Surprising Hydrodynamic Results Discovered by means of Direct Simulation Monte Carlo

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von Karman Institute for Fluid Dynamics

Discoveries made by DSMC

This lecture will describe four interesting discoveries made using Direct Simulation Monte Carlo (DSMC).

First two occur due to Knudsen number effects:

* Anomalous Poiseuille Flow
* Anomalous Couette Flow

The other two occur due to thermal fluctuations:

* Anomalous Temperature Gradient Flow
* Anomalous Diffusion Flow

Outline

- Direct Simulation Monte Carlo
- Anomalous Poiseuille Flow
- Anomalous Couette Flow
- Anomalous Temperature Gradient Flow
- Anomalous Diffusion Flow

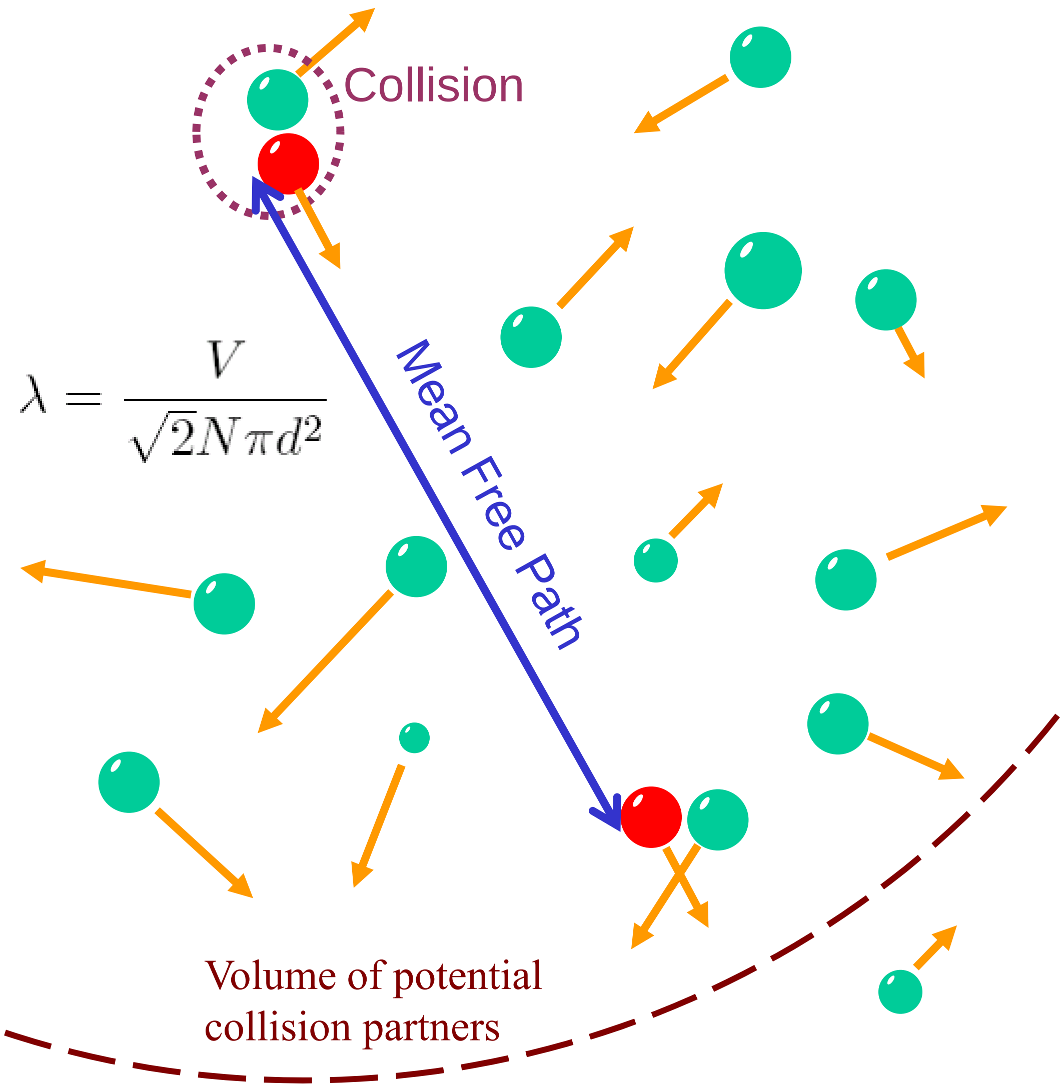
Molecular Dynamics for Dilute Gases

Molecular dynamics inefficient for simulating the kinetic scale.

Relevant time scale is mean free time but MD computational time step limited by time of collision.

DSMC time step is large because collisions are evaluated stochastically.

$$\lambda = \frac{V}{\sqrt{2} N \pi d^2}$$



Direct Simulation Monte Carlo

Development of DSMC

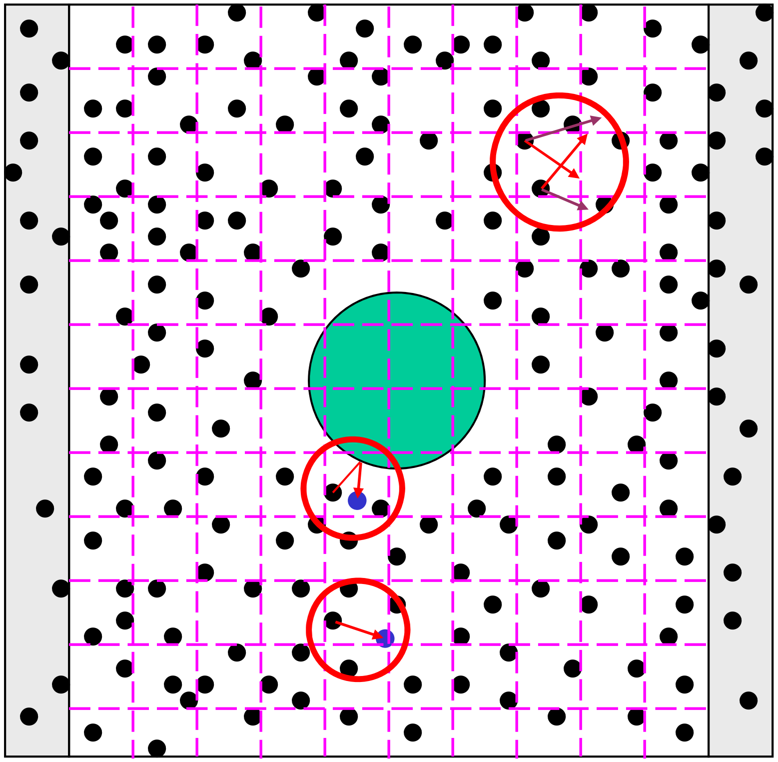
- DSMC developed by Graeme Bird (late 60's)
- Popular in aerospace engineering (70's)
- Variants & improvements (early 80's)
- Applications in physics & chemistry (late 80's)
- Used for micro/nano-scale flows (early 90's)
- Extended to dense gases & liquids (late 90's)
- Granular gas simulations (early 00's)
- Multi-scale modeling of complex fluids (late 00's)

DSMC is the dominant numerical method for molecular simulations of dilute gases

DSMC Algorithm

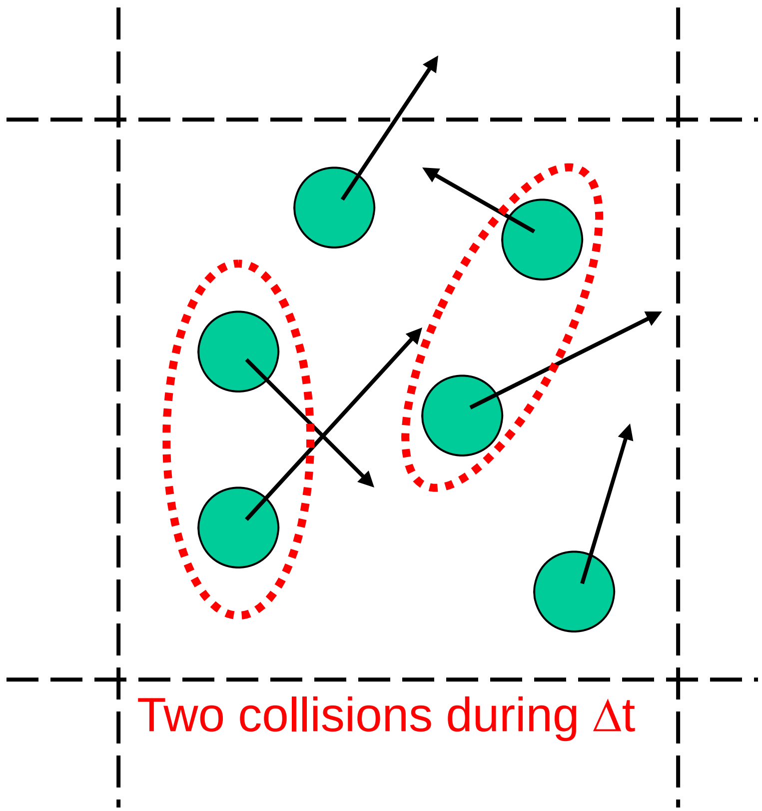
- Initialize system with particles
- Loop over time steps
  - Create particles at open boundaries
  - Move *all* the particles
  - Process any interactions of particle & boundaries
  - Sort particles into cells
  - Select and execute random collisions
  - Sample statistical values

Example: Flow past a sphere



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



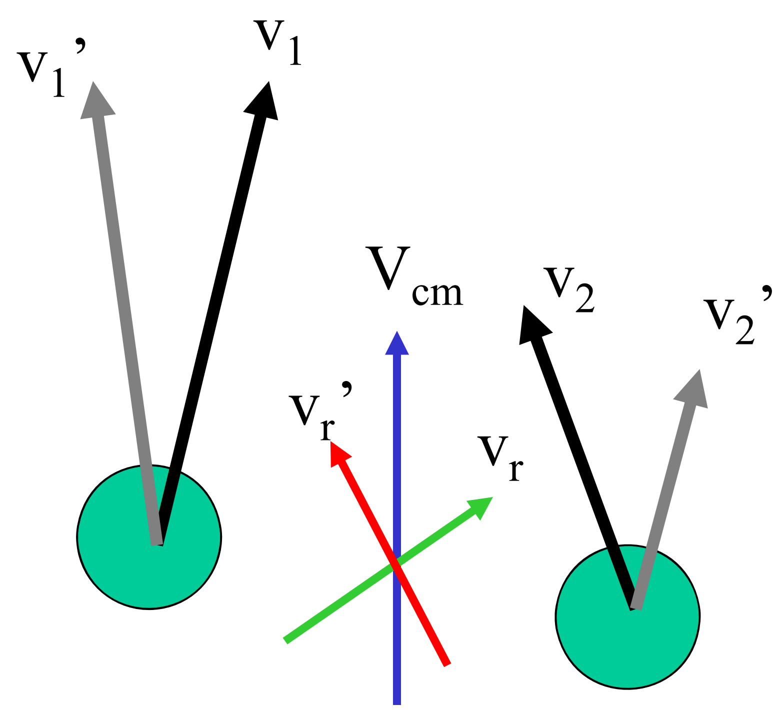
Probability that a pair collides only depends on their relative velocity.

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)



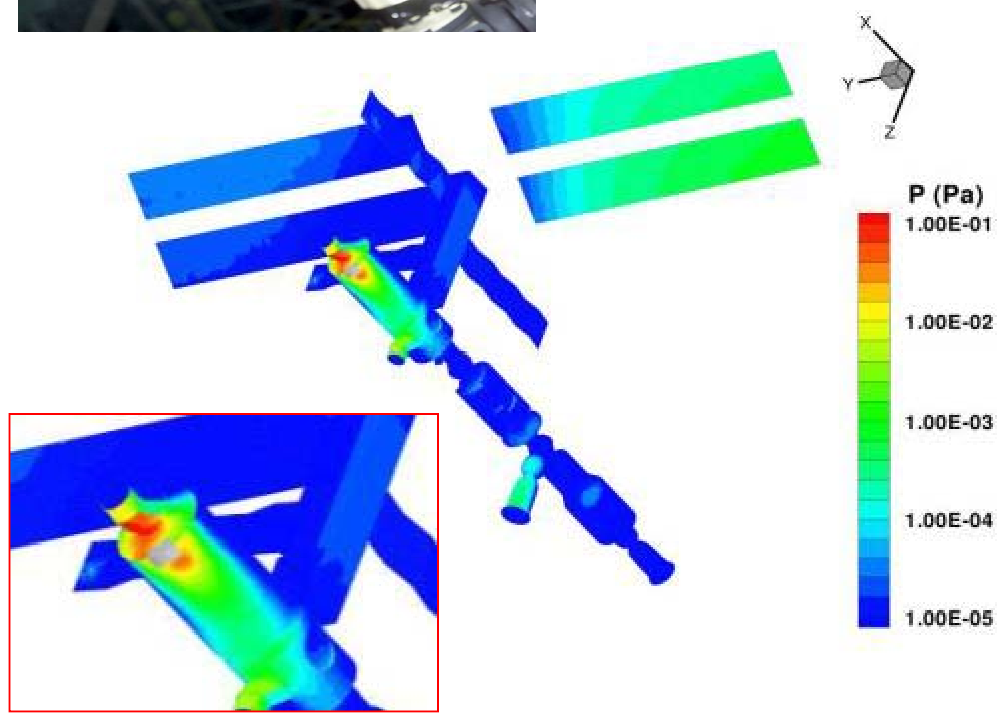
Direction of v_r' is uniformly distributed in the unit sphere

DSMC in Aerospace Engineering

International Space Station experienced an unexpected 20-25 degree roll about its X-axis during usage of the U.S. Lab vent relief valve.

Mean free path
~ 1 m @ 10^{-1} Pa

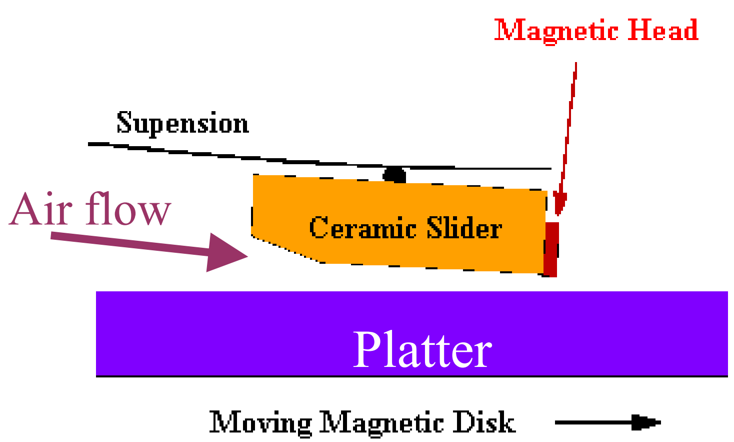
Analysis using DSMC provided detailed insight into the anomaly and revealed that the “zero thrust” T-vent imparts significant torques on the ISS when it is used.

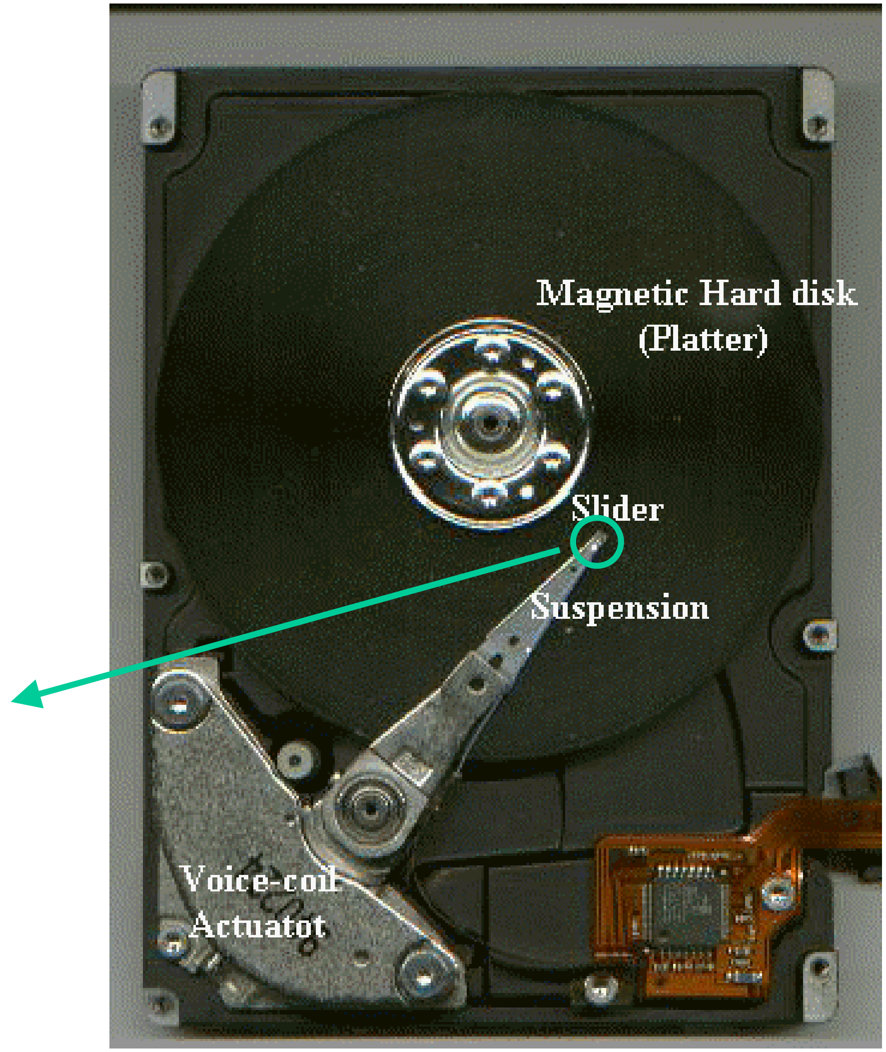


NASA DAC (DSMC Analysis Code)

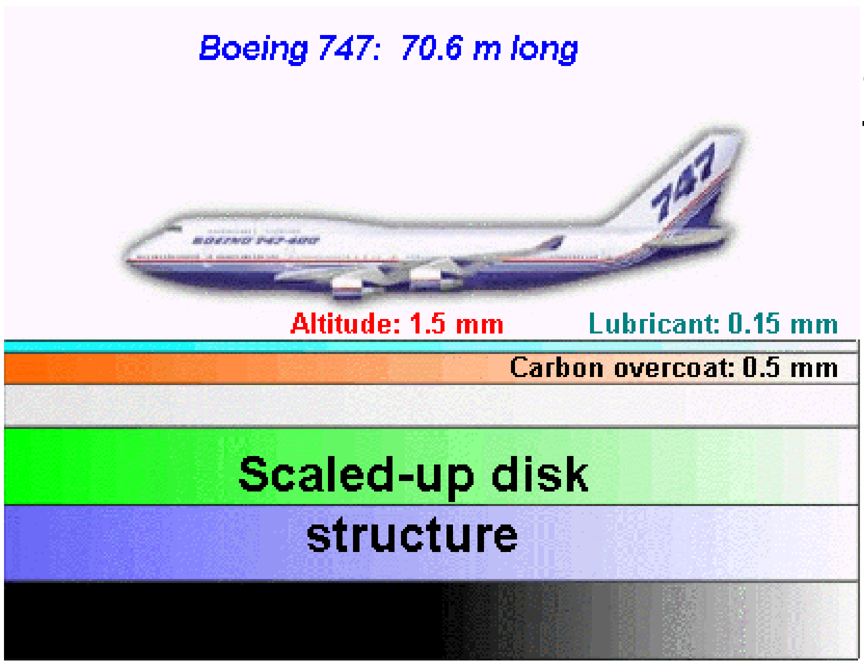
Computer Disk Drives

Mechanical system resembles phonograph, with the read/write head located on an air bearing slider positioned at the end of an arm.

