Direct Simulation Monte Carlo:
theory, methods, & open challenges

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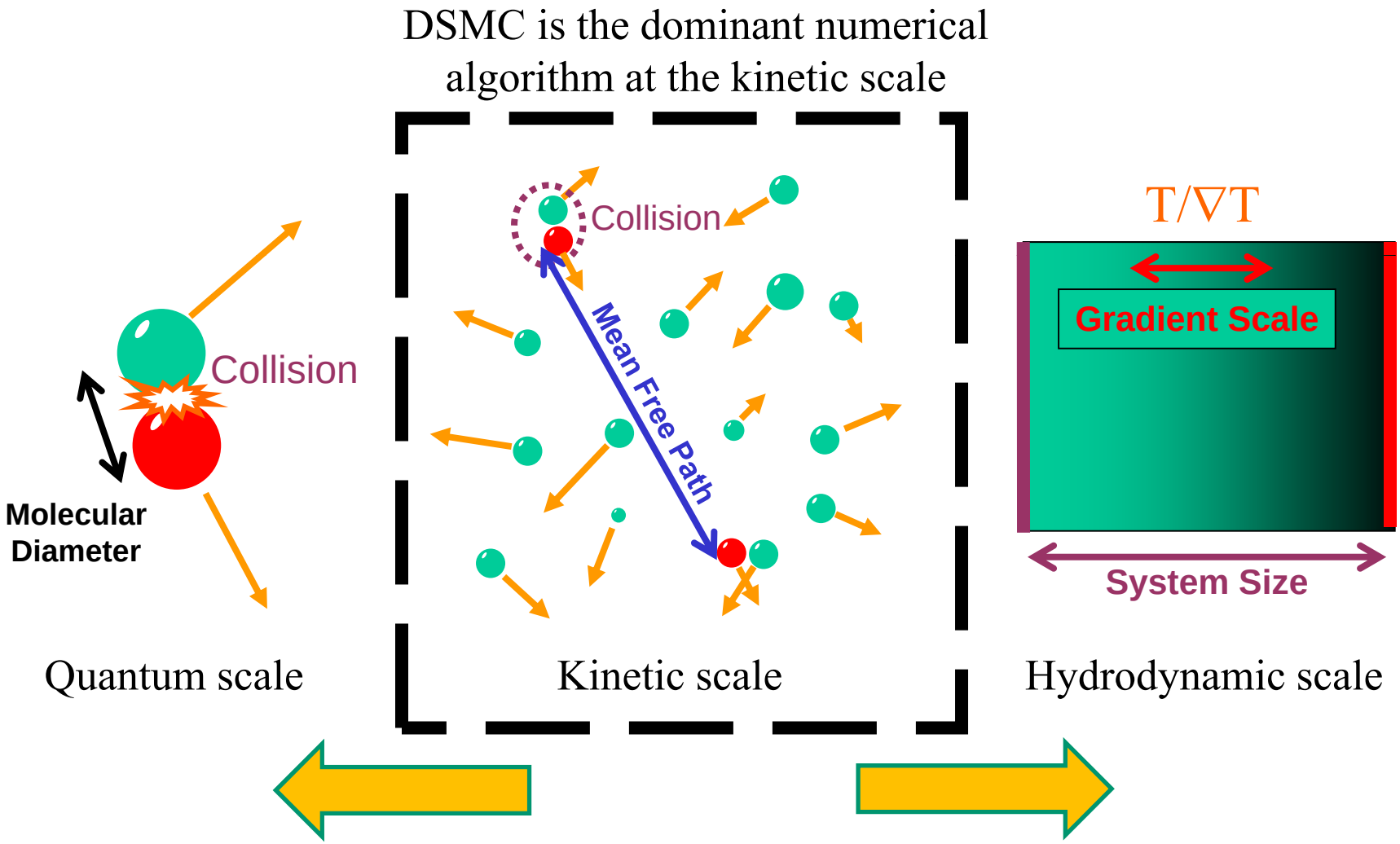
Physical Scales for Dilute Gases

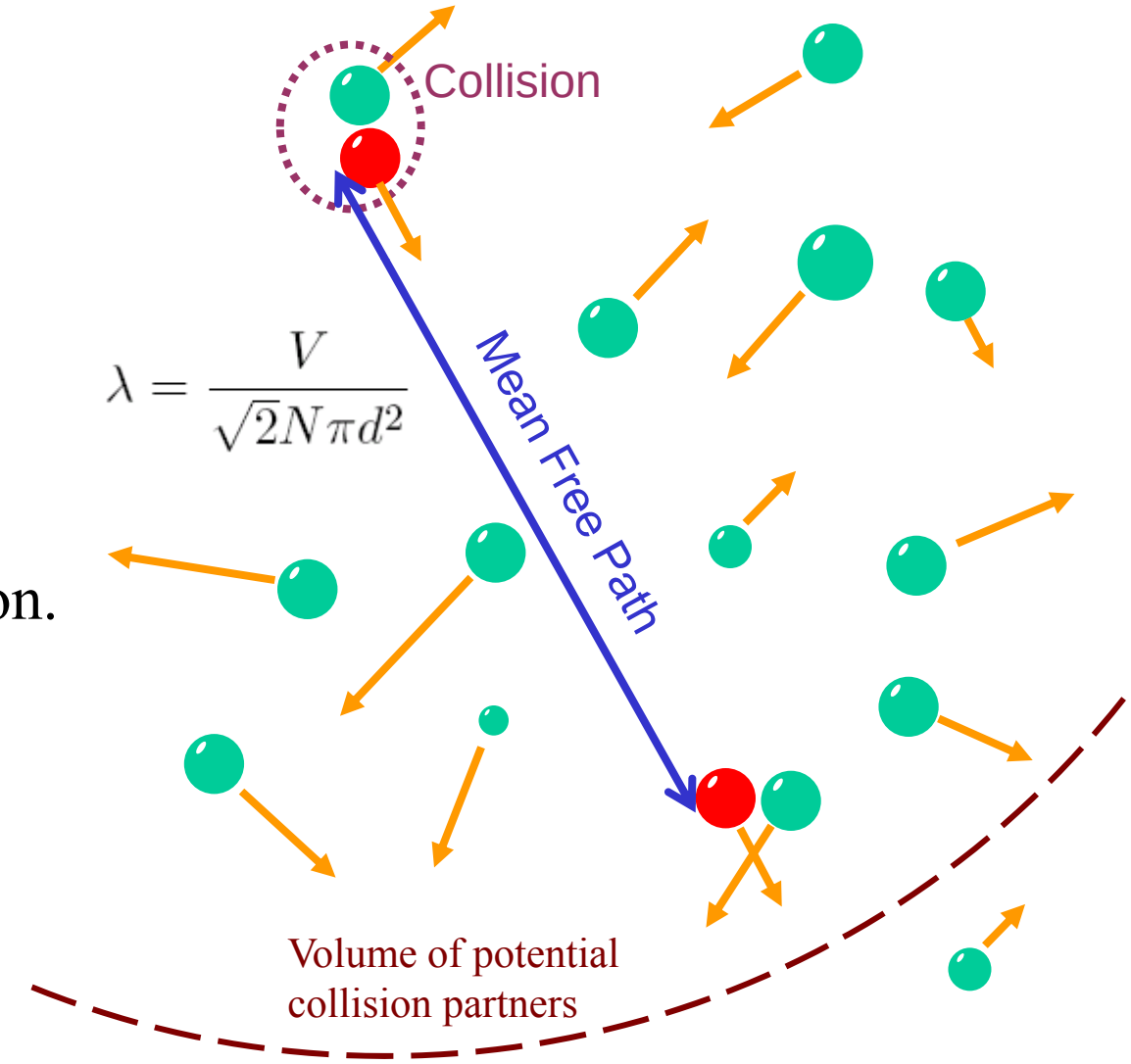


Molecular Dynamics for Dilute Gases

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.



