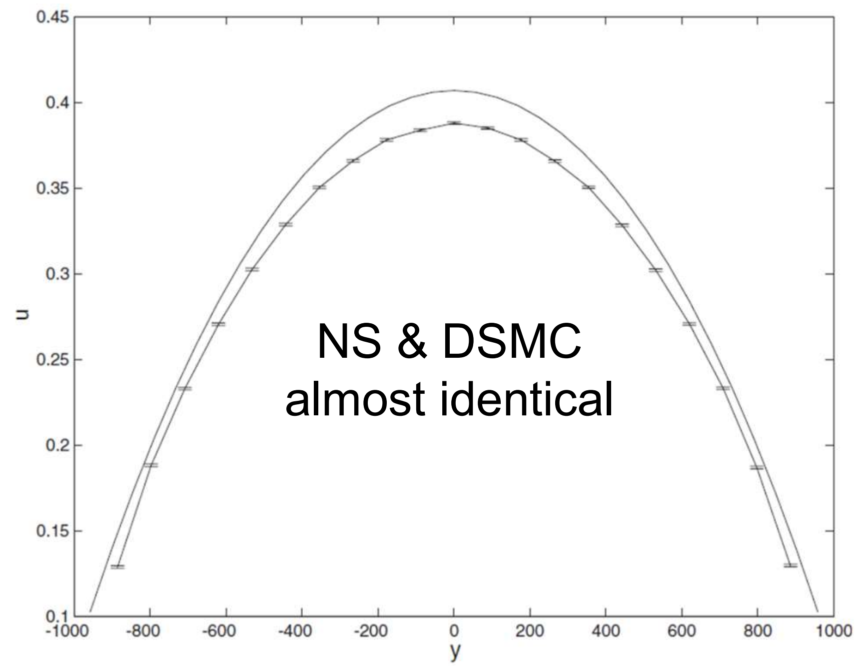
Channel widths roughly 10 to 100 mean free paths ($Kn \approx 0.1$ to 0.01)

Fluid Velocity

Velocity profile across the channel (wall-to-wall)



Acceleration Driven

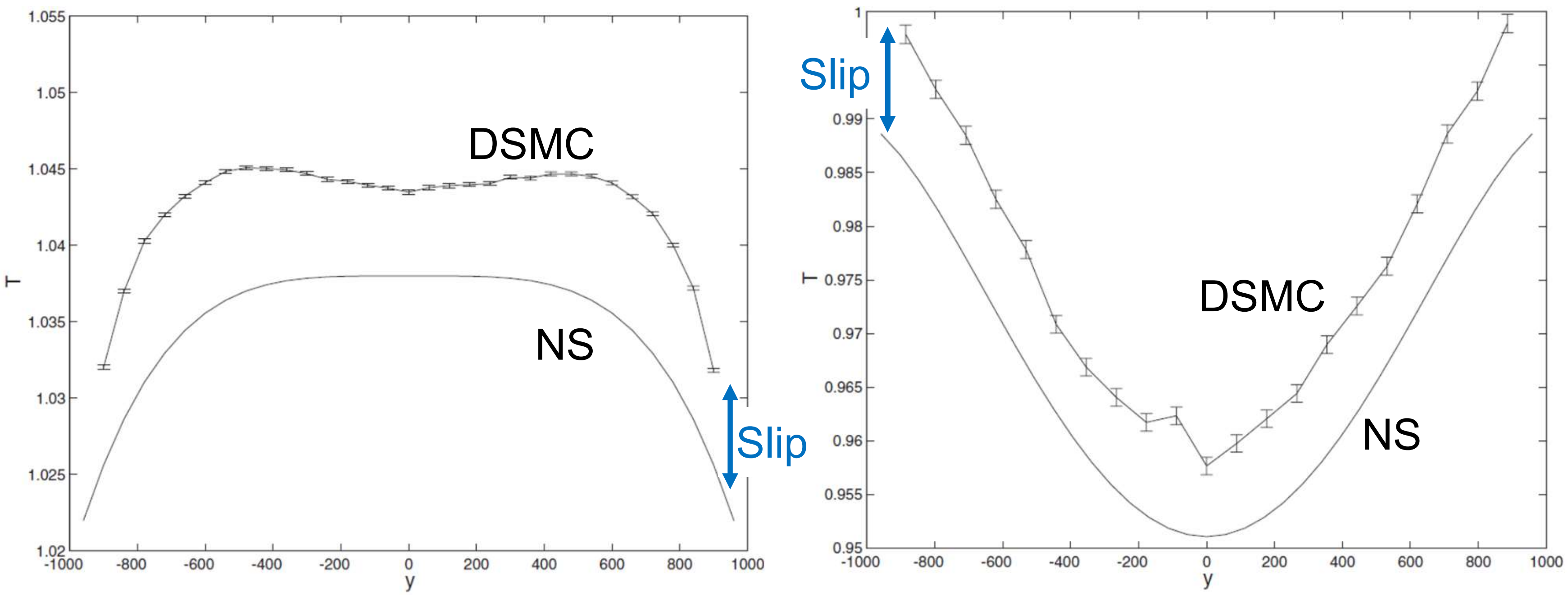


Pressure Driven

Note: Flow is subsonic & low Reynolds number (Re = 5)

Temperature

Temperature profile across the channel (wall-to-wall)



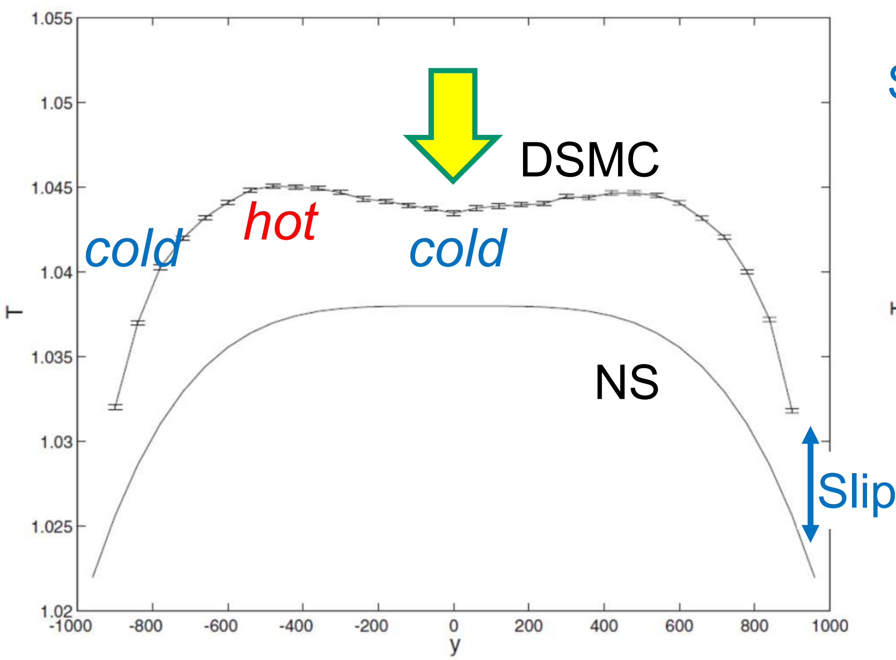
Acceleration Driven

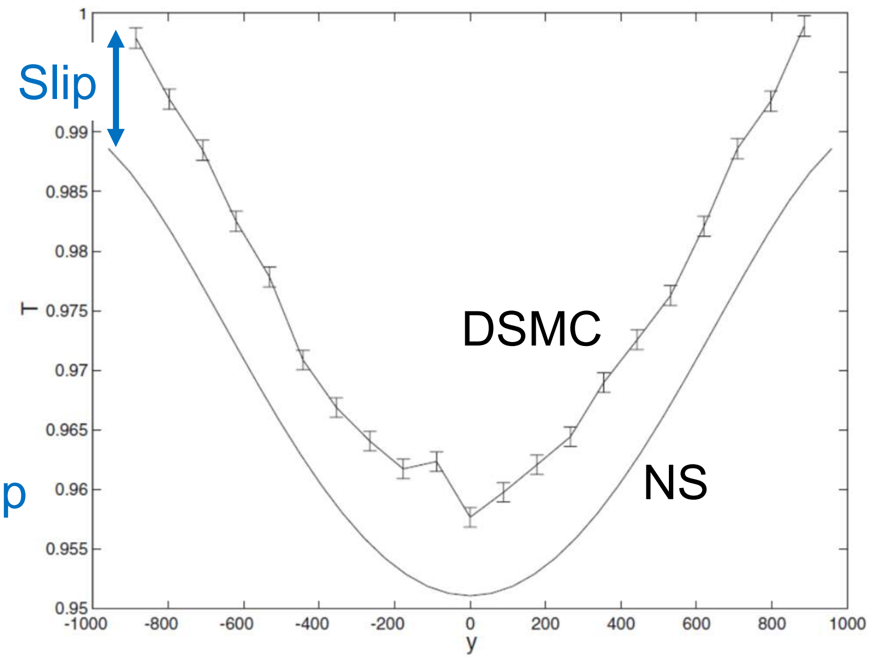
Pressure Driven

M. Malek Mansour, F. Baras and ALG, *Physica A* **240** 255 (1997).
Y. Zheng, ALG, and B. Alder, *J. Stat. Phys.* **109** 495-505 (2002).

Temperature

Temperature profile across the channel (wall-to-wall)





Acceleration Driven

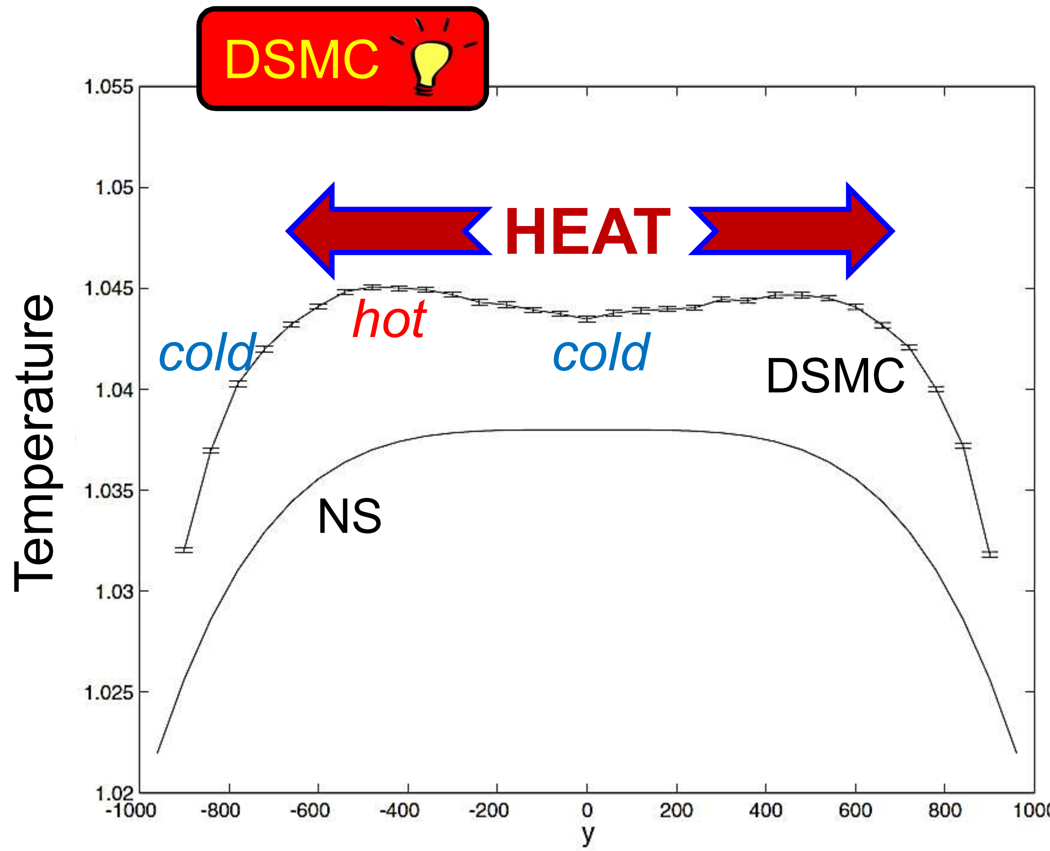
Pressure Driven

M. Malek Mansour, F. Baras and ALG, *Physica A* **240** 255 (1997).
Y. Zheng, ALG, and B. Alder, *J. Stat. Phys.* **109** 495-505 (2002).

Heat Flux & Temperature Gradient

Heating occurs inside the system by viscous shear and heat flows to the walls.