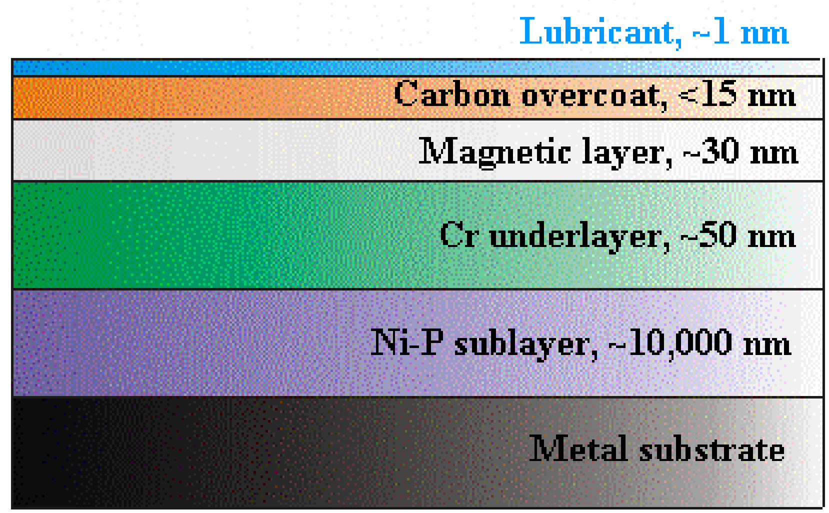




Multi-scales of Air Bearing Slider



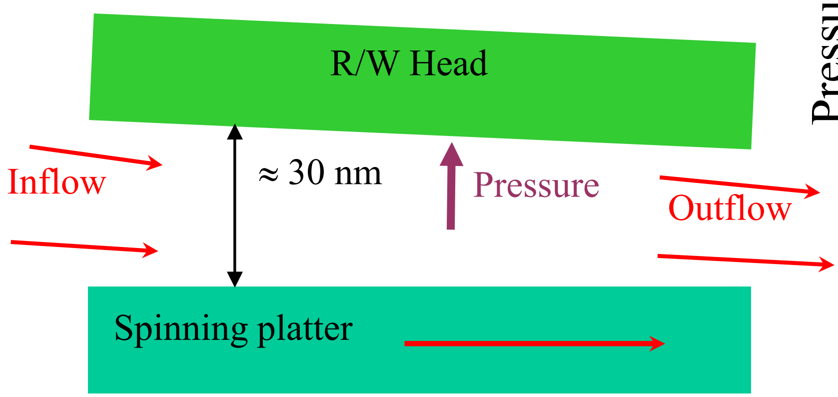
Slider (1 mm long) flies about 30 nm above platter. This is like a 747 flying 1.5 millimeters above ground

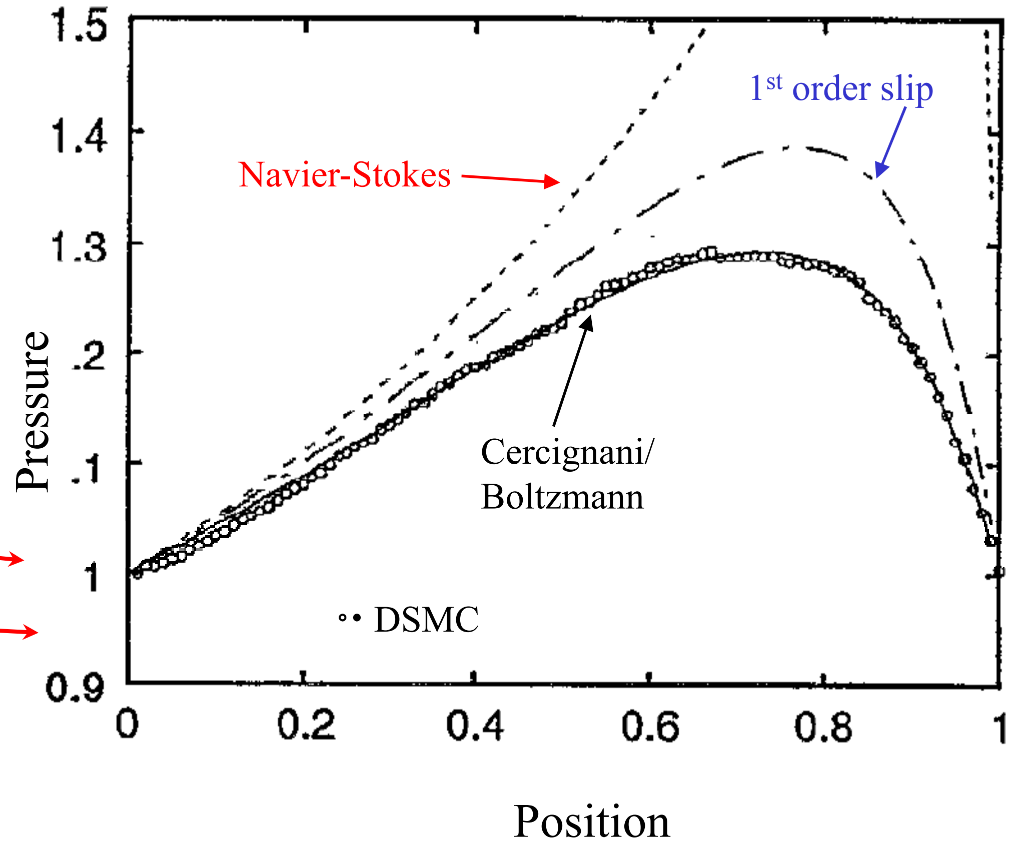


Sensitivity decreases exponentially with height

DSMC Simulation of Air Slider

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





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

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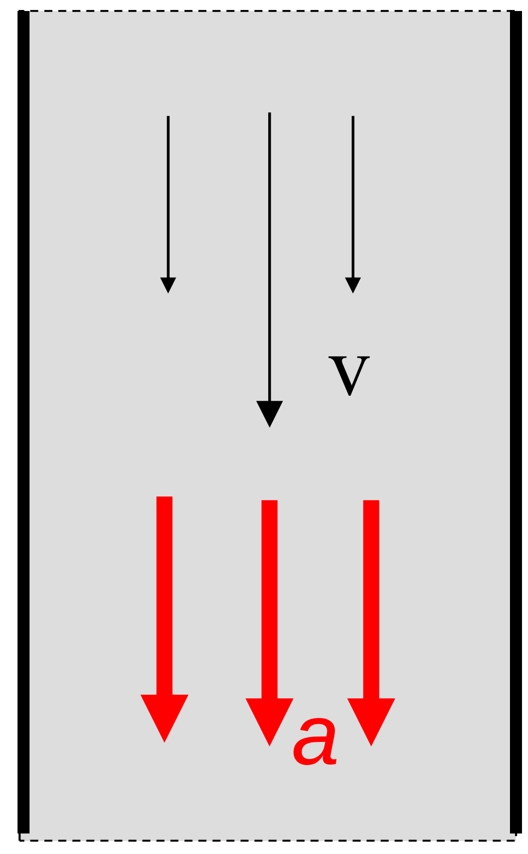
- Anomalous Poiseuille Flow
- Anomalous Couette Flow
- Anomalous Temperature Gradient Flow
- Anomalous Diffusion Flow

Acceleration Poiseuille Flow

Similar to pipe flow but between pair of flat planes (thermal walls).

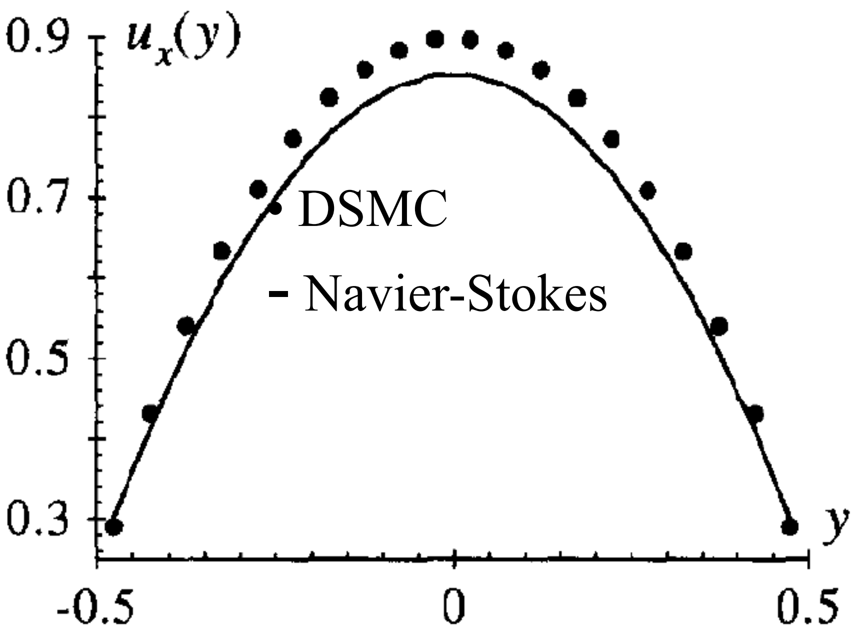
Push the flow with a body force, such as gravity.

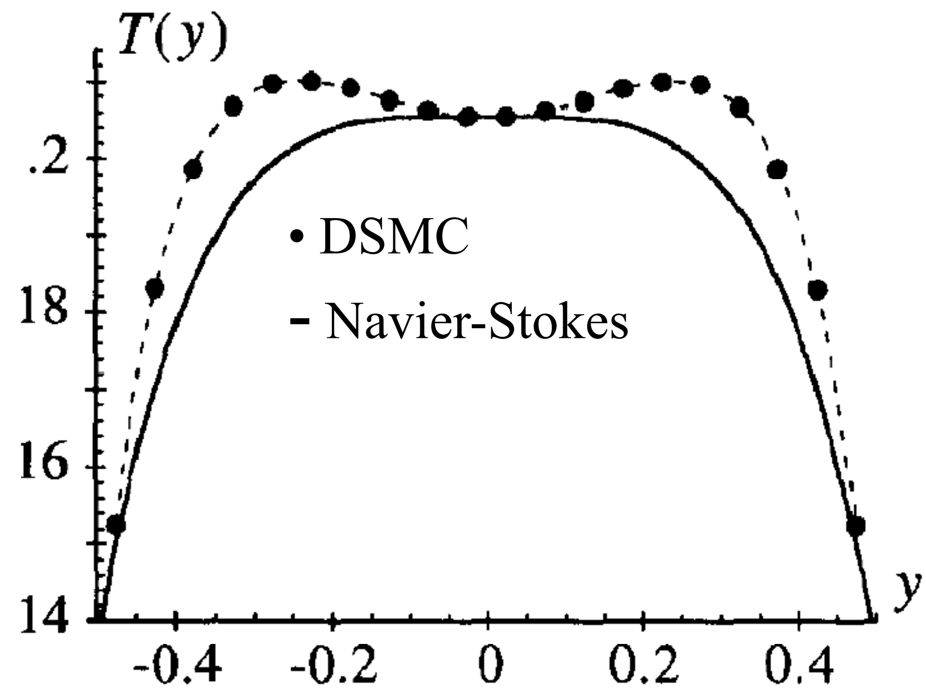
Channel widths roughly 10 to 100 mean free paths (Kn ≈ 0.1 to 0.01)



Anomalous Temperature

Velocity profile in qualitative agreement with Navier-Stokes but temperature has anomalous dip in center.



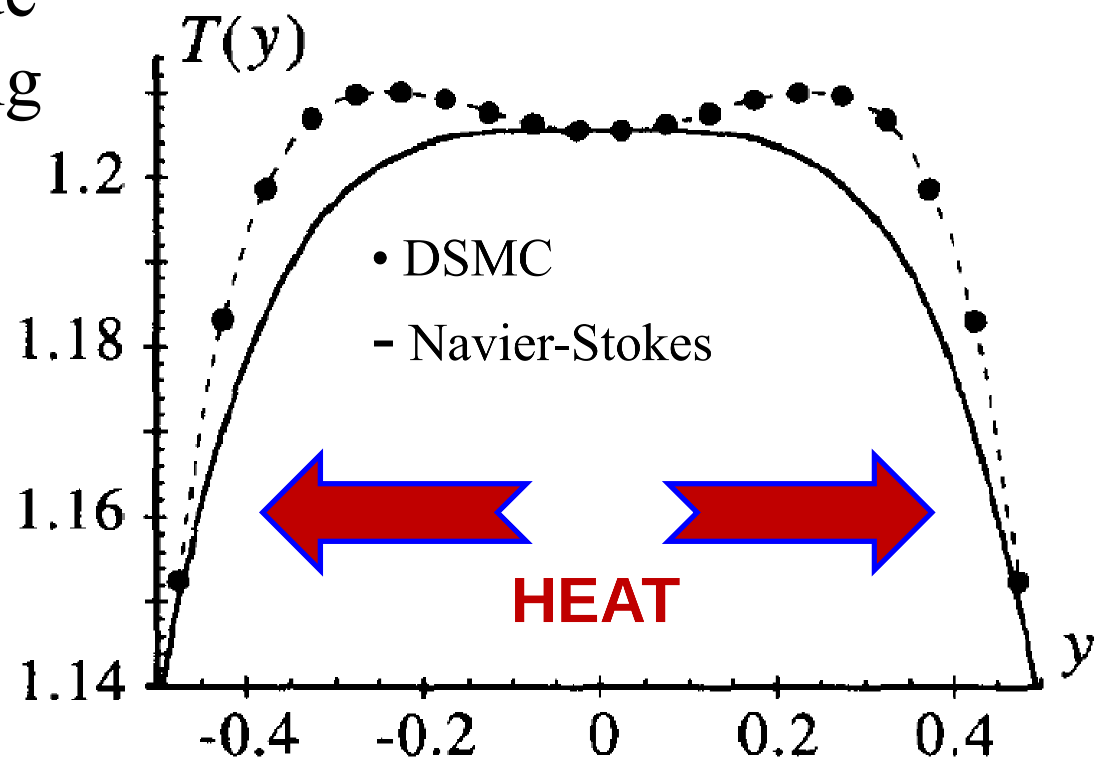


M. Malek Mansour, F. Baras and A. Garcia, *Physica A* **240** 255 (1997).

Heat Flux &Temperature Gradient

Heat is generate inside the system by shearing and it is removed at the walls.

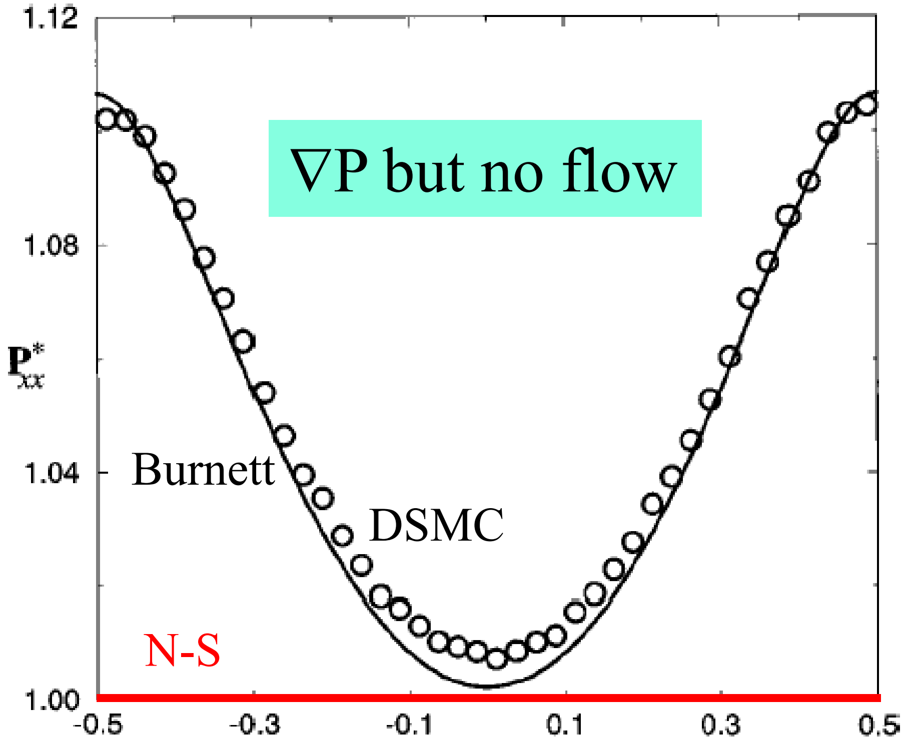
Heat is flowing from cold to hot near the center.