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)
- Used for 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

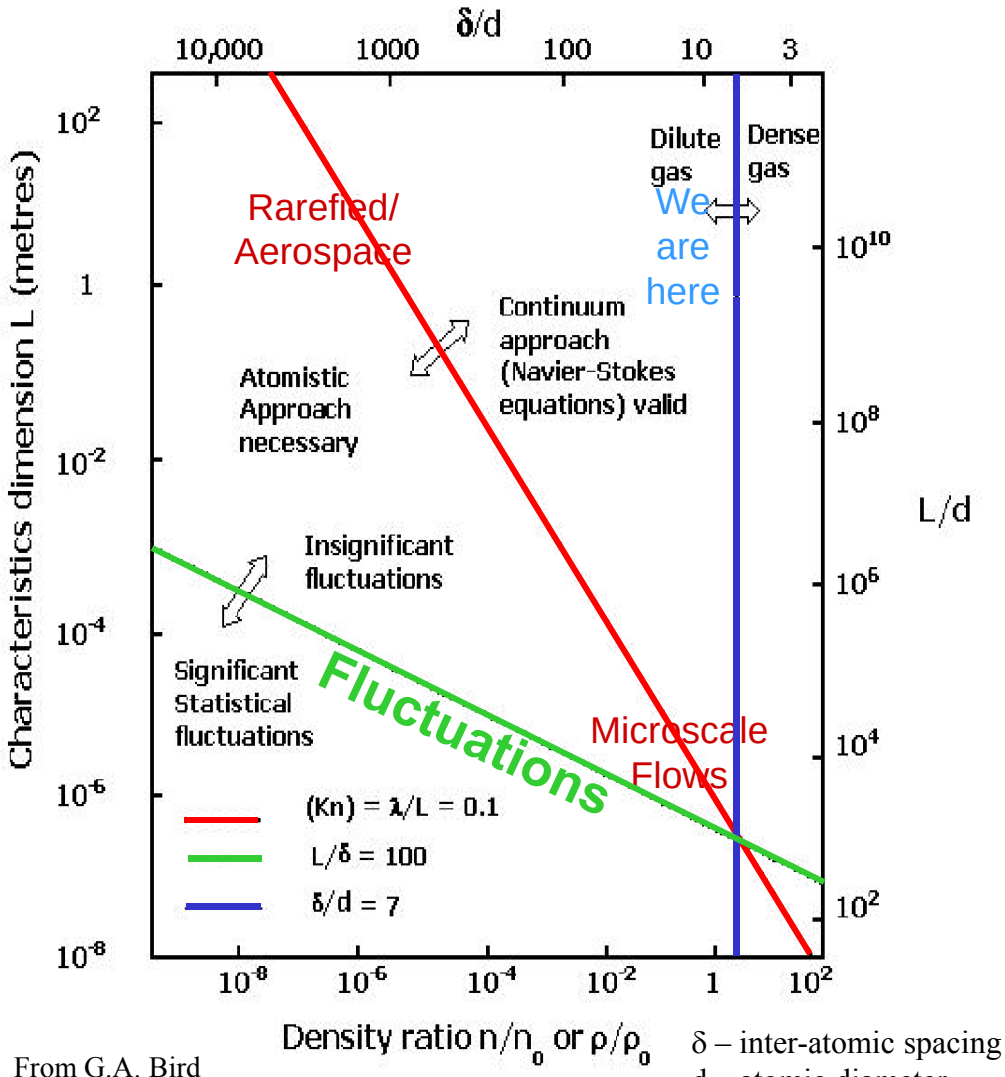
Particle vs. Continuum

When is the continuum description of a gas not accurate?

$$\text{Knudsen Number} = \frac{\text{Mean Free Path}}{\text{System Length}}$$

When Kn > 0.1, continuum description is not accurate

Equilibrium fluctuations are noticeable when the number of particles < 10^6 .



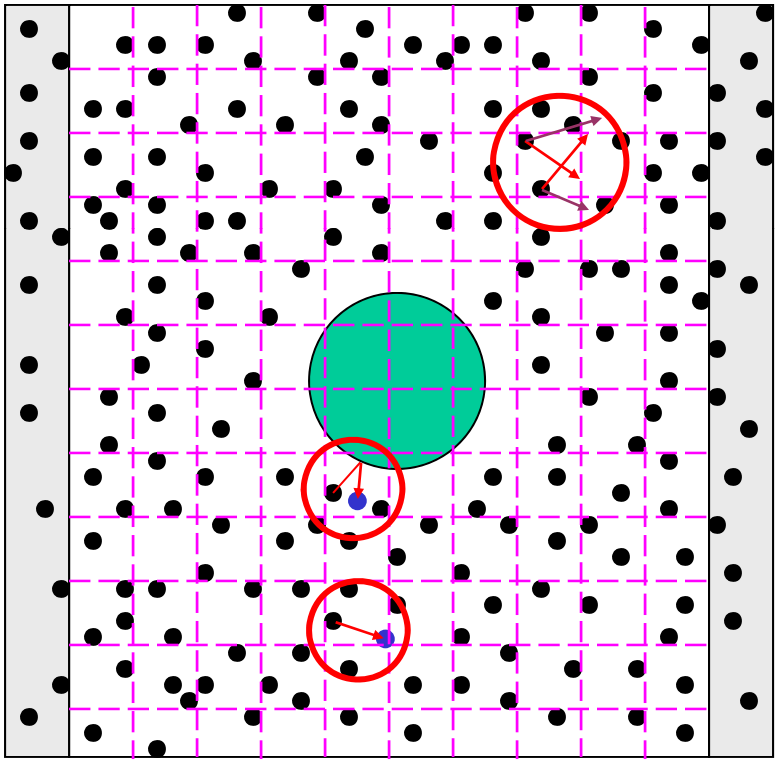
From G.A. Bird

δ – inter-atomic spacing
d – atomic diameter

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
  - Sample statistical values
  - Select and execute random collisions

Example: Flow past a sphere



G.A. Bird, *Molecular Gas Dynamics and Direct Simulation of Gas Flows*, Clarendon, Oxford (1994)
F. Alexander and A. Garcia, *Computers in Physics*, **11** 588 (1997)

Random Numbers

Need a high-quality random number generator for the uniform (0,1) distribution, such as Mersenne Twister.

Many distributions (e.g., Gaussian, exponential) may be generated by the inversion method:

Generate random value x with distribution $P(x)$ as
$x = f(R)$ where R is uniformly distributed in (0,1).

Most other distributions are generated by the accept-reject method:

Draw x_{try} uniformly in the range of x;
Accept it if $P(x_{try}) > \max\{P(x)\}R$ else draw again.

Be careful to use high-quality algorithms and be sure that you verify your implementation with independent testing.

Initialization

Divide the system into cells and generate particles in each cell according to desired density, fluid velocity, and temperature.

From density, determine number of particles in cell volume, N, either rounding to nearest integer or from Poisson distribution.

Assign each particle a position in the cell, either uniformly or from the linear distribution using the density gradient.

From fluid velocity and temperature, assign each particle a velocity from Maxwell-Boltzmann distribution $P(\mathbf{v};\ \{\mathbf{u},T\})$ or from the Chapman-Enskog distribution $P(\mathbf{v};\{\mathbf{u},T,\nabla\mathbf{u},\nabla T\})$.

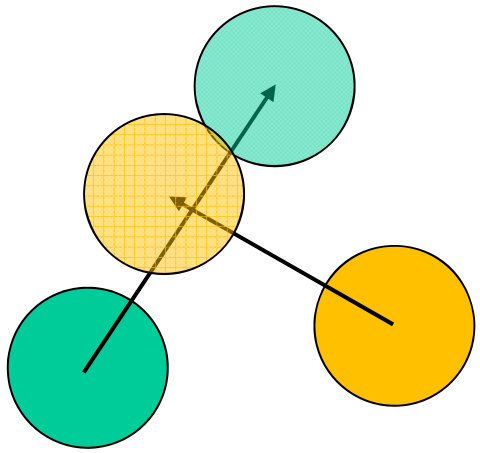
Be careful initializing particles for initial value problems.

Ballistic Motion

Particles motion is ballistic; during a time step, τ, particle positions are updated as,

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\,\tau$$

The particles move without interaction and can even overlap.

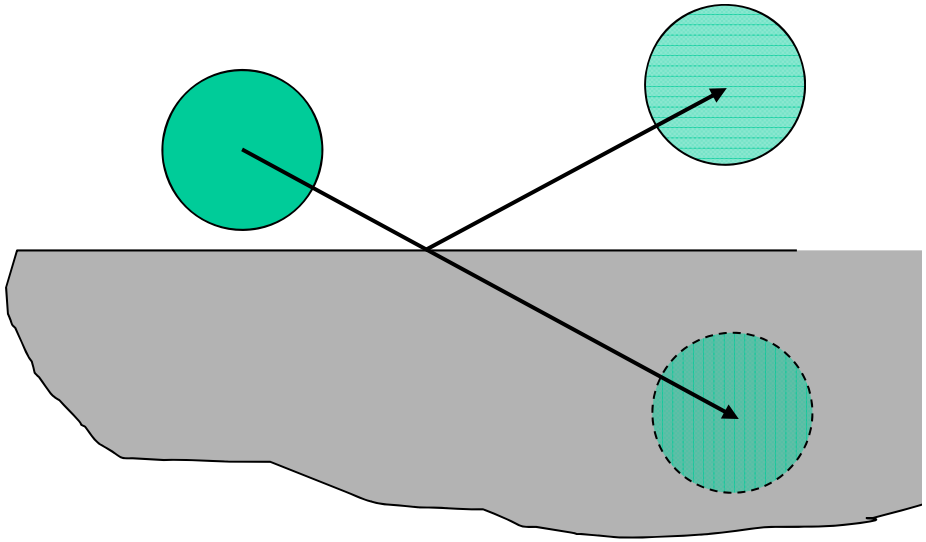


For transient flows, on the first time step use ½ τ (Strang splitting) to maintain accuracy. If measuring non-conserved variables (e.g., fluxes) then time-center the sampling (half move, sample, half move, collisions) for all steps.