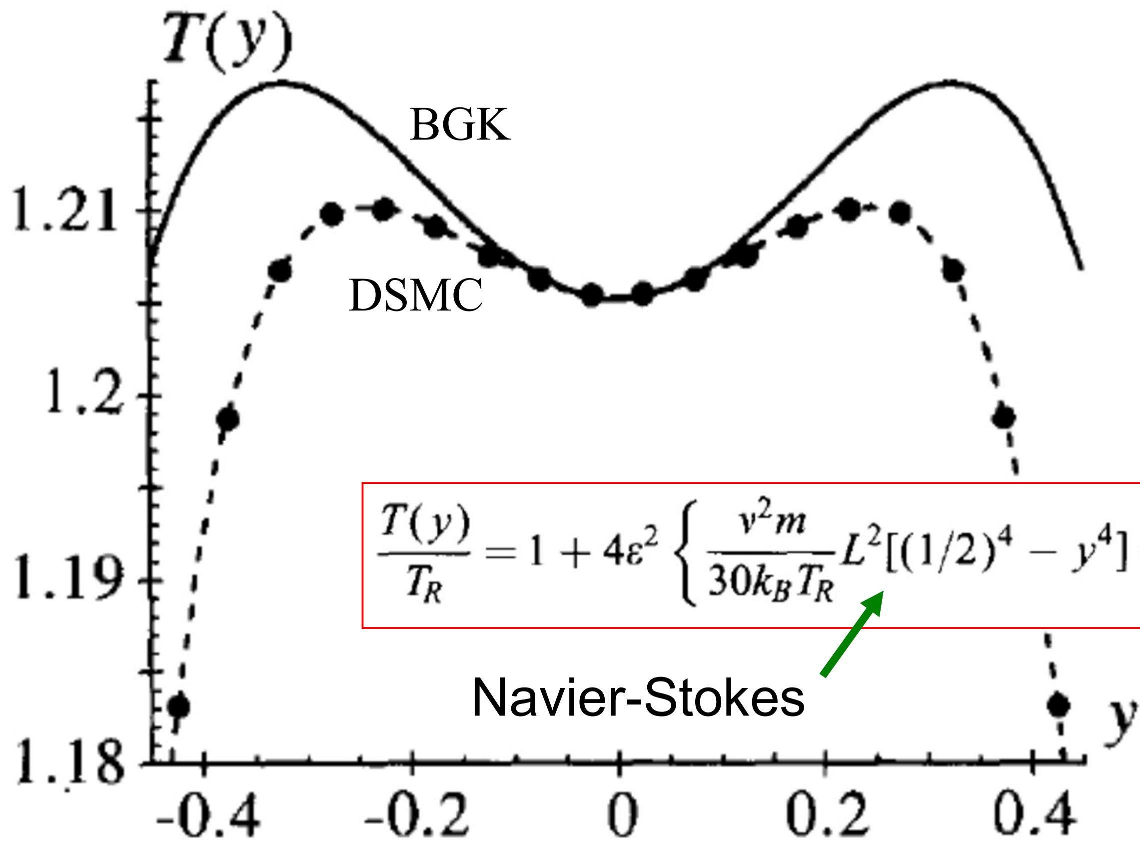
Near the center of the channel the heat is flowing from *cold to hot* !



Acceleration Driven

Kinetic Theory - BGK model

Kinetic theory calculations using BGK model predicts the dip.



"Dip" term

$$\frac{T(y)}{T_R} = 1 + 4\varepsilon^2 \left\{ \frac{v^2 m}{30 k_B T_R} L^2 [(1/2)^4 - y^4] - \frac{19}{25}[(1/2)^2 - y^2] \right\} + O(\varepsilon^4)$$

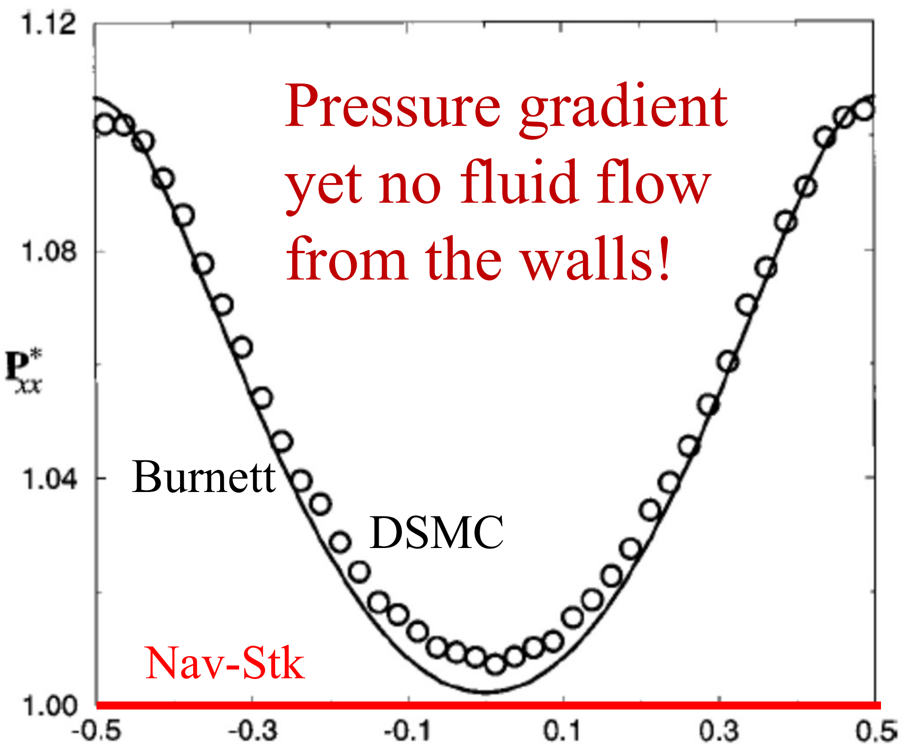
Navier-Stokes

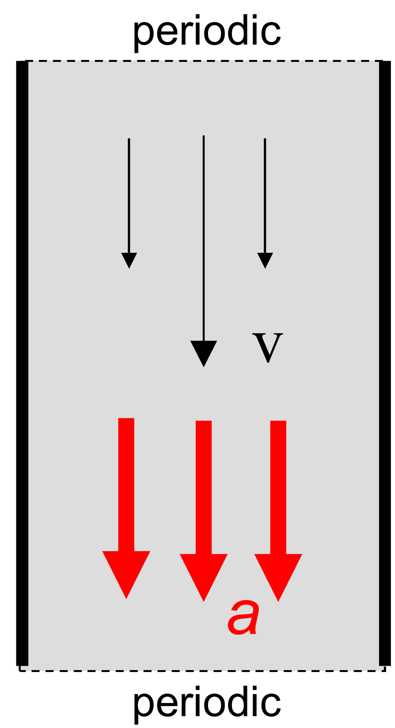
$$\varepsilon \equiv \frac{amL}{2k_B T_R}$$

M. Tij, A. Santos, *J. Stat. Phys.* **76** 1399 (1994)
M. Malek Mansour, F. Baras and ALG, *Physica A* **240** 255 (1997).

Burnett Theory for Poiseuille

Pressure profile also anomalous with a gradient normal to the walls. Agrees with Burnett's hydrodynamic theory.





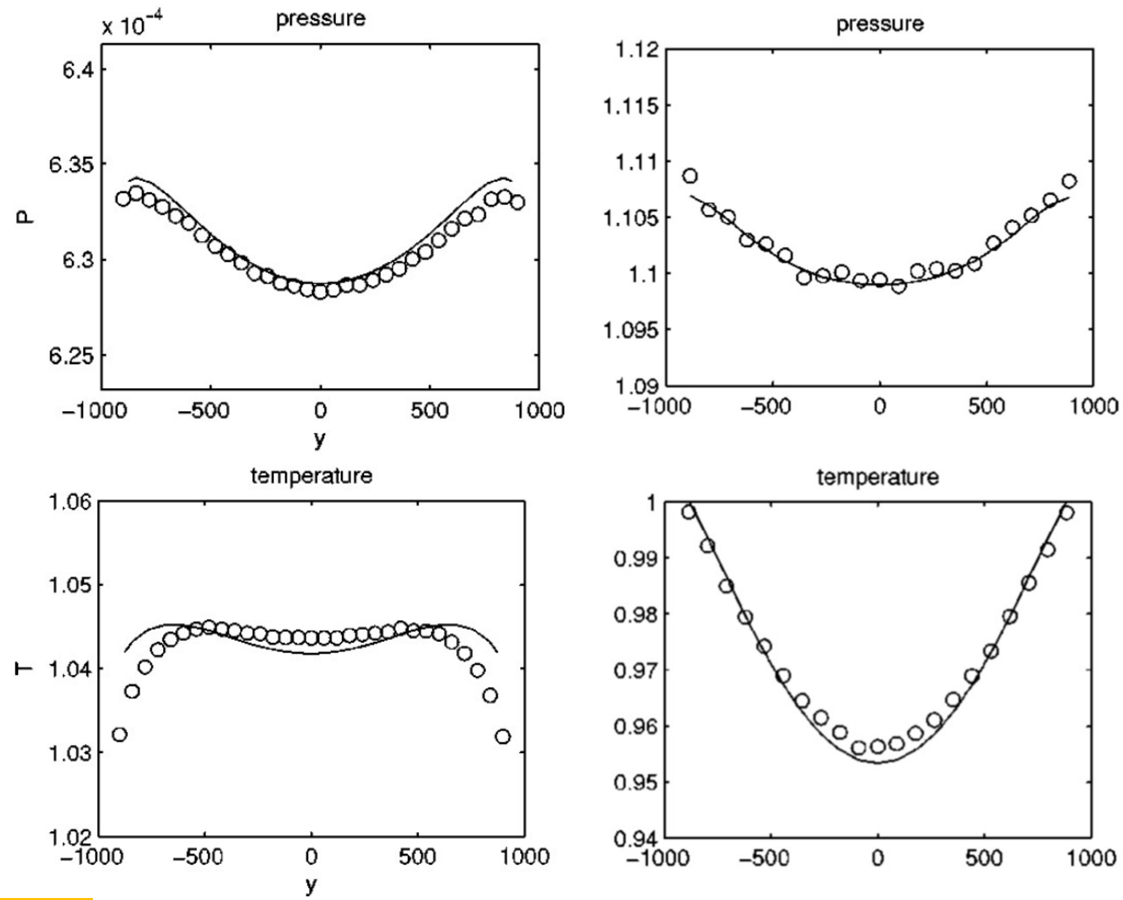
Acceleration Driven

F. Uribe and ALG, *Phys. Rev. E* **60** 4063 (1999)

Super-Burnett Theory

Pressure
Profile

Temperature
Profile



Super-Burnett – Lines
DSMC – Symbols

Acceleration Driven

Pressure Driven

Xu, Phys. Fluids **15** 2077 (2003)

Outline

- Direct Simulation Monte Carlo
- Surprising Poiseuille Flow
- **Surprising Couette Flow**
- Surprising “Phantom” Flow
- Surprising Diffusive Mixing
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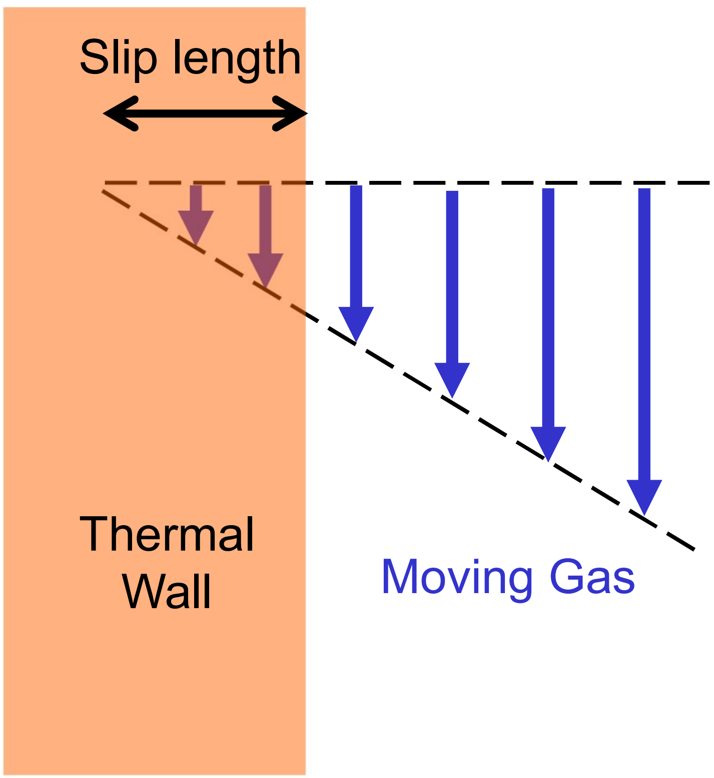
Slip Length

The velocity of a gas moving over a stationary, thermal wall has a “slip length.”



This effect was predicted by Maxwell; confirmed by Knudsen.

Physical origin is difference between impinging and reflected velocity distributions of the gas molecules.

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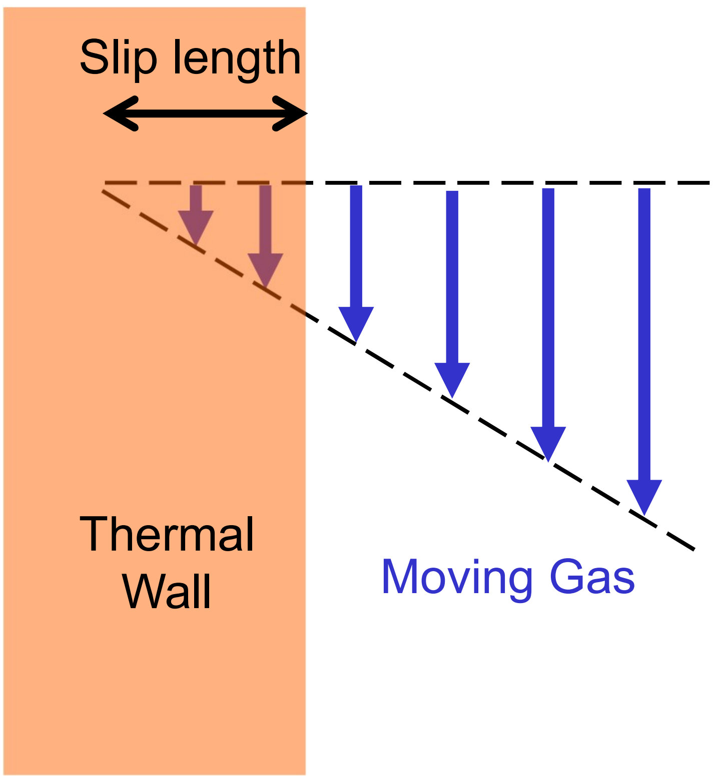


This effect was predicted by Maxwell; confirmed by Knudsen.

