How I Broke DSMC
A Cautionary Tale

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DSFD 2016 - Shenzhen
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The Story Arc

This story is in three acts:

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Act I – The Rise (The Ego Trip)

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Act II – The Fall

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This story is in three acts:

Act I – The Rise (The Ego Trip)

Act II – The Fall

Act III – The Redemption

Act I

The Rise (The Ego Trip)

In which the speaker discovers the power of DSMC and uses it to his great advantage.

Ascension of the procession
Gustave Dore (1890)

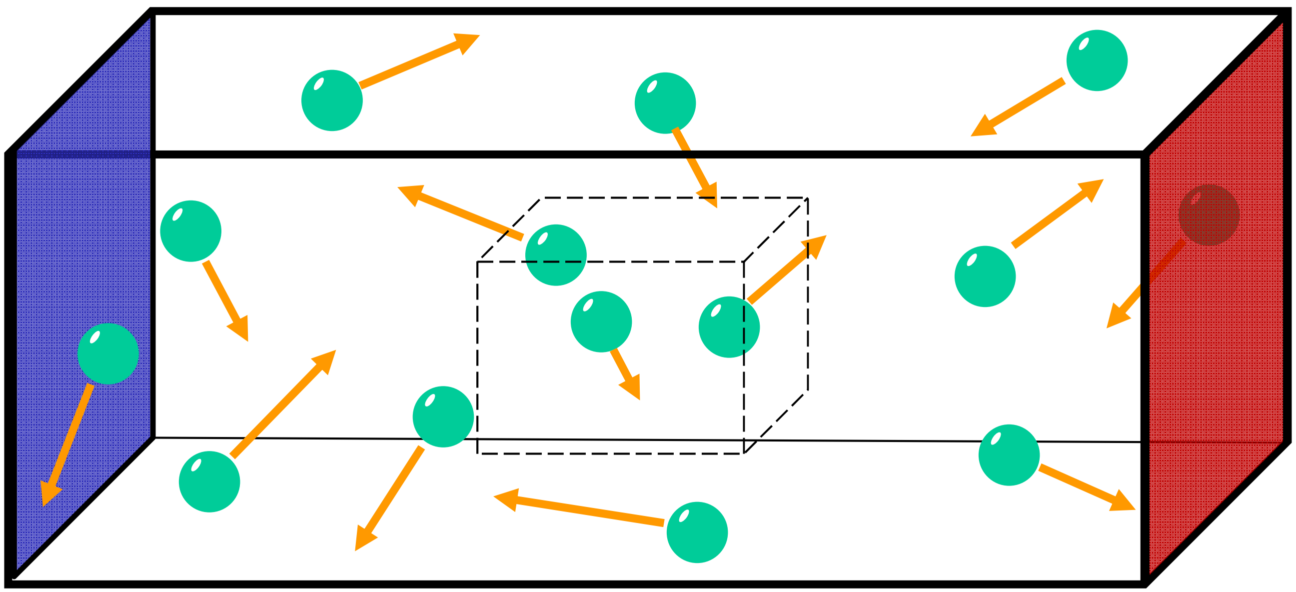
Brussels, 1985

Shortly before finishing a doctorate in physics at UT Austin, my thesis adviser shows me Graeme Bird's book.

Working as a post-doc in Ilya Prigogine's group I start using DSMC to study non-equilibrium effects in simple fluids.

With Lar Hannon and Malek Mansour

Hydrodynamic Fluctuations



My DSMC simulations investigated fluctuations

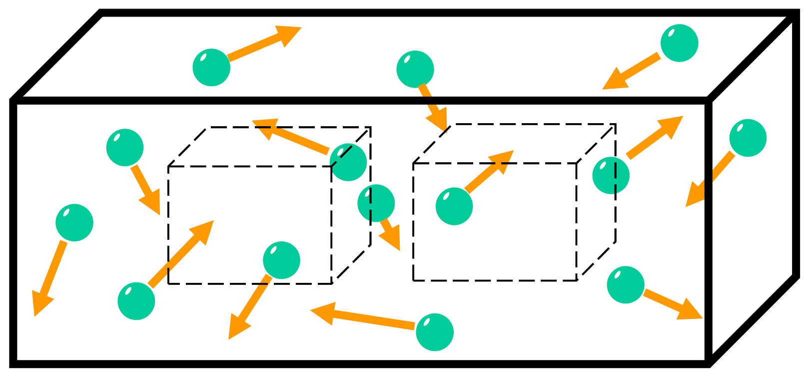
$$\delta\rho(x,t) = \rho(x,t) - \langle\rho(x)\rangle$$

(Density fluctuation) = (Density) – (Average Density)

Correlations of Fluctuations

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

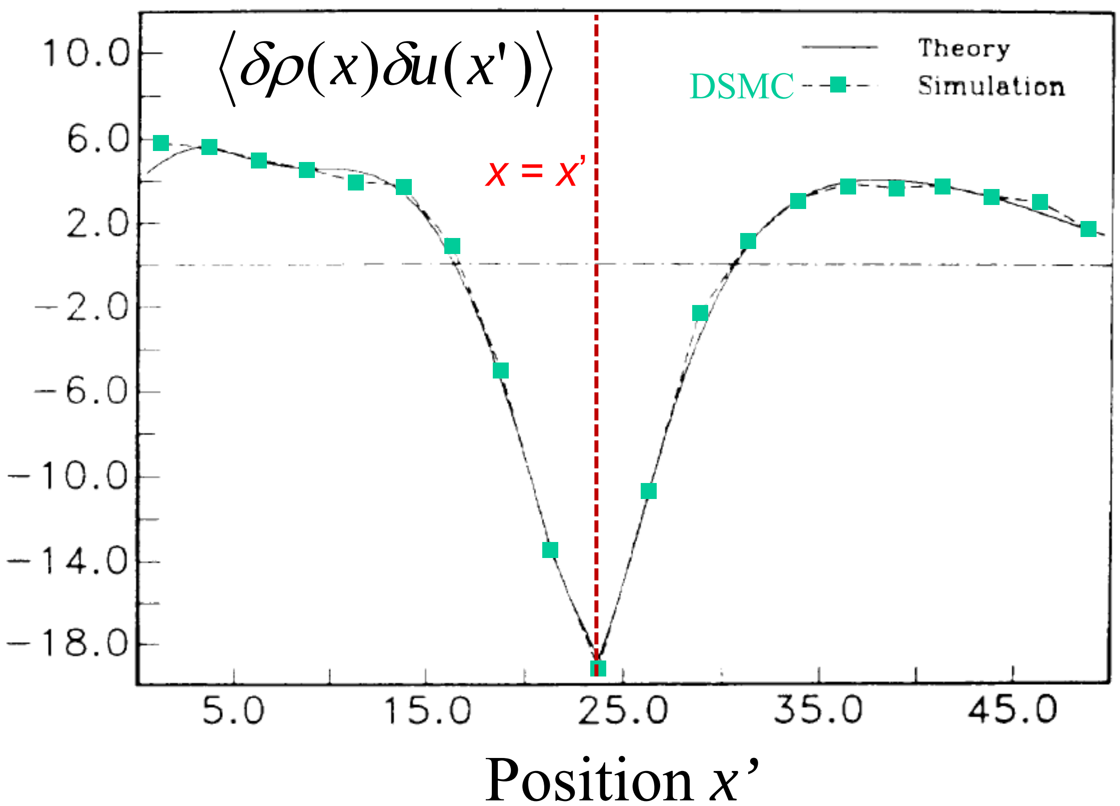
$$\left\langle \delta\rho(x,t)\,\delta u(x',t)\right\rangle = 0$$



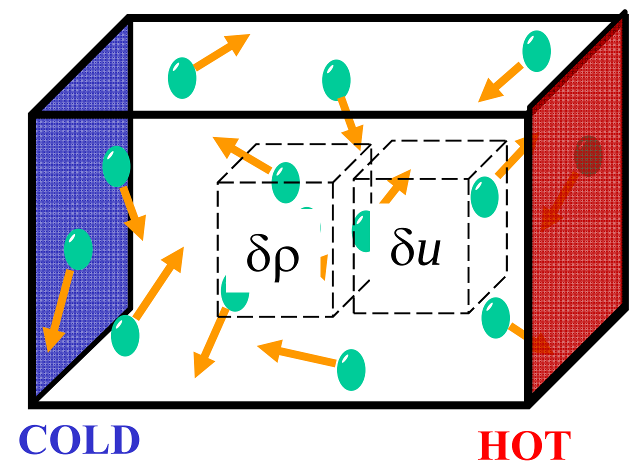
Out of equilibrium, (e.g., gradient of temperature) long-ranged correlations appear in a fluid.

Density-Velocity Correlation

Correlation of density-velocity fluctuations under ∇T



Theory is Landau-Lifshitz fluctuating hydrodynamics



"Nonequilibrium Fluctuations studied by a Rarefied Gas Simulation", ALG, *Phys. Rev. A* **34** 1454 (1986)

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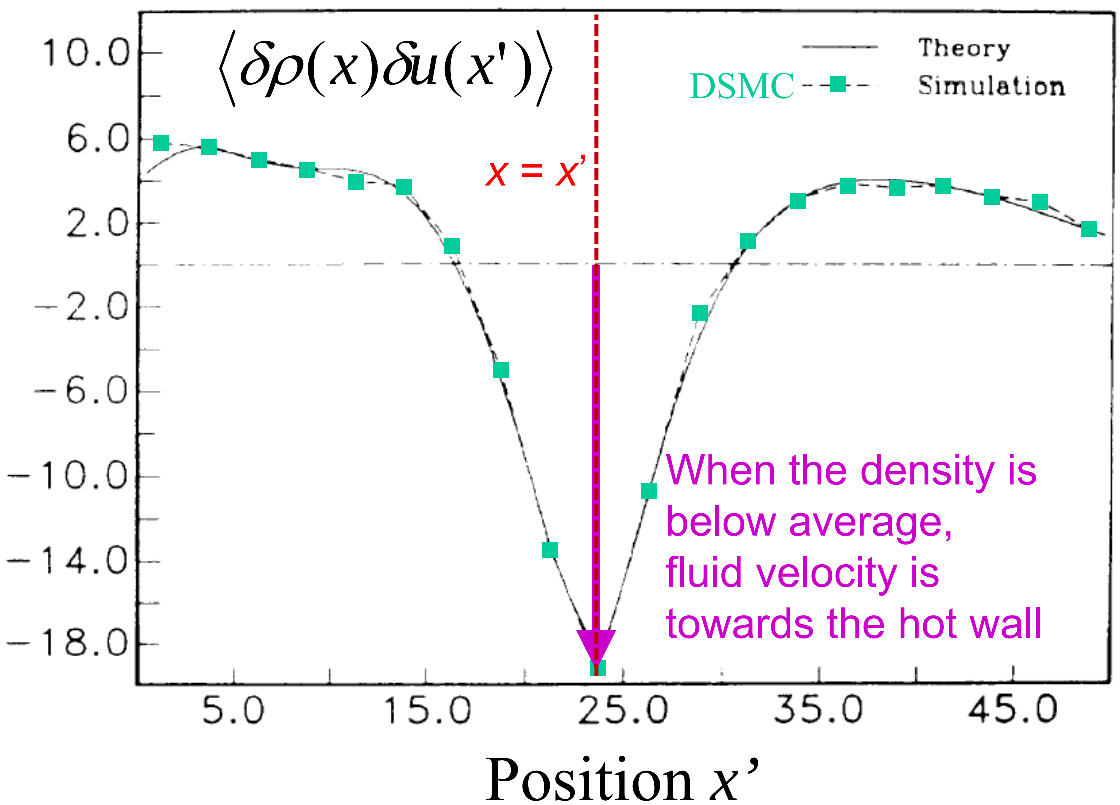