Simple Boundaries

With periodic boundaries particles are re-introduced on the opposite side of the system.

Specular surfaces modeled by ballistic (mirror) reflection of point particles.



Be careful with corners.

Be careful with body forces.

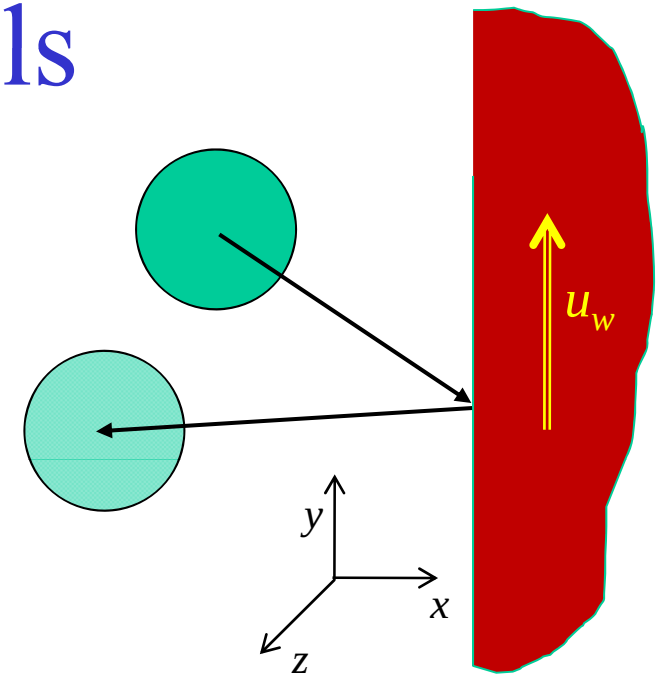
Thermal Walls

A more realistic treatment of a material surface is a thermal wall, which resets the velocity of a particle as a biased-Maxwellian distribution,

$$P_{v_x}(v_x) = \pm\frac{m}{kT_{\rm w}} v_x e^{-mv_x^2/2kT_{\rm w}}$$

$$P_{v_y}(v_y) = \sqrt{\frac{m}{2\pi kT_{\rm w}}} e^{-m(v_y-u_{\rm w})^2/2kT_{\rm w}}$$

$$P_{v_z}(v_z) = \sqrt{\frac{m}{2\pi kT_{\rm w}}} e^{-mv_z^2/2kT_{\rm w}}$$



These distributions (exponential and Gaussian) are simple to generate by inversion.

Walls can also be part-thermal, part-specular (accommodation).

Reservoir Boundary

Inflow/outflow boundary conditions commonly treated as a reservoir with given density, fluid velocity, temperature.

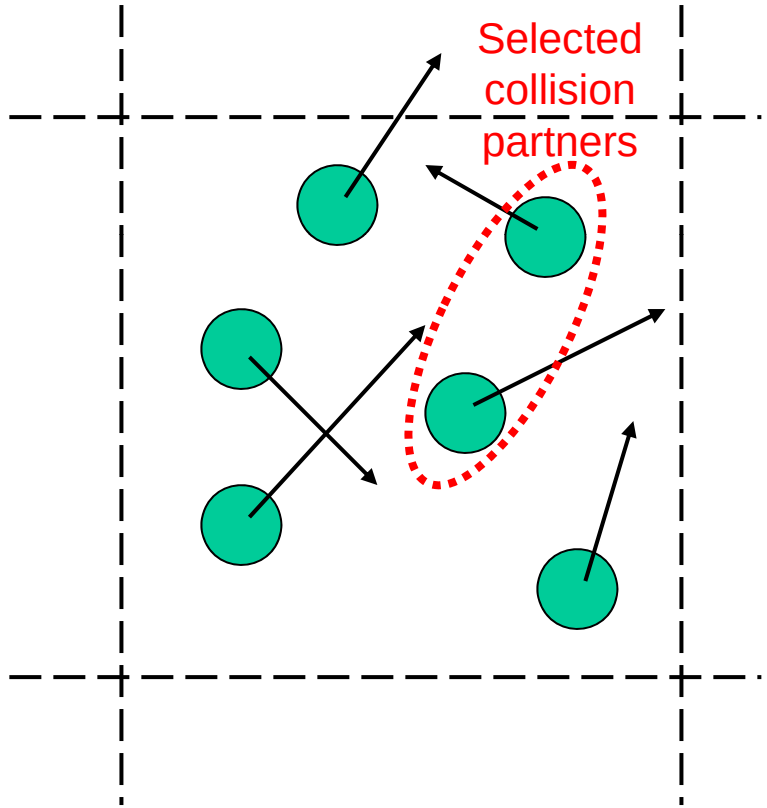
Particles in the main system are removed if they cross the boundary into the reservoir.

Particles injected from reservoir to main system by either:

- Surface generator: From number flux determines number to be injected; generate particle velocities from surface distribution (e.g., inflow Maxwellian).
- Volume generator: Initialize a "ghost cell" with particles before the ballistic move; discard any that do not cross the boundary into the main system during the move phase.

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

Collision Rate

Number of collisions that should occur during time step is

$$M_{coll} = \tau \, R\left(N, V, d, \langle v_r \rangle, \ldots\right)$$

where the functional form of the collision rate, R, depends on the intermolecular model.

For hard spheres of diameter d, the collision rate is,

$$R\left(N, V, d, \langle v_r \rangle\right) = \frac{N(N-1)\pi d^2 \langle v_r \rangle}{2V}$$

where is $\langle v_r \rangle$ the average relative velocity.

Early DSMC implementations used $N\,N_{\mathrm{av}}$ instead of $N(N-1)$, where N_{av} is an estimated average value of N.

Collision Selections

To avoid having to compute the average relative velocity for all particle pairs in a cell, a larger number of attempted collisions are selected and some are rejected.

Number of collisions attempted during a time step is,

$$M_{cand} = \tau \, R\left(N, V, d, v_{\max}\right)$$

where $v_{\max} \geq \max\{v_r\}$ is estimated maximum relative velocity. An attempted collision is accepted with probability,

$$P(\mathbf{v}_i, \mathbf{v}_j) = \frac{R\left(N, V, d, v_r = \left|\mathbf{v}_i - \mathbf{v}_j\right|\right)}{R\left(N, V, d, v_{\max}\right)}$$

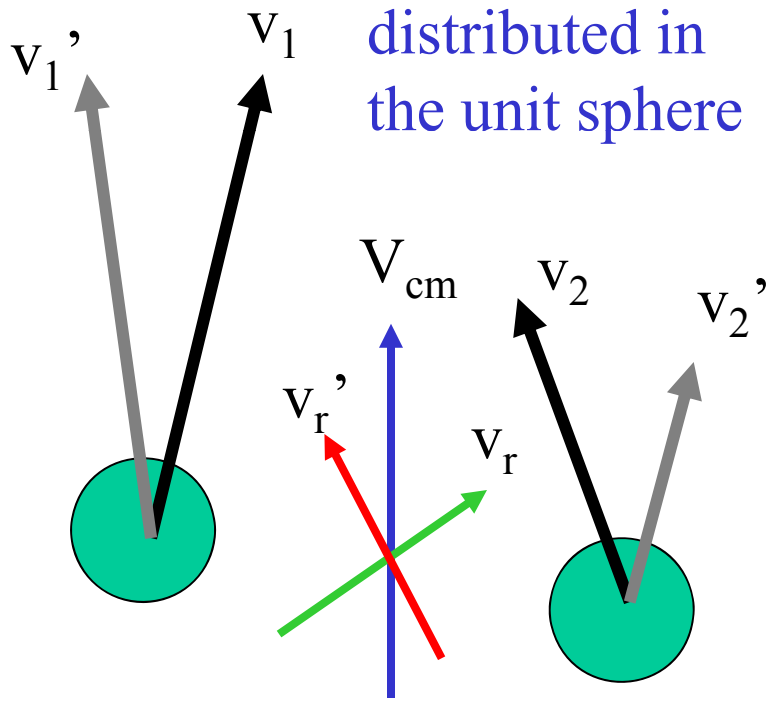
Early DSMC implementations rounded M_{cand} down and carried fraction to next time step. Modern approach is to randomly round to nearest integer (or use Poisson dist.).

Post-Collision Velocities

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

Selection of the post-collision velocities must satisfy detailed balance.