M. Malek Mansour, F. Baras and A. Garcia, *Physica A* **240** 255 (1997).

Burnett Theory for Poiseuille

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



Navier-Stokes

$$\mathbf{P}^{\mathrm{NS}} = p\,\mathbf{I} - 2\,\mu\,\overset{\circ}{\overline{\overline{\nabla \mathbf{c}_0}}},$$

Burnett

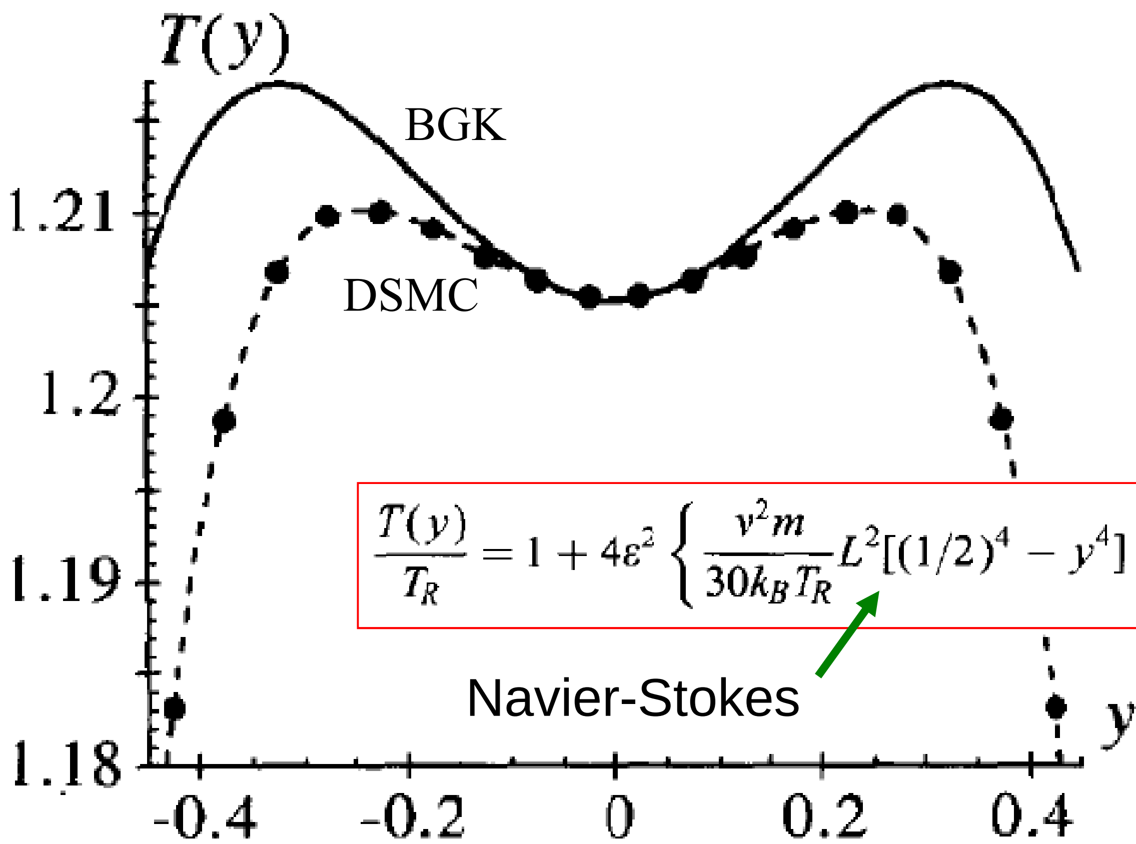
$$\omega_1 \frac{\mu^2}{p}\Delta\mathring{\mathbf{e}} + \omega_2 \frac{\mu^2}{p}\left\{\frac{D_0}{Dt}\,\mathring{\mathbf{e}} - 2\,\overset{\circ}{\overline{\overline{\nabla \mathbf{c}_0 \cdot \mathring{\mathbf{e}}}}}\right\} + \omega_3 \frac{\mu^2}{\rho T}\overset{\circ}{\overline{\overline{\nabla\nabla T}}}$$

$$+ \omega_4 \frac{\mu^2}{\rho p T}\overset{\circ}{\overline{\overline{\nabla p \nabla T}}} + \omega_5 \frac{\mu^2}{\rho T^2}\overset{\circ}{\overline{\overline{\nabla T \nabla T}}} + \omega_6 \frac{\mu^2}{\rho T}\overset{\circ}{\overline{\overline{\mathring{\mathbf{e}} \cdot \mathring{\mathbf{e}}}}},$$

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

BGK Theory for Poiseuille

Kinetic theory calculations using BGK theory predict the dip.



"Dip" term

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

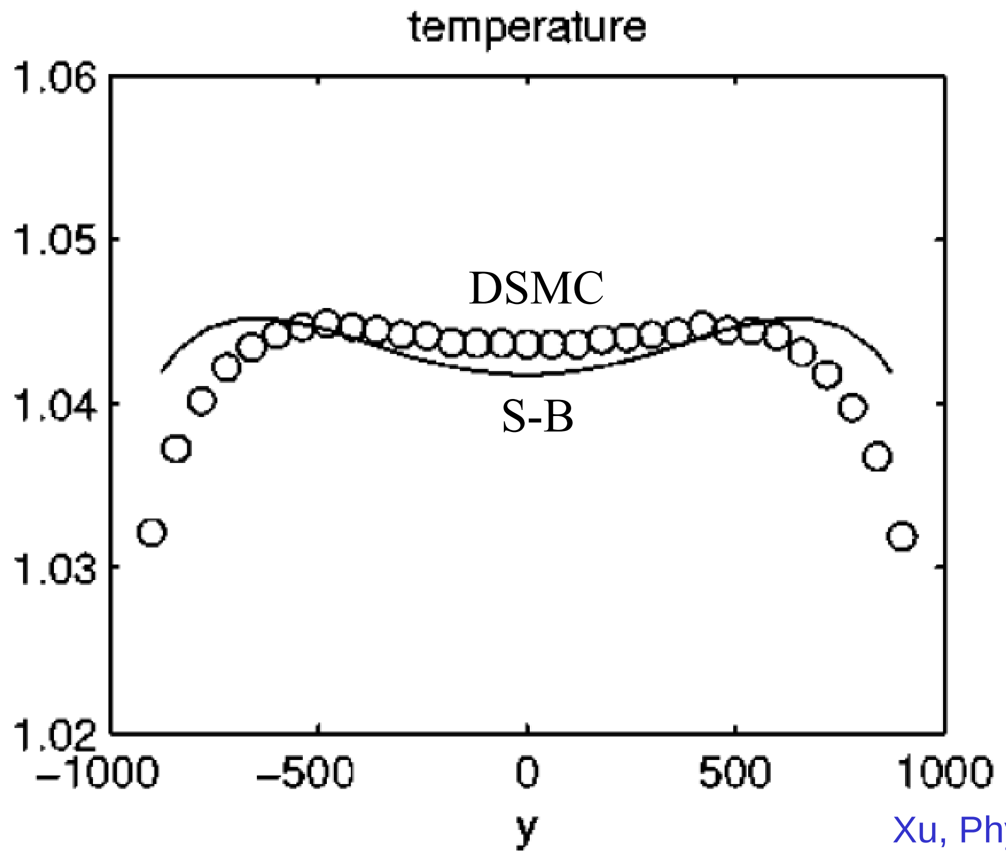
Navier-Stokes

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

M. Tij, A. Santos, *J. Stat. Phys.* **76** 1399 (1994)

Super-Burnett Calculations

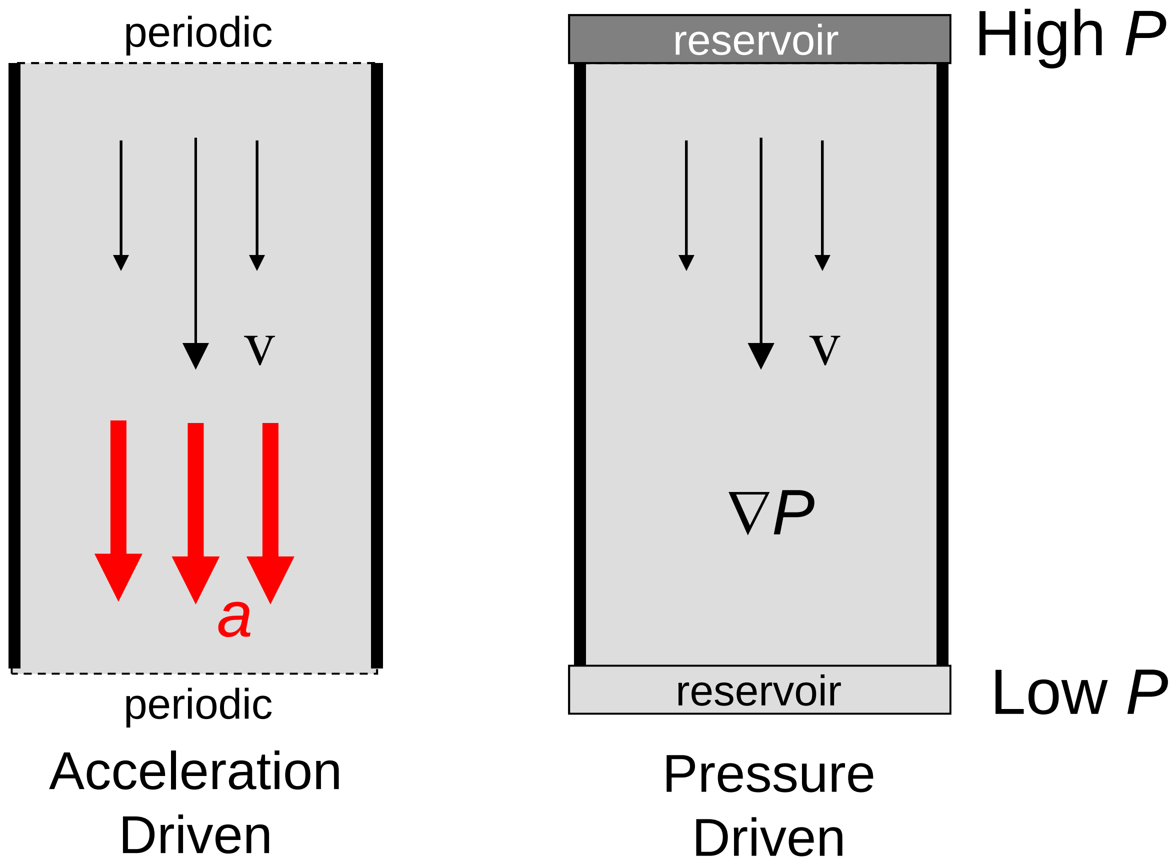
Burnett theory does not get temperature dip but it is recovered at Super-Burnett level.



Xu, Phys. Fluids 15 2077 (2003)