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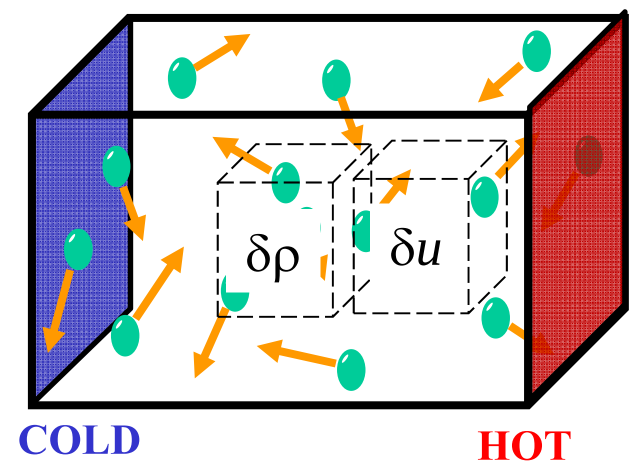

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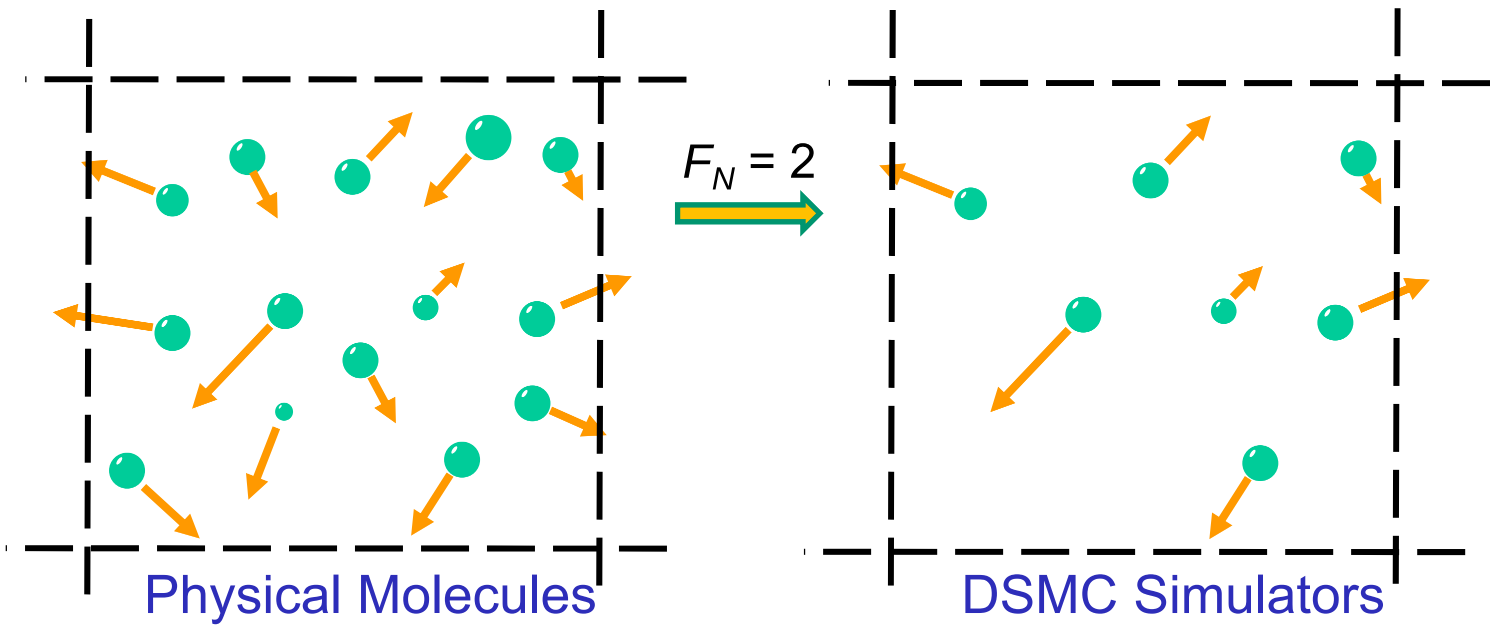
Molecules & “Simulators”

In DSMC the fluctuations are typically amplified because the number of simulation particles (“simulators”) is typically a small fraction of the number physical molecules.

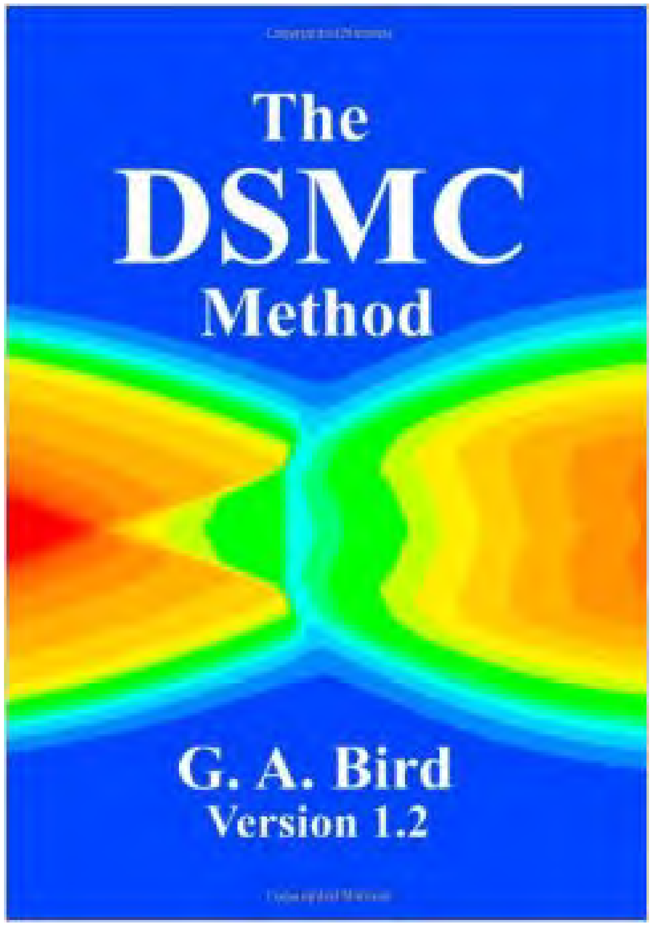
Each simulator represents F_N physical molecules.
Each simulator collision represents F_N physical collisions.



Fluctuations & DSMC

Graeme Bird liked these results on thermodynamic fluctuations in DSMC.

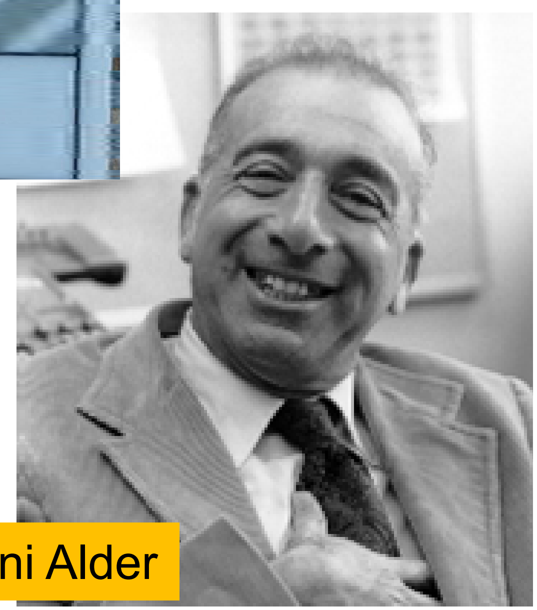
In his newest book, he writes, “While the fluctuations are unphysical when F_N is large, they are physically realistic … (with) a one-to-one correspondence between real and simulated molecules. This is another instance of DSMC going beyond the Boltzmann equation because fluctuations are neglected in the Boltzmann model.



Livermore Lab, 1993

A few years later I join San Jose State and meet Berni Alder, one of the pioneers of molecular simulations.

Berni takes an interest in DSMC and working with him at Livermore Lab we publish 16 papers, most of them on ways to extend the DSMC algorithm.



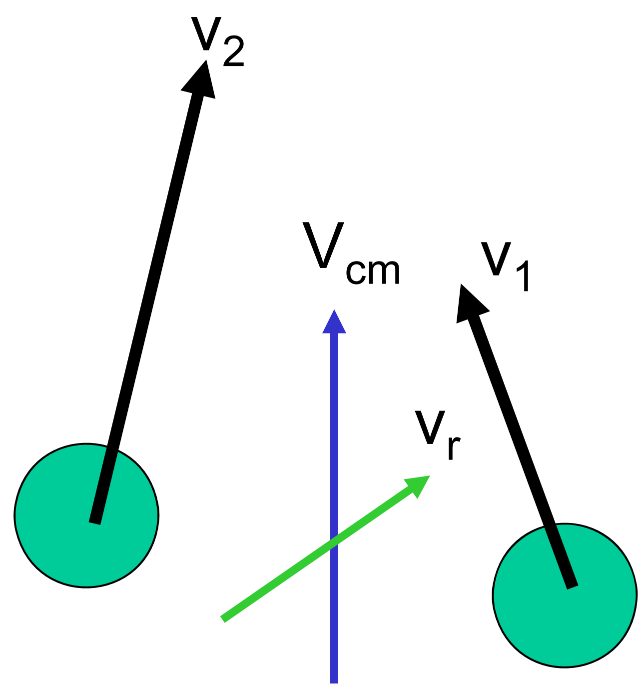
Berni Alder

Standard DSMC Collisions

Post-collision velocities

(6 variables) are given by:

- Conservation of momentum – Center of mass velocity (3 constraints)
- Conservation of energy – Magnitude of the relative velocity (1 constraint)
- Random solid angle – Direction of the apse line (2 choices)



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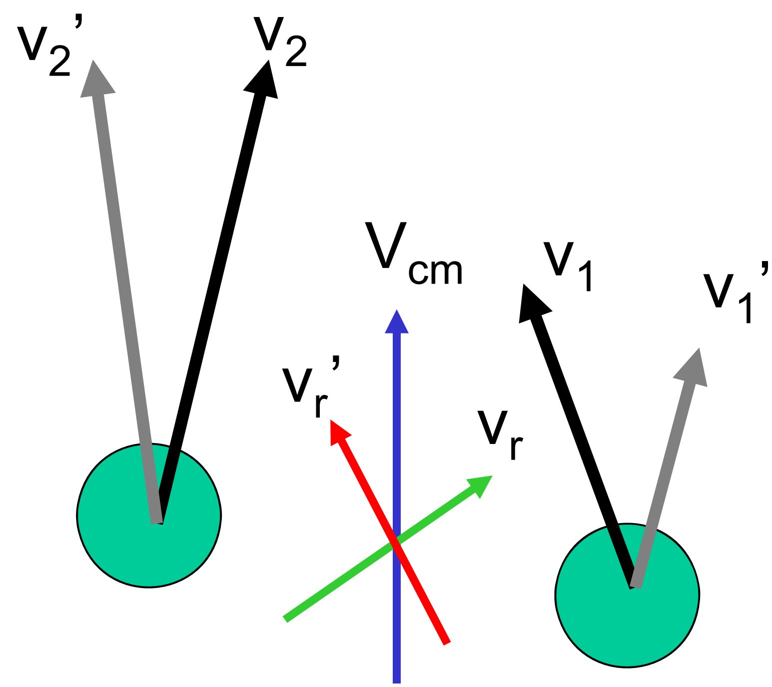
For hard spheres the direction of v_r' is uniformly distributed.