Random Solid Angle

Post-collision relative velocity is,

$$\mathbf{v}_{\mathrm{r}}^{*} = v_{\mathrm{r}}[(\sin\theta\cos\phi)\hat{\mathbf{x}} + (\sin\theta\sin\phi)\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}}]$$

The azimuthal angle is just,

$$\phi = 2\pi\Re_1$$

Polar angle distribution is,

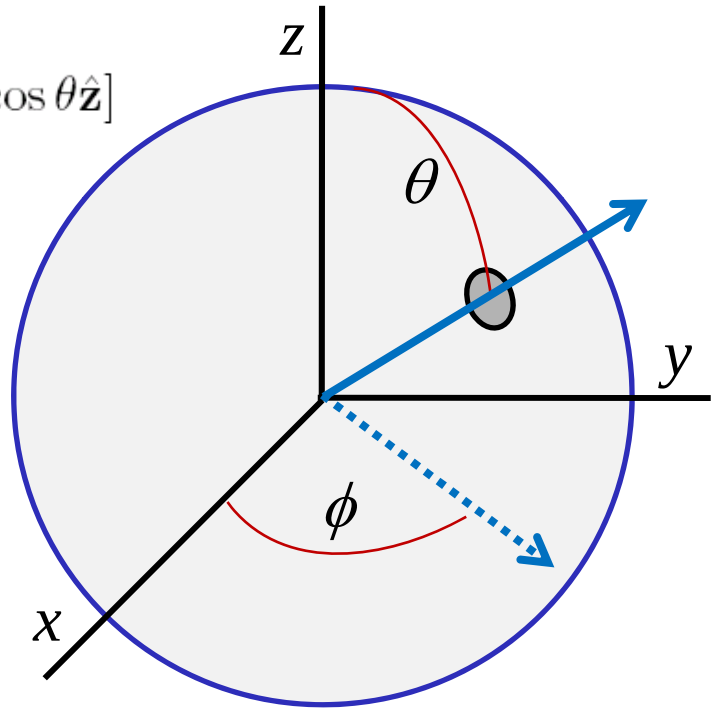
$$P_\theta(\theta)\,d\theta = \tfrac{1}{2}\sin\theta\,d\theta$$

But with change of variable,

$$P_q(q)\,dq = (\tfrac{1}{2})\,dq$$

So,

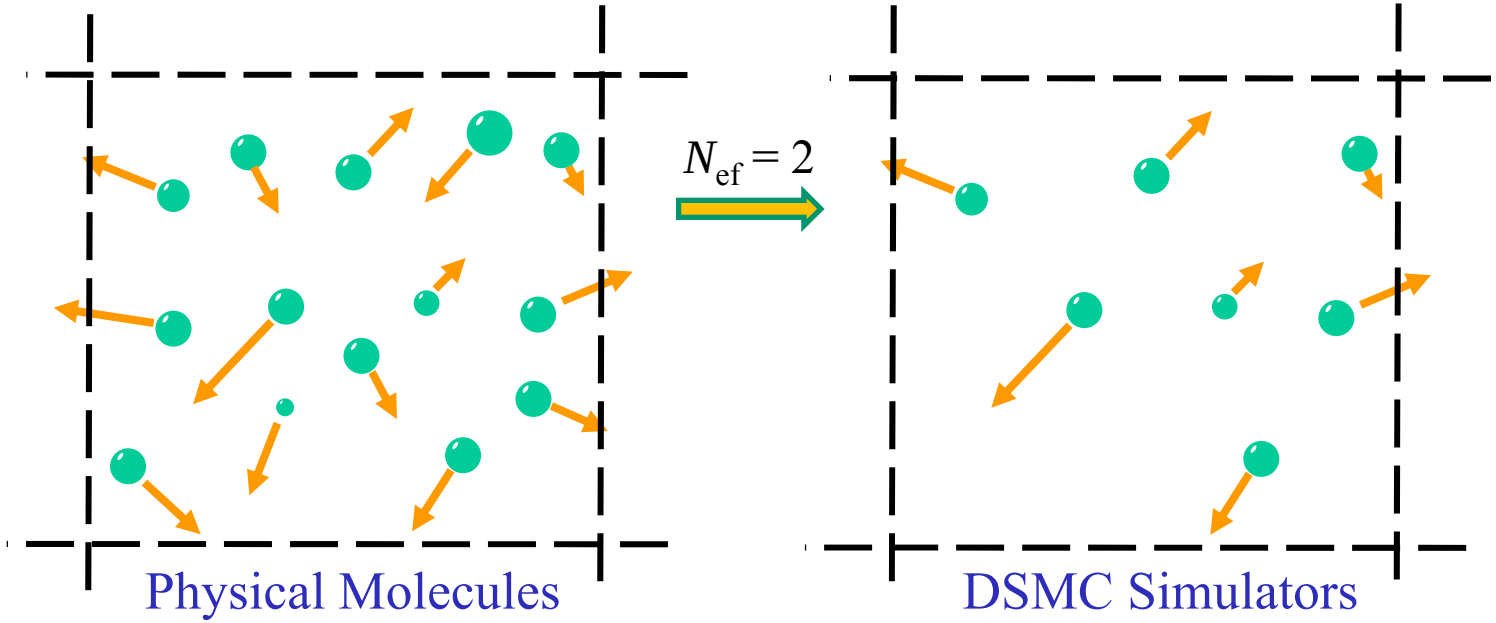
$$\begin{aligned} q &= 2\Re_2 - 1 \\ \cos\theta &= q \\ \sin\theta &= \sqrt{1-q^2} \end{aligned}$$



Generated by inversion method

Molecules & "Simulators"

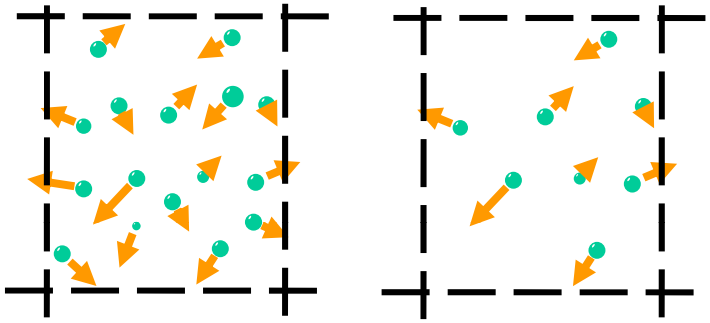
In DSMC the number of simulation particles ("simulators") is typically a small fraction of the number physical molecules. Each simulator represents N_{ef} physical molecules.



Accuracy of DSMC goes as $1/N$; for traditional DSMC about 20 particles per collision cell is the rule-of-thumb.

DSMC "Parliament"

DSMC dynamics is correct if:

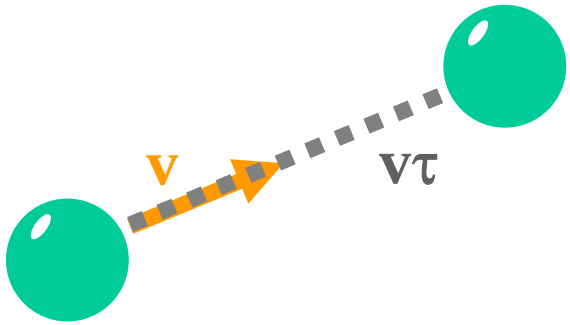


- The DSMC simulators are an unbiased sample of the physical population (unbiased parliament).
- Collision rate is increased by N_{ef} so the number of collisions per unit time for a simulator is same as for a physical molecule.
- In sampling, each simulator counts as N_{ef} physical molecules.

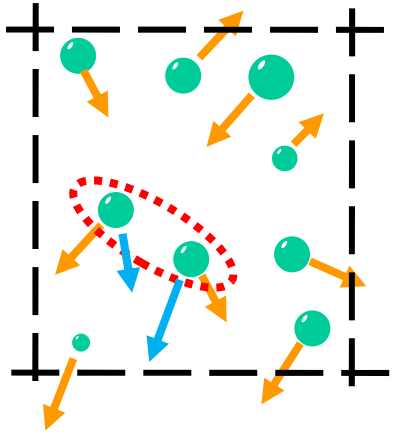
Early DSMC implementations used a different representation, rescaling the simulator diameter and mass to maintain the same physical mean free path and mass density.

Ballistic & Collisional Transport

By their ballistic motion particles carry mass, momentum and energy. In a dilute gas, this is the *only* source of transport.



In DSMC, momentum and energy are also transported by the collisions. The larger the collision cell, the more collisional transport (greater average separation between particle pairs).



Cell Size and Time Step

Can calculate collisional transport by Green-Kubo theory; error is quadratic in cell size and time step.

Collisional transport is incorrect so to minimize it the cell size in DSMC is limited to a fraction of a mean free path.

For similar reasons, the time step is limited to a fraction of a mean collision time.

Due to symmetry, the collisional transport does not affect the pressure. However, if we restrict collisions to only particles moving towards each other then this symmetry is broken and DSMC has a non-ideal gas equation of state.

Nearest Particle Collision Partner

New DSMC implementations minimize collisional transport error by choosing collision partner as closest particle in cell.

To avoid bias due to re-collisions, a particle pair is not allowed to collide twice (choose next-nearest particle).