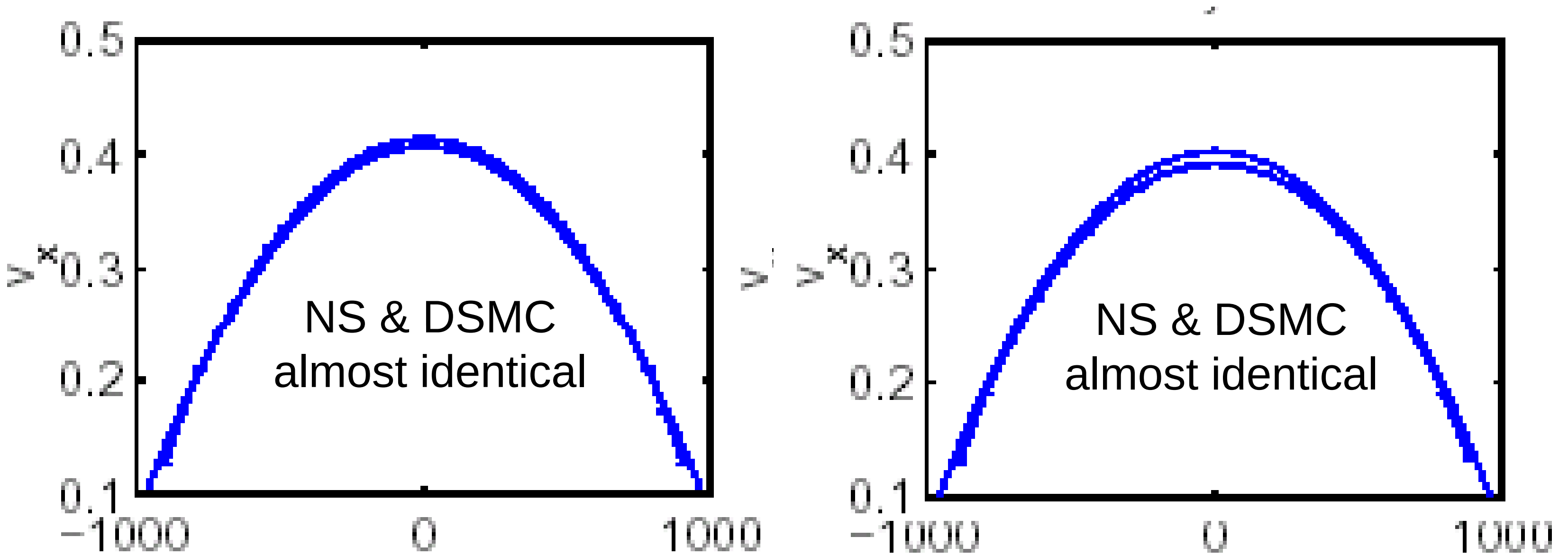
Pressure-driven Poiseuille Flow

Compare acceleration-driven and pressure-driven Poiseuille flows



Poiseuille: Fluid Velocity

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



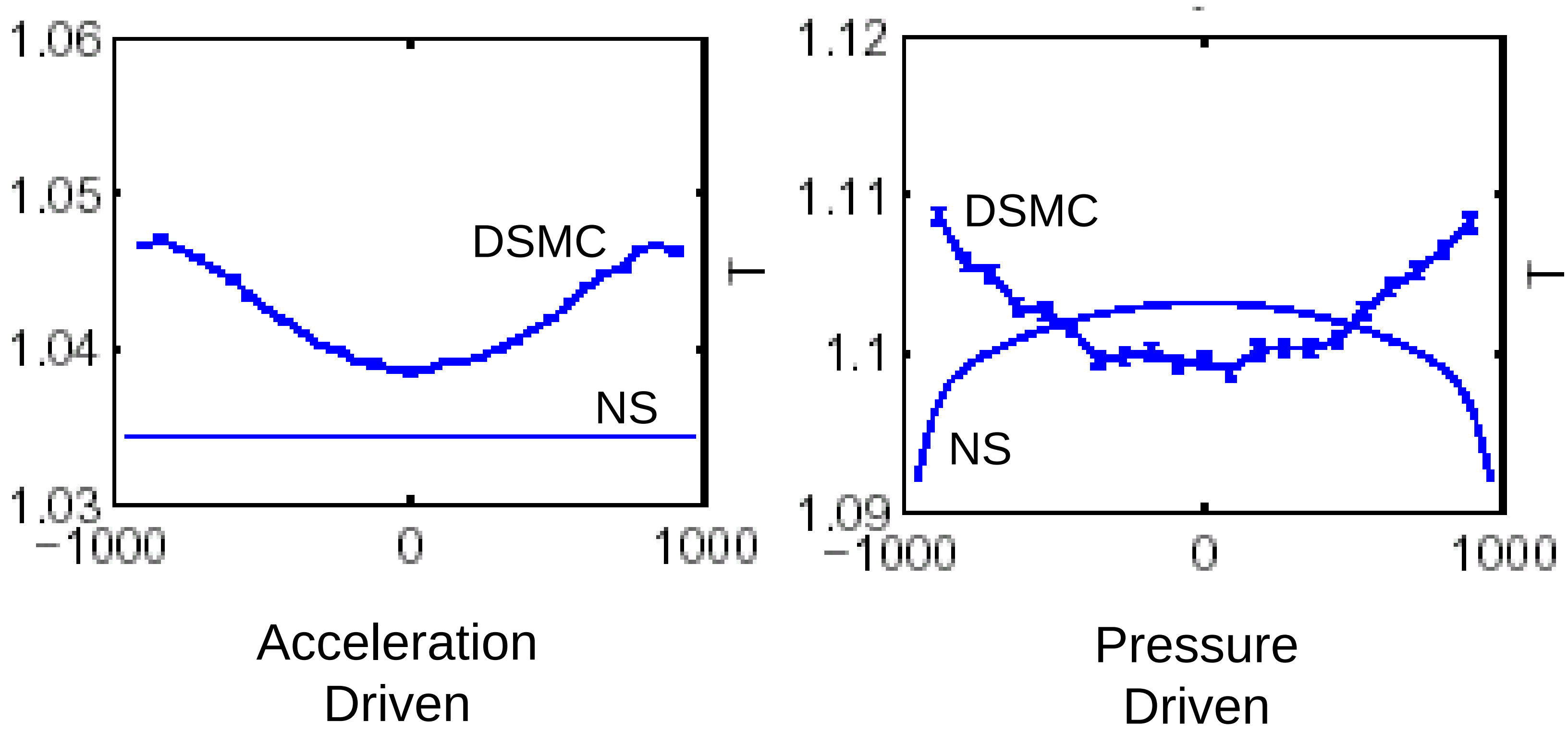
Acceleration Driven

Pressure Driven

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

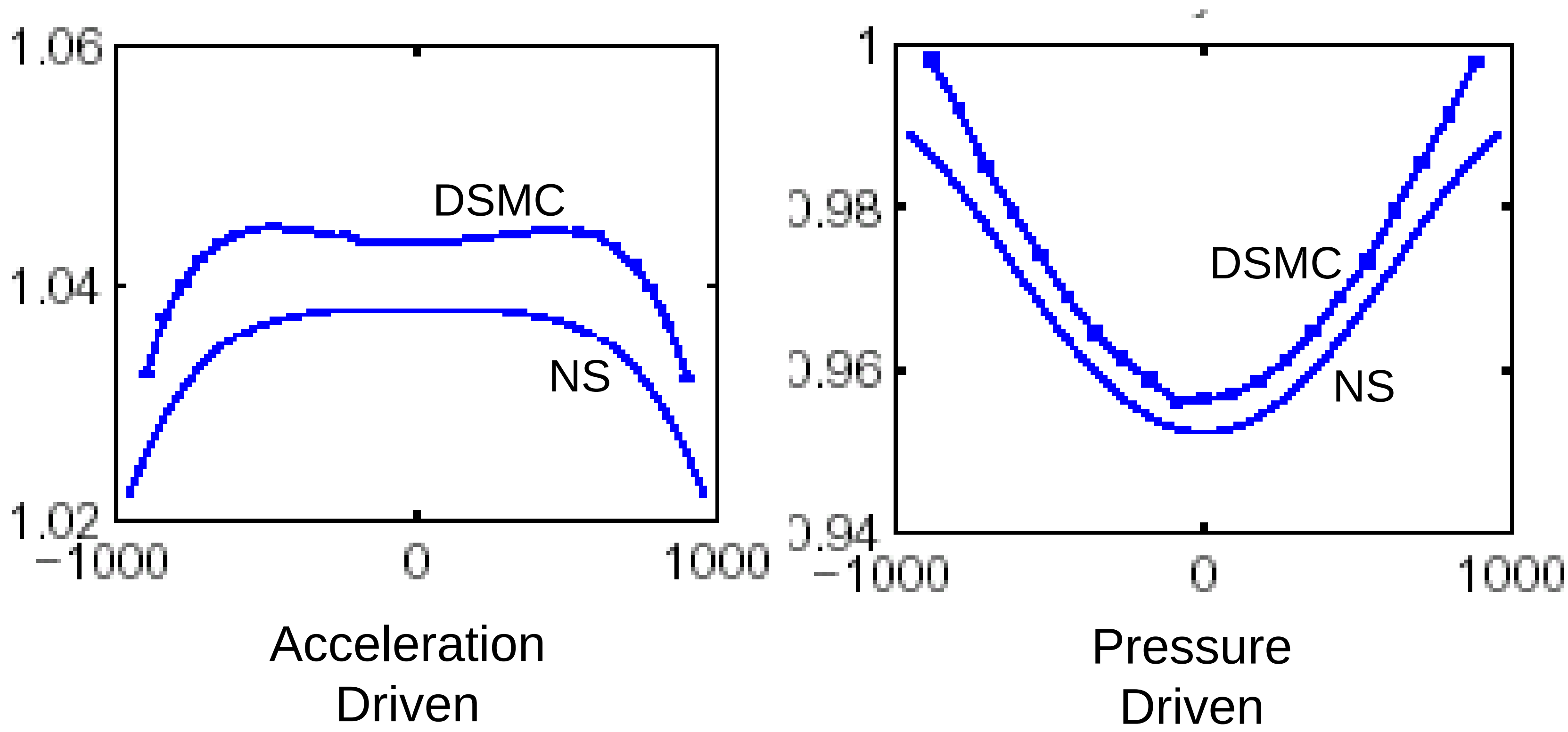
Poiseuille: Pressure

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



Y. Zheng, A. Garcia, and B. Alder, *J. Stat. Phys.* **109** 495-505 (2002).

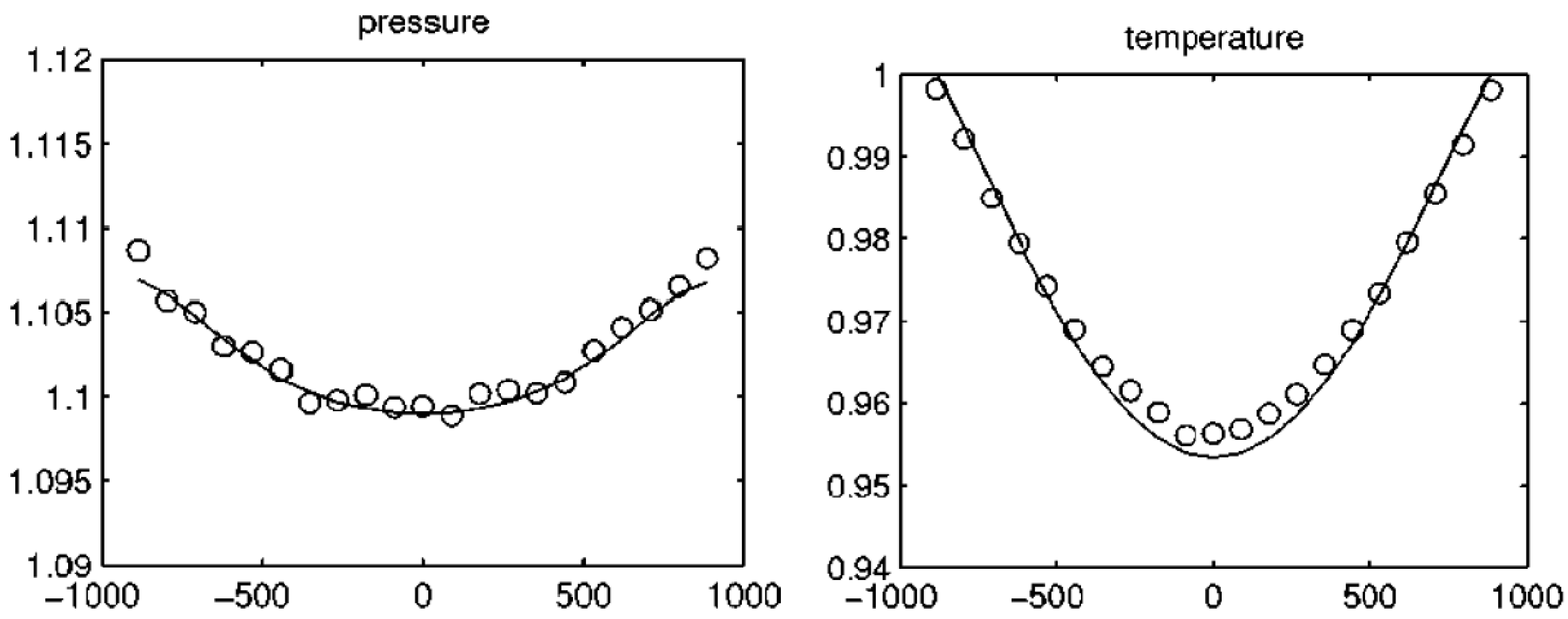
Poiseuille: Temperature



Y. Zheng, A. Garcia, and B. Alder, *J. Stat. Phys.* **109** 495-505 (2002).

Super-Burnett Theory

Super-Burnett accurately predicts profiles.



Xu, Phys. Fluids 15 2077 (2003)

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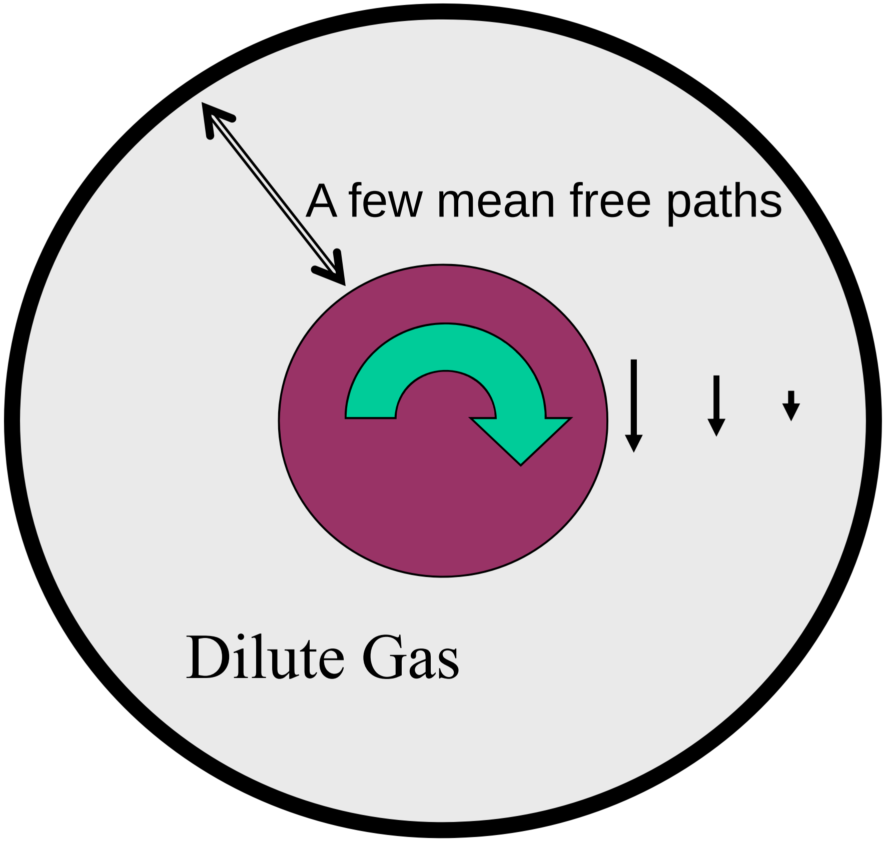
Couette Flow

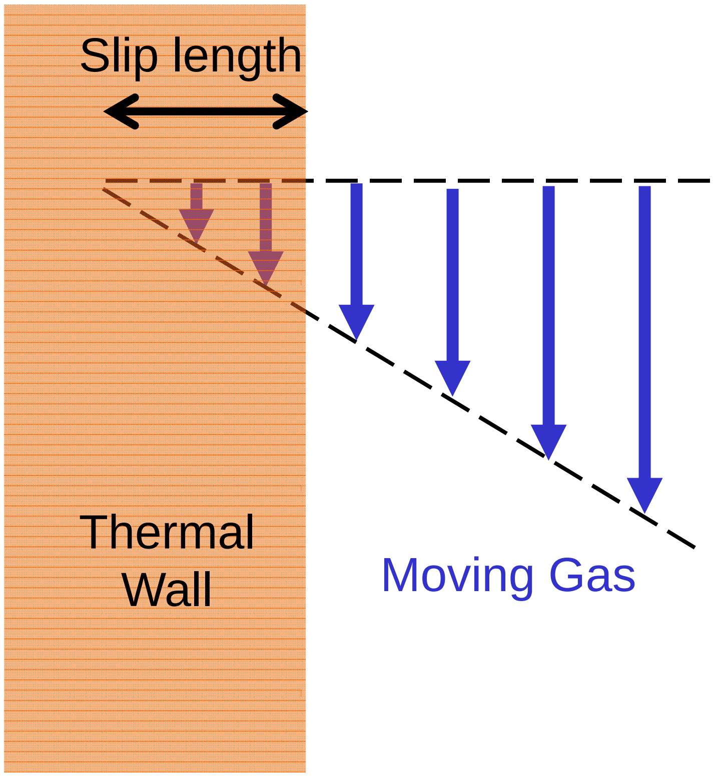
Dilute gas between concentric cylinders. Outer cylinder fixed; inner cylinder rotating.

Low Reynolds number ($Re \approx 1$) so flow is laminar; also subsonic.



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.

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

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

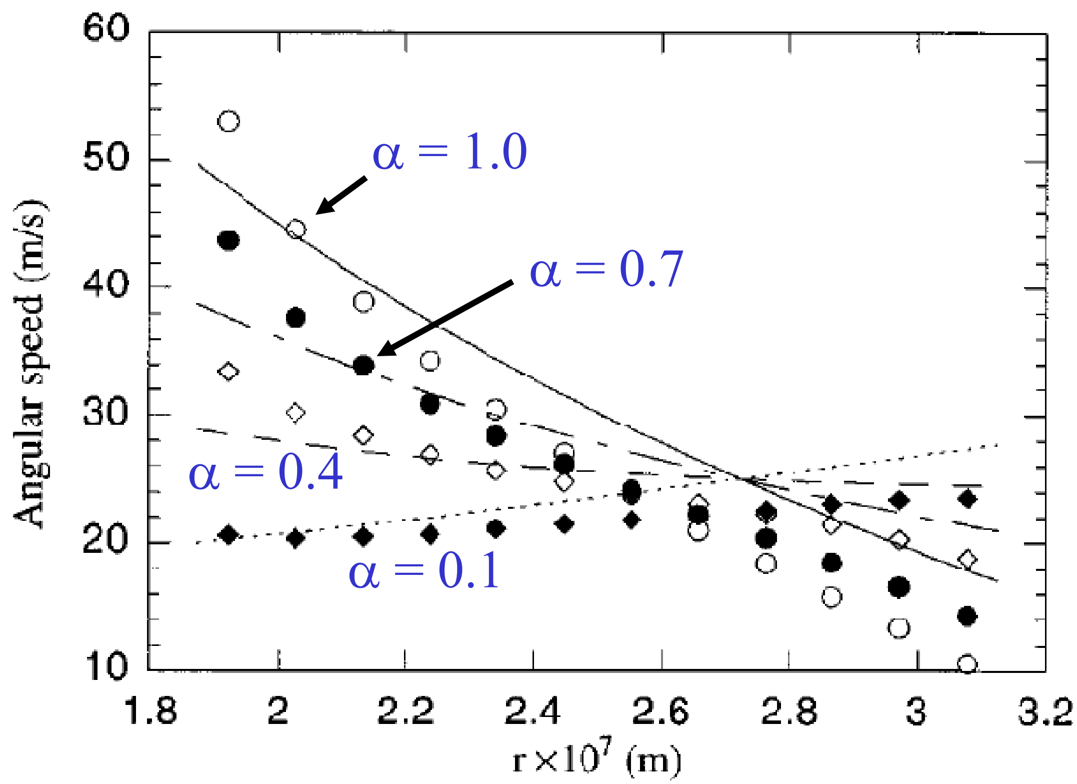
Slip in Couette Flow

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

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

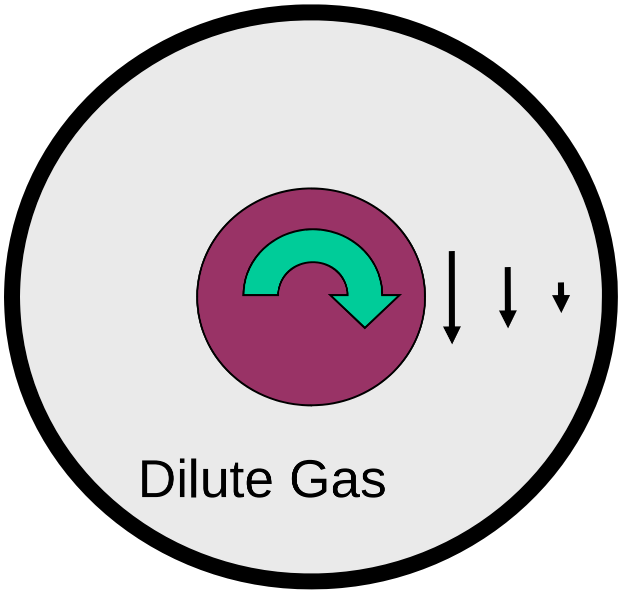
$$A = \frac{1}{R_2^2}\left(1 - 2\frac{\zeta_0}{R_2}\right); \quad B = \frac{1}{R_1^2}\left(1 + 2\frac{\zeta_0}{R_1}\right)$$

ζ is the slip length.



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

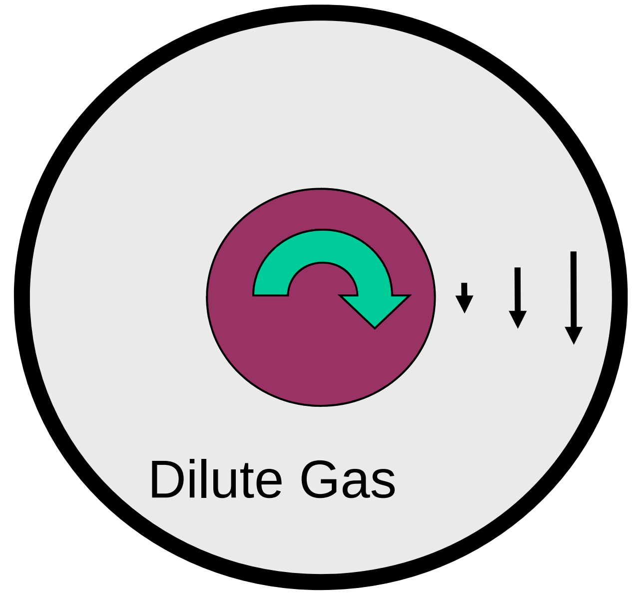
Diffusive and Specular Walls



Diffusive Walls

Outer wall stationary

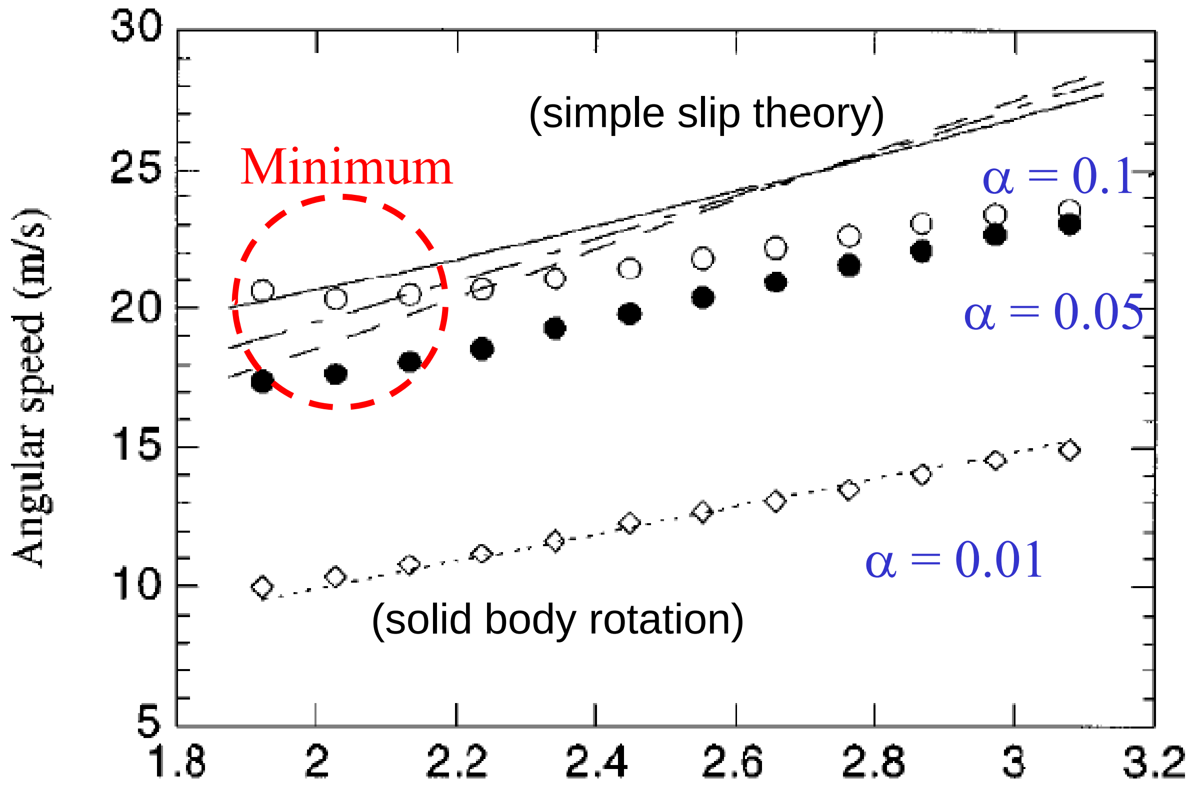
When walls are completely specular the gas undergoes solid body rotation so $v = \omega r$