Dense Gas Eqn. of State

The virial expansion gives the first order correction for the ideal gas law as,

$$p = nk_BT\,(1 + B(T)\,n)$$

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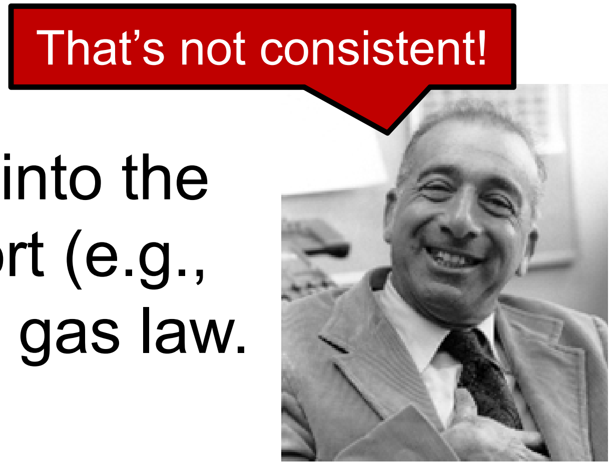

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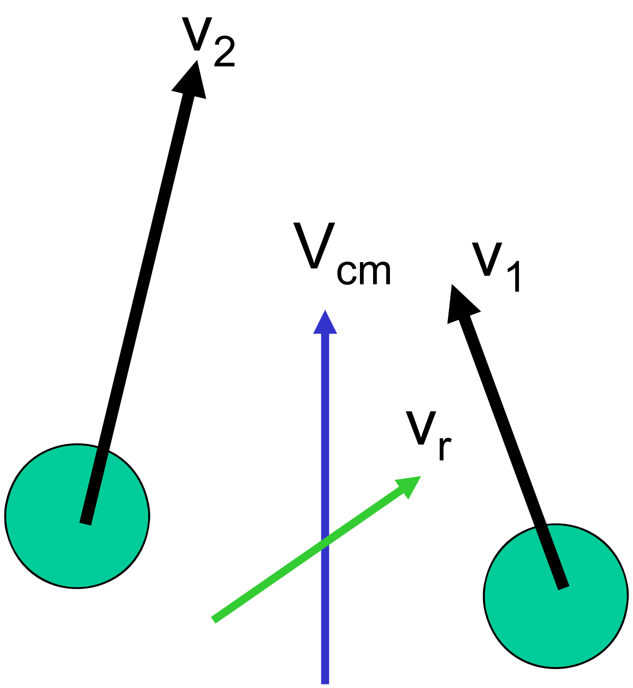
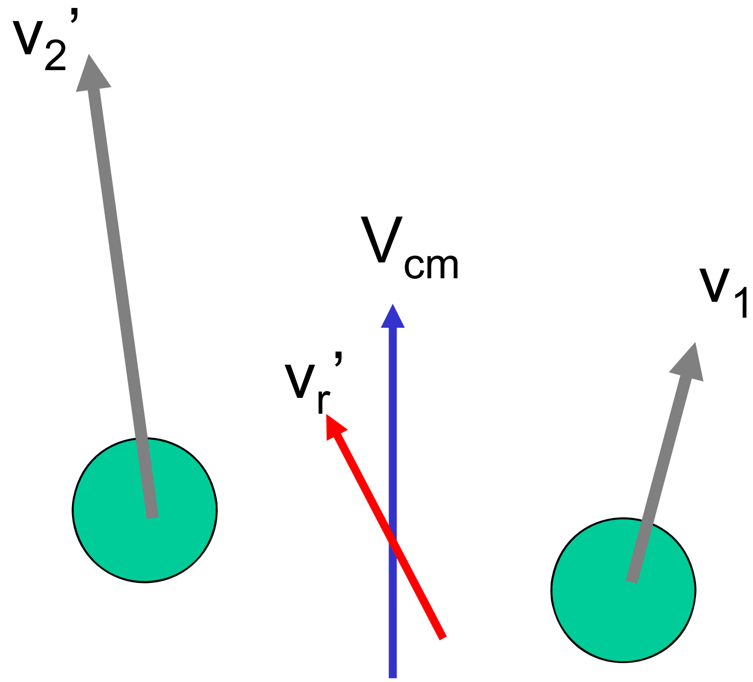
Frank Alexander

Consistent Boltzmann Algorithm (CBA)



Pre-collision velocities



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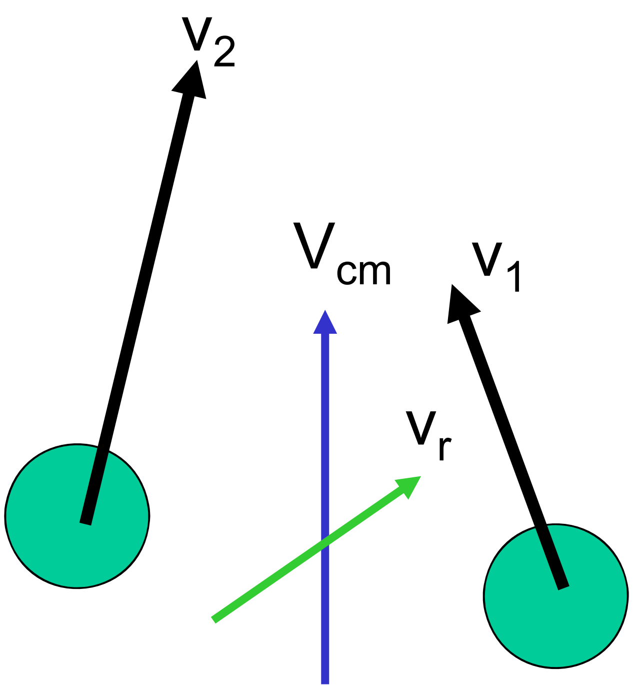

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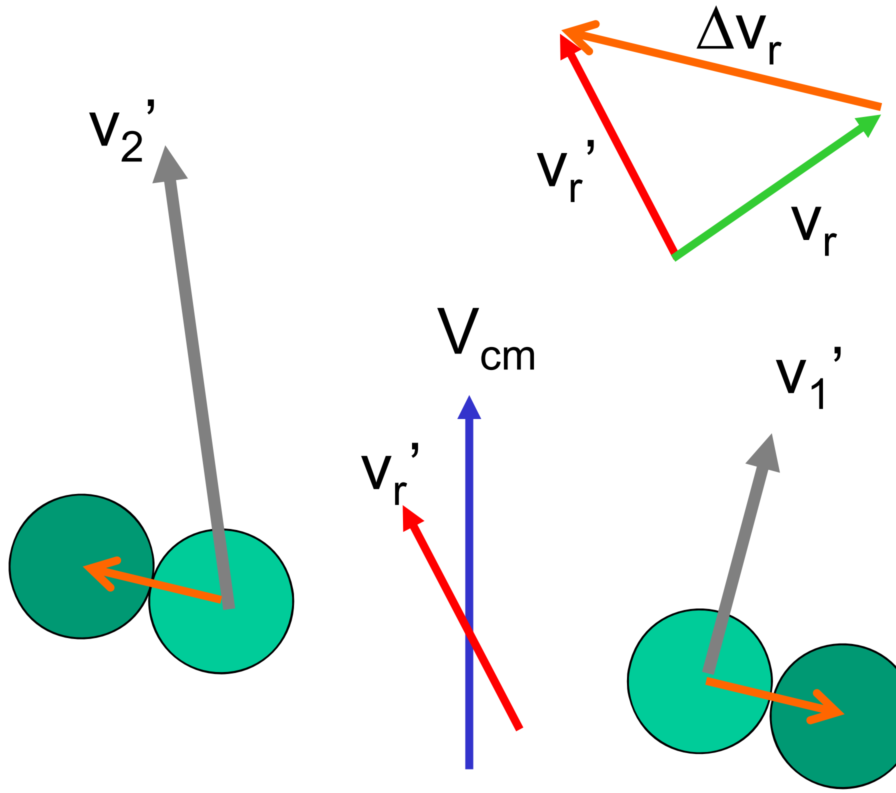

Post-collision velocities
Post-collision positions

Virial Coefficient & CBA

The CBA model gives the correct hard-sphere equation of state because the virial coefficient is,

$$B(T) = {}^{1}\!/_{12}\,\pi\left(\langle \boldsymbol{r}_{ij} \cdot \Delta\widehat{\boldsymbol{v}}_r \rangle\right)^3$$

where $\boldsymbol{r}_{ij}$ is the separation between colliding particles and $\Delta\boldsymbol{v}_r$ is the change in the relative velocity on colliding.

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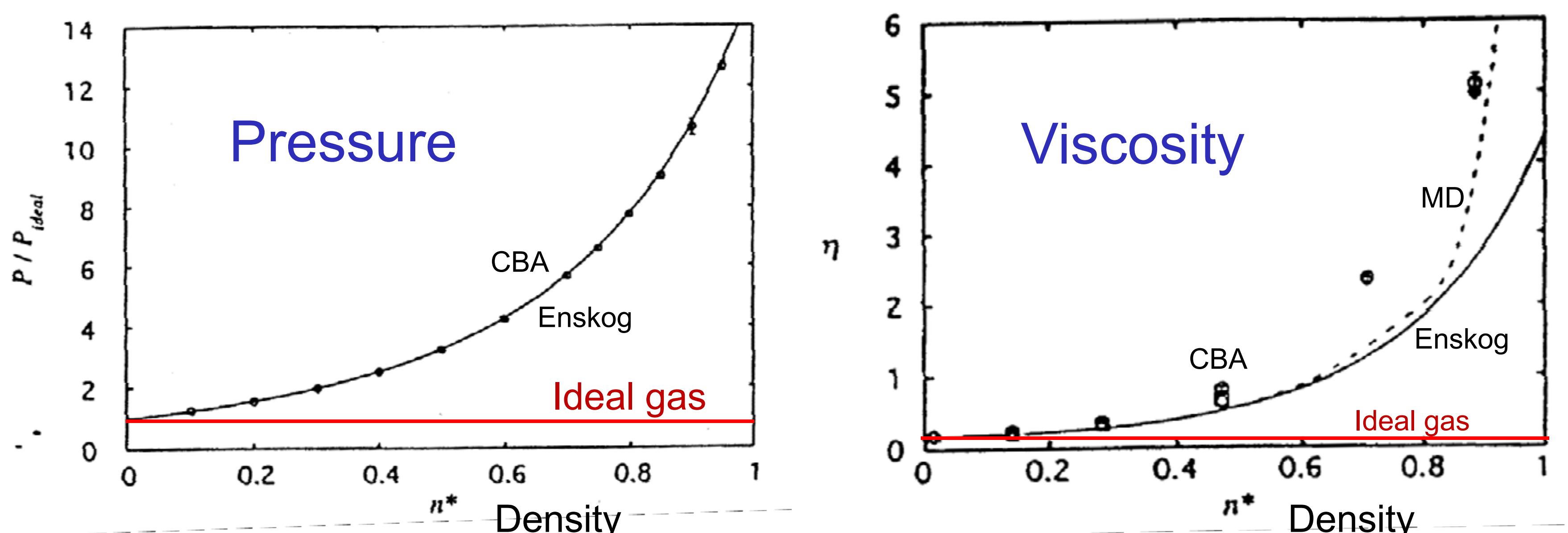
where $\boldsymbol{r}_{ij}$ is the separation between colliding particles and $\Delta\boldsymbol{v}_r$ is the change in the relative velocity on colliding.