Two common implementations are:

- Transient Adaptive Sub-cells (introduced by Bird)
- Virtual Sub-cells (introduced by LeBeau, et al)

M.A. Gallis, J.R. Torczynski, D.J. Rader, G.A. Bird, *J. Comp. Phys.*, **228** 4532-48 (2009)

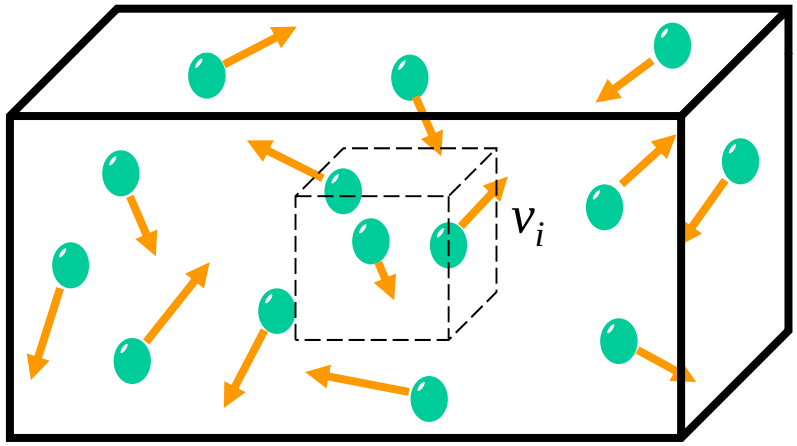
Fluctuations in DSMC

- Hydrodynamic fluctuations (density, temperature, etc.) have *nothing* to do with Monte Carlo aspect of DSMC.
- Variance of fluctuations in DSMC is exact at equilibrium (due to uniform distribution for position and Maxwell-Boltzmann for velocity).
- Time-correlations correct (at hydrodynamic scale)
- Non-equilibrium fluctuations correct (at hydrodynamic scale)

Sampling and Fluctuations

Measurements in DSMC are done by statistical sampling.

For volume measurements the particles are sorted into sampling cells and polled.



For surface measurements, particles crossing a surface during a time interval are counted.

Many sample measurements are required due to fluctuations.

Error Bars

Error bars may be estimated by equilibrium variances since non-equilibrium corrections are small.

In general, the standard deviation for sampled valued goes as $1/\sqrt{N}$ where N is the number of *simulators*.

If each simulator represents one molecule then the fluctuations are the same as in the physical system.

If $N_{ef} >> 1$ then the fluctuations are much greater than in the physical system, with correspondingly larger error bars.

Statistical Error (Fluid Velocity)

Fractional error in fluid velocity

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

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

For desired accuracy of $E_u = 1\%$ with $N = 100$ simulators/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, A. Garcia, M. Bazant, and G. He, *J. Comp. Phys.* **187** 274-297 (2003).

Statistical Error (Other Variables)

Fractional error in density, temperature, pressure

$$E_\rho = \frac{1}{\sqrt{SN}} \qquad E_T = \frac{C}{\sqrt{SN}} \qquad E_P = \frac{C'}{\sqrt{SN}} \qquad C, C' = O(1)$$

Fractional error in temperature *difference*

$$E_{\Delta T} \approx \frac{\mathrm{Br}}{\mathrm{Ma}^2} \frac{1}{\sqrt{SN}}$$

where Brinkman number; $\mathrm{Br} \approx 1$, if ΔT due to viscous heating

For given $E_{\Delta T}$, number of samples $S \propto 1/\mathrm{Ma}^4$

Statistical Error (Fluxes)

Fractional error in stress and heat flux

$$E_\tau \approx \frac{1}{\mathrm{Kn}\,\mathrm{Ma}} \frac{1}{\sqrt{SN}} \qquad E_q \approx \frac{\mathrm{Br}}{\mathrm{Kn}\,\mathrm{Ma}^2} \frac{1}{\sqrt{SN}}$$

Comparing state versus flux variables

$$E_\tau \approx \frac{E_u}{\mathrm{Kn}} \qquad E_q \approx \frac{E_{\Delta T}}{\mathrm{Kn}}$$

Typically Kn < 0.1 so error bars for fluxes significantly greater; measurements such as drag force are difficult for low Mach number flows.

Variance Reduction in DSMC

Variance reduction in DSMC has been difficult to achieve, in part because DSMC is already an importance sampling algorithm for the Boltzmann equation.

Attempts to mollify the fluctuations in DSMC, while preserving accuracy at kinetic scales, have been mostly unsuccessful.

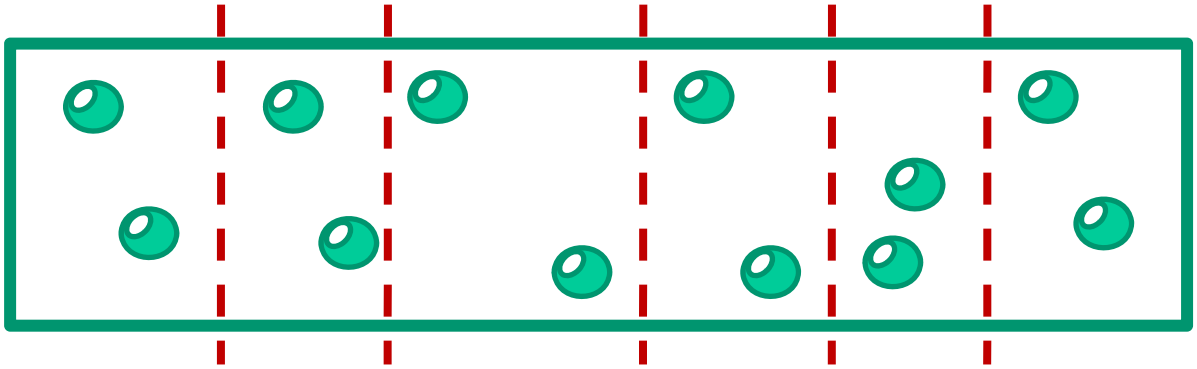
A promising approach is Hadjiconstantinou's low-variance algorithm, which is loosely based on DSMC.

Fluctuations and Statistical Bias

Given the presence of fluctuations in DSMC, we need to be careful to avoid all sources of statistical bias.

Suppose we dynamically vary the cell sizes so that each cell has the same number of particles.

This is helpful in that DSMC is not accurate when N is too small.



Yet there could be unintended consequences when we replace fluctuations in N with fluctuations in V.

DSMC Collision Rate

The average number of collisions in a cell is

$$\langle M \rangle = \langle M_{TRY} P_{ACCEPT} \rangle$$

$$= \left\langle \frac{N(N-1)\sigma [v_r]_{MAX} \tau}{2V} \times \frac{v_r}{[v_r]_{MAX}} \right\rangle$$

Use this

Want this

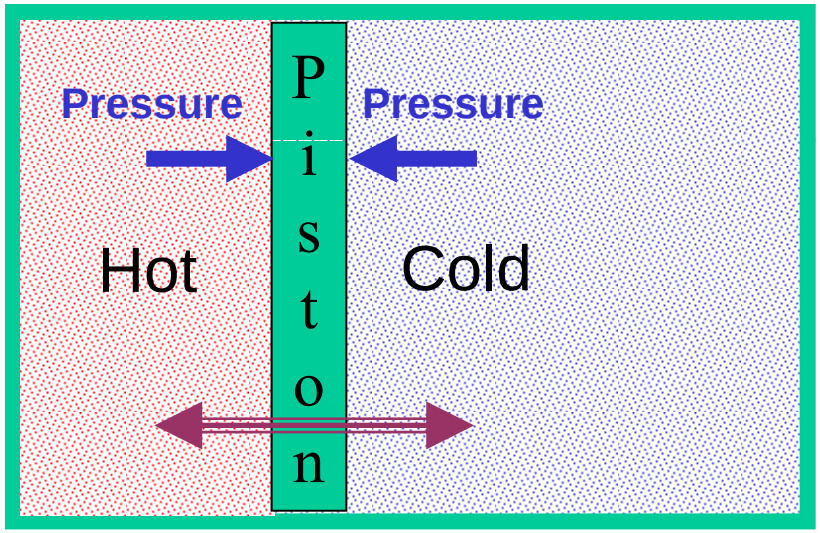
$$= \left\langle \frac{N(N-1)\sigma v_r \tau}{2V} \right\rangle \stackrel{?}{=} \frac{\langle N \rangle^2 \sigma \langle v_r \rangle \langle \tau \rangle}{2\langle V \rangle}$$

In general $\langle 1/V \rangle \neq 1/\langle V \rangle$
so equality does not hold.

For Poisson
$\langle N(N-1) \rangle = \langle N \rangle^2$

Brownian Systems

Fluctuations in DSMC are not always a nuisance; there are interesting phenomena that rely on fluctuations.



"Adiabatic" Piston Problem

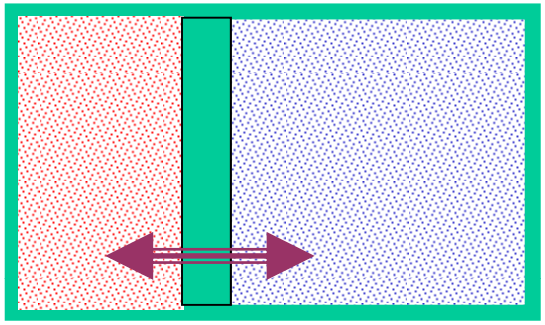
Chambers have gases at different temperatures, equal pressures. Walls are perfectly elastic yet gases come to common temperature.