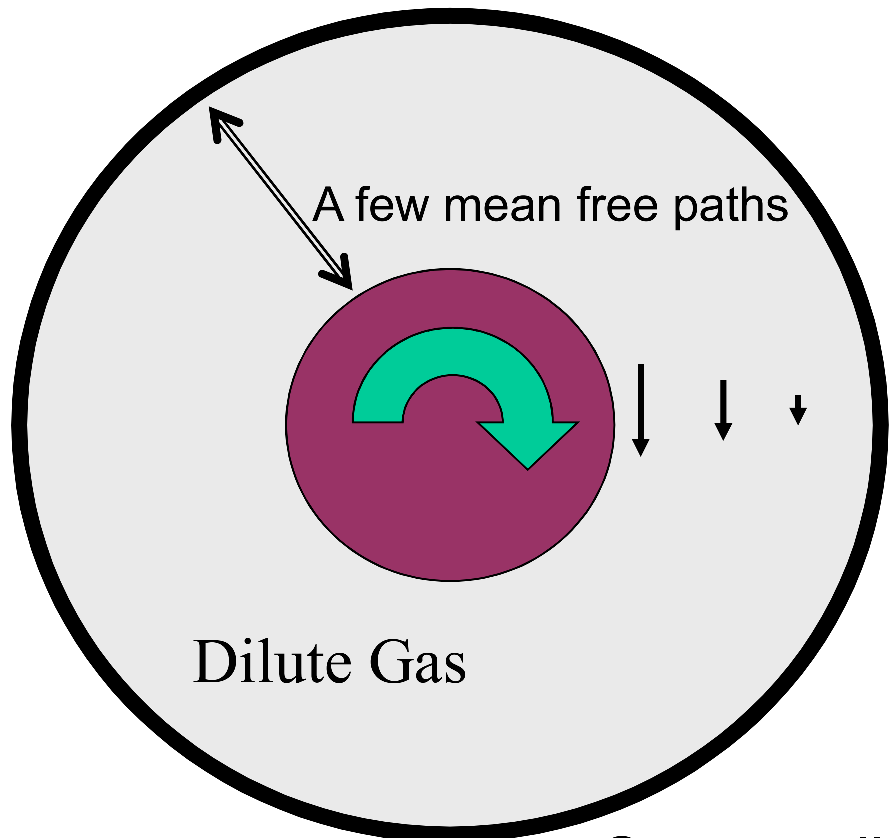
Physical origin is difference between impinging and reflected velocity distributions of the gas molecules.

Slip length for thermal wall is about one mean free path.

Slip increases if some particles reflect specularly; define accommodation coefficient, α, as fraction of thermalize (non-specular) reflections.

Cylindrical Couette Flow

- Dilute gas between concentric cylinders. Outer cylinder fixed; inner cylinder rotating.
- Low Reynolds number ($Re \approx 1$) so flow is laminar; also subsonic.



Outer wall stationary

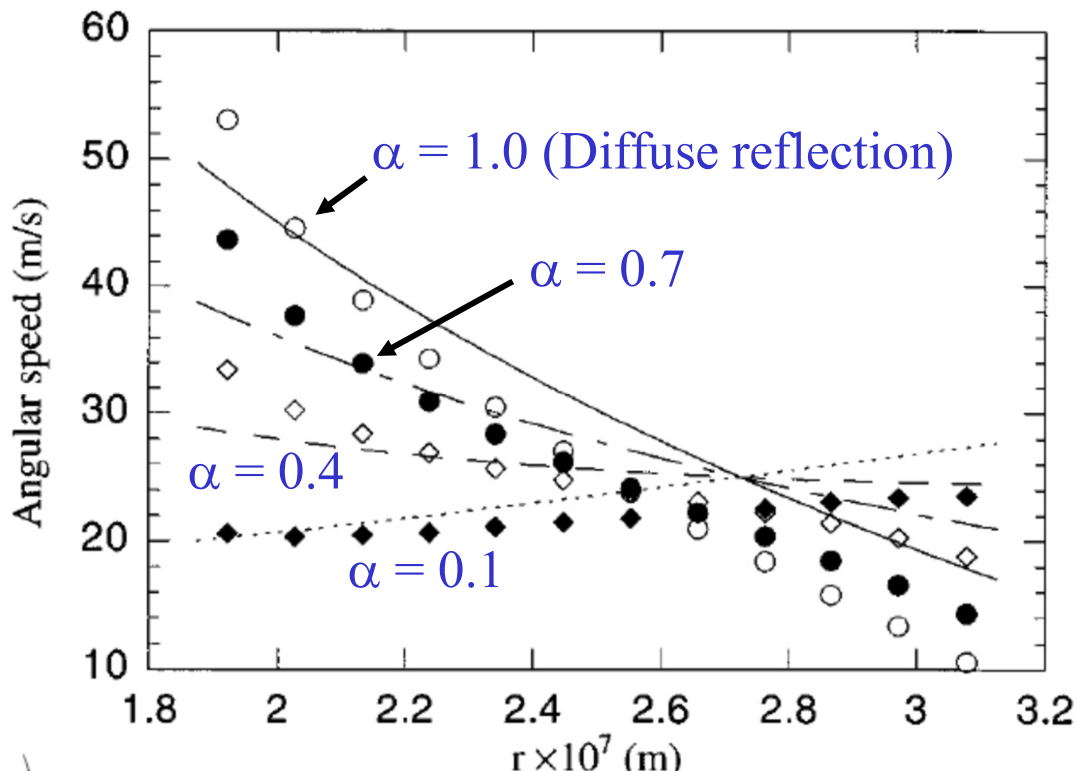
Velocity Slip in Couette Flow

Simple prediction of angular velocity including slip is mostly in qualitative agreement with DSMC data.

$$v_\theta = \frac{\omega}{A-B}\left(Ar - \frac{1}{r}\right)$$

$$A = \frac{1}{R_2^2}\left(1 - 2\frac{\zeta_0}{R_2}\right); \quad B = \frac{1}{R_1^2}\left(1 + 2\frac{\zeta_0}{R_1}\right)$$

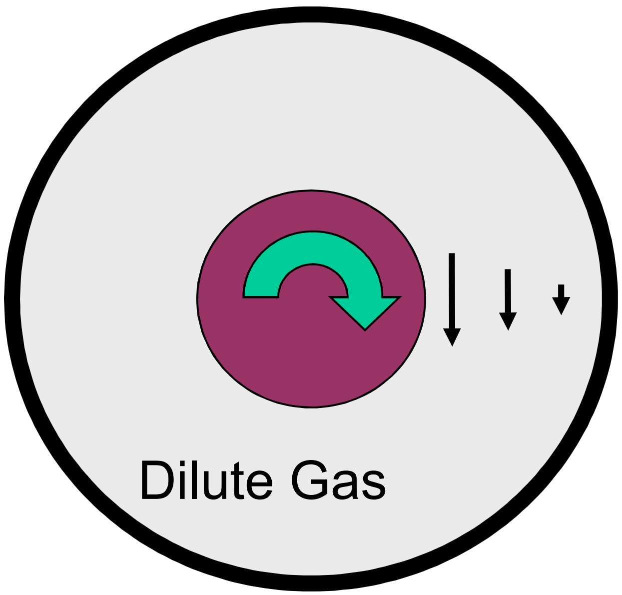
ζ is the slip length.



Not shown: α = 0.0 (Specular reflection)

K. Tibbs, F. Baras, ALG, *Phys. Rev. E* **56** 2282 (1997)

Diffusive and Specular Walls

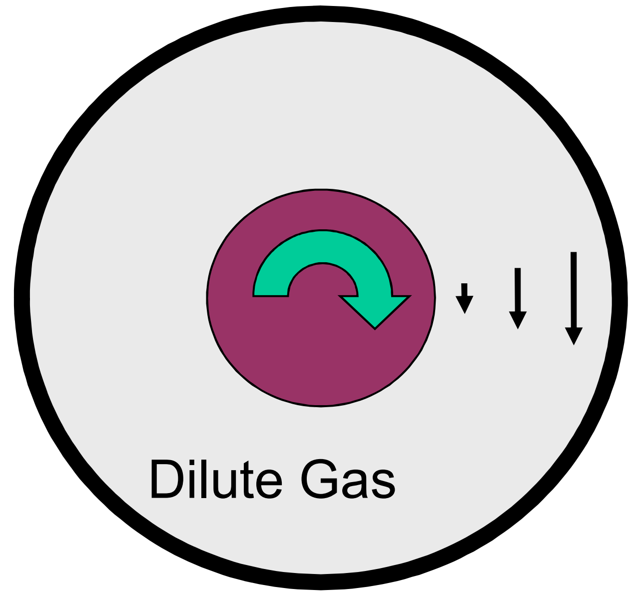


Diffusive Walls

$\alpha = 1.0$

Outer wall stationary

When walls are completely specular the gas undergoes solid body rotation so $v = \omega r$