Specular Walls

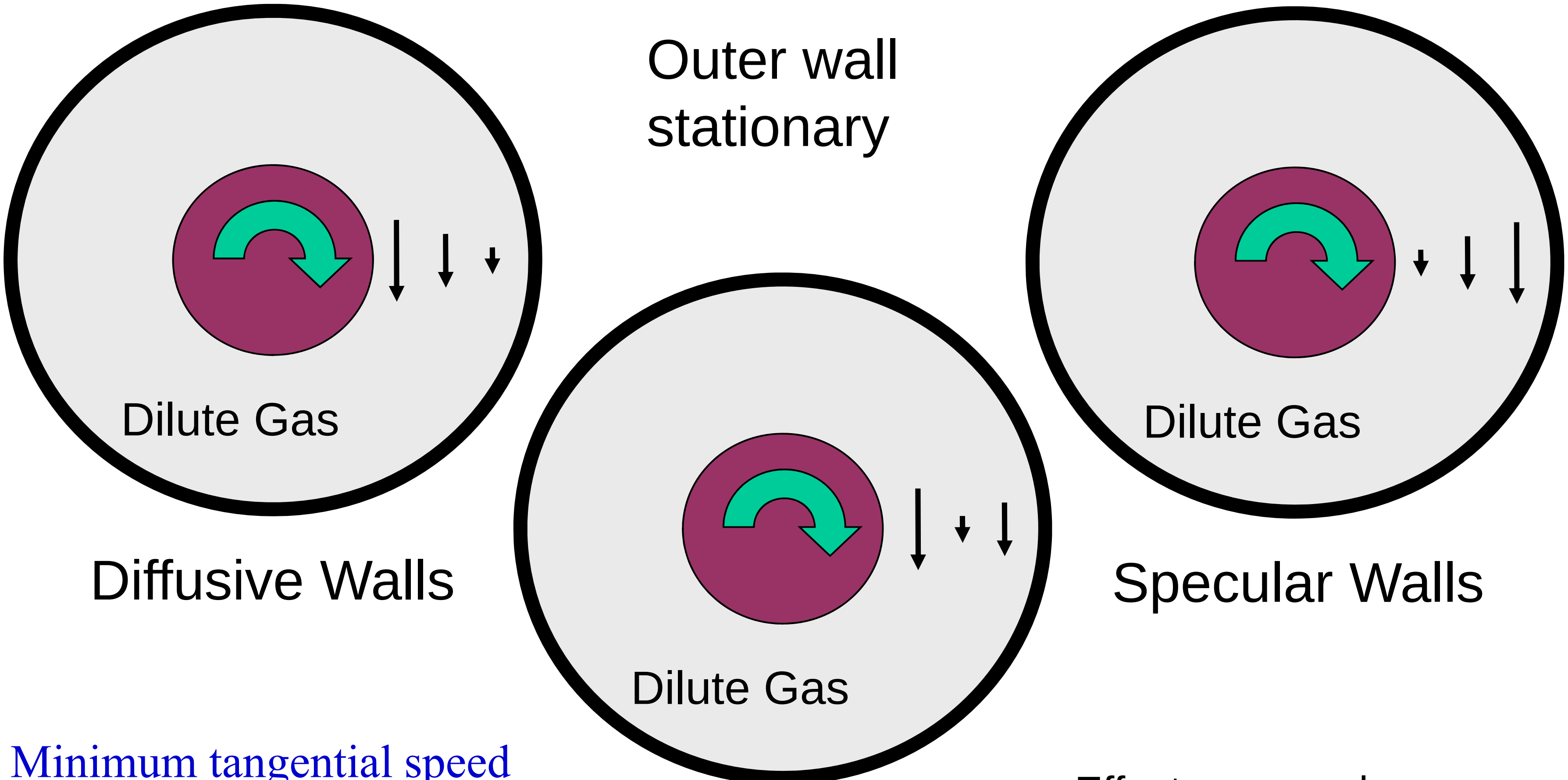
Anomalous Couette Flow

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



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

Anomalous Rotating Flow



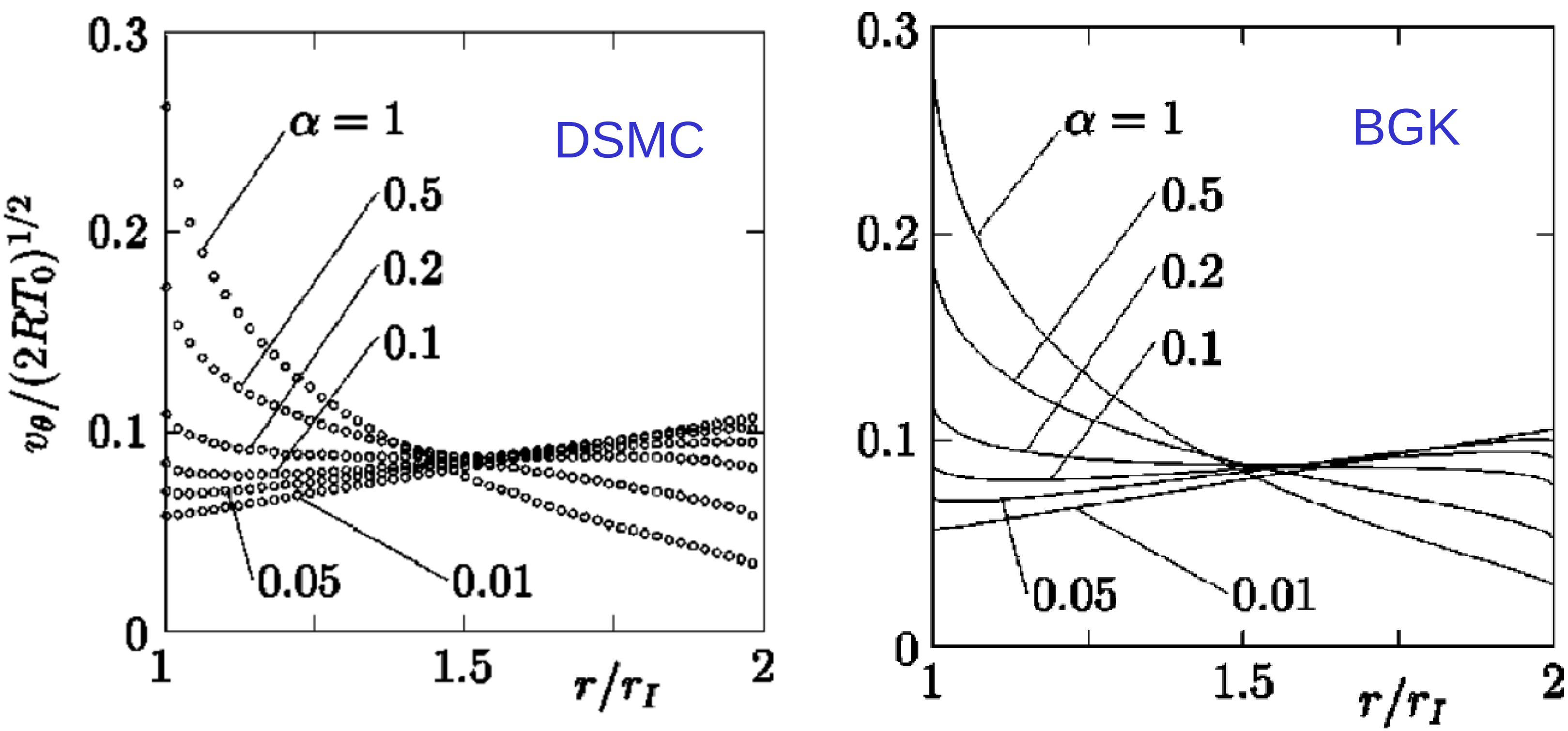
Intermediate Case

Minimum tangential speed occurs *in between* the walls

Effect occurs when walls ~80-90% specular

BGK Theory

Excellent agreement between DSMC data and BGK calculations; the latter confirm velocity minimum at low accommodation.



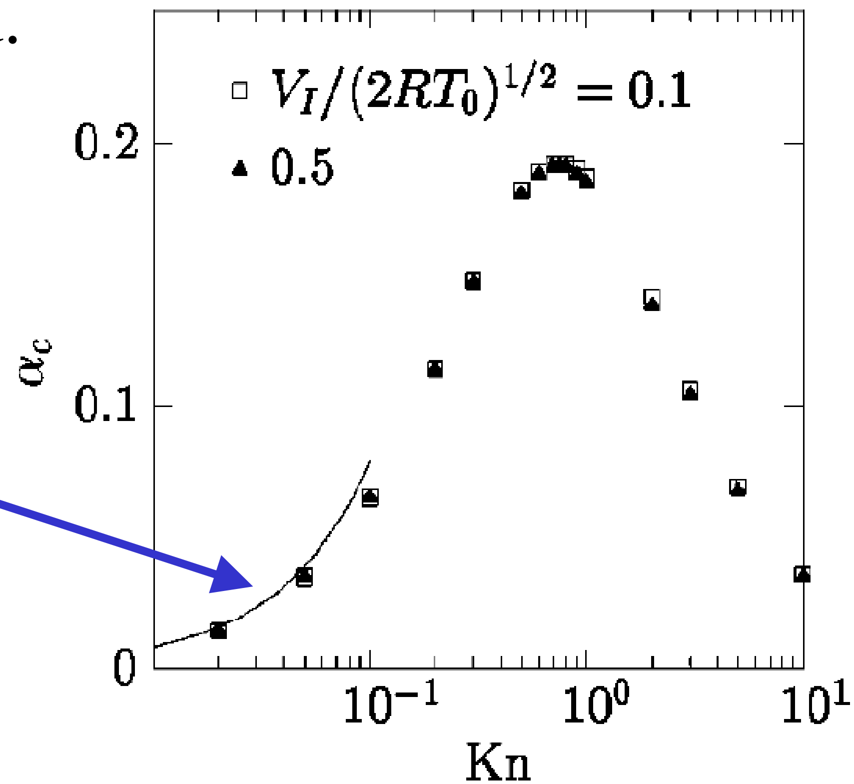
K. Aoki, H. Yoshida, T. Nakanishi, A. Garcia, *Physical Review E* **68** 016302 (2003).

Critical Accommodation for Velocity Minimum

BGK theory allows accurate computation of critical accommodation at which the velocity profile has a minimum within the fluid.

Approximation is

$$\alpha_c \approx \frac{\pi}{2} \frac{r_I}{r_O} \text{Kn}$$



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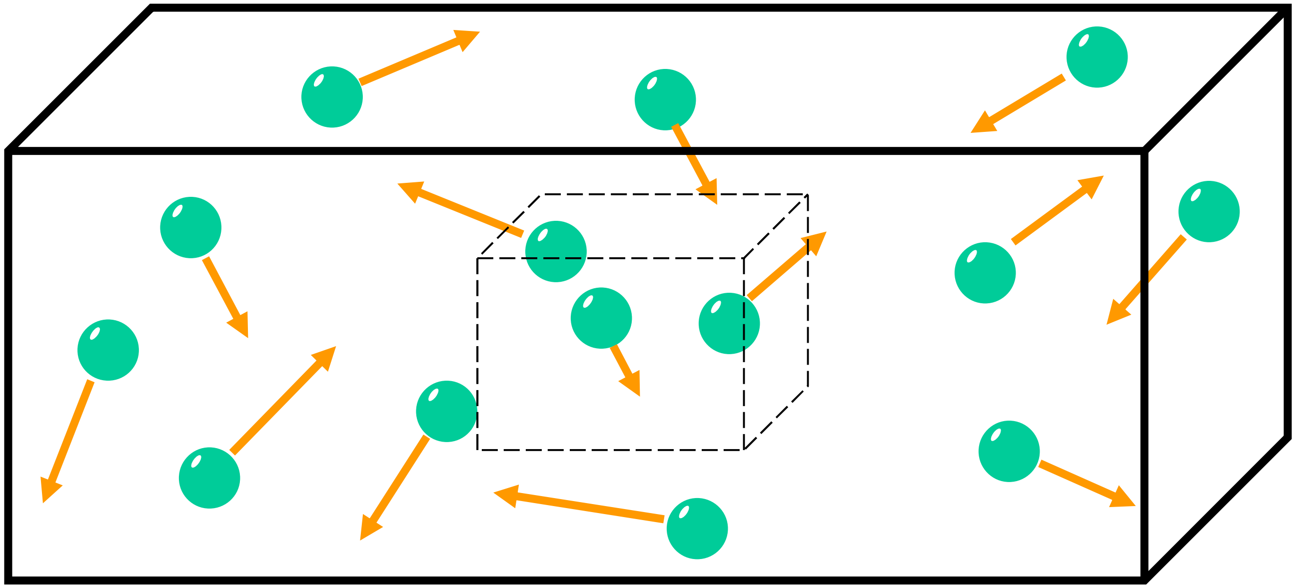
Fluid Velocity



How should one measure local fluid velocity from particle velocities?

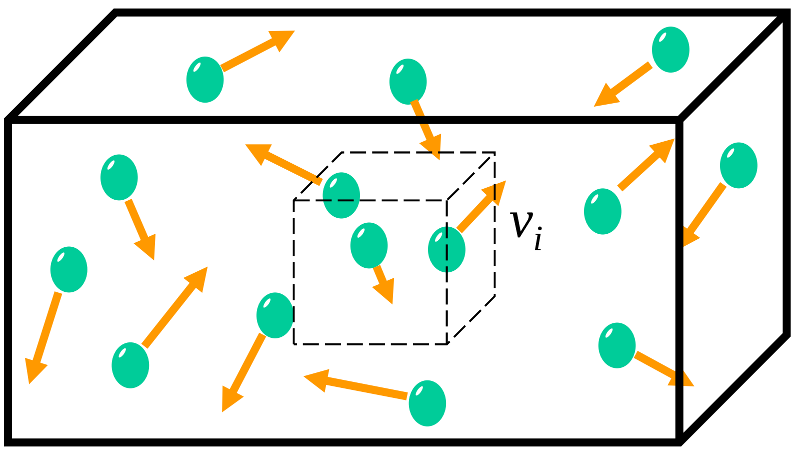
Instantaneous Fluid Velocity

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

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



Note that $u = \bar{v}$

Estimating Mean Fluid Velocity

Mean of instantaneous fluid velocity

$$\langle u \rangle = \frac{1}{S}\sum_{j=1}^{S} u(t_j) = \frac{1}{S}\sum_{j=1}^{S}\left(\frac{1}{N(t_j)}\sum_{i\in C}^{N(t_j)} v_i(t_j)\right)$$

where S is number of samples

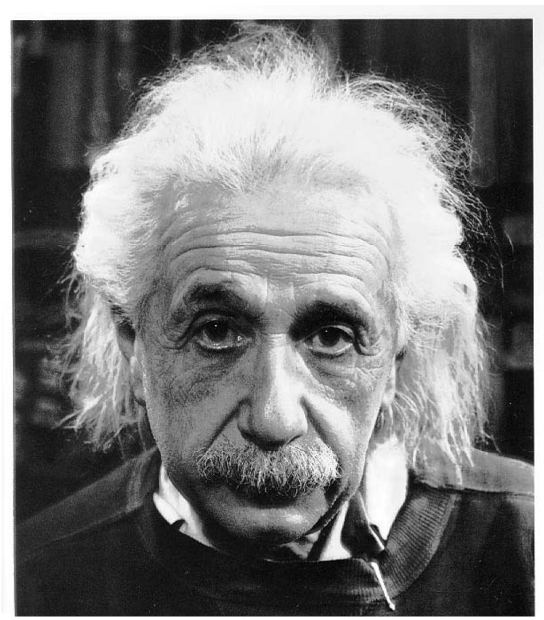
Alternative estimate is cumulative average

$$\langle u \rangle_* = \frac{\sum_j^S \sum_{i\in C}^{N(t_j)} v_i(t_j)}{\sum_j^S N(t_j)}$$

Landau Model for Students

Simplified model for university students:

Genius



Intellect = 3

Not Genius

Intellect = 1

Three Semesters of Teaching

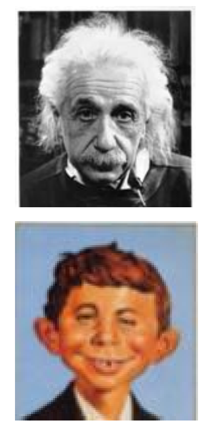
First semester

Average = 3

Second semester

Average = 1

Third semester



Average = 2

Sixteen students in three semesters

Total value is 2x3+14x1 = 20.

Average Student?

How do you estimate the intellect of the average student?