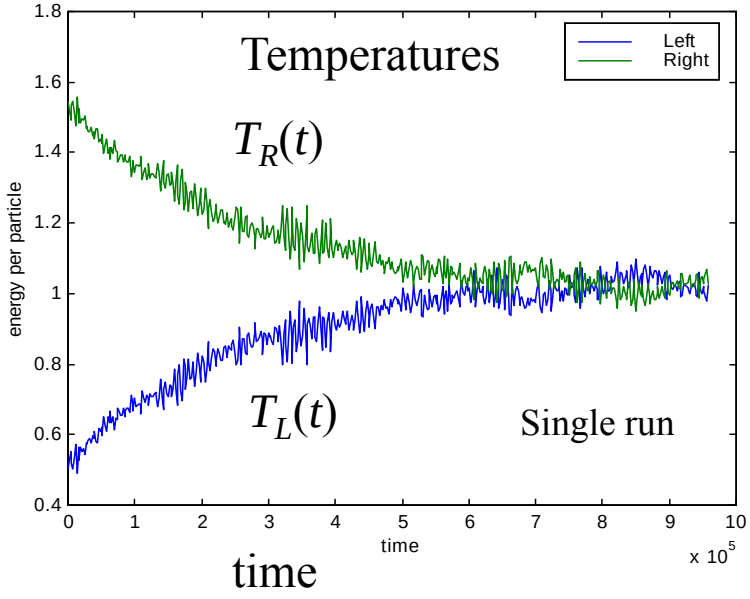
How? Heat is conducted between the chambers by the non-equilibrium Brownian motion of the piston.

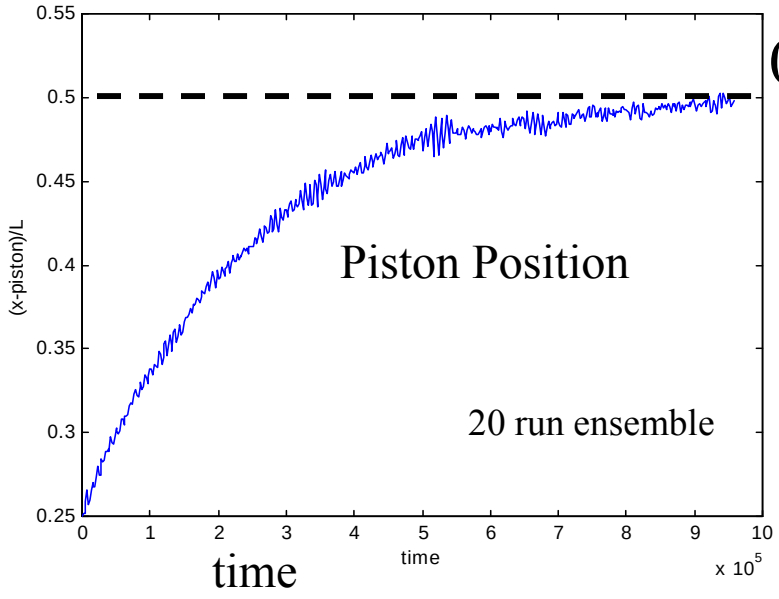
Adiabatic Piston by DSMC

Initial State: $X = L/4$, $M = 64\ m$

$N_L = N_R = 320$, $T_R = 3\ T_L$







Feynman's Ratchet & Pawl

Carnot* engine driven by fluctuations

Brownian motors and nanoscale machines

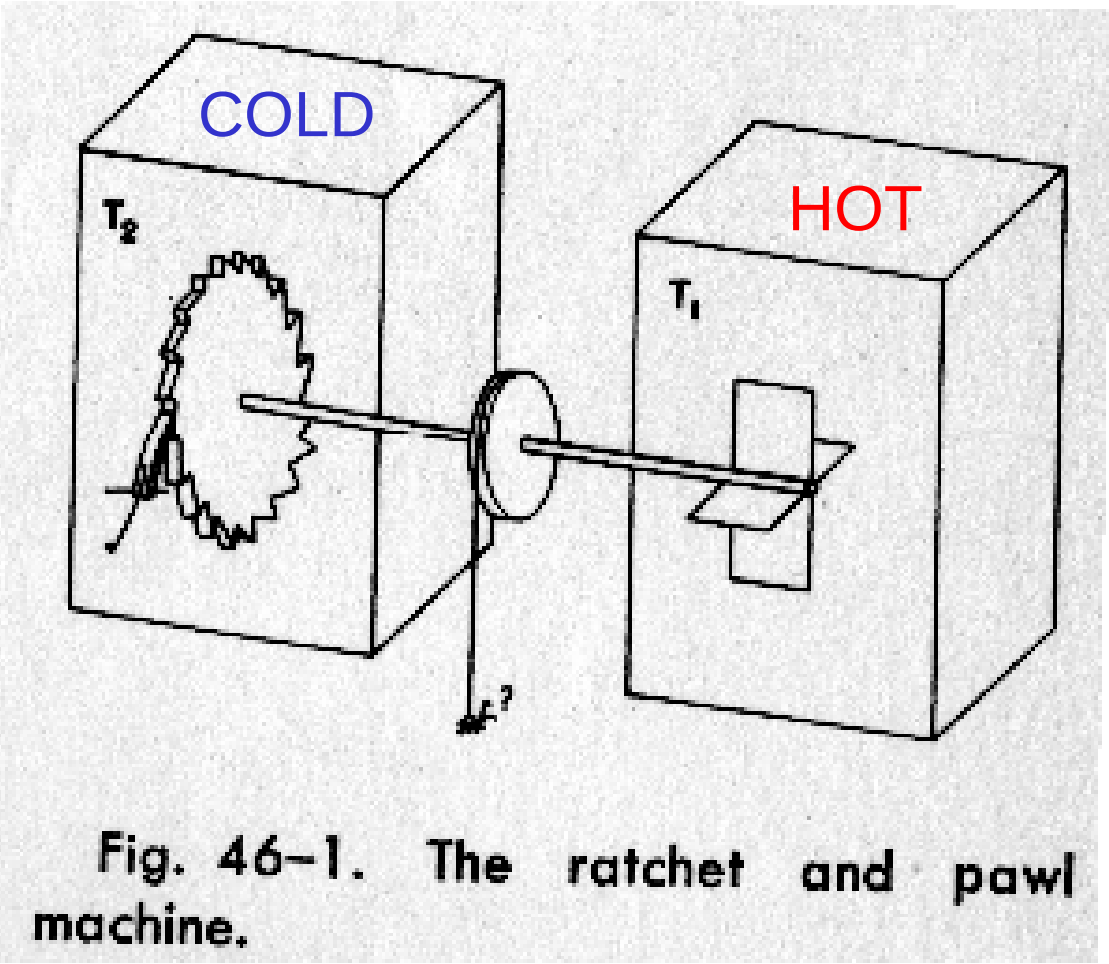
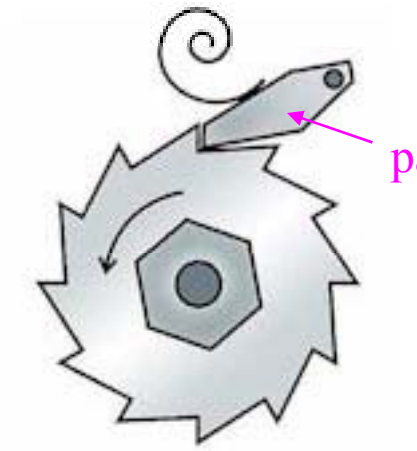


Fig. 46–1. The ratchet and pawl machine.

* almost

Violate 2nd Law of Thermo?

NO. Fluctuations also lift the pawl, dropping the weight back down.