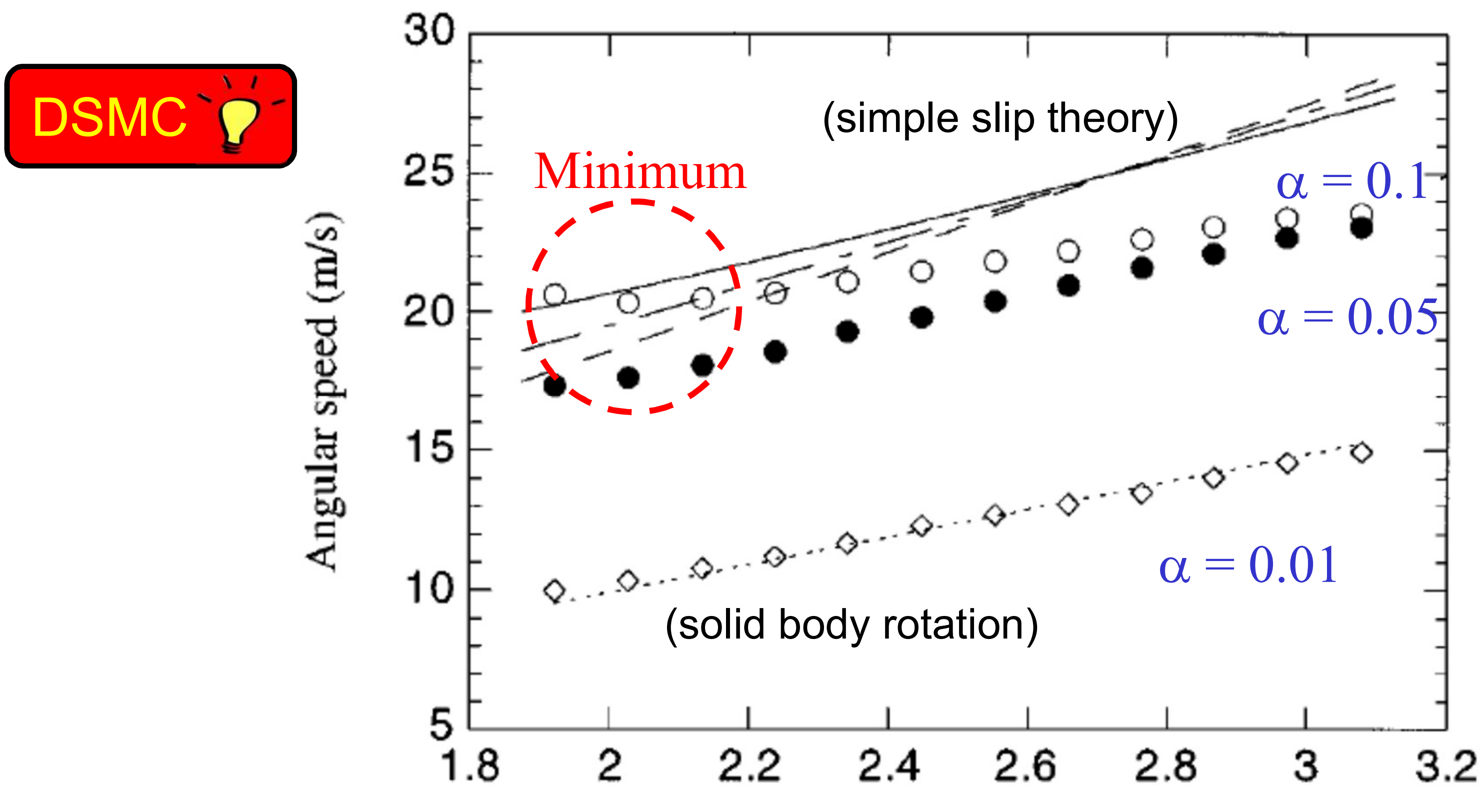


Specular Walls

$\alpha = 0.0$

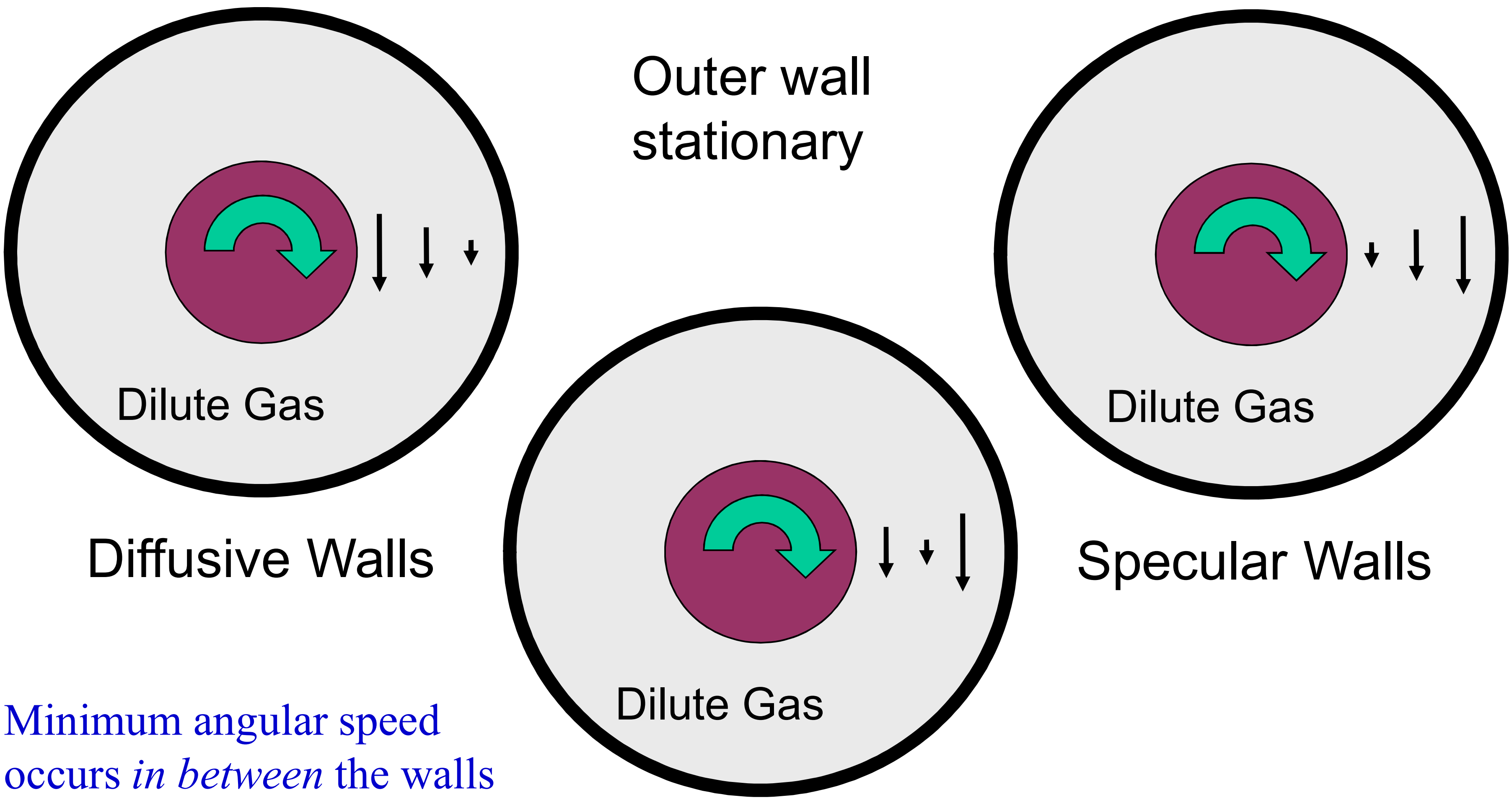
Anomalous Couette Flow

At certain values of accommodation, the angular fluid speed is minimum ***within*** the fluid.



K. Tibbs, F. Baras, ALG, *Phys. Rev. E* **56** 2282 (1997)

Anomalous Rotating Flow



Diffusive Walls

Specular Walls

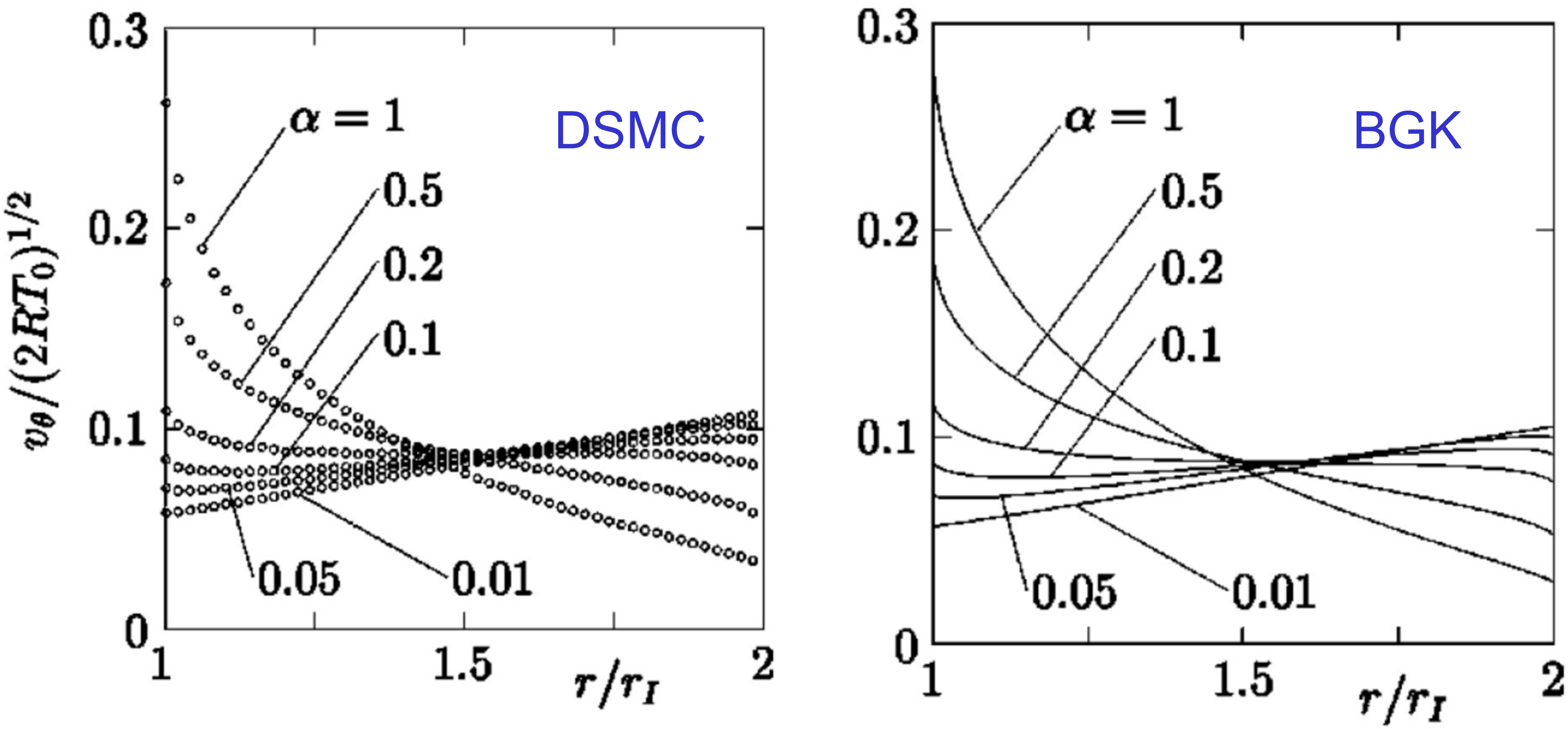
Intermediate Case

Minimum angular speed
occurs *in between* the walls

Effect occurs when
walls ~80-90% specular

BGK Theory

Excellent agreement between DSMC data and BGK calculations and BGK theory confirms the velocity minimum at low accommodation.



K. Aoki, H. Yoshida, T. Nakanishi, ALG, *Physical Review E* **68** 016302 (2003)

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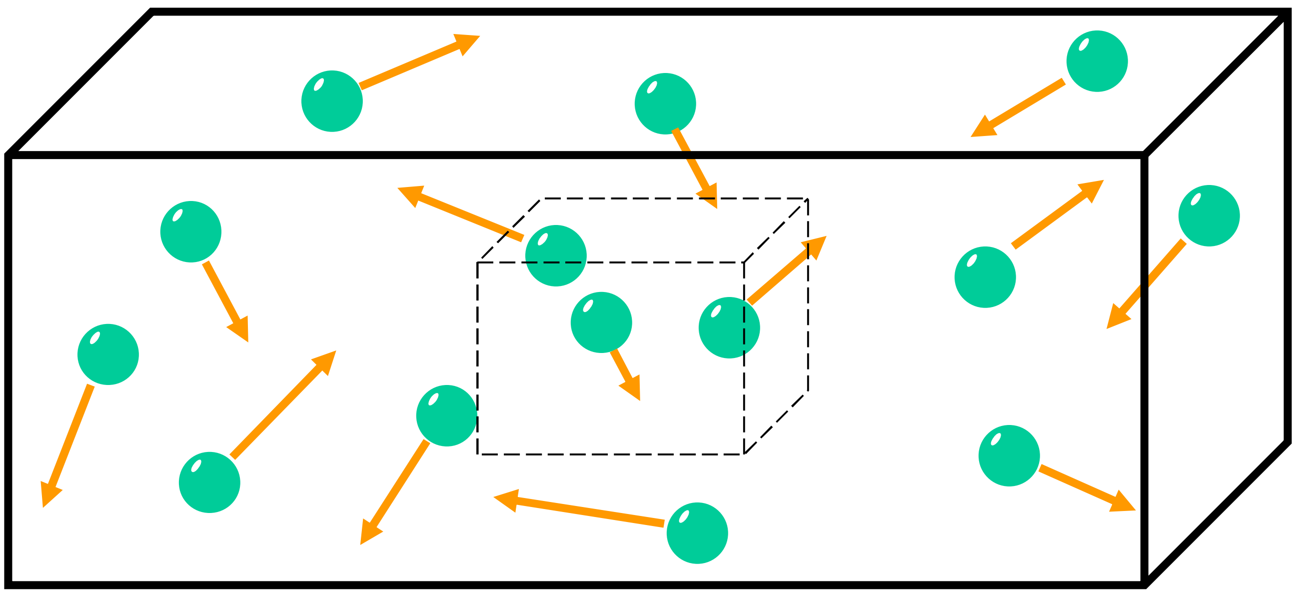
Calculating Fluid Velocity



How should one calculate local fluid velocity from particle velocities in DSMC (or in MD)?

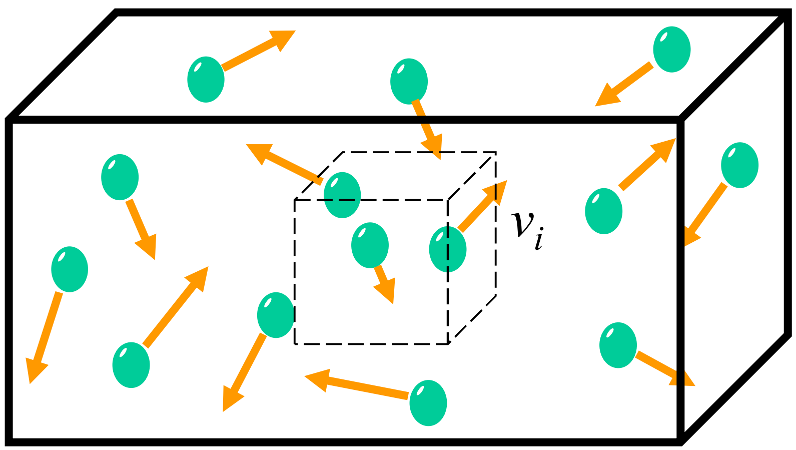
Instantaneous Fluid Velocity

Center-of-mass velocity in a cell *C*

$$u = \frac{J}{M} = \frac{\sum_{i \in C}^{N} m v_i}{mN}$$

Average particle velocity

$$\overline{v} = \frac{1}{N} \sum_{i \in C}^{N} v_i$$



Note that $u = \overline{v}$ so these are equivalent

Mean Fluid Velocity

Instantaneous fluid velocity is defined as,

$$u = \frac{J}{M} = \frac{\sum_{i \in C}^{N} m v_i}{mN} = \frac{1}{N} \sum_{i \in C}^{N} v_i$$

But we have two ways to define mean fluid velocity, averaged over independent samples:

$$\langle u \rangle = \left\langle \frac{J}{M} \right\rangle \qquad \langle u \rangle_* = \frac{\langle J \rangle}{\langle M \rangle}$$

Mean Instantaneous Mean Cumulative

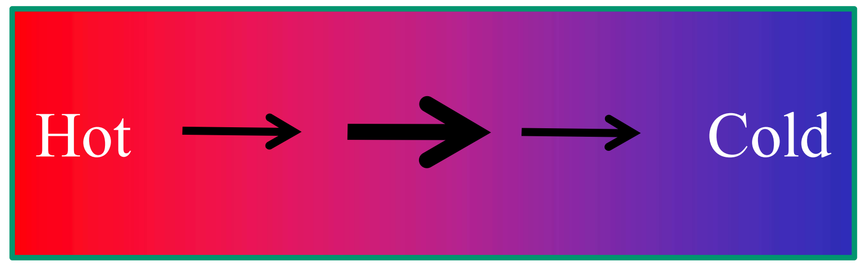
Which definition gives the correct hydrodynamic fluid velocity?