Average of values for the three semesters:

$(3 + 1 + 2)/3 = 2$

Or

Cumulative average over all students:

$(2 \times 3 + 14 \times 1)/16 = 20/16 = 1.25$

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

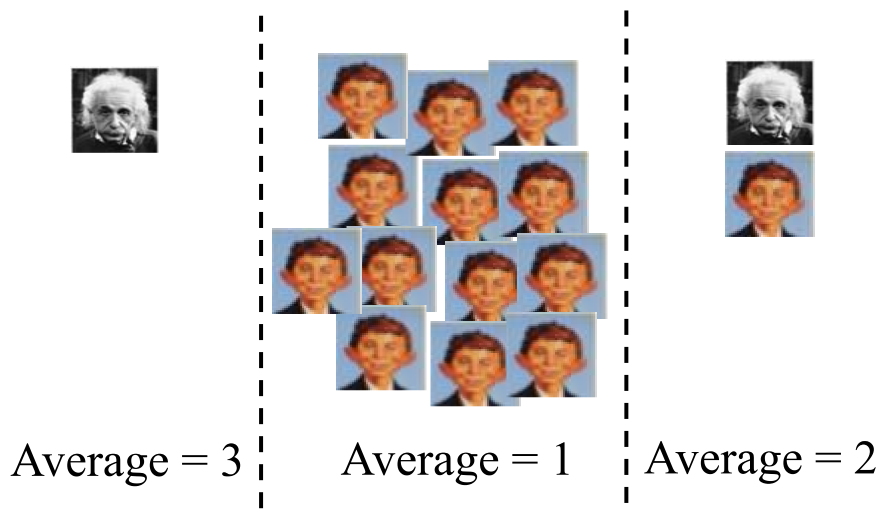
Relation to Student Example

$$\langle u \rangle = \frac{1}{S}\sum_{j=1}^{S}\left(\frac{1}{N(t_j)}\sum_{i\in C}^{N(t_j)} v_i(t_j)\right)$$

$$\langle u \rangle_* = \frac{\sum_j^S \sum_{i\in C}^{N(t_j)} v_i(t_j)}{\sum_j^S N(t_j)}$$

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

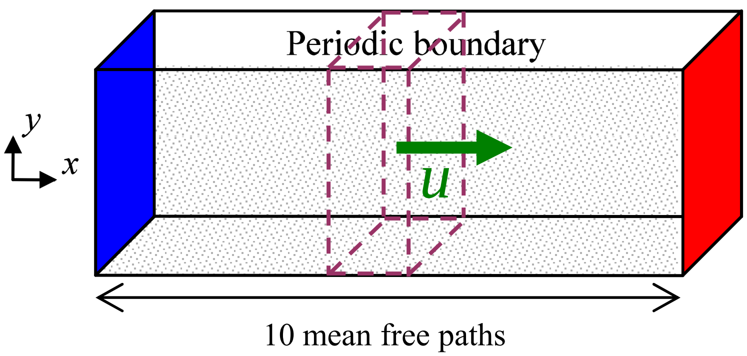
$$\langle u \rangle_* = \frac{2\times 3+14\times 1}{16} = 1.25$$



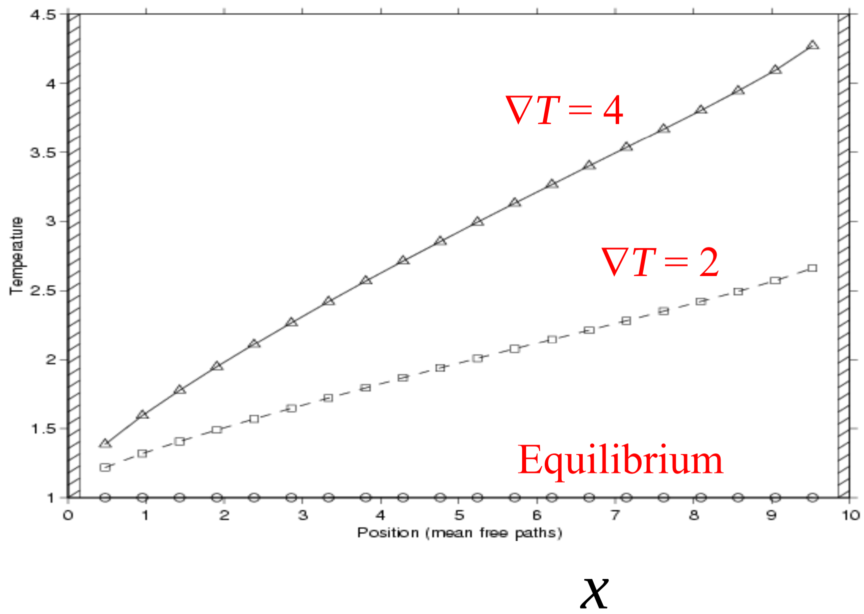
DSMC Simulations

Measured fluid velocity using both definitions. Expect no flow in *x* for closed, steady systems

∇T system



Temperature profiles



20 sample cells

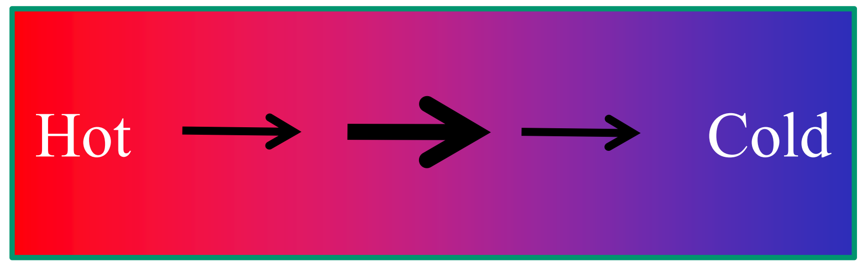
$N = 100$ particles per cell

Anomalous Fluid Velocity

Mean instantaneous fluid velocity measurement gives an anomalous flow in a closed system at steady state with ∇T.

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

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

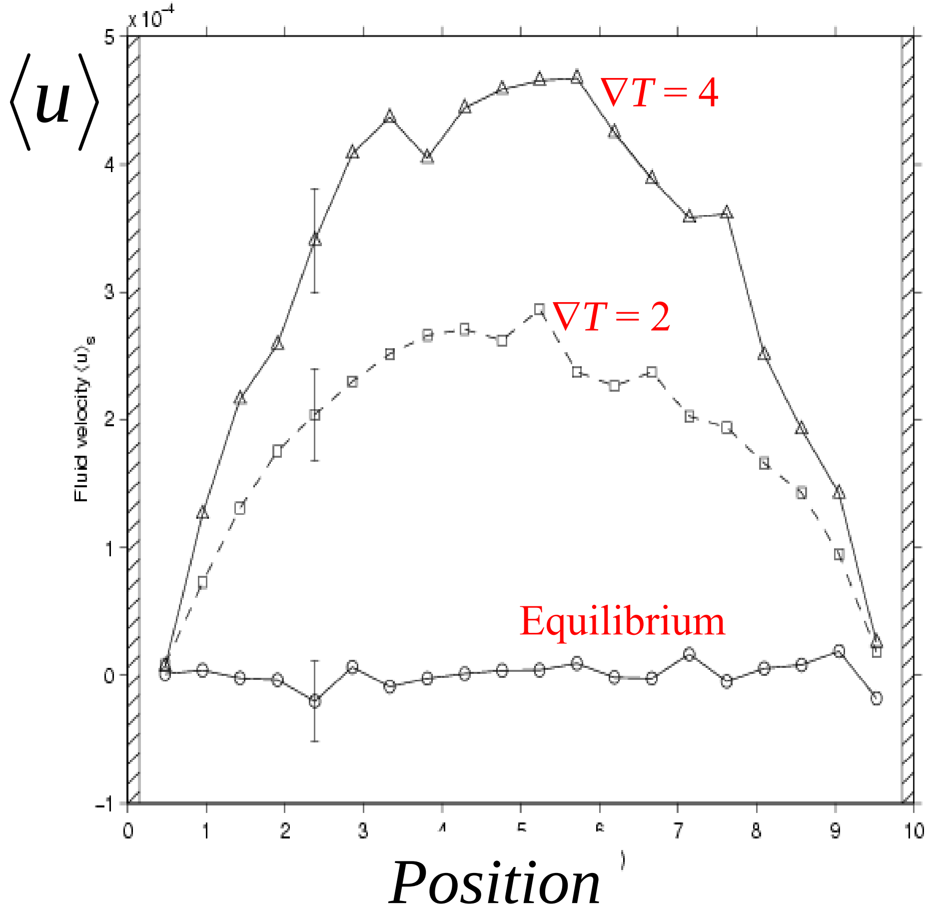


$$\langle u \rangle_* = \frac{\langle J \rangle}{\langle M \rangle} = 0$$

Anomalous Fluid Velocity

Mean instantaneous fluid velocity measurement gives an anomalous flow in the closed system.

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



Properties of Flow Anomaly

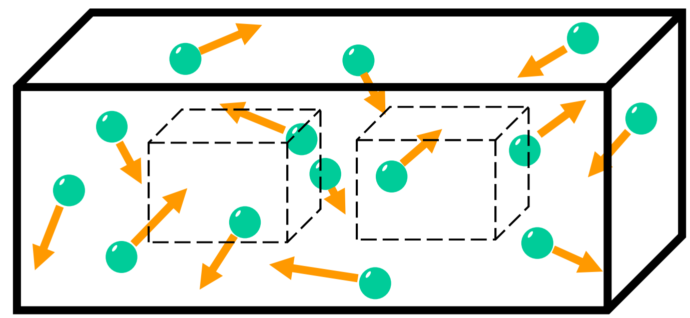
- Small effect. In this example $\langle u \rangle \approx 10^{-4}\sqrt{\frac{kT}{m}}$
- Anomalous velocity goes as $1/N$ where N is number of particles per sample cell (in this example $N = 100$).
- Velocity goes as gradient of temperature.
- Does not go away as number of samples increases.
- Similar anomaly found in plane Couette flow.

Correlations of Fluctuations

At equilibrium, fluctuations of conjugate hydrodynamic quantities are uncorrelated. For example, density is uncorrelated with fluid velocity and temperature,

$$\langle \delta\rho(x,t)\delta u(x',t)\rangle = 0$$

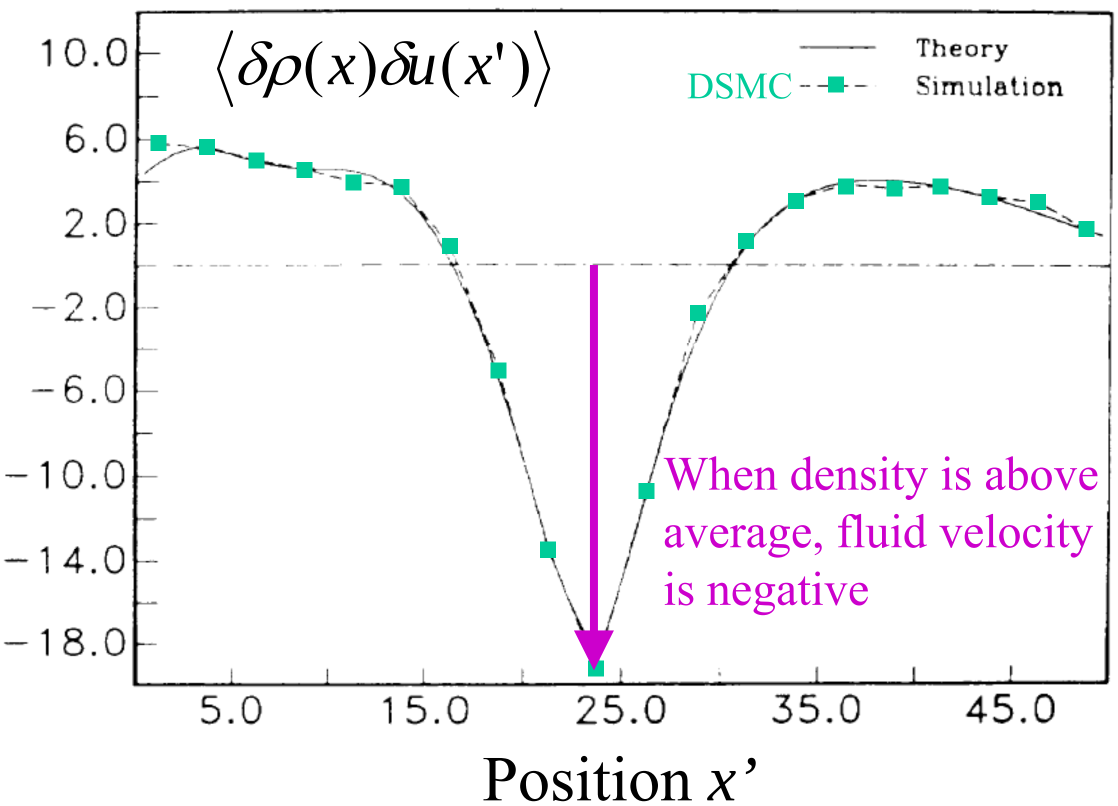
$$\langle \delta\rho(x,t)\delta T(x',t)\rangle = 0$$



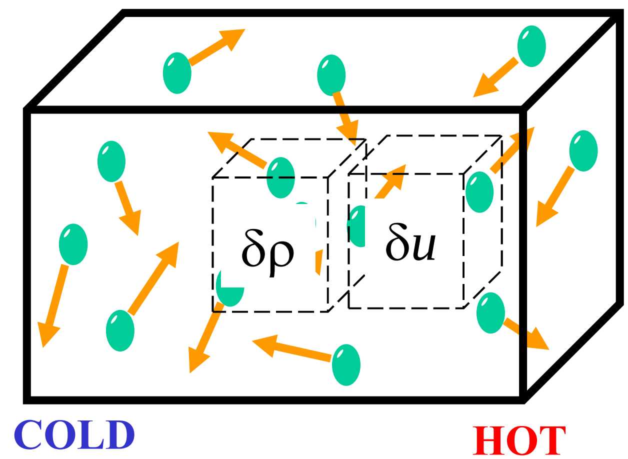
Out of equilibrium, (e.g., gradient of temperature or shear velocity) correlations appear.

Density-Velocity Correlation

Correlation of density-velocity fluctuations under ∇T



Theory is Landau fluctuating hydrodynamics



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

Relation between Means of Fluid Velocity

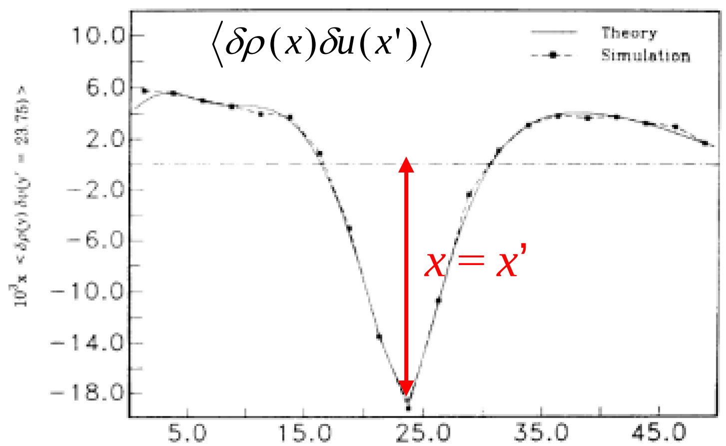
From the definitions,

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

From correlation of non-equilibrium fluctuations,

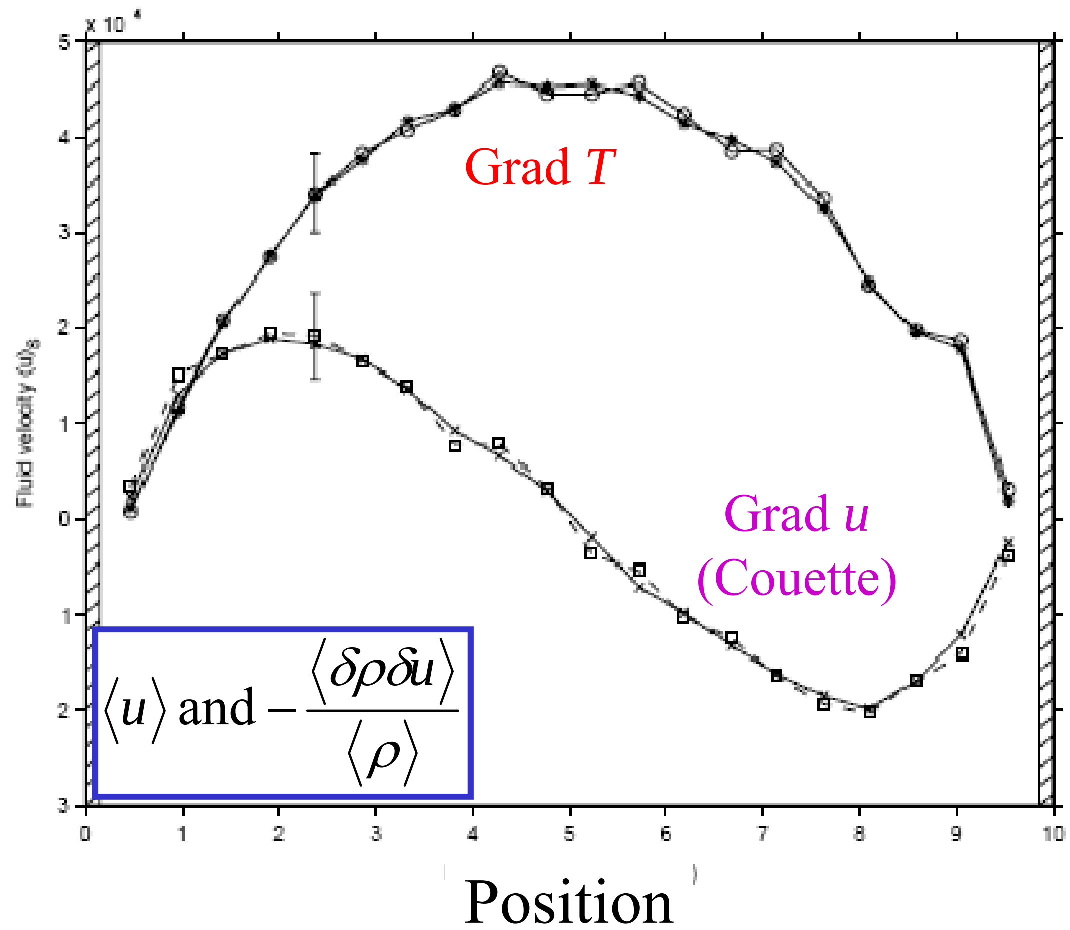
$$\langle \delta\rho(x)\delta u(x) \rangle \propto -x(L-x)\nabla T$$

This prediction agrees perfectly with observed bias.



Comparison with Prediction

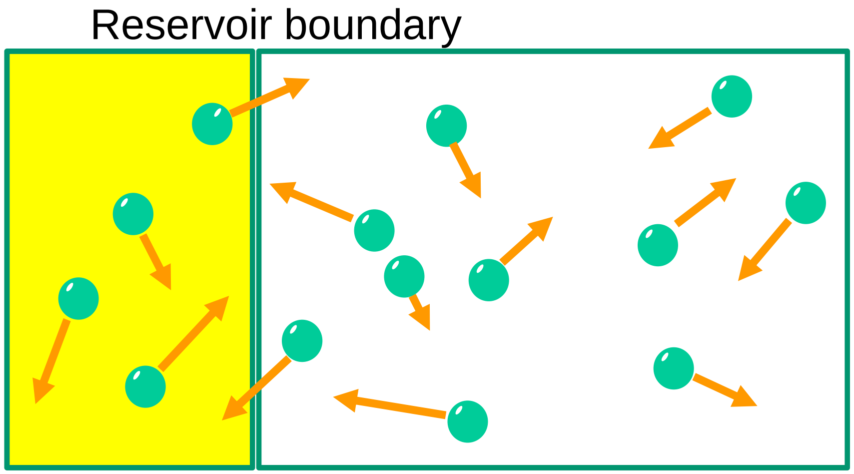
Perfect agreement between mean instantaneous fluid velocity and prediction from correlation of fluctuations.