In ordinary DSMC collisions this average is zero due to symmetry; the CBA displacement correlates positions with the change of velocities due to collisions.

CBA Properties

Measurements of pressure and transport coefficients in CBA were in very good agreement with hard sphere kinetic theory and molecular dynamics measurements.



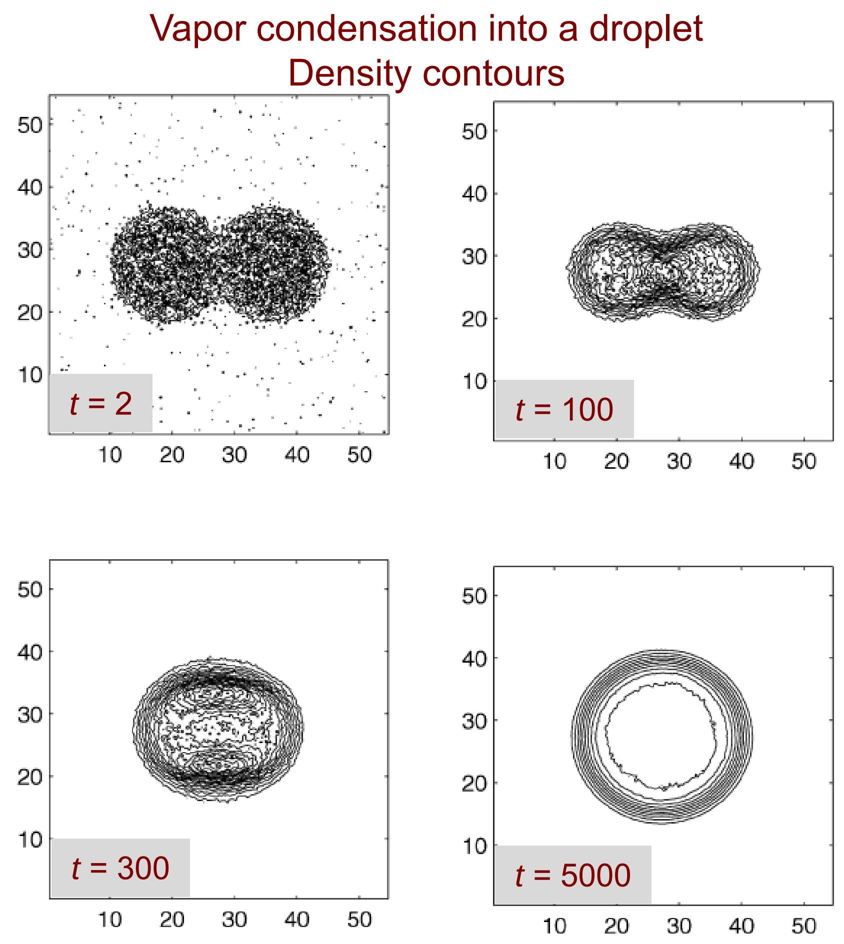
$n^* = n\, d^3$

F. Alexander, ALG, and B. Alder, *Phys. Rev. Lett.* **74** 5212 (1995)

Consistent Universal Boltzmann Algorithm (CUBA)

Making CBA displacement a function of density and temperature allows you to choose the equation of state.

Using van der Waals EoS we were able to simulate the condensation of vapor into a liquid droplets.



F. Alexander, ALG, and B.J. Alder, *Physica A* **240** 196 (1997).
N. Hadjiconstantinou, ALG, and B.J. Alder, *Physica A* **281** 337-47 (2000).

Act II

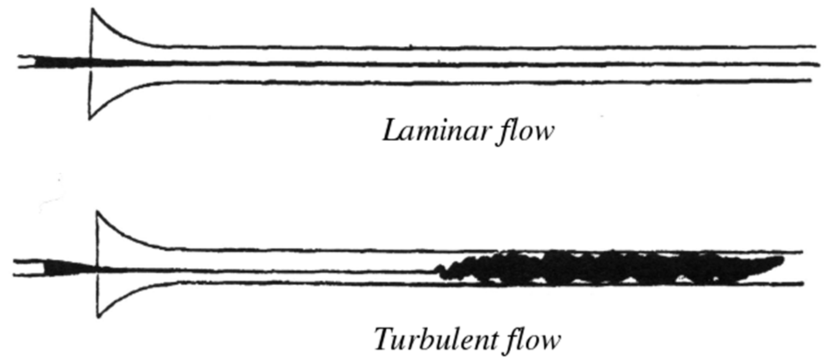
The Fall

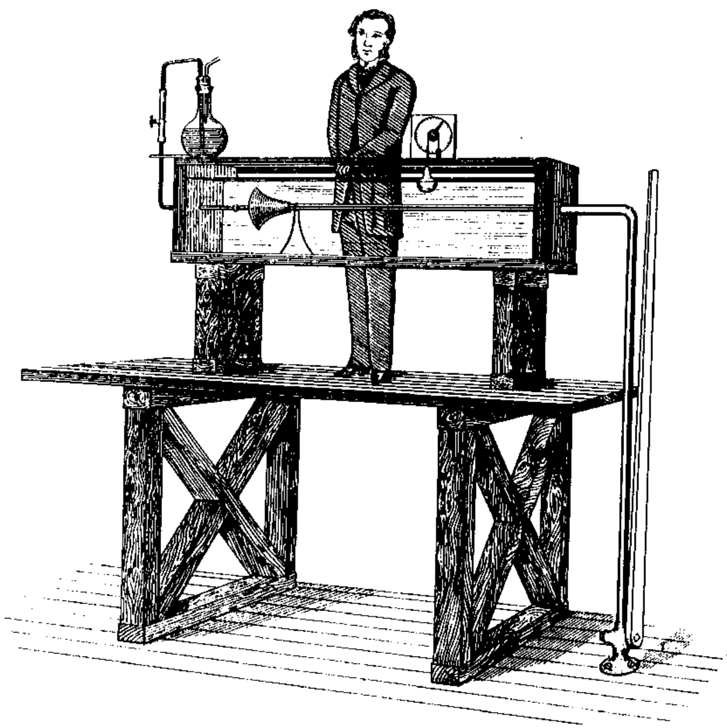
In which the speaker abuses the theoretical foundations of DSMC and produces an abomination.

Fall of a Sinner (Alichino and Ciampolo)
Gustave Dore (1890)

Holy Grail of Fluid Simulation

In 1883 Reynolds reported experimental results on the transition from laminar to turbulent flow in pipes.





Reynolds Number

The dimensionless number relevant to turbulence is the Reynolds number,

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In a dilute gas the kinematic viscosity is roughly,

$$\nu \cong {}^{1}/_{2}\,(\text{Sound speed})(\text{Mean free path})$$

and so,

$$\mathrm{Re} \cong 2\ (\text{Mach number})/(\text{Knudsen number})$$

Turbulence & DSMC

For subsonic (Ma = 0.5) fluid flow at Re = 1000 requires a system with Kn = 10^{-3} .

For a 3D calculation of isotropic turbulence this needs a system volume of 10^9 cubic mean free paths.

Such a DSMC simulation would require roughly 10^{11} to 10^{12} simulation particles.

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This is possible using the Sandia Sparta code running on modern exo-scale computers but we were trying to do it in 1994!

Controlling Viscosity

To attain high Reynolds number we tried various ways of lowering the viscosity:

- Manipulating the collision rate

  "Microscopic simulation of dilute gases with adjustable transport coefficients", F. Baras, M. Malek Mansour, and ALG, *Phys. Rev. E* **49** 3512 (1994).

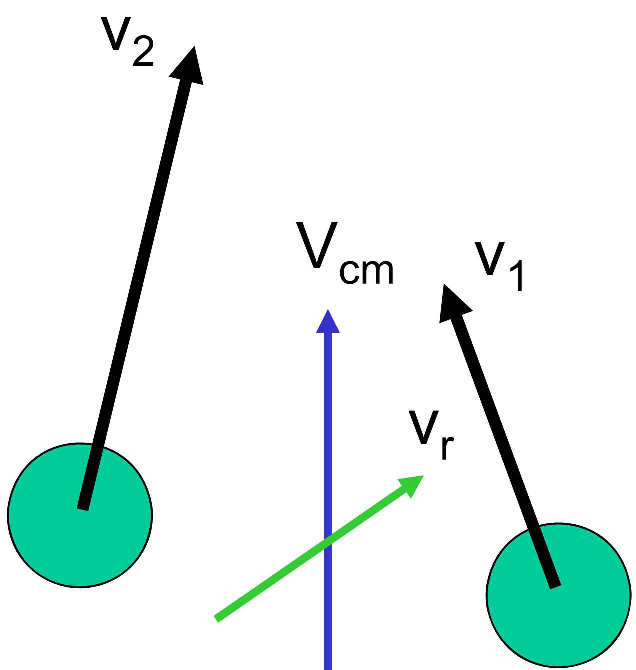
- Manipulating the CBA displacement

  "A Particle Method with Adjustable Transport Properties- The Generalized Consistent Boltzmann Algorithm", ALG, F. Alexander and B. Alder, *J. Stat. Phys.* **89** 403 (1997).

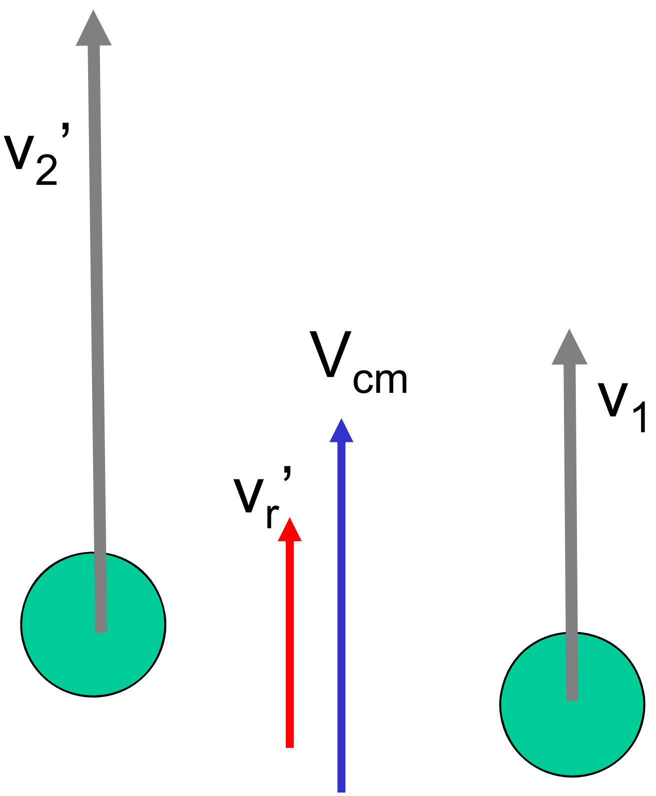
These helped but not enough. We were desperate.