“Phantom” Fluid Velocity

DSMC

Mean instantaneous fluid velocity, $\langle u \rangle$, measurement gives an anomalous flow in a <u>closed</u> system at steady state with ∇T.

$$\langle u \rangle = \left\langle \frac{J}{M} \right\rangle \propto x(L-x)\nabla T$$



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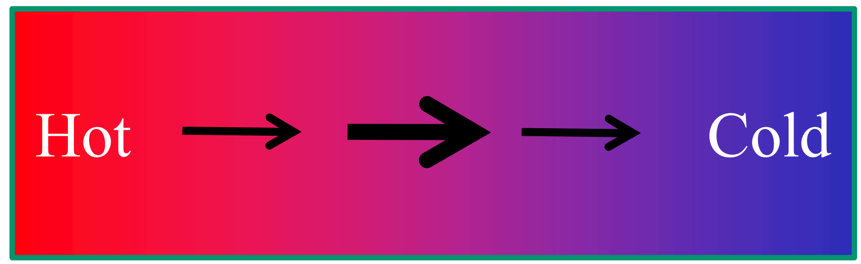


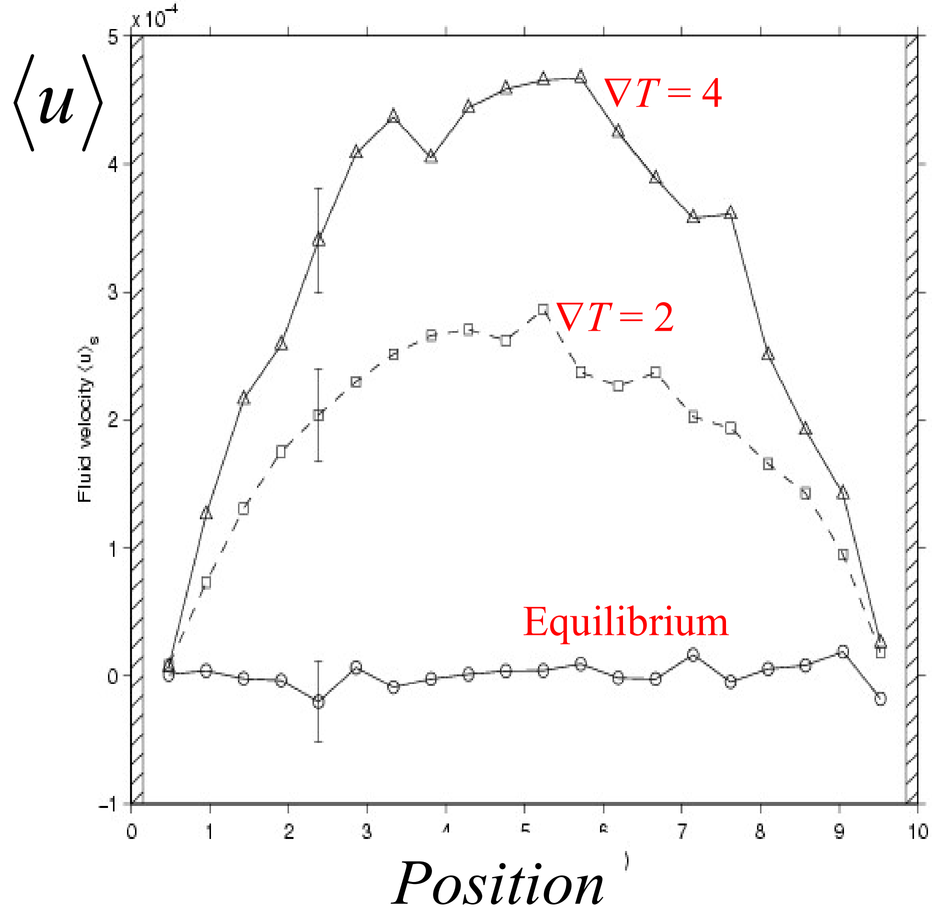
Using the cumulative mean, $\langle u \rangle_*$, gives the expected result of zero fluid velocity.

$$\langle u \rangle_* = \frac{\langle J \rangle}{\langle M \rangle} = 0$$

Measured Fluid Velocity

Mean instantaneous fluid velocity, $\langle u \rangle$, measurement gives an anomalous flow in a <u>closed</u> system at steady state with ∇T.

Using the cumulative mean, $\langle u \rangle_*$, gives the expected result of zero fluid velocity.

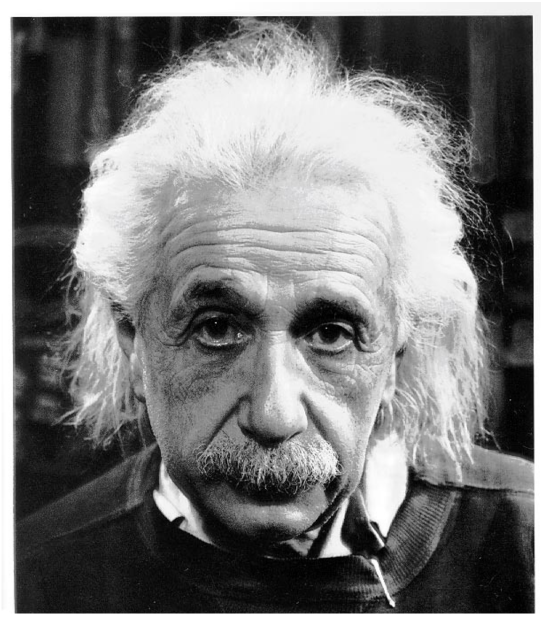


M. Tysanner and ALG,
J. Comp. Phys. **196** 173-83 (2004).

Landau Model for Intelligence

Apply the Landau model to university students:

Genius



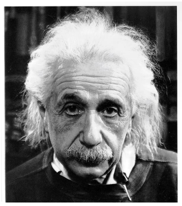
Intellect = 3

Not Genius

Intellect = 1

Three Semesters of Teaching

First semester



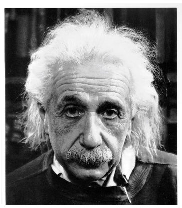
Average = 3

Second semester

Third semester

Three Semesters of Teaching

First semester



Average = 3

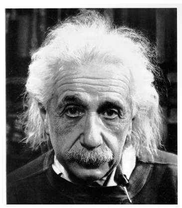
Second semester

Average = 1

Third semester

Three Semesters of Teaching

First semester

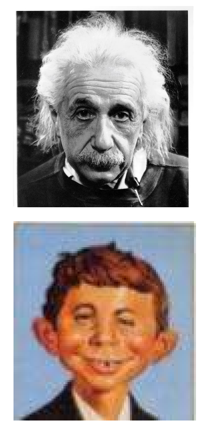


Average = 3

Second semester

Average = 1

Third semester



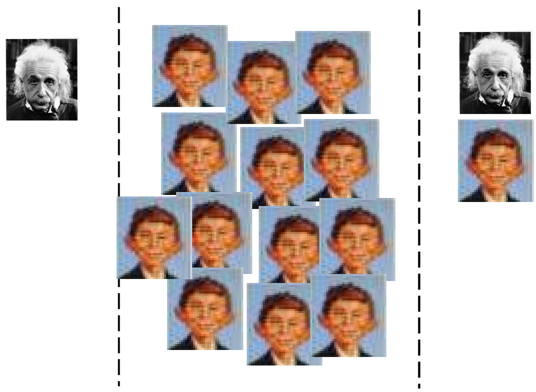
Average = 2

Average Student?

How do you estimate the intellect of the average student?

* Average of instantaneous values for the three semesters:

$$\boxed{\langle u \rangle = \frac{3+1+2}{3} = 2}$$



<u>Or</u>

* Cumulative average over all students:

$$\boxed{\langle u \rangle_* = \frac{2\times 3 + 14\times 1}{16} = 1.25}$$

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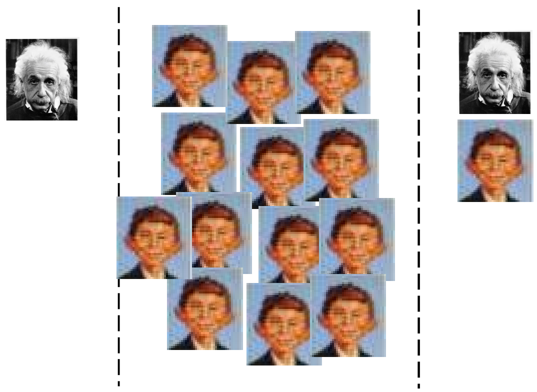
How do you estimate the intellect of the average student?

* Average of instantaneous values for the three semesters:

$$\boxed{\langle u \rangle = \frac{3+1+2}{3} = 2}$$



Or

* Cumulative average over all students:

$$\boxed{\langle u \rangle_* = \frac{2\times 3+14\times 1}{16} = 1.25}$$

Significant difference because there is a *correlation* between class size and quality of students in the class.

Bias in Instantaneous Fluid Velocity

From the definitions,

$$\langle u \rangle \approx \langle u \rangle_* \left(1 + \frac{\langle \delta N^2 \rangle}{\langle N \rangle^2} \right) - \frac{\langle \delta J \delta N \rangle}{m \langle N \rangle^2} = \langle u \rangle_* - \frac{\langle \delta \rho \delta u \rangle}{\langle \rho \rangle}$$

Fluctuating hydrodynamics theory predicts a correlation,

$$\langle \delta\rho(x) \delta u(x) \rangle \propto -x(L-x)\nabla T$$

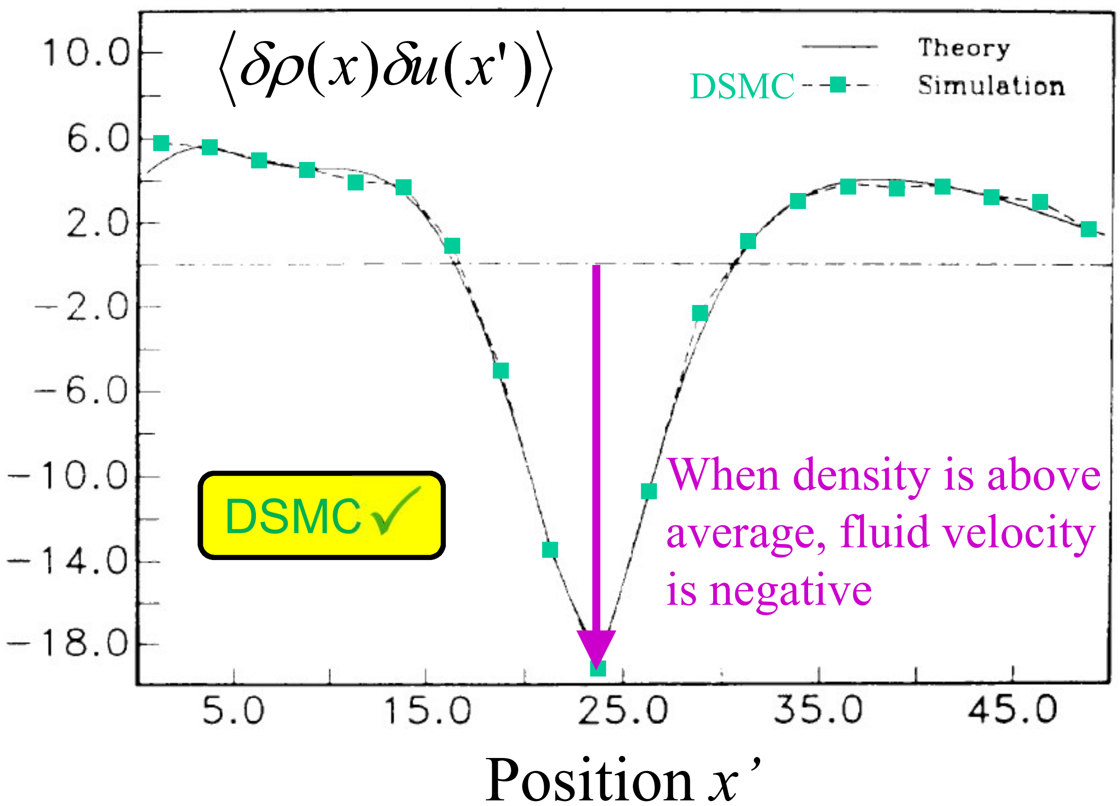
This prediction agrees perfectly with observed effect.

Similar effect occurs with temperature, pressure, etc.

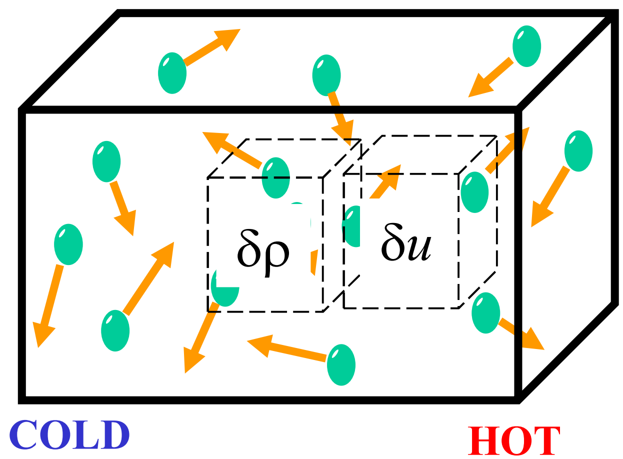
M. Tysanner and ALG, *J. Comp. Phys.* **196** 173-83 (2004)

Density-Velocity Correlation

Correlation of density-velocity fluctuations under ∇T



Theory is fluctuating hydrodynamics



ALG, *Phys. Rev. A* **34** 1454 (1986).