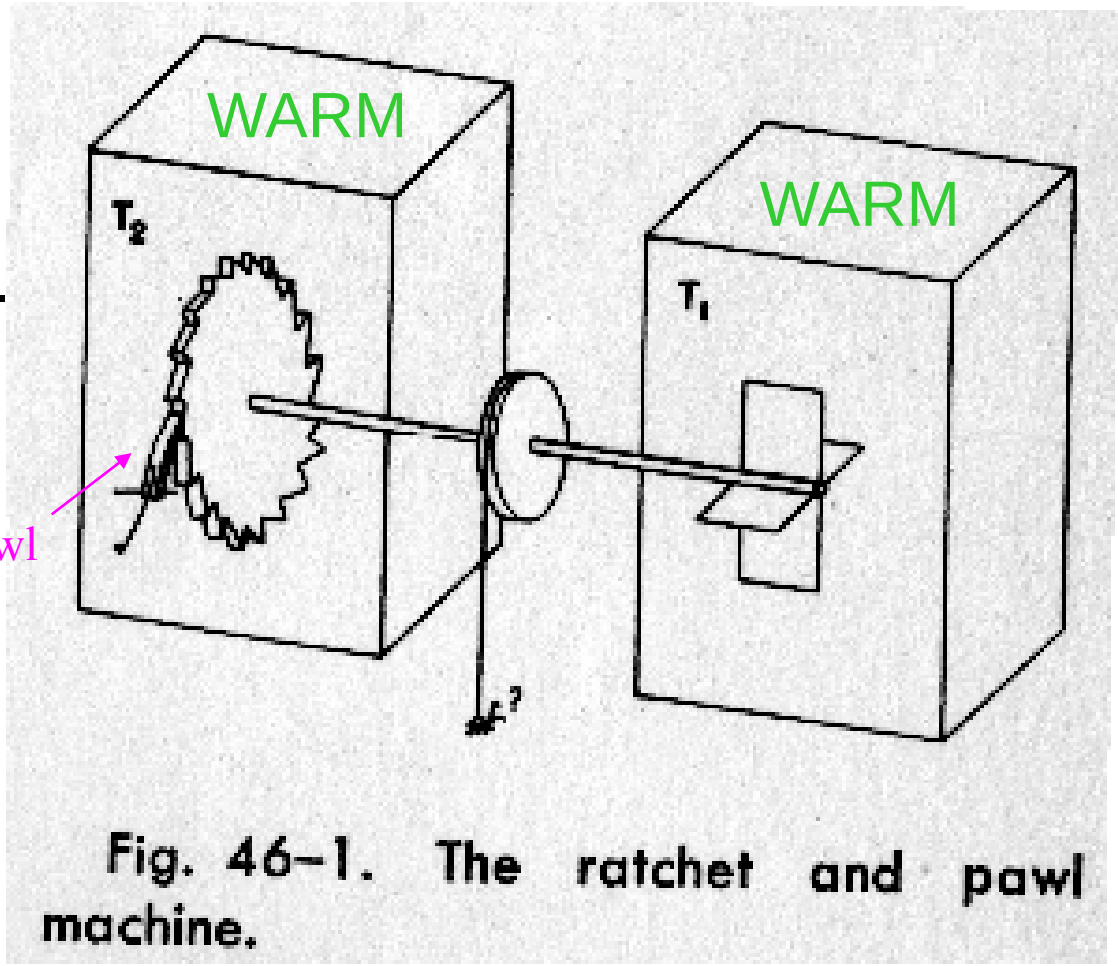
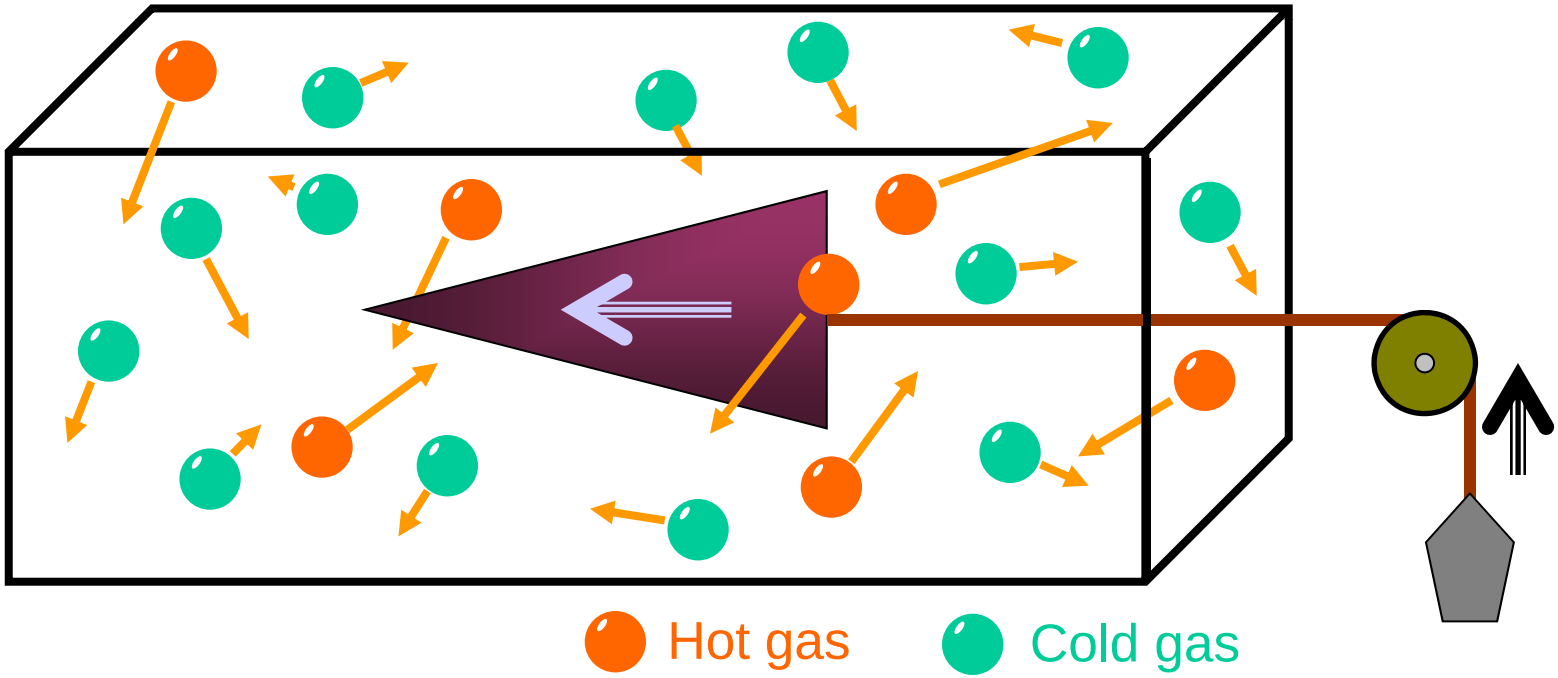


Fig. 46–1. The ratchet and pawl machine.

Triangula Brownian Motor

Feynman's complicated mechanical geometry not needed.

An asymmetrically shaped Brownian object in a non-equilibrium system (e.g., dual-temperature distribution) is enough.



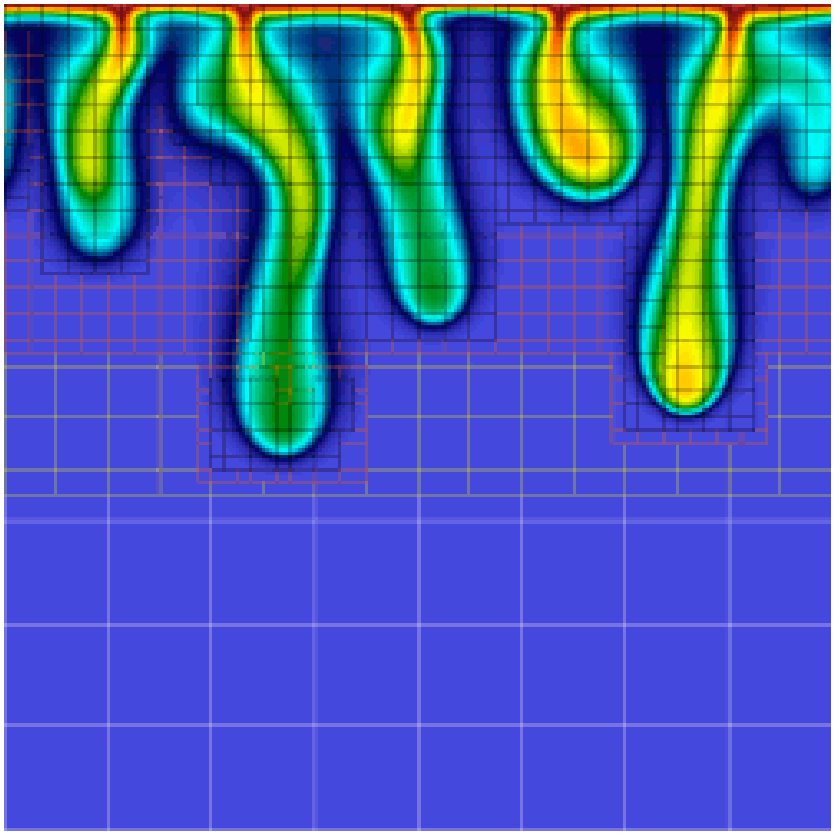
P. Meurs, C. Van den Broeck, and A. Garcia, *Physical Review E* **70** 051109 (2004).

Algorithm Refinement

Algorithm Refinement is a multi-algorithm hybrid methodology based on Adaptive Mesh Refinement.

At the finest level or resolution, instead of refining the mesh you “refine” the algorithm (change to a model with more physics).