“With The Flow” Model

Direction of the post-collision relative velocity is parallel to the center of mass velocity.



Pre-collision velocities



Post-collision velocities

“With The Flow” Model

A few remarks regarding “With The Flow” (WTF):

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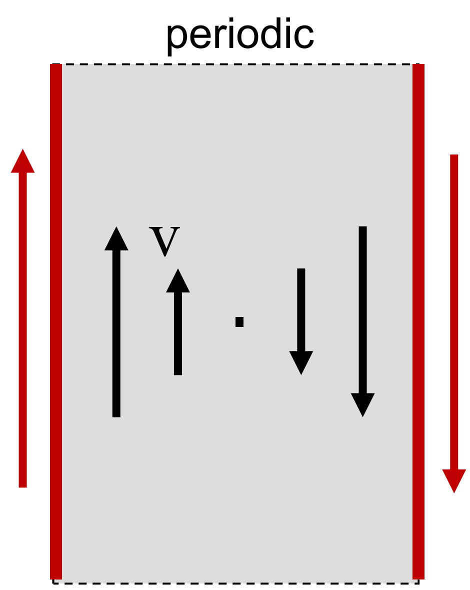
- The WTF rule violates the symmetry of forward and reverse collisions however DSMC collisions are *not* elementary events since typically $F_N >> 1$.
- The WTF collisions tend to lower entropy, which is favorable since, by irreversible thermodynamics, entropy production is proportional to viscosity.

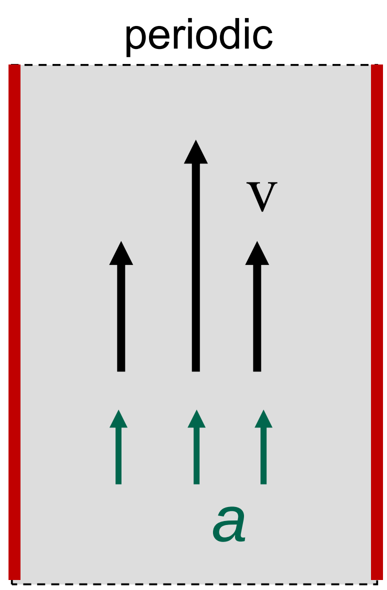
Measuring Viscosity

Couette Flow



Viscosity ∝
Wall drag force

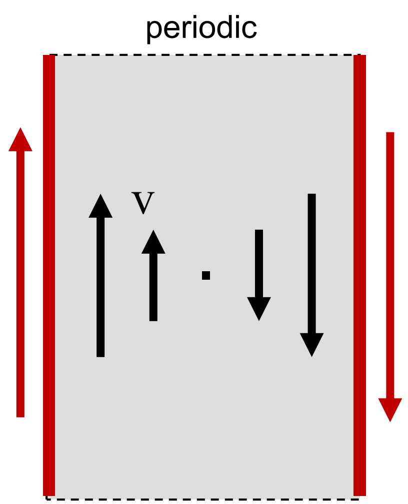
Poiseuille Flow

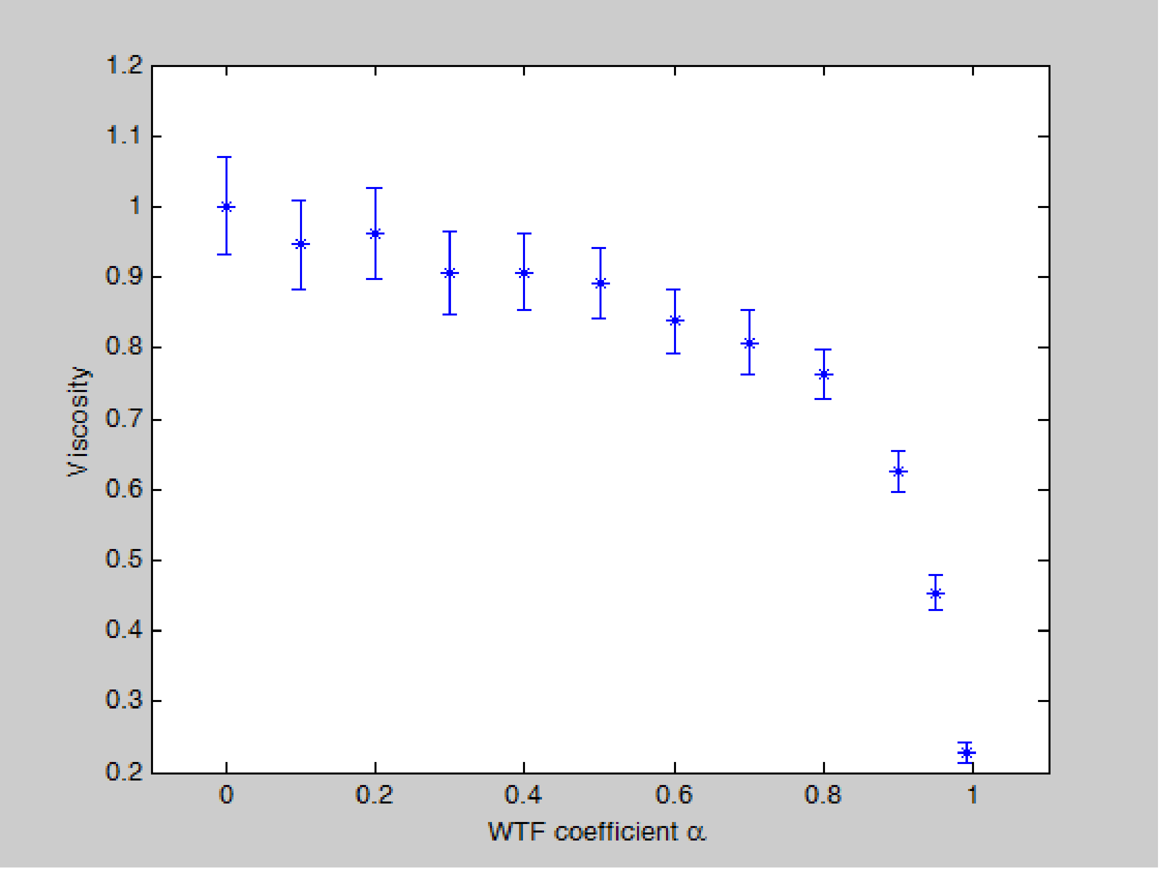


Viscosity ∝
Peak velocity

Viscosity in Couette Flow

Couette flow measurement of viscosity looked promising.

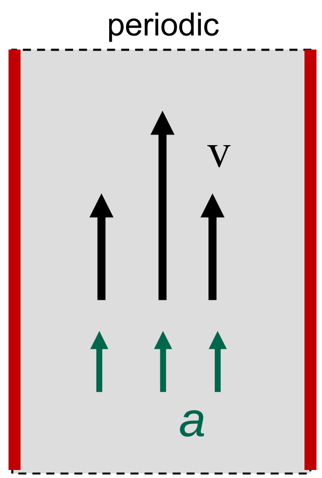


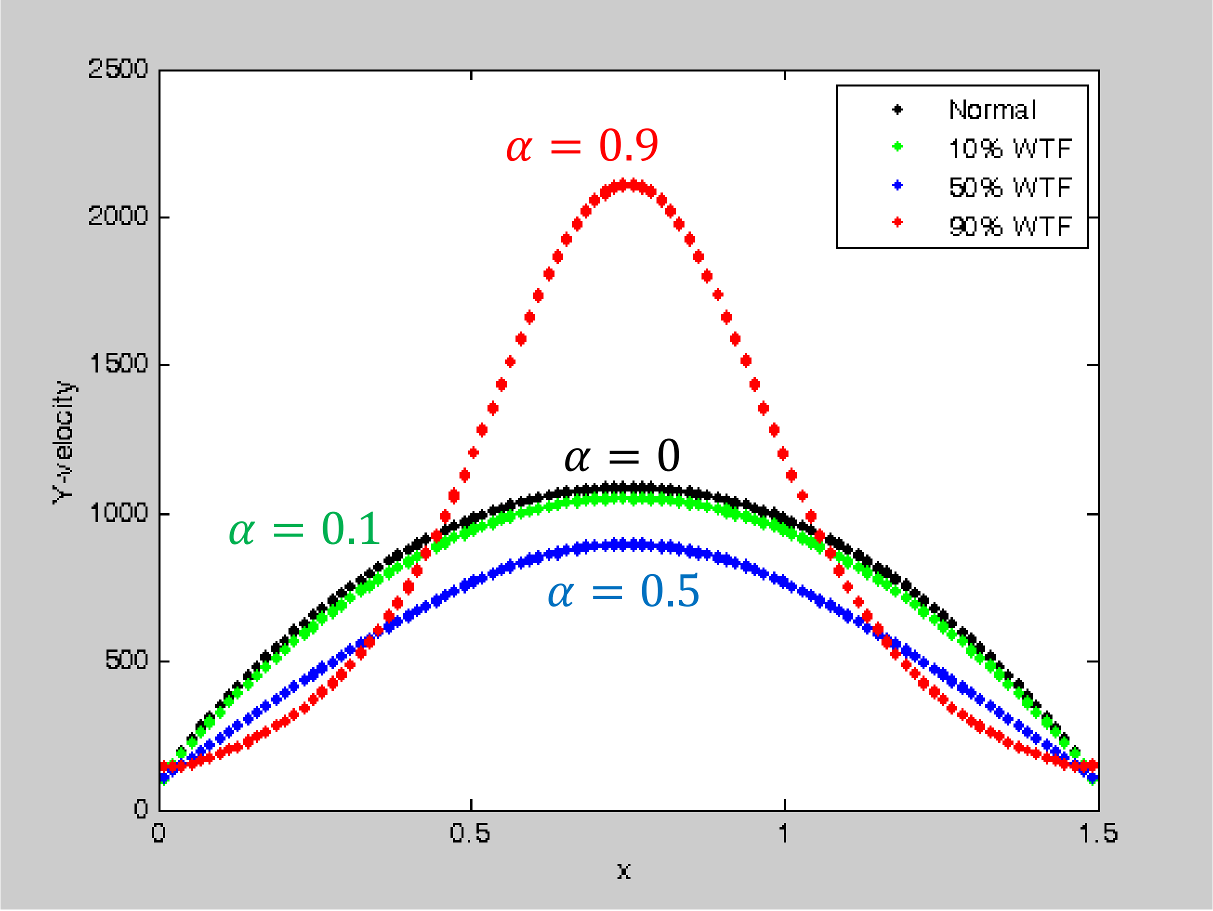


Viscosity goes down as $\alpha \to 1$

Viscosity in Poiseuille Flow

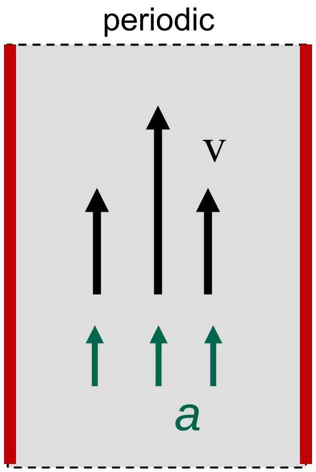
Velocity profile for Poiseuille flow looked strange.