Outline

- Direct Simulation Monte Carlo
- Surprising Poiseuille Flow
- Surprising Couette Flow
- Surprising “Phantom” Flow
- Surprising Diffusive Mixing
- Surprising Brownian Motion

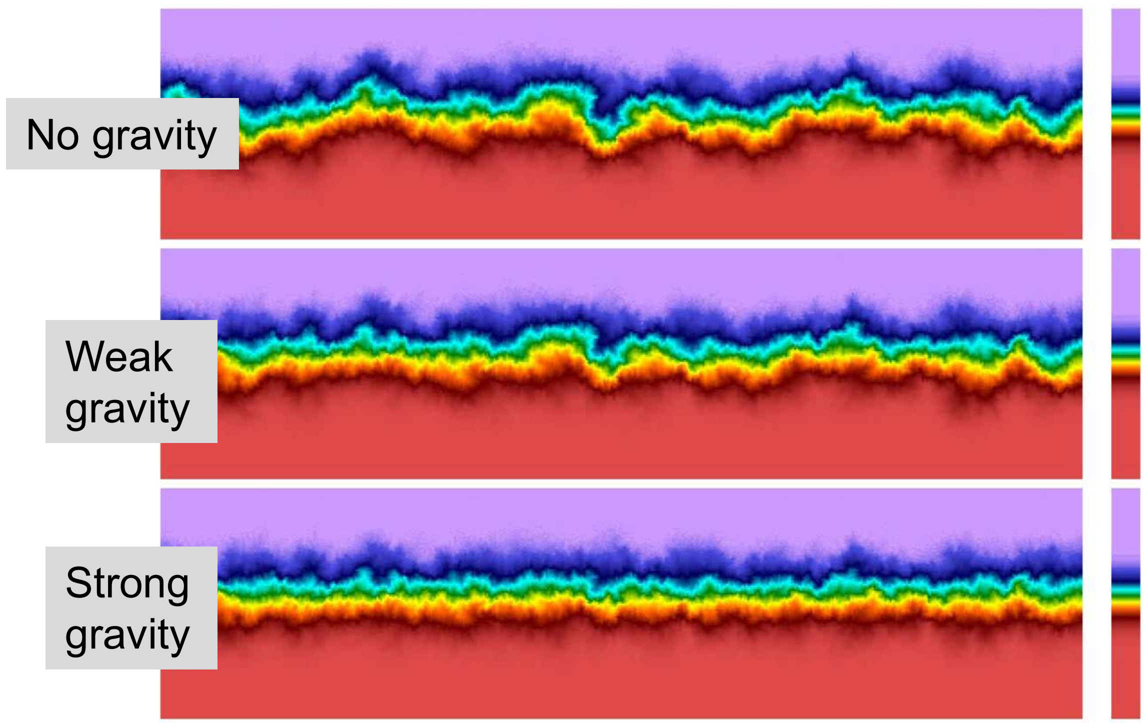
Giant Fluctuations in Mixing

Fluctuations grow large during mixing even when the two species are identical (e.g., red & blue hard spheres).

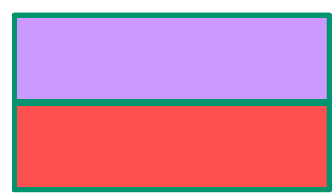
The effect is driven by a coupling of concentration and velocity fluctuations.

This is **not** a hydrodynamic instability!

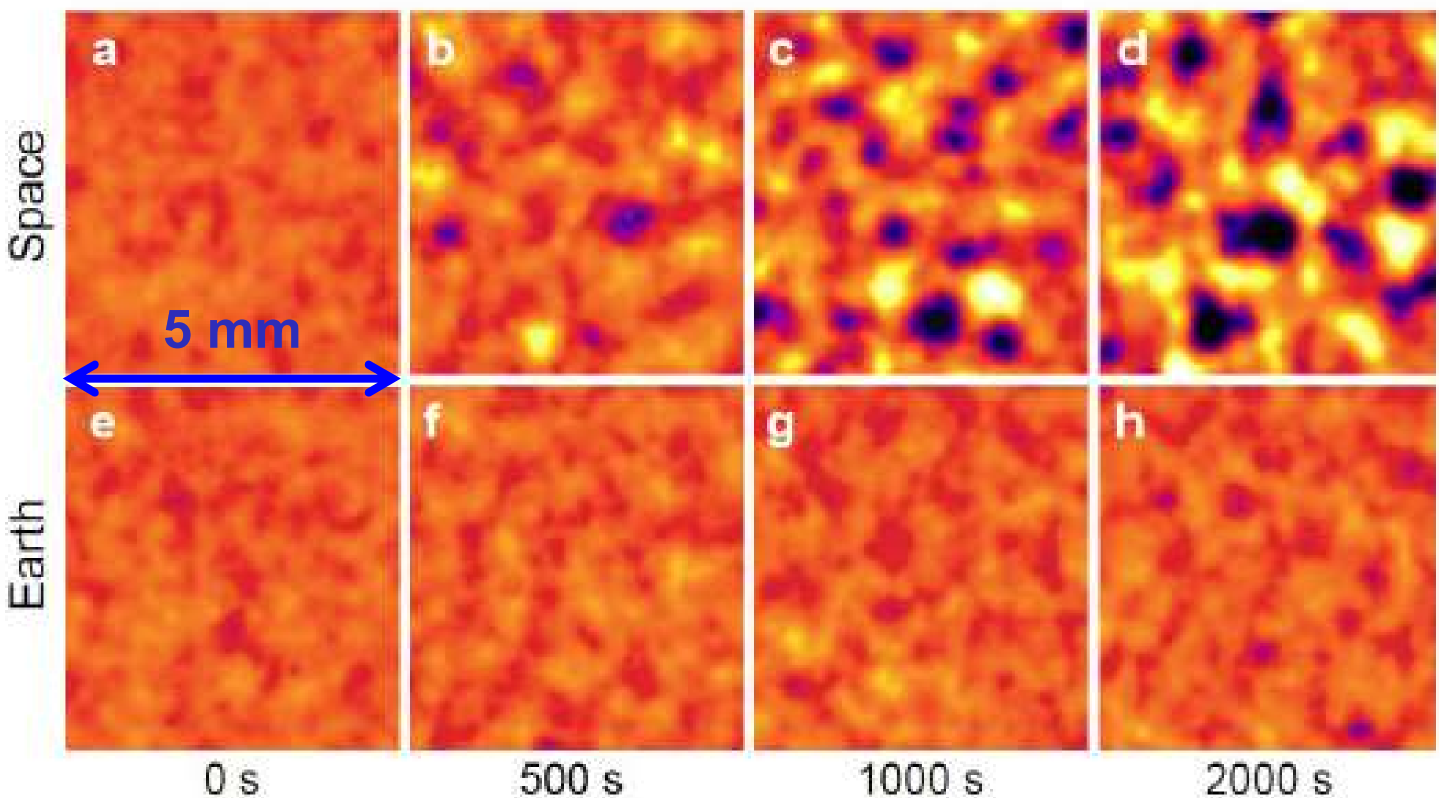
Color indicates concentration

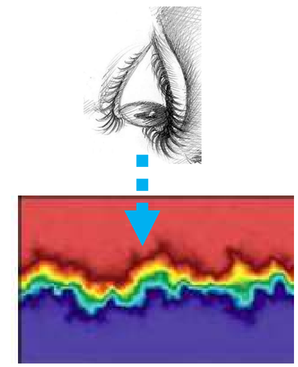


Initial State

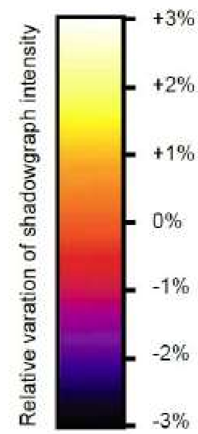


Experimental Observations





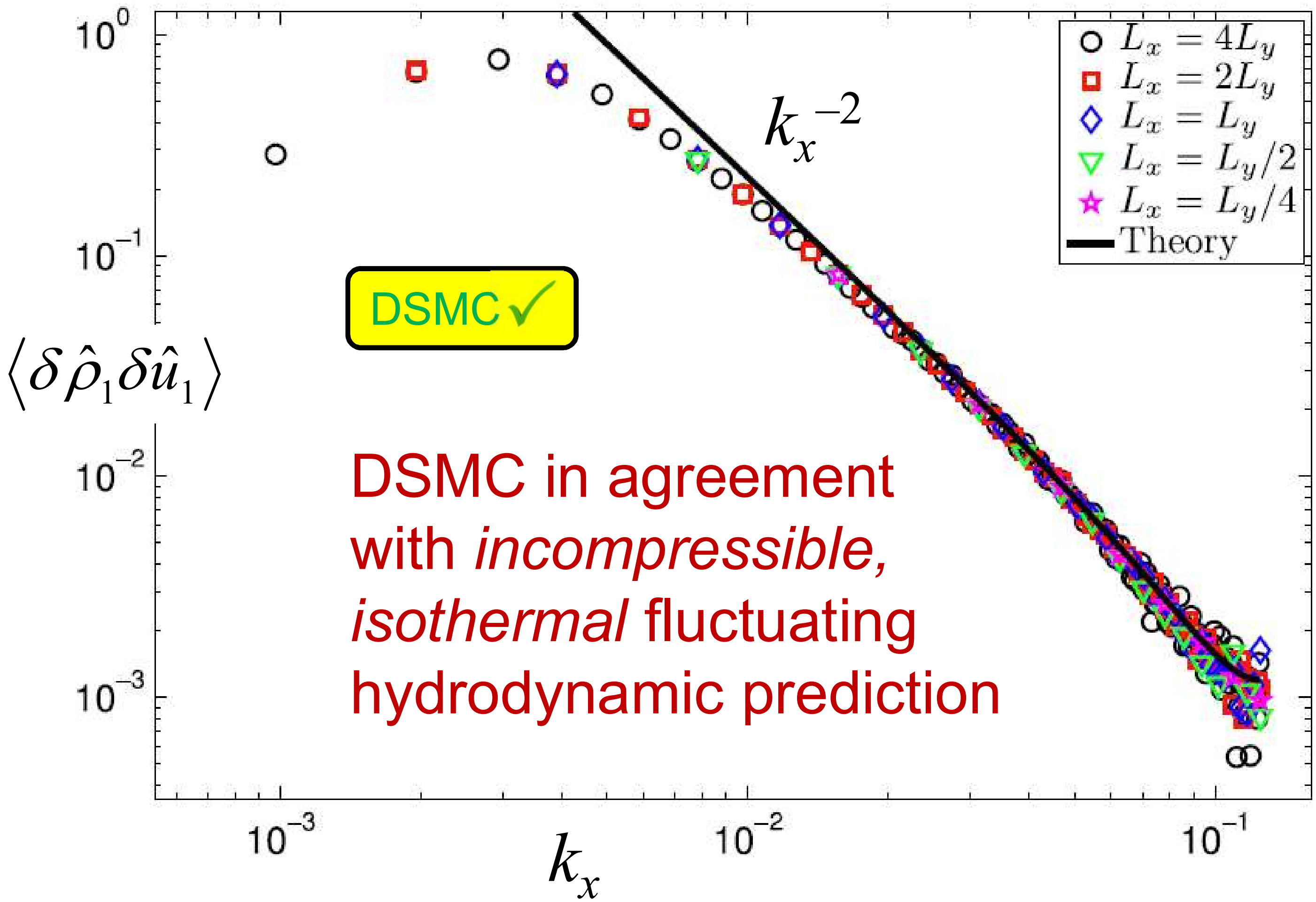
Top-down view of density fluctuations during mixing



In microgravity experiments fluctuations during mixing grow to millimeter size

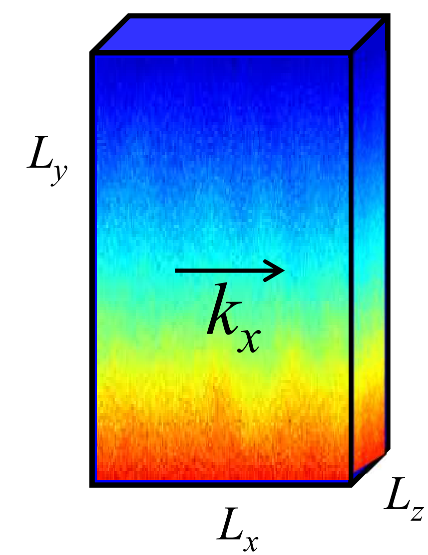
Vailati, et al., Nature Comm., 2:290 (2011).

Concentration-Velocity Correlation



DSMC in agreement with *incompressible, isothermal* fluctuating hydrodynamic prediction

Symbols are DSMC;
$k_y = 0$

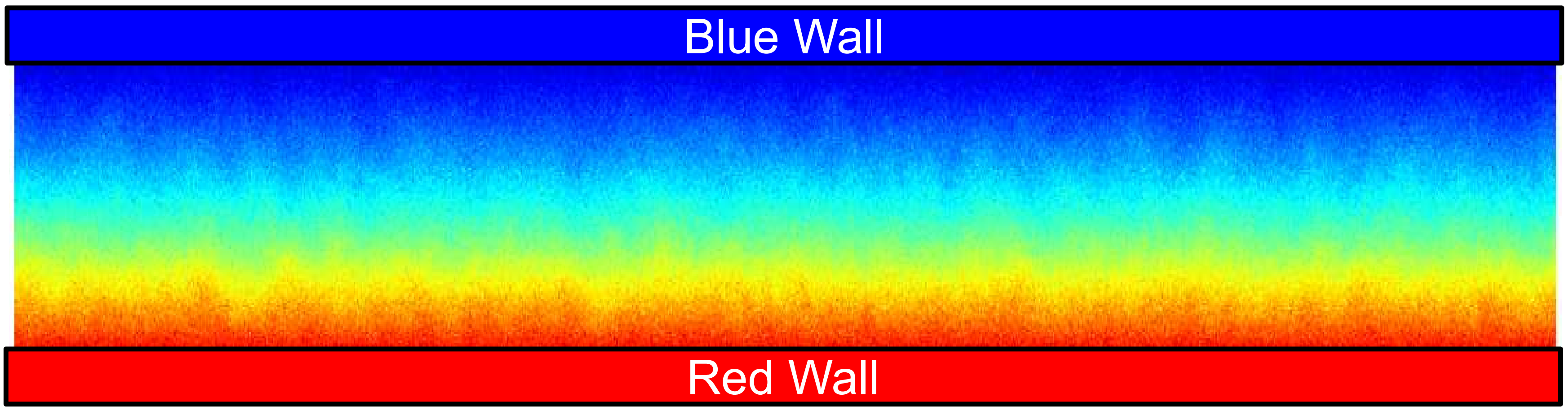


$L_y = 512\ \lambda$; $L_z = 2\ \lambda$

A. Donev, ALG, A. de la Fuente, and J.B. Bell, *J. Stat. Mech.* 2011:P06014 (2011)

Diffusion Flux & Fluctuations

Consider a monatomic gas of “red” and “blue” particles with a steady state gradient imposed by wall boundaries.