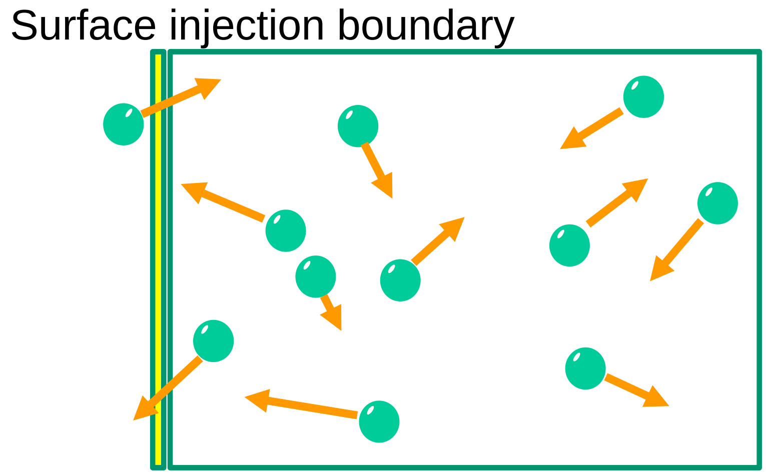
M. Tysanner and A. Garcia,
J. Comp. Phys. **196** 173-83 (2004).

Inflow / Outflow Boundaries

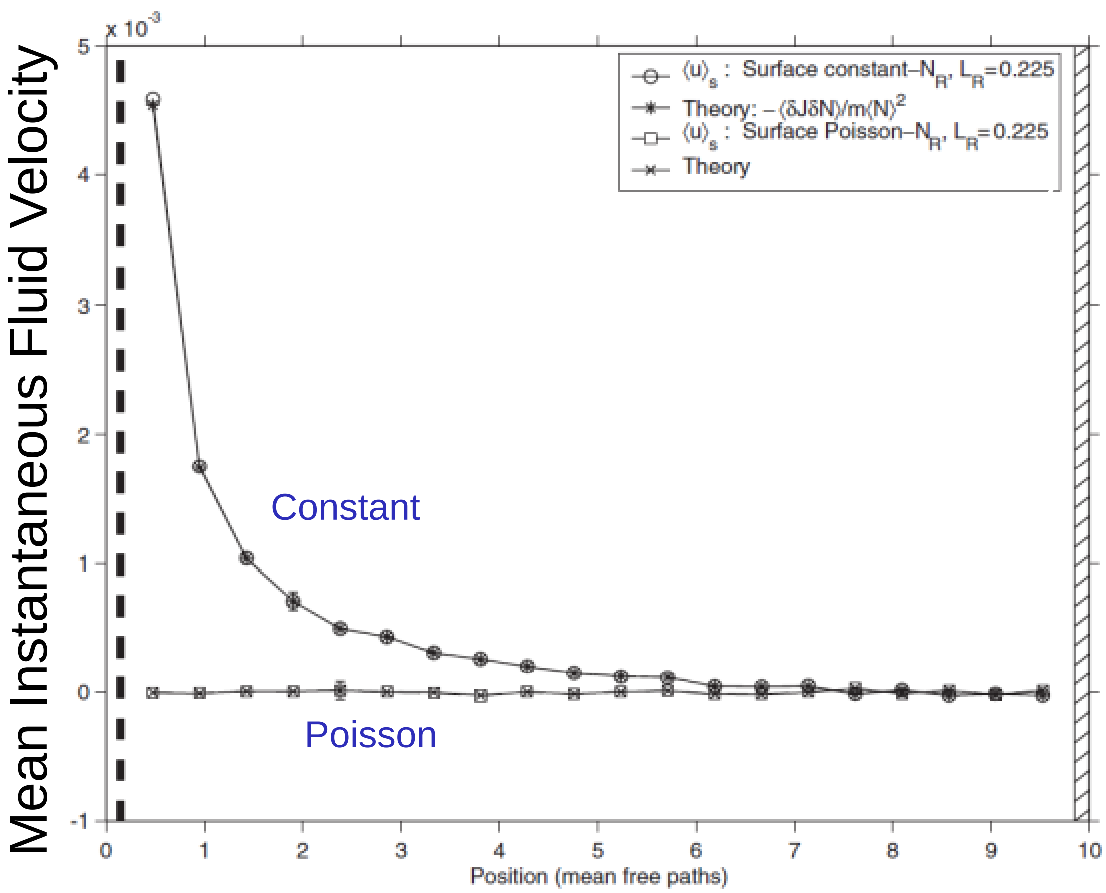
Unphysical fluctuation correlations also appear boundary conditions are not thermodynamically correctly.



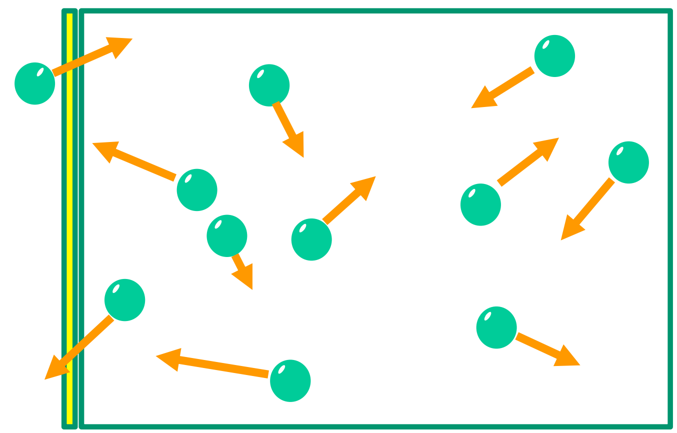
For example, number of particles crossing an inflow / outflow boundary are Poisson distributed.



Anomalous *Equilibrium* Flow



Surface injection boundary



Mean instantaneous fluid velocity is non-zero *even at equilibrium* if boundary conditions not treated correctly with regards to fluctuations.

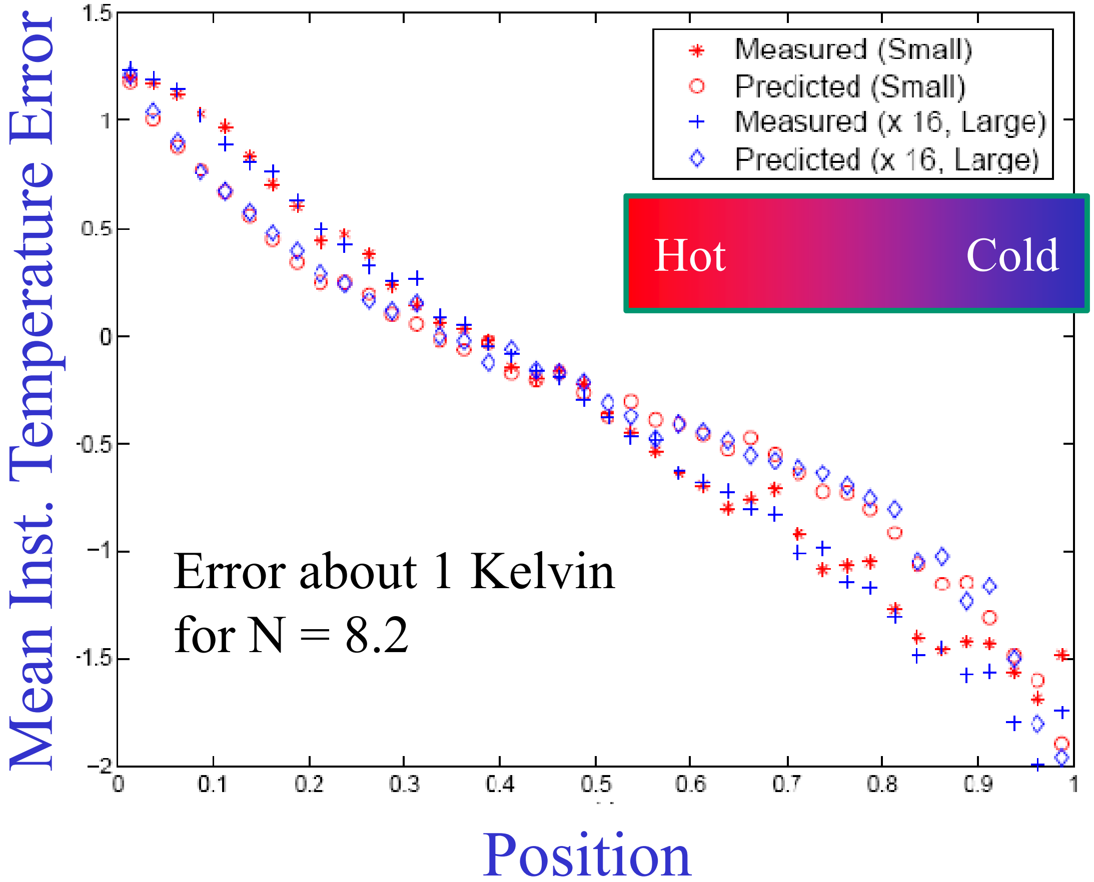
M. Tysanner and A. Garcia, *Int. J. Num. Meth. Fluids* **48** 1337-49 (2005)

Instantaneous Temperature

Measured error in mean instantaneous temperature for small and large *N*. (N = 8.2 & 132)

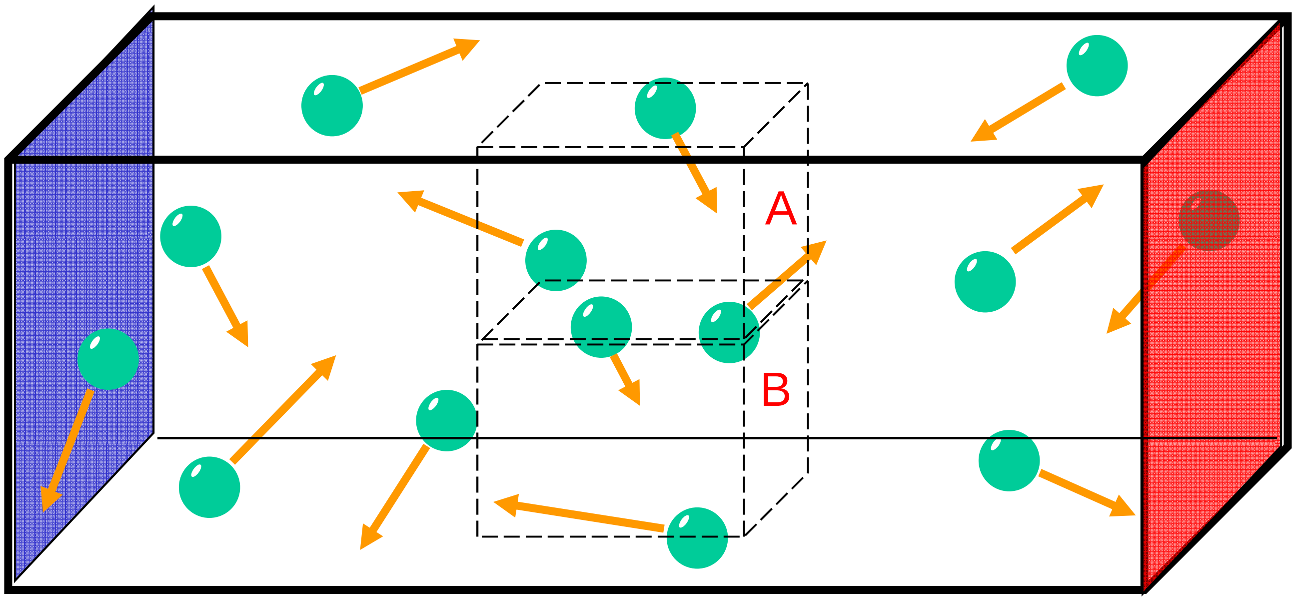
Error goes as $1/N$

Predicted error from density-temperature correlation in good agreement.



A. Garcia, *Comm. App. Math. Comp. Sci.* **1** 53-78 (2006)

Non-intensive Temperature



Mean instantaneous temperature has bias that goes as $1/N$, so it is not an intensive quantity.

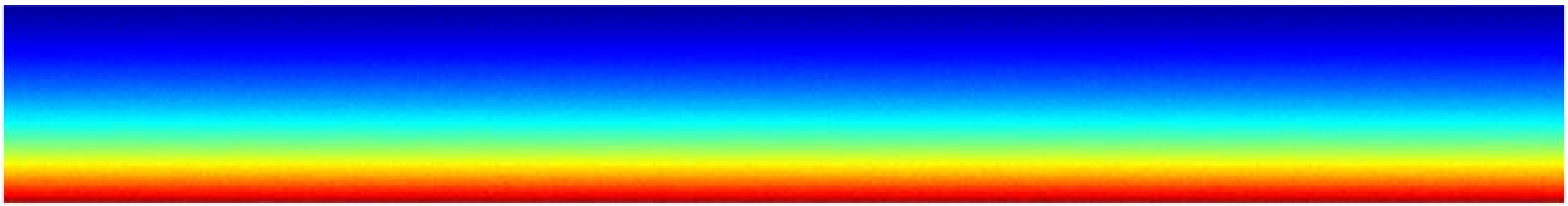
Temperature of cell A = temperature of cell B yet *not* equal to temperature of super-cell (A U B)

Outline

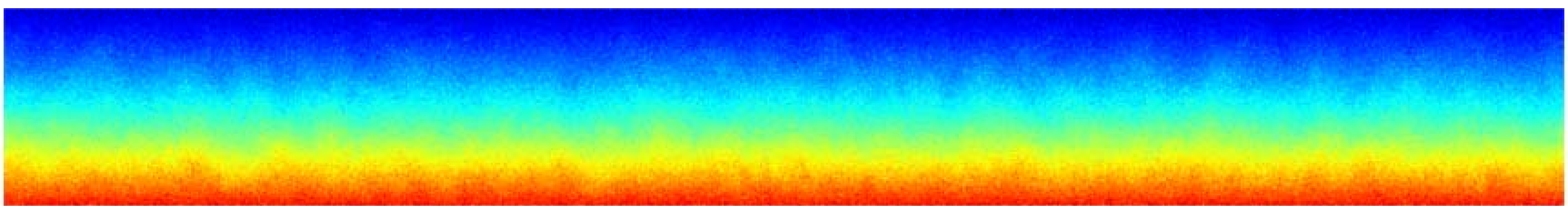
- Direct Simulation Monte Carlo
- Anomalous Poiseuille Flow
- Anomalous Couette Flow
- Anomalous Temperature Gradient Flow
- Anomalous Diffusion Flow

Diffusion & Fluctuations

As we've seen, fluctuations are enhanced when a system is out of equilibrium, such as under a gradient imposed by boundaries.



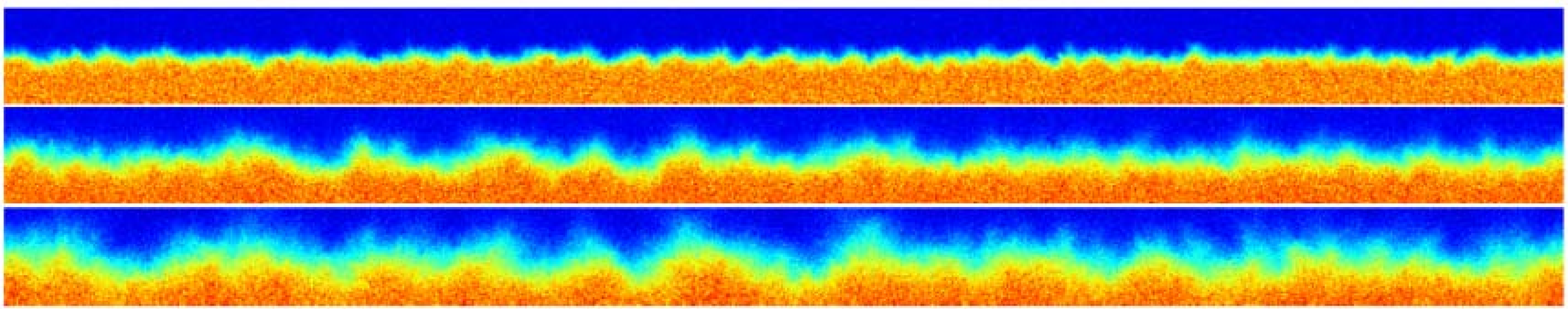
Equilibrium concentration gradient (induced by gravity)



Steady-state concentration gradient (induced by boundaries)

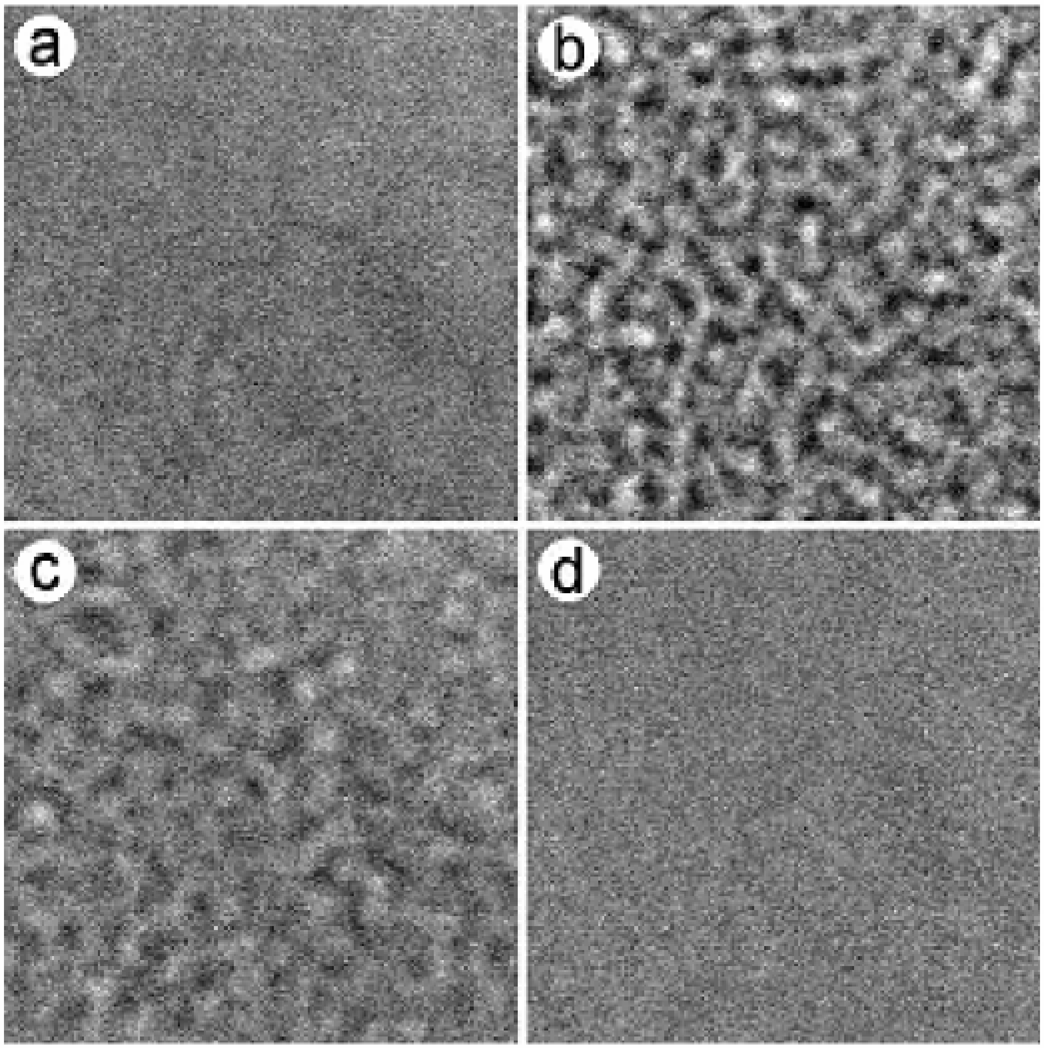
Giant Fluctuations in Mixing

Fluctuations grow large during mixing even when the two species are identical (red & blue).