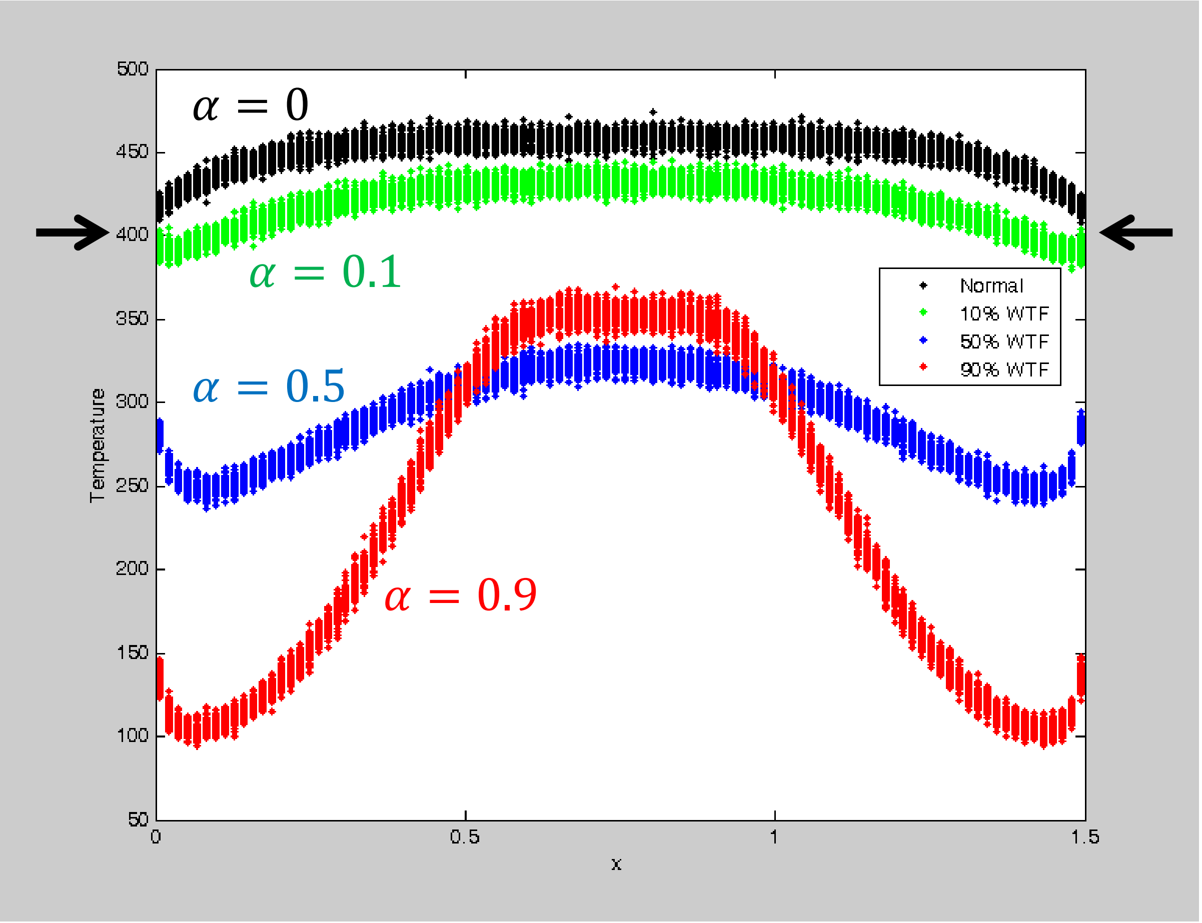




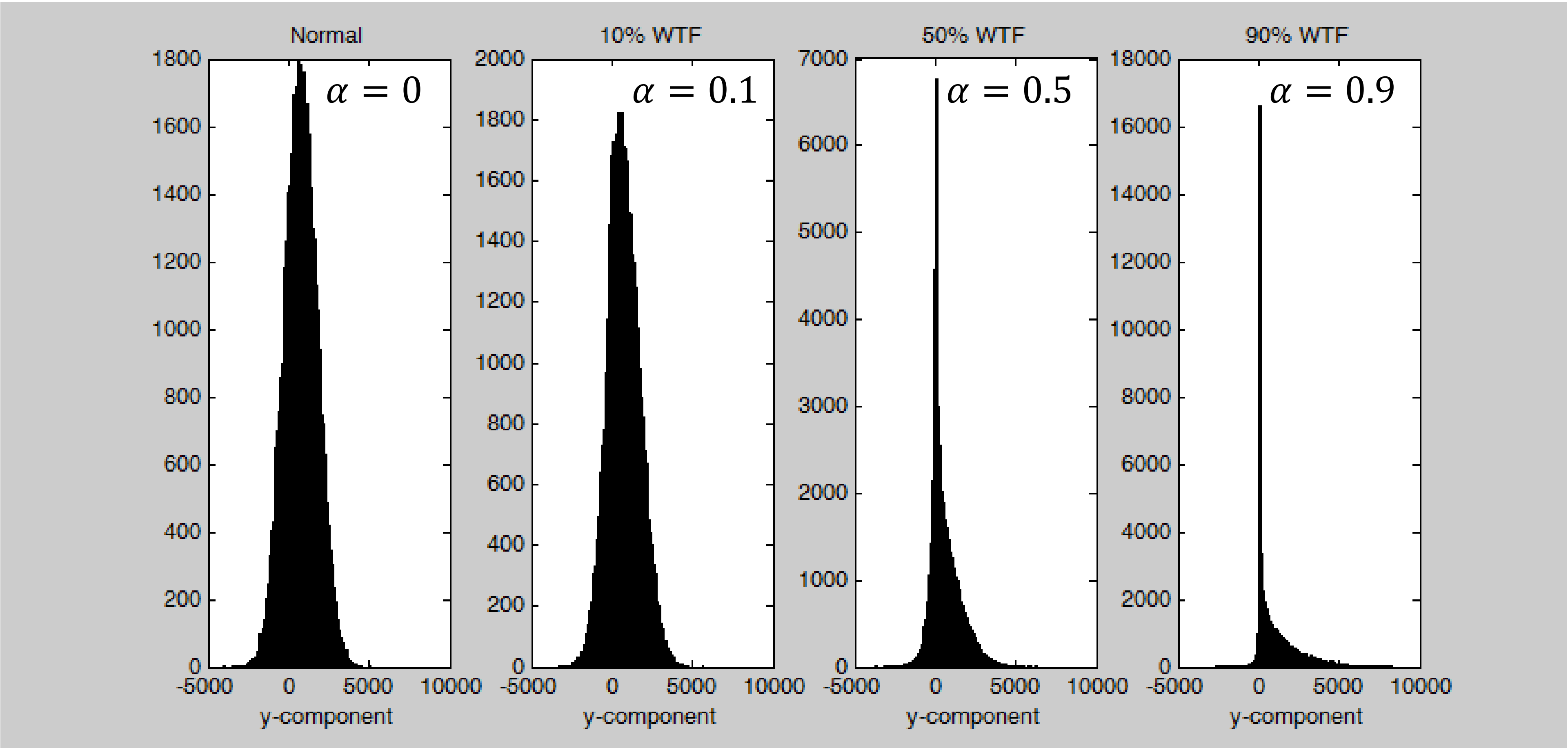
Temperature in Poiseuille Flow

Temperature profile for Poiseuille flow looked *very* strange, with anomalous *viscous cooling*.





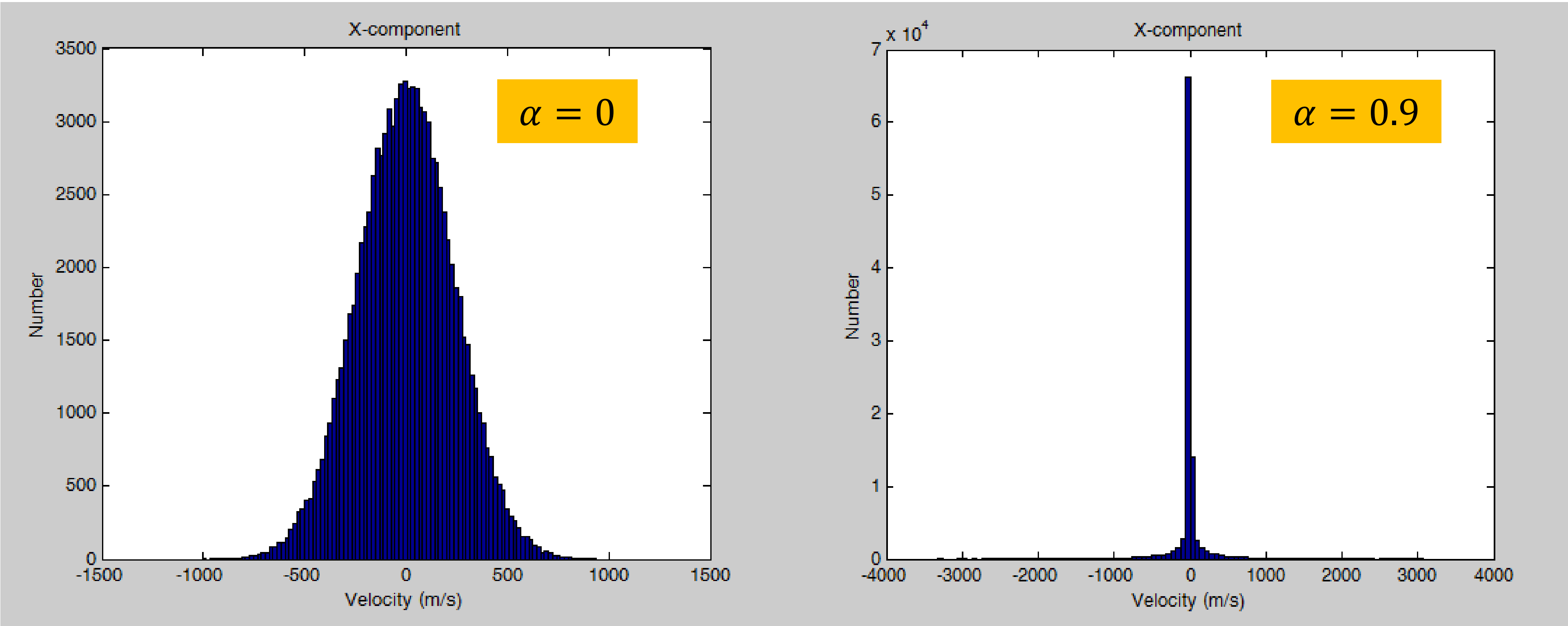
Poiseuille Flow
Velocity Distribution Function