The non-equilibrium correlation $\left\langle \delta\hat{c}\,\delta\hat{u}_{\parallel} \right\rangle$ enhances the effective flux of concentration even at this steady state.

A. Donev, ALG, A. de la Fuente, and J.B. Bell, *Phys. Rev. Lett.*, 106(20): 204501 (2011)

Fluctuation Enhanced Diffusion

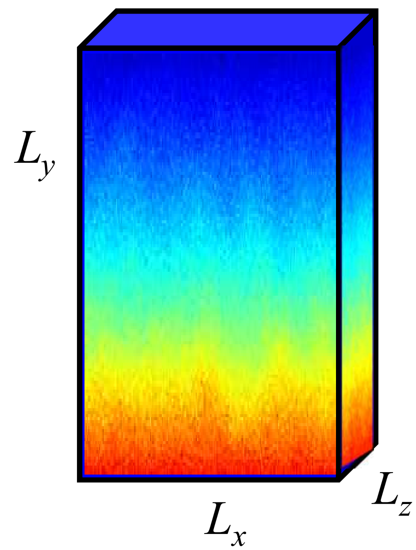
Can separate the contributions to the concentration flux as,

$$\langle \boldsymbol{F} \rangle = \underbrace{\langle \rho_1 \mathbf{u}_1 \rangle}_{D_{\text{eff}} \nabla c} = \underbrace{\langle \rho_1 \rangle \langle \mathbf{u}_1 \rangle}_{D_0 \nabla c} + \underbrace{\langle \delta\rho_1 \delta\mathbf{u}_1 \rangle}_{\Delta D \nabla c}$$

In DSMC we can easily measure

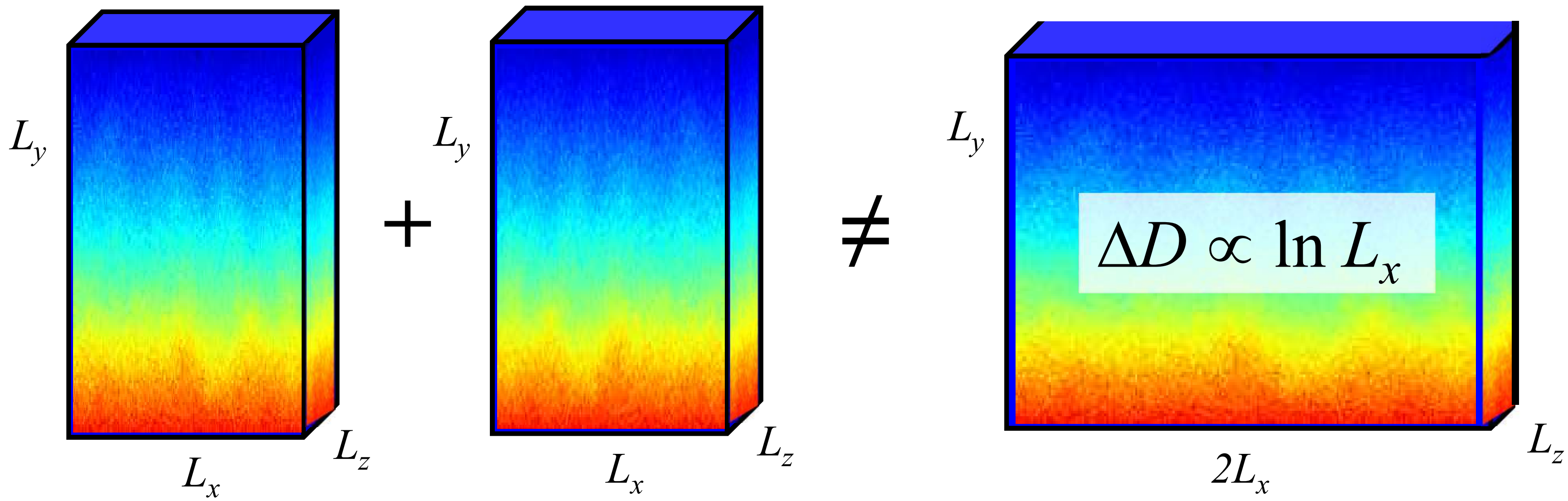
$$\langle \rho_1 \rangle, \langle \mathbf{u}_1 \rangle, \langle \rho_1 \mathbf{u}_1 \rangle \text{ and } \nabla c$$

Find the bare diffusion coefficient D_0 and the total effective diffusion coefficient D_{eff}



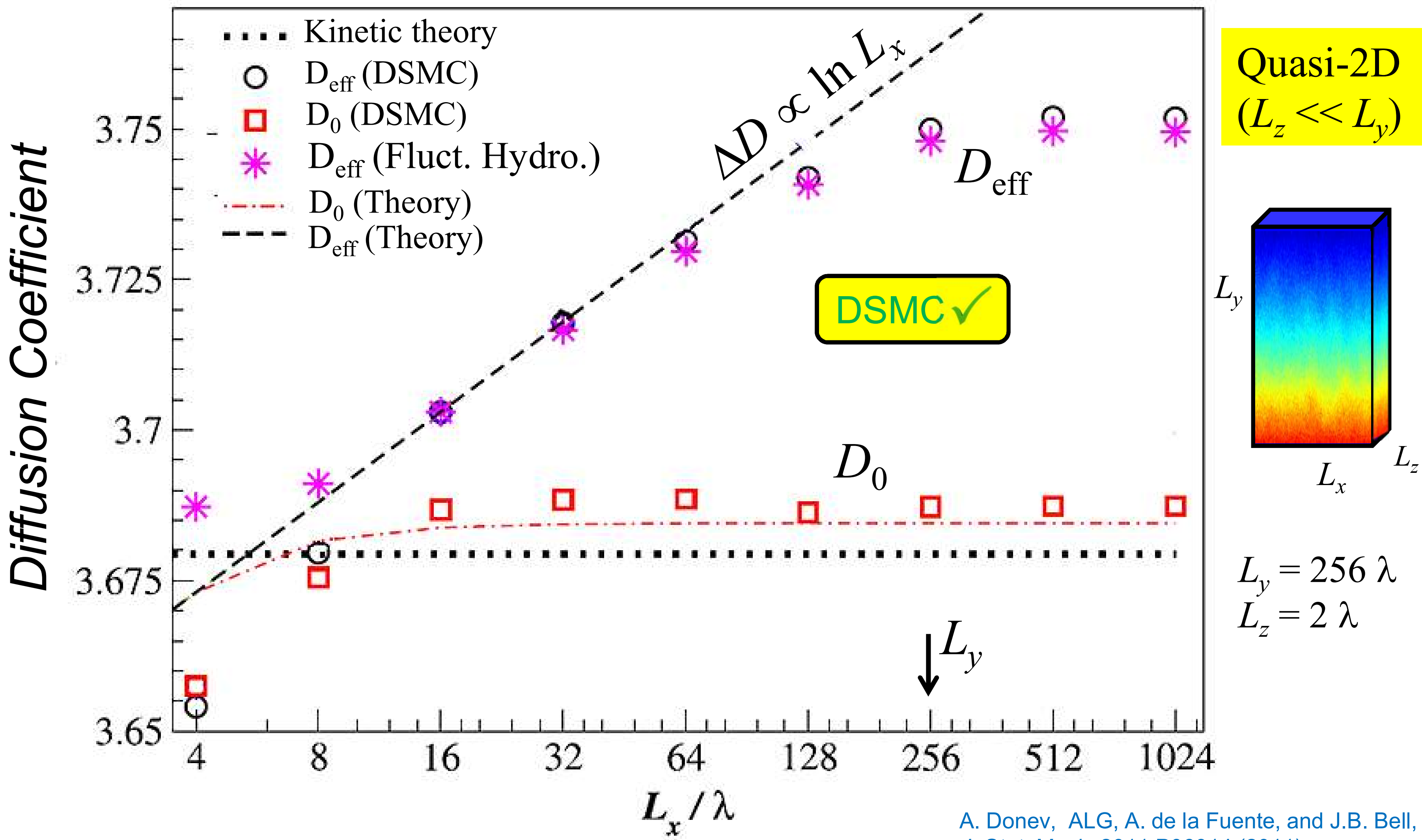
Surprising Diffusion

Spectrum of hydrodynamic fluctuations is truncated at wavenumbers given by the size of the physical system.



The wider system can accommodate long wavelength fluctuations, thus it has an enhanced diffusion rate.
Diffusion coefficient depends on system width!

DSMC and FNS Results (Quasi-2D)



A. Donev, ALG, A. de la Fuente, and J.B. Bell,
J. Stat. Mech. 2011:P06014 (2011)

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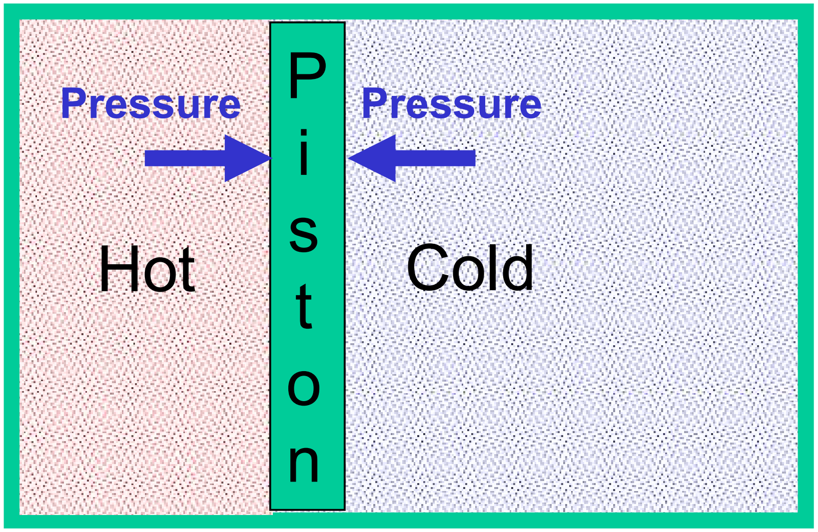
Adiabatic Piston

Fluctuations in DSMC can model phenomena, like Brownian motion, that rely on fluctuations.

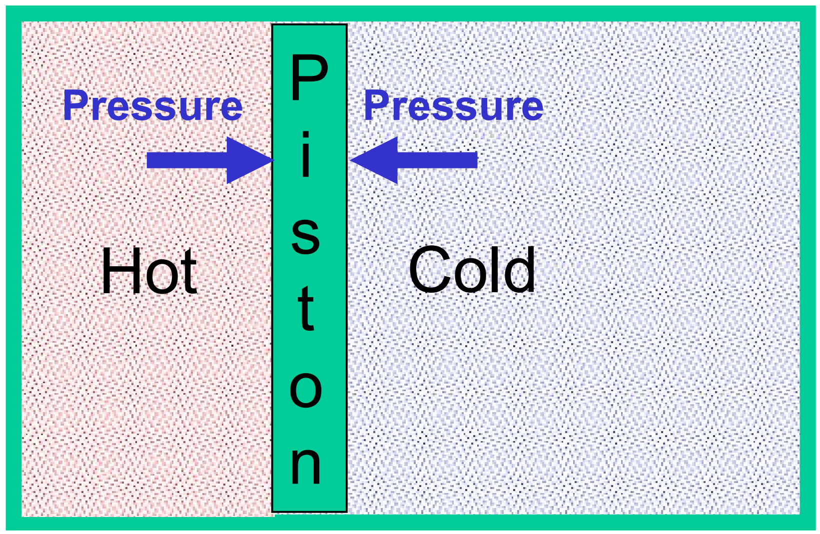


"Adiabatic" Piston Problem

Chambers have gases at different temperatures, equal pressures.
Walls are perfectly elastic (specular reflection, accommodation α = 0)

Adiabatic Piston

Fluctuations in DSMC can model phenomena, like Brownian motion, that rely on fluctuations.