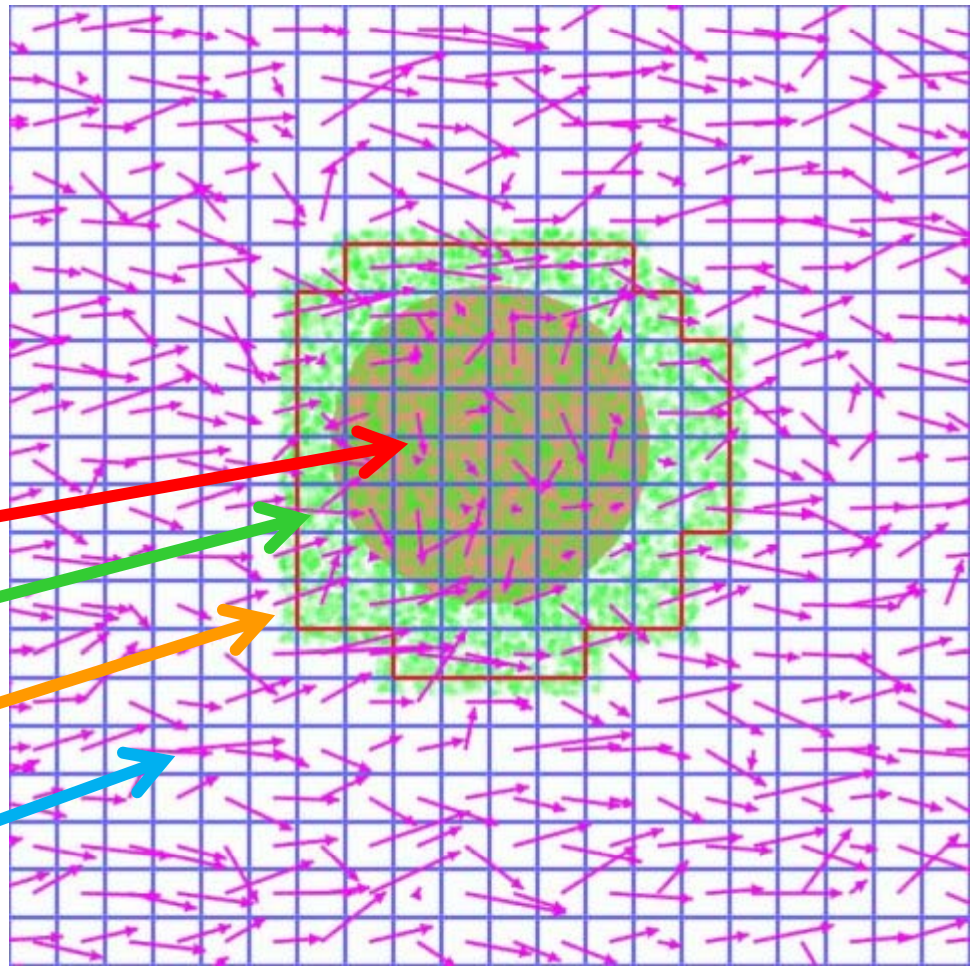
This refinement may be adaptive.



Particle/PDE AR Hybrid

http://cims.nyu.edu/~donev/FluctHydro/Hybrid.2D.sphere.plug.inst.mov

Particle/PDE Algorithm Refinement for flow past a sphere.



Stationary particle

Molecular simulation of solvent fluid

Interface

Continuum simulation of solvent fluid

Note: Continuum calculation done everywhere

Advances in Algorithms Refinement

Stochastic Particle Algorithms – Our original AR method was limited to dilute gases using the Direct Simulation Monte Carlo scheme. Have developed more advanced stochastic particle schemes for non-ideal fluids.

Stochastic Continuum Algorithms – Our original AR method used a deterministic, explicit scheme for the full Navier-Stokes equations. Have developed stochastic PDE schemes to capture hydrodynamic fluctuations.

Coupling Issues – Perfecting the coupling of particle and PDE schemes is challenging due to fluctuations.

Stochastic Navier-Stokes PDEs

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

$$\mathbf{F} = \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v}\mathbf{v} + P\mathbf{I} \\ (E+P)\mathbf{v} \end{pmatrix}$$

Parabolic Fluxes

$$\mathbf{D} = \begin{pmatrix} 0 \\ \tau \\ \kappa \nabla T + \tau \cdot \mathbf{v} \end{pmatrix}$$

Stochastic Fluxes

$$\mathbf{S} = \begin{pmatrix} 0 \\ \mathcal{S} \\ \mathcal{Q} + \mathbf{v} \cdot \mathcal{S} \end{pmatrix},$$

$$\langle \mathcal{S}_{ij}(\mathbf{r},t)\mathcal{S}_{k\ell}(\mathbf{r}',t') \rangle = 2k_B\eta T \left(\delta^K_{ik}\delta^K_{j\ell} + \delta^K_{i\ell}\delta^K_{jk} - \tfrac{2}{3}\delta^K_{ij}\delta^K_{k\ell} \right) \delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

$$\langle \mathcal{Q}_i(\mathbf{r},t)\mathcal{Q}_j(\mathbf{r}',t') \rangle = 2k_B\kappa T^2 \delta^K_{ij}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

Fluctuating Hydrodynamic Solvers

We now have simple, accurate, and efficient finite volume schemes for solving the stochastic Navier-Stokes PDEs of fluctuating hydrodynamics.

$$
\begin{aligned}
\boldsymbol{U}_j^{n+\frac{1}{3}} &= \boldsymbol{U}_j^n + \Delta \boldsymbol{U}_j(\boldsymbol{U}^n, \boldsymbol{W}_1) \text{ (estimate at } t = (n+1)\Delta t \text{)} \\
\boldsymbol{U}_j^{n+\frac{2}{3}} &= \frac{3}{4}\boldsymbol{U}_j^n + \frac{1}{4}\left[\boldsymbol{U}_j^{n+\frac{1}{3}} + \Delta \boldsymbol{U}_j(\boldsymbol{U}_j^{n+\frac{1}{3}}, \boldsymbol{W}_2)\right] \text{ (estimate at } t = (n+\frac{1}{2})\Delta t \text{)} \\
\boldsymbol{U}_j^{n+1} &= \frac{1}{3}\boldsymbol{U}_j^n + \frac{2}{3}\left[\boldsymbol{U}_j^{n+\frac{2}{3}} + \Delta \boldsymbol{U}_j(\boldsymbol{U}^{n+\frac{2}{3}}, \boldsymbol{W}_3)\right],
\end{aligned}
$$

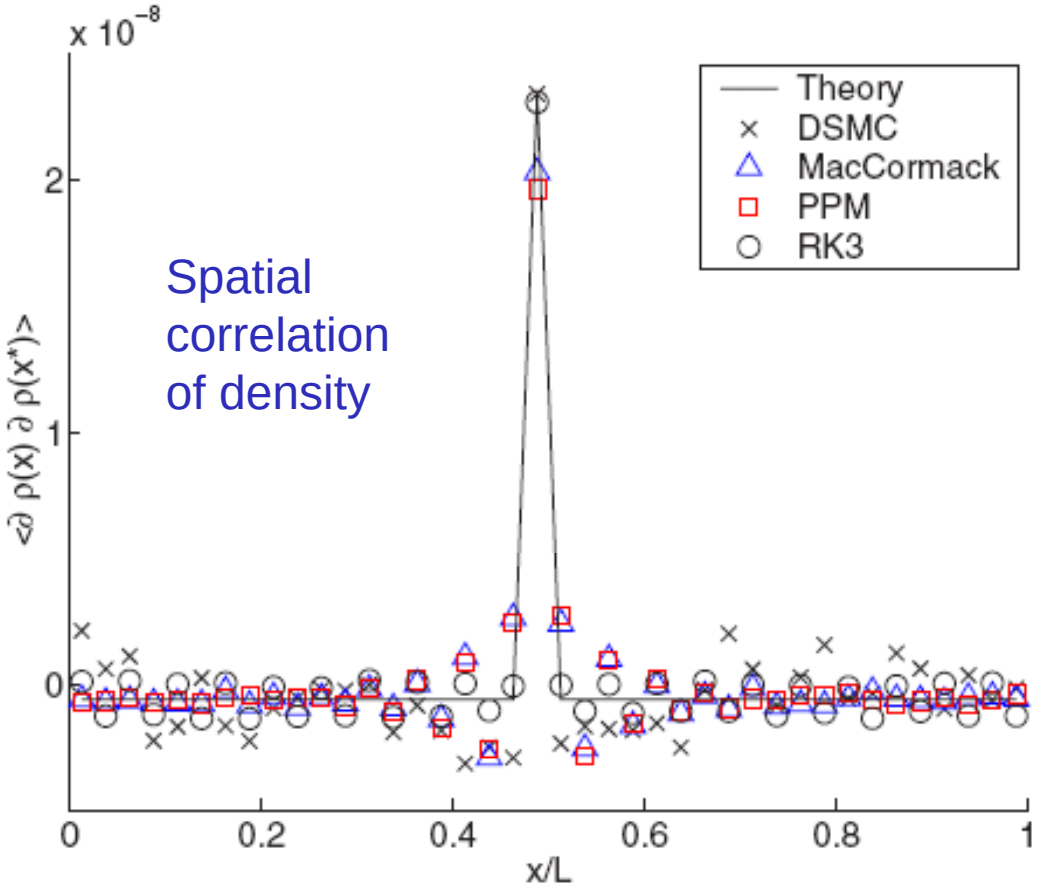
where