Snapshots of the concentration during the diffusive mixing of two fluids (red and blue) at t = 1 (top), t = 4 (middle), and t = 10 (bottom), starting from a flat interface (phase-separated system) at t = 0.

Experimental Observations



Giant fluctuations in diffusive mixing seen in lab experiments.

Experimental images (1mm side) of scatterring from the interface between two miscible fluids (from A. Vailati & M. Giglio, *Nature* 1997)

Diffusion & Fluctuations

Using Landau-Lifshitz fluctuating hydrodynamics in the isothermal, incompressible approximation we may write,

$$(\delta c)_t + \mathbf{v} \cdot \boldsymbol{\nabla} c_0 = -D\boldsymbol{\nabla}^2 (\delta c) + \sqrt{2Dk_B T}\,(\boldsymbol{\nabla} \cdot \mathcal{W}_c)$$

$$\rho \mathbf{v}_t = \eta \boldsymbol{\nabla}^2 \mathbf{v} - \boldsymbol{\nabla}\pi + \sqrt{2\eta k_B T}\,(\boldsymbol{\nabla} \cdot \mathcal{W}) \text{ and } \boldsymbol{\nabla} \cdot \mathbf{v} = 0$$

for the fluctuations of concentration and velocity.

Solving in Fourier space gives the correlation function,

$$\widehat{S}_{c,v_y}(\boldsymbol{k}) = \langle (\widehat{\delta c})(\widehat{v}_y^\star) \rangle \sim -\left[k_\perp^2 \left(\nabla_y c\right)\right] k^{-4}$$

Diffusion & Fluctuations

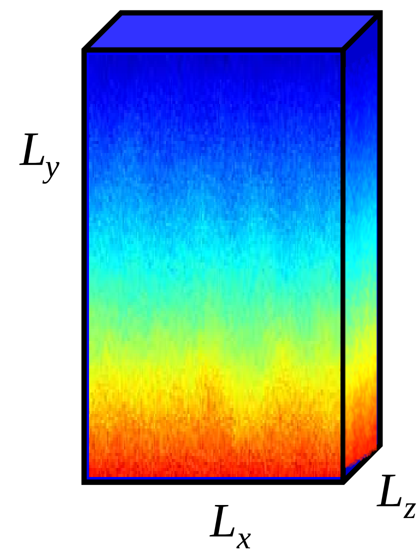
The total mass flux for concentration species is,

$$\langle \mathbf{j} \rangle \approx (D_0 + \Delta D)\, \nabla c_0 = \left[D_0 - (2\pi)^{-3} \int_{\mathbf{k}} \widehat{S}_{c,v_y}(\mathbf{k})\, d\mathbf{k} \right] \nabla c_0$$

where there are two contributions, the "bare" diffusion coefficient and the contribution due to correlation of fluctuations.

For a slab geometry ($L_z \ll L_x \ll L_y$) we have,

$$\Delta D \approx k_B T \left[4\pi\rho(D_0 + \nu) L_z \right]^{-1} \ln \frac{L_x}{L_{mol}}$$



Notice that diffusion enhancement goes as $\ln L_x$

DSMC Measurements

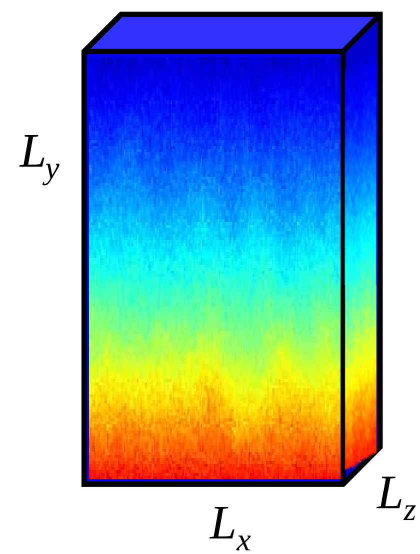
Can separate the contributions to the concentration flux as,

$$\langle j_y \rangle = \langle \rho_1 v_{1,y} \rangle = \langle \rho_1 \rangle \langle v_{1,y} \rangle + \langle (\delta \rho_1)(\delta v_{1,y}) \rangle$$

$$= D_{\mathrm{eff}} \nabla c \quad = \quad D_0 \nabla c \quad + \quad \Delta D \nabla c$$

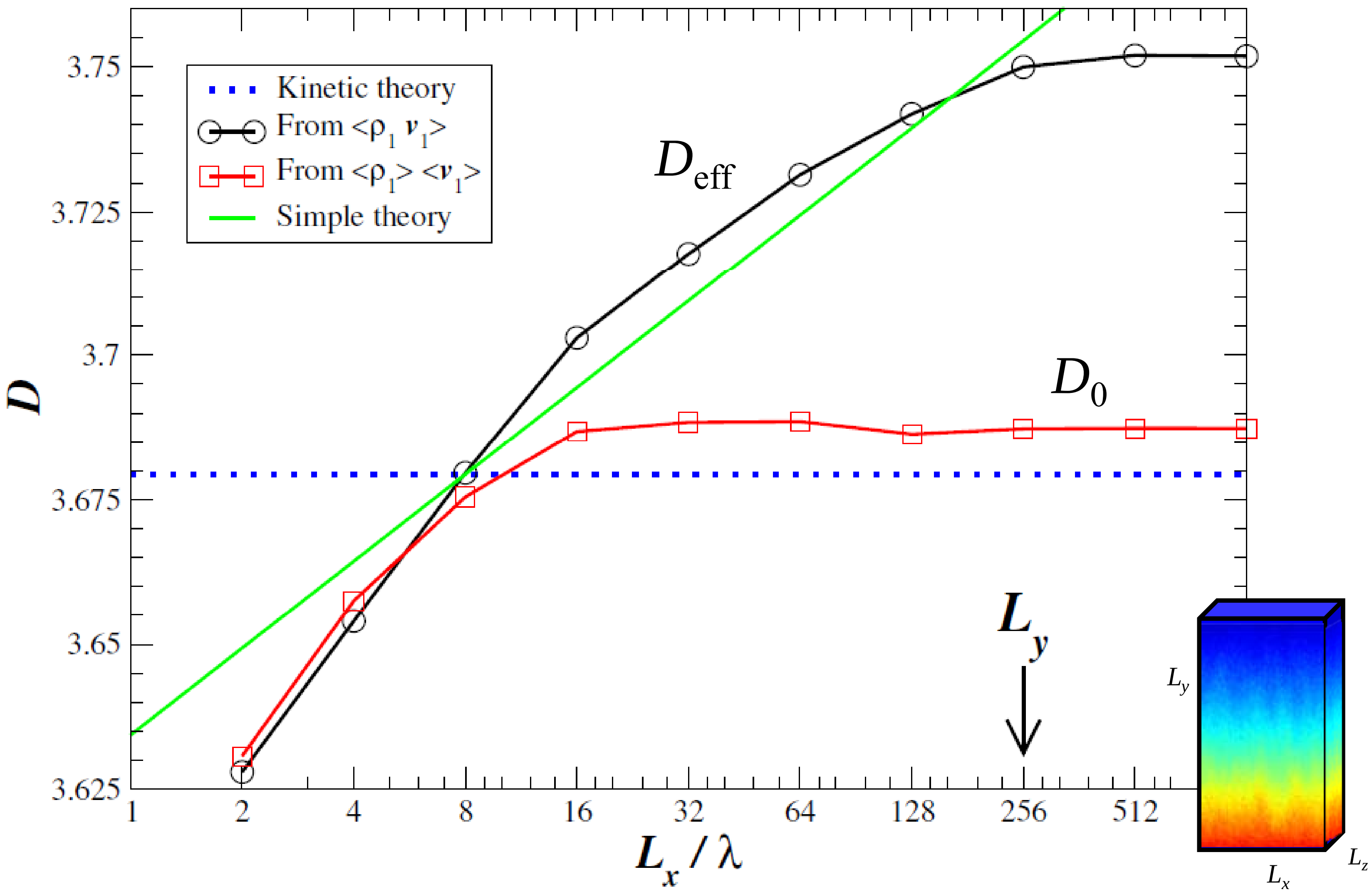
In DSMC we can easily measure

$$\langle \rho_1 \rangle \quad \langle v_{1,y} \rangle \quad \langle \rho_1 v_{1,y} \rangle \text{ and } \nabla c$$



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

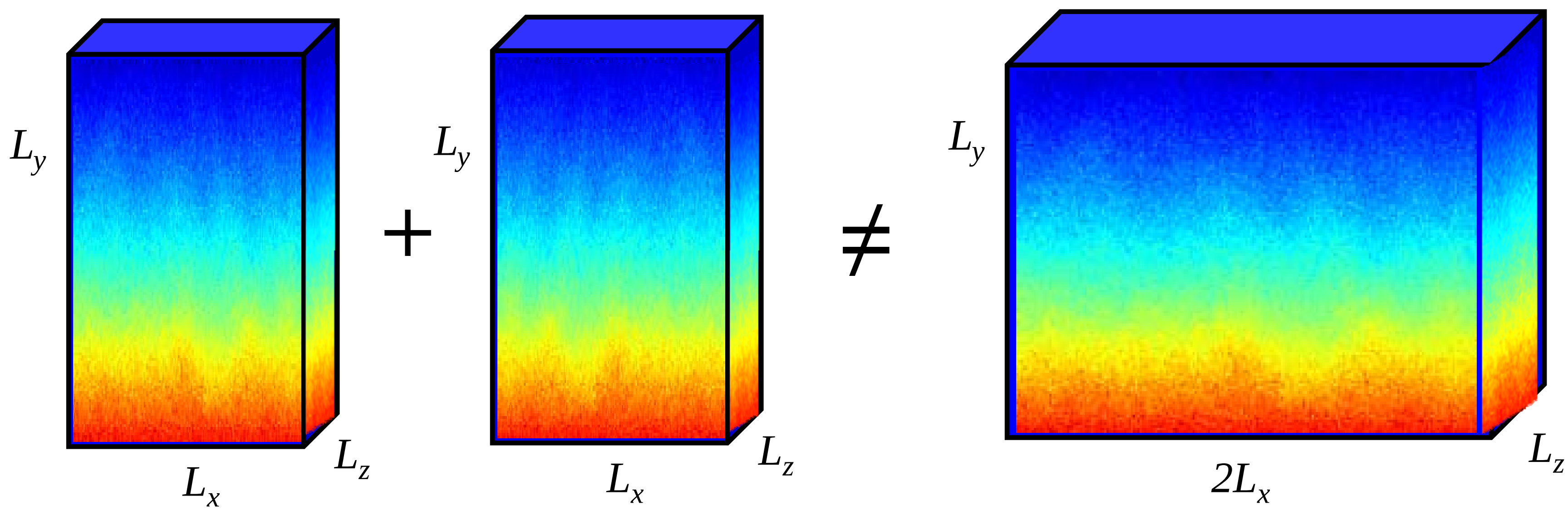
DSMC Results for D_{eff} and D_0



A. Donev, J. Bell, A. Garcia, J. Goodman, E. Vanden-Eijnden, in preparation

Global Enhancement of Diffusion

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



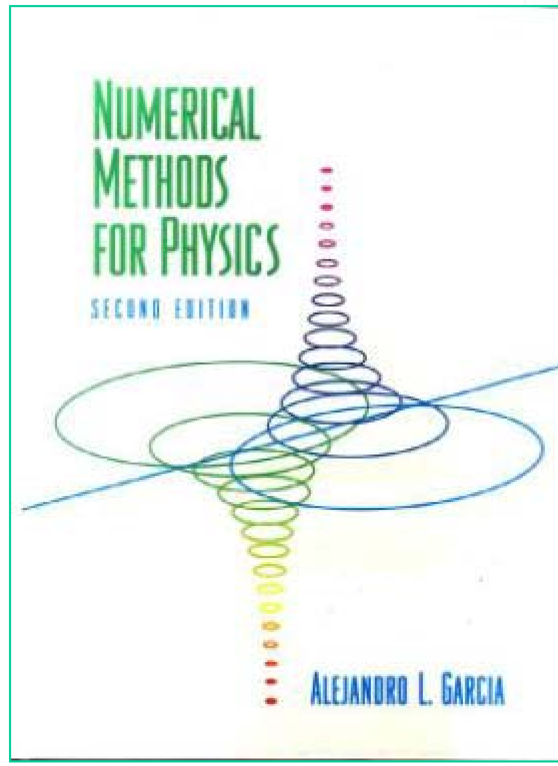
The wider system can accommodate long wavelength fluctuations, thus it has enhanced diffusion.

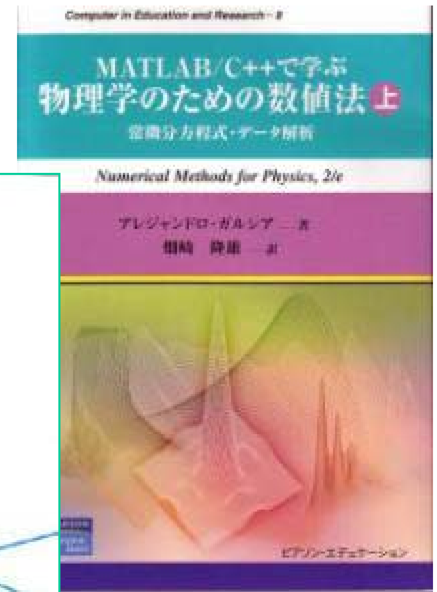
References and Spam

Reprints, pre-prints and slides available:

www.algarcia.org

DSMC tutorial & programs in my textbook.





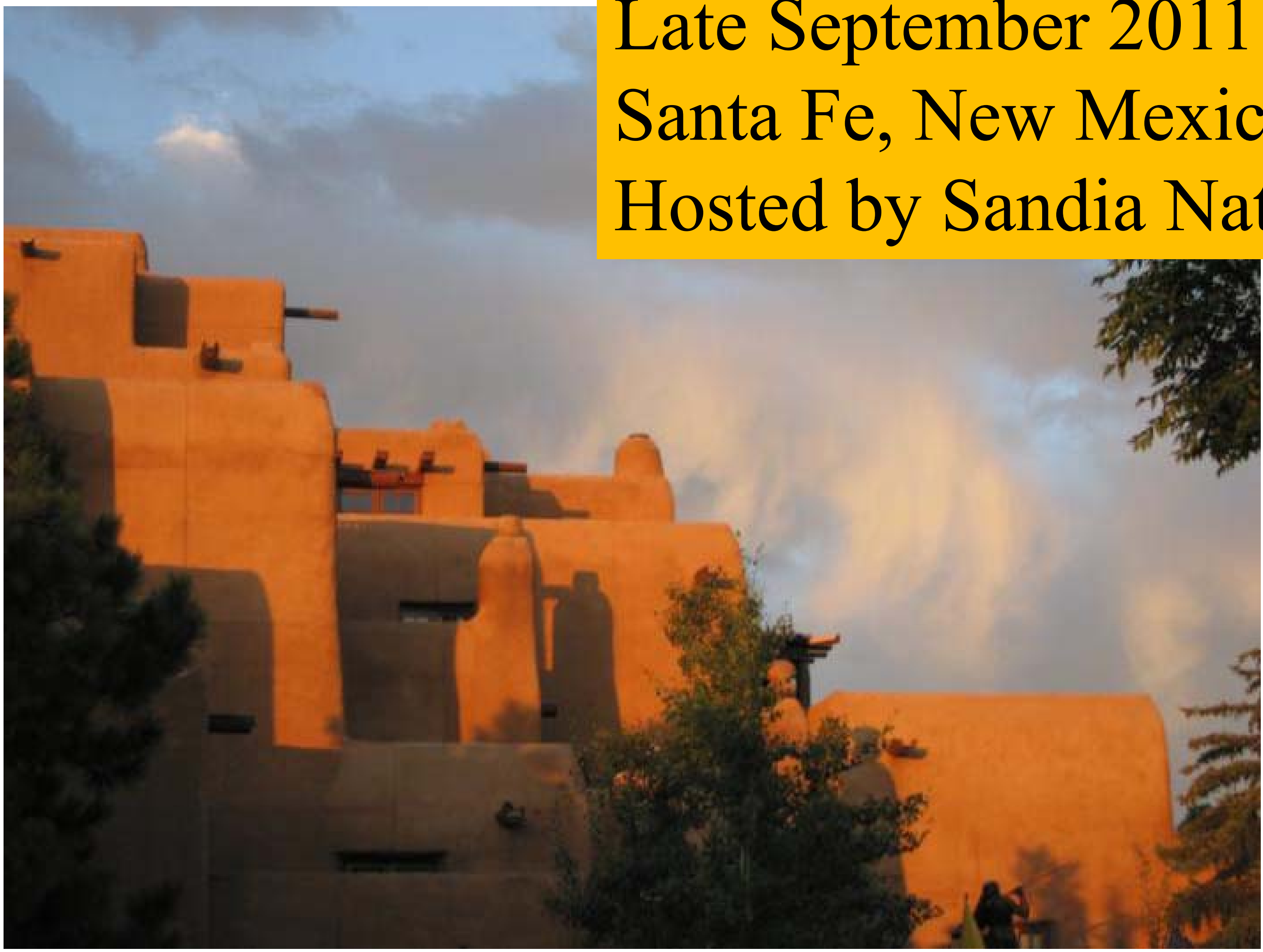
Japanese

RGD 2012 in Zaragoza, Spain

Hosted by ZCAM, the Spanish node of the European Centers for Atomic and Molecular Calculations (CECAM)

DSMC 2011 Workshop

Late September 2011
Santa Fe, New Mexico
Hosted by Sandia Nat. Lab.



Von Neumann Symposium on Multi-scale Algorithms

July 4-8, 2011
Snowmass, Utah

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