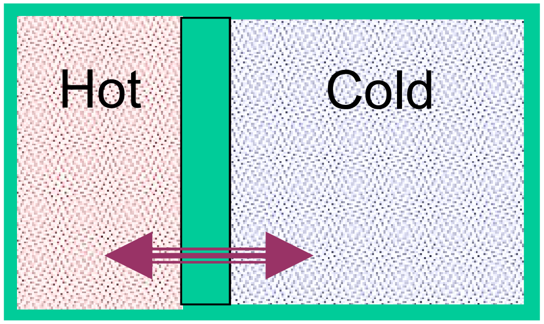
"Adiabatic" Piston Problem

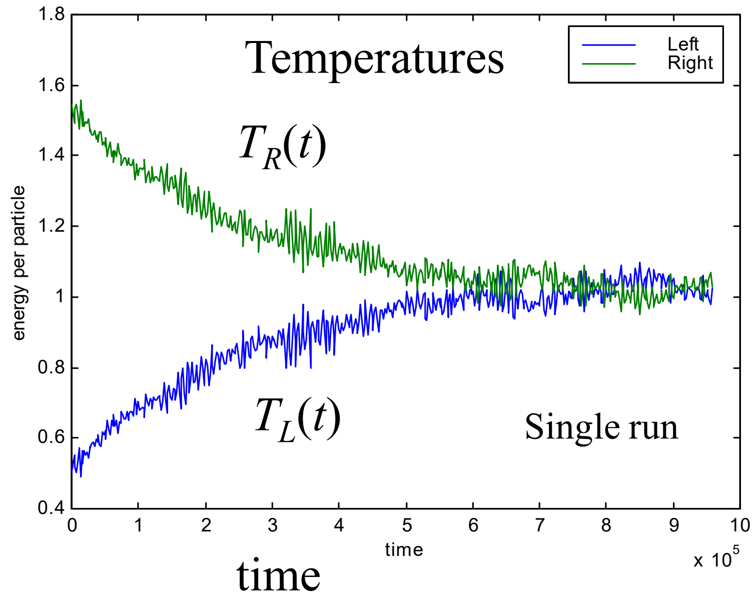
Chambers have gases at different temperatures, equal pressures.
Walls are perfectly elastic (specular reflection, accommodation α = 0)

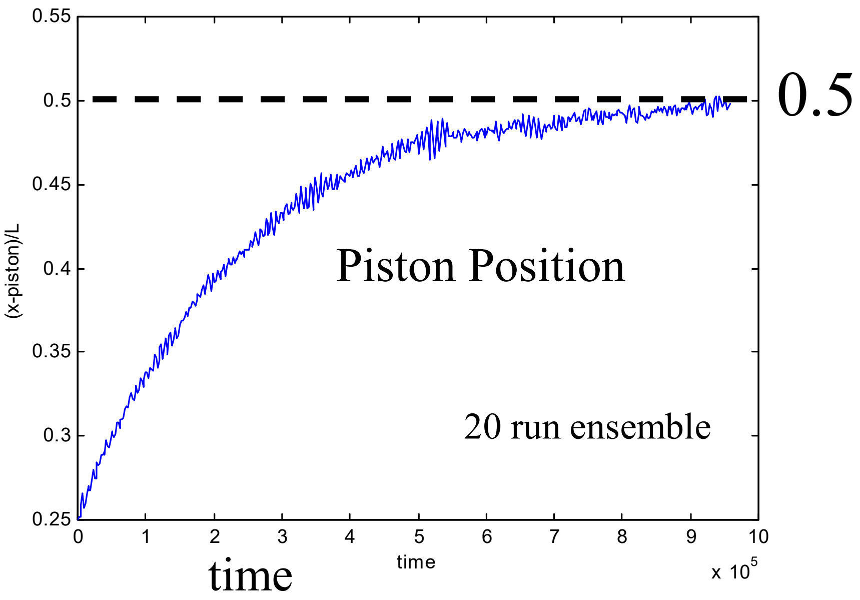
The piston moves (despite equal pressures) and the gases on the two sides reach a common temperature!

Adiabatic Piston by DSMC

Heat is conducted between the chambers by the non-equilibrium Brownian motion of the adiabatic piston.







M. Malek Mansour, ALG, and F. Baras, *Phys. Rev. E* **73** 016121 (2006)

DSMC / PDE Hybrids

Each approach has its own relative advantages

PDE Solvers

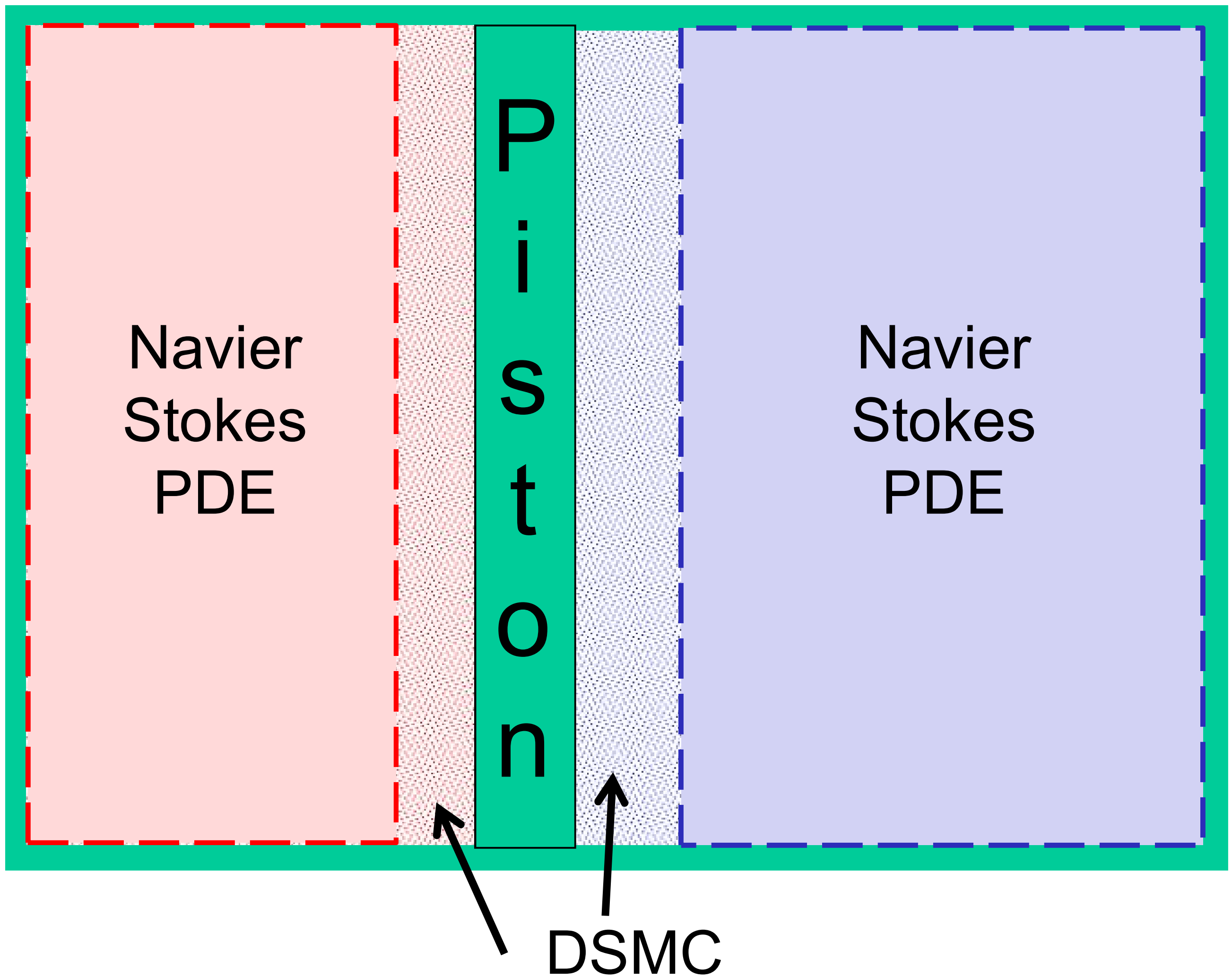
- **Fast (few variables, simple relations)**
- Efficient and accurate (high order CFD methods)
- Approximations available (incompressible, inviscid)

DSMC

- **More Physics (molecular details)**
- Thermal fluctuations
- Stable (H-theorem)

DSMC / PDE Hybrids use Navier-Stokes solver in flow regions where DSMC is not required.

Hybrid for Adiabatic Piston



Fluctuating Hydrodynamics

Landau introduced fluctuations into the Navier-Stokes equations by adding white noise fluxes of stress and heat.

$$\partial \mathbf{U}/\partial t + \nabla \cdot \mathbf{F} = \nabla \cdot \mathbf{D} + \nabla \cdot \mathbf{S} \quad \text{where} \quad \mathbf{U} = \begin{pmatrix} \rho \\ \mathbf{J} \\ E \end{pmatrix}$$

Hyperbolic Fluxes | Parabolic Fluxes | Stochastic Fluxes

$$\mathbf{F} = \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v}\mathbf{v} + P\mathbf{I} \\ (E+P)\mathbf{v} \end{pmatrix} \quad \mathbf{D} = \begin{pmatrix} 0 \\ \tau \\ \kappa \nabla T + \tau \cdot \mathbf{v} \end{pmatrix} \quad \mathbf{S} = \begin{pmatrix} 0 \\ \mathcal{S} \\ \mathcal{Q} + \mathbf{v} \cdot \mathcal{S} \end{pmatrix},$$

We have adapted standard numerical schemes from CFD to solve these stochastic PDEs.

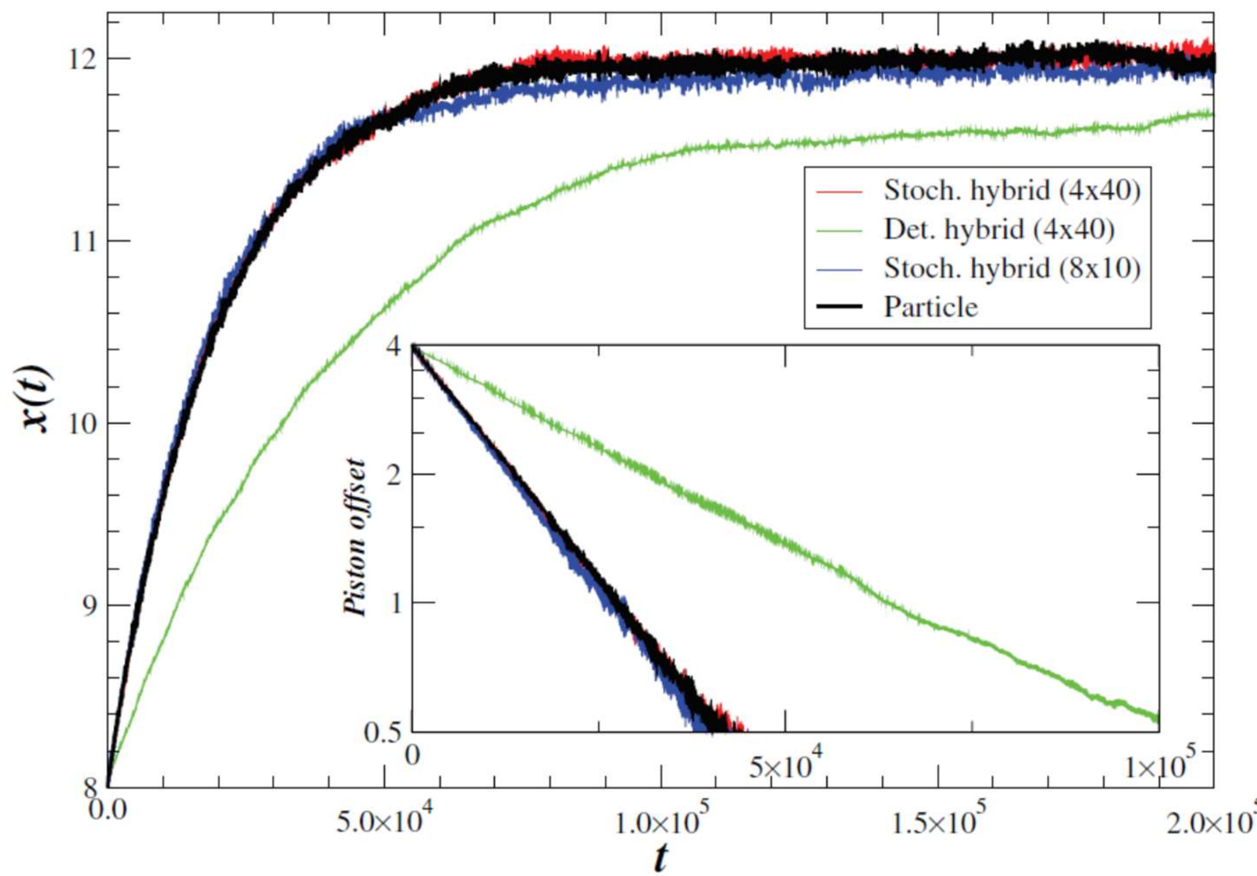
J.B. Bell, ALG, and S. Williams, Physical Review E 76 016708 (2007)

A. Donev, E. Vanden-Eijnden, ALG, and J.B. Bell, *Comm. in Applied Math. & Comp. Sci.* **5** 149–197 (2010)

Stochastic vs. Deterministic PDEs

Compare results from an all-DSMC simulation with hybrids DSMC/PDE simulations.

Long-time relaxation of the piston position is *wrong* using deterministic PDEs in the hybrid.



DSMC

A. Donev, J.B. Bell, ALG, and B. Alder, *SIAM Multiscale Model. Sim.* **8** 871-911 (2010)

Conclusions

- DSMC is a powerful engineering design tool (e.g., disk drive)
- DSMC has discovered interesting hydrodynamic effects in Poiseuille and Couette flows.
- DSMC has confirmed theoretical predictions for the enhancement of diffusion due to non-equilibrium fluctuations.
- DSMC must be used carefully due to these fluctuations (e.g., measuring fluid velocity; Brownian effects in hybrids).

Thank you for your attention

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