Particle velocity distribution function in the center-line of the channel

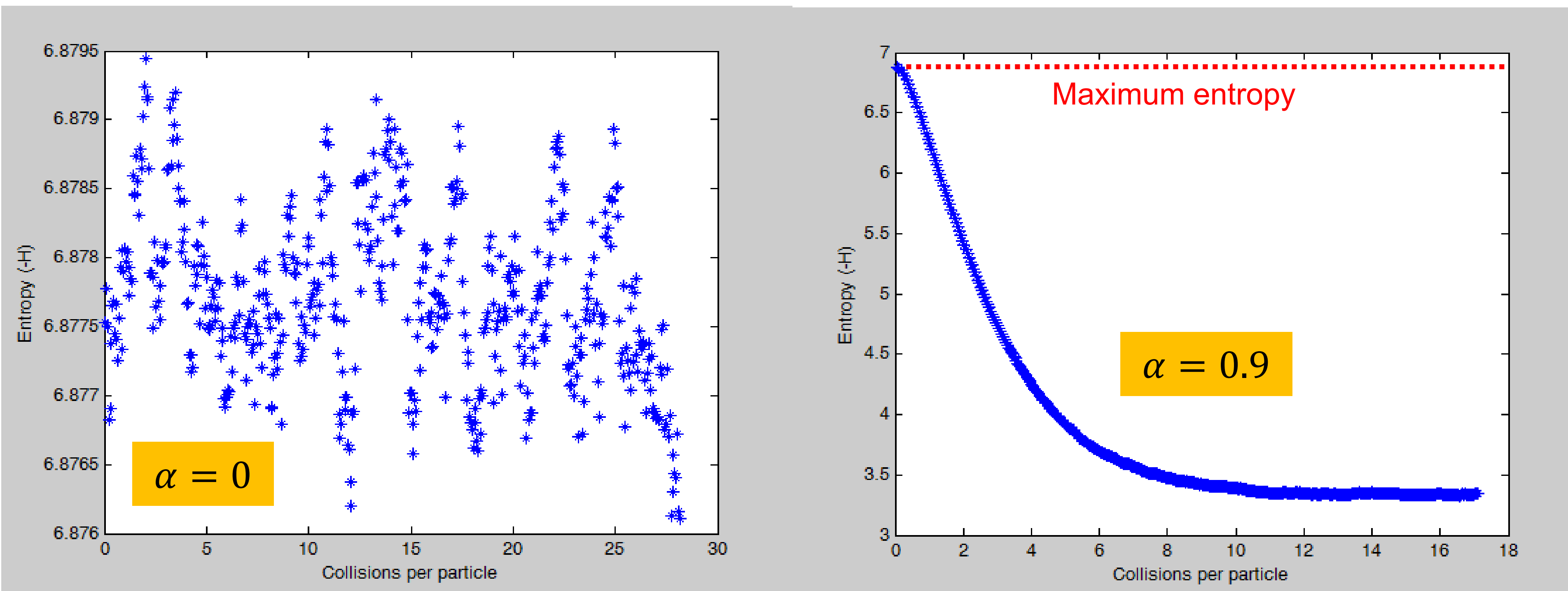
Equilibrium Distribution

At thermodynamic equilibrium the WTF model does *not* relax to the Maxwell-Boltzmann velocity distribution.



Entropy & Equilibrium

At thermodynamic equilibrium the WTF model is *not* at a state of maximum entropy, violating 2nd Law of Thermodynamics.



Entropy measured using the Boltzmann H-function

Act III

The Redemption

In which the speaker attempts to redeem himself with a cautionary tale for his comrades.

Dante and Virgil emerging from Hell
Gustave Dore (1890)

Breaking DSMC

The DSMC algorithm has evolved over the past 50 years.

- Collision rate (Time counter, NTC, Bernoulli trials, …)
- Basic collisions (VHS, VSS, Lennard-Jones models, …)
- Complex collisions (Internal energy, chemistry models, …)
- Particle motion (Adaptive time step, …)
- Boundary conditions (Surface models, Inflow/Outflow, …)
- Statistical analysis (Filters, Variance-reduction, …)
- Other innovations (Hybrids with CFD, …)

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How do we know that we've not violated any fundamental physical laws?

Laws of Thermodynamics

The First Law of Thermodynamics is easy to verify in DSMC by checking that energy is conserved.

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How do you verify that your DSMC code also satisfies the Second Law of Thermodynamics?

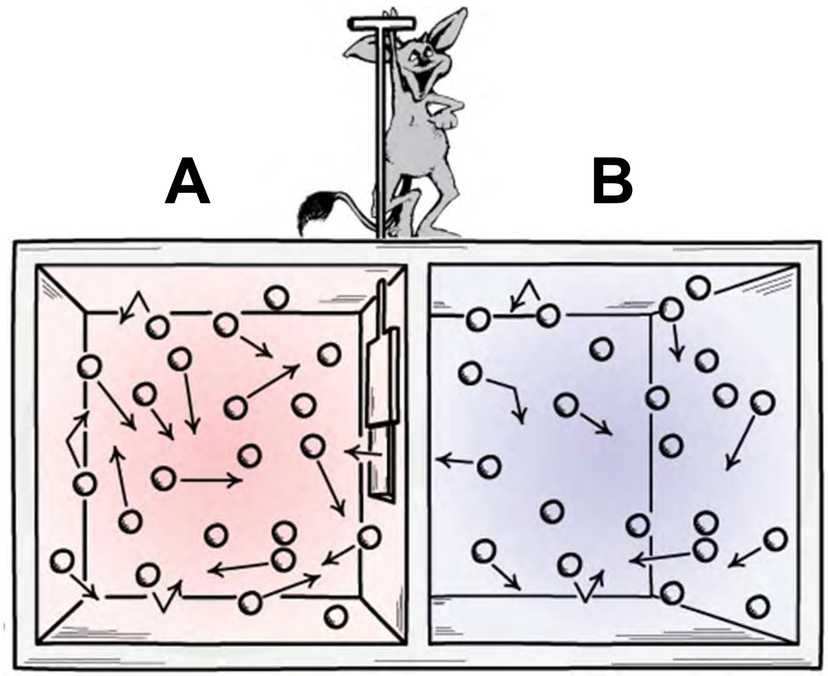
We believe that the basic DSMC algorithm is sound but how do you test that your implementation, with advanced collision models, boundary models, etc., has maximum entropy at equilibrium?

Maxwell's Demon

In 1887 Maxwell presented this thought experiment,

… conceive of a being whose faculties are so sharpened that he can follow every molecule in its course … so as to allow only the swifter molecules to pass from A to B, and only the slower molecules to pass from B to A.

He will thus, without expenditure of work, raise the temperature of B and lower that of A, in *contradiction to the second law of thermodynamics*.



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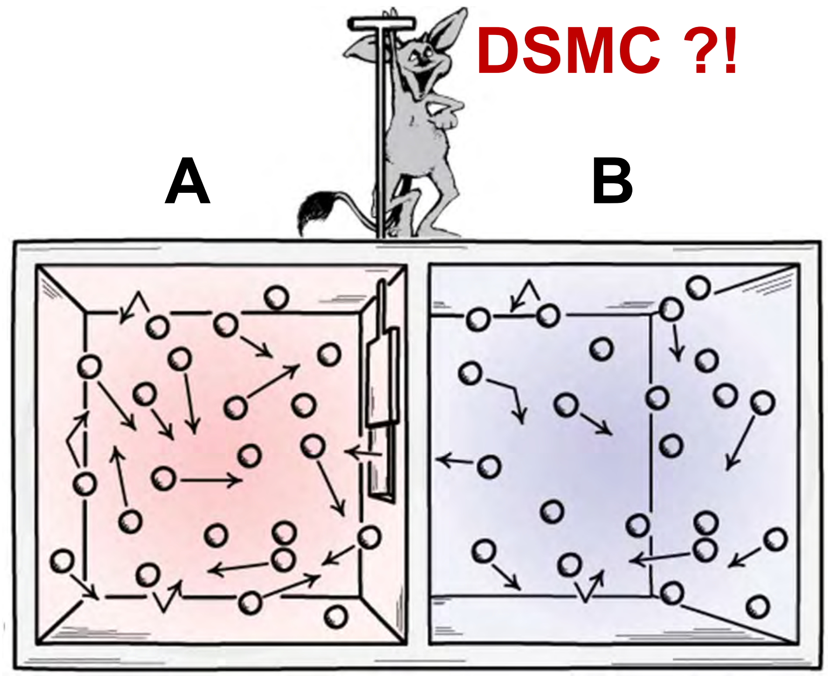
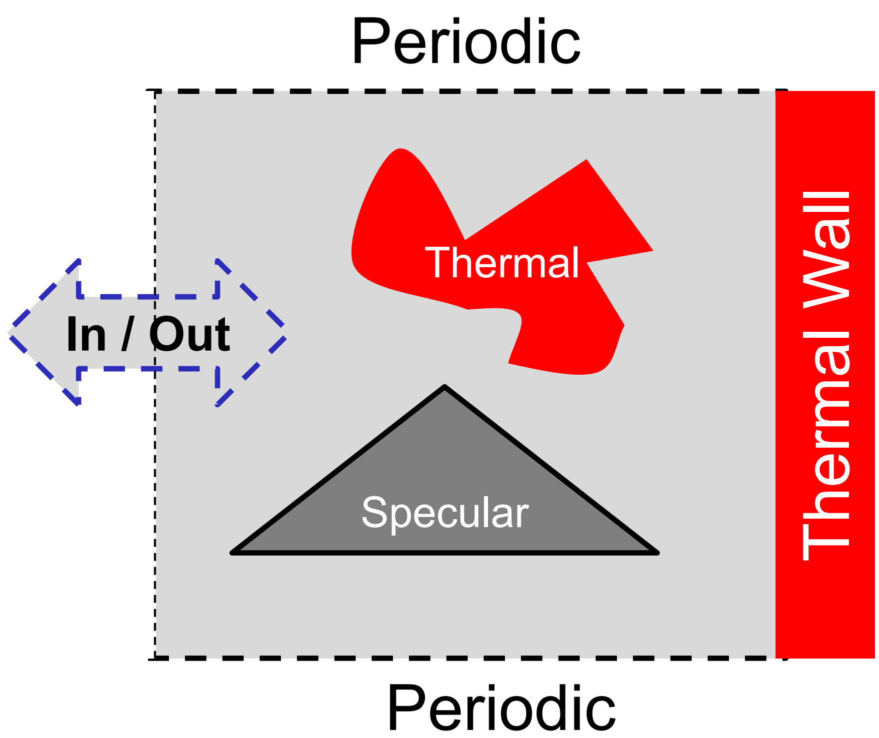


DSMC *does* follow every molecule and affects its motion.

Entropy & Equilibrium

The entropy measured in DSMC at thermodynamic equilibrium should match the theoretical prediction of statistical mechanics.



This validation requires an accurate measurement of the probability distribution,

$$P(\boldsymbol{r}_1, \dots, \boldsymbol{r}_N, \boldsymbol{v}_1, \dots, \boldsymbol{v}_N)$$

It is <u>not</u> enough to measure just $P(\boldsymbol{r})$ and $P(\boldsymbol{v})$.

Equilibrium Fluctuations

A simple way to test the full probability distribution is to measure thermal fluctuations and compare with equilibrium statistical mechanics predictions. For example,

$$\langle \delta\rho_i \delta\rho_j \rangle = \frac{\langle \rho \rangle^2}{\langle N_i \rangle} \delta_{i,j} \qquad \langle \delta\rho_i \delta u_j \rangle = 0$$

with similar expressions for other hydrodynamic correlations, such as $\langle \delta u_i \delta u_j \rangle, \langle \delta u_i \delta T_j \rangle, \text{etc.}.$

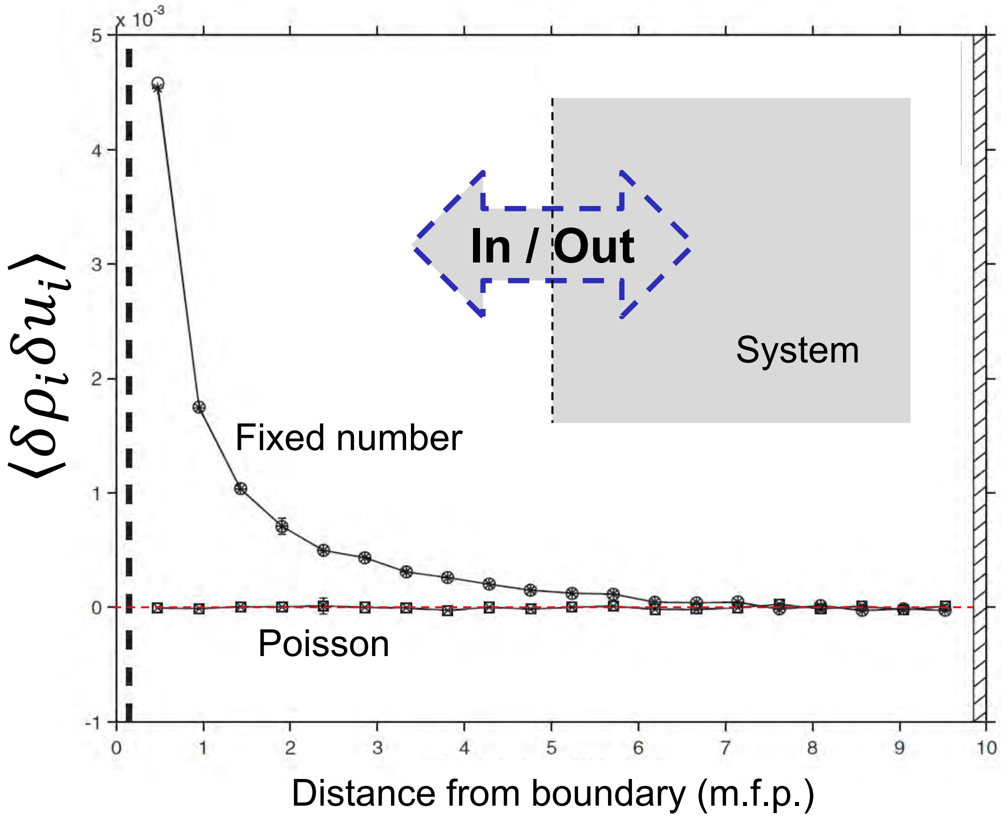
Note that these results are *independent* of F_N.

"Estimating Hydrodynamic Quantities in the Presence of Microscopic Fluctuations", ALG, *CAMCoS* **1** 53-78(2006).

Inflow / Outflow Boundary

An inflow / outflow boundary models an infinite reservoir of particles with an equilibrium density and temperature.

Number of particles generated at the boundary should be Poisson distributed to match equilibrium.



"Non-equilibrium behavior of equilibrium reservoirs in molecular simulations", M. Tysanner and ALG, *Int. J. Num. Meth. Fluids* **48** 1337-1349 (2005).

Who Cares?

You may be thinking to yourself,
“That’s all interesting but … who cares?”

Who Cares?

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"That's all interesting but … who cares?"

Home > Publishers > AIP Publishing > Physics of Fluids (1994-present) > Volume 28, Issue 6 > Article

AIP | Physics of Fluids

F Brownian relaxation of an inelastic sphere in air CrossMark

G. A. Bird[1,a)]

+ VIEW AFFILIATIONS

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Phys. Fluids **28**, 062005 (2016); http://dx.doi.org/10.1063/1.4953151

June 2016 issue

"The paper concentrates on the transfer of energy from the air to an initially stationary sphere as it acquires Brownian motion. …
The implications of Brownian relaxation for the second law of thermodynamics are discussed."

Brownian Motors

Heat engine is driven by thermal fluctuations.

Introduced by Smoluchowski and later popularized by Feynman.

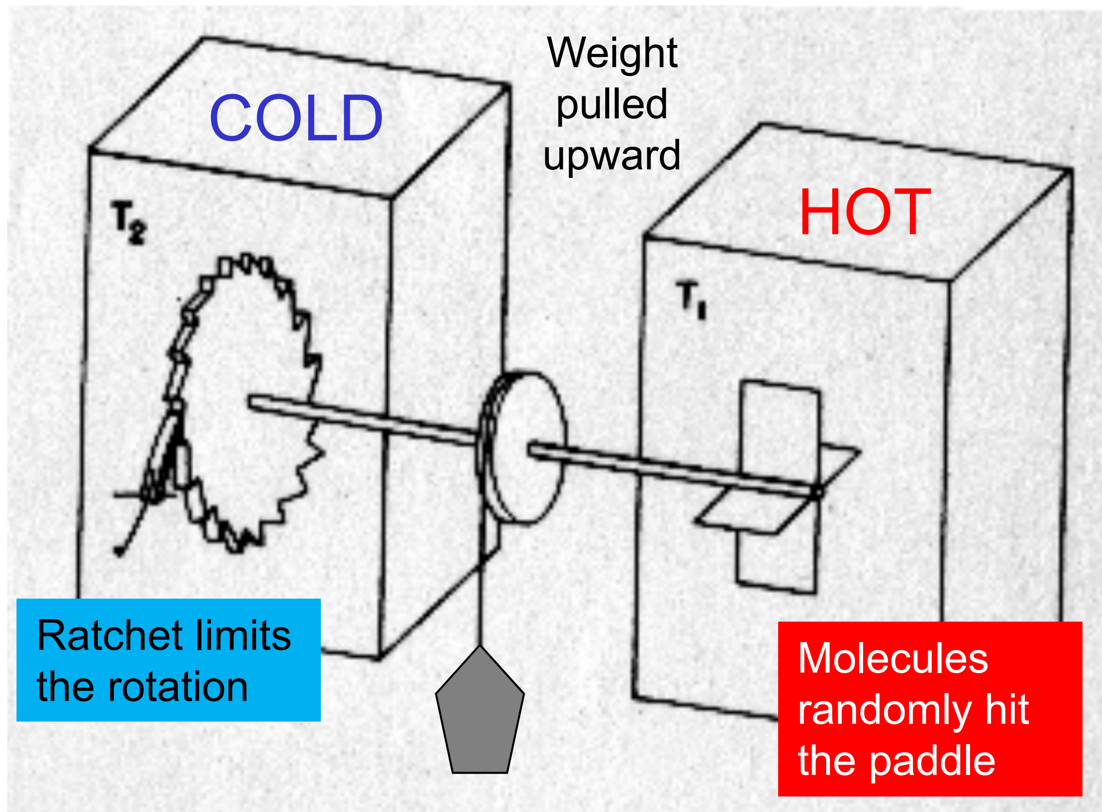


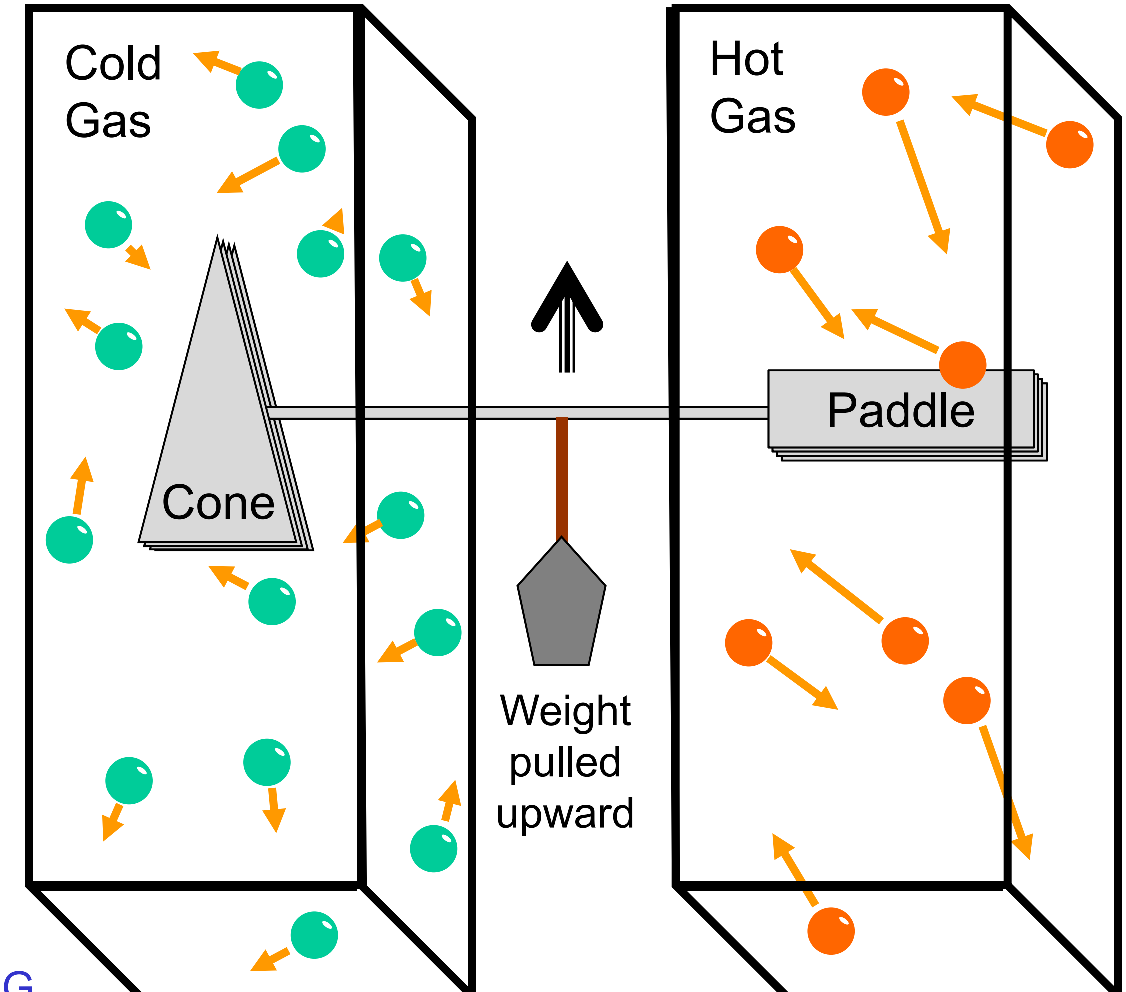
Fig. 46-1. The ratchet and pawl machine.

Living cells have Brownian motors powered by chemical potential gradients

Triangula Brownian Motor

Feynman's complex ratchet and pawl mechanism is not necessary.

Heat engine can be made using simple, asymmetrically shaped Brownian objects, such as a triangular cone.



P. Meurs, C. Van den Broeck, and ALG, *Physical Review E* **70** 051109 (2004).

Second Law, Revisited

From the September 2015 issue of *Physics Today*

From Maxwell's demon to Landauer's eraser

Eric Lutz and Sergio Ciliberto

Thought experiments that long puzzled the thermodynamics community are now being performed in the lab—and they're forging a deeper understanding of the second law.

DSMC is ideally suited for numerical experiments in this important and vibrant field of theoretical physics

Closing Thoughts

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- DSMC is not fool-proof.
- DSMC implementations may violate the 2^{nd} Law of Thermodynamics.
- There are applications where this matters (e.g., Brownian motors).
- Hydrodynamic fluctuations are a useful validation test of thermal equilibrium.
- The 2^{nd} Law is a hot topic in physics.

Maxwell's demon is in the details.

Thank you for your attention.

Satan
Gustave Dore (1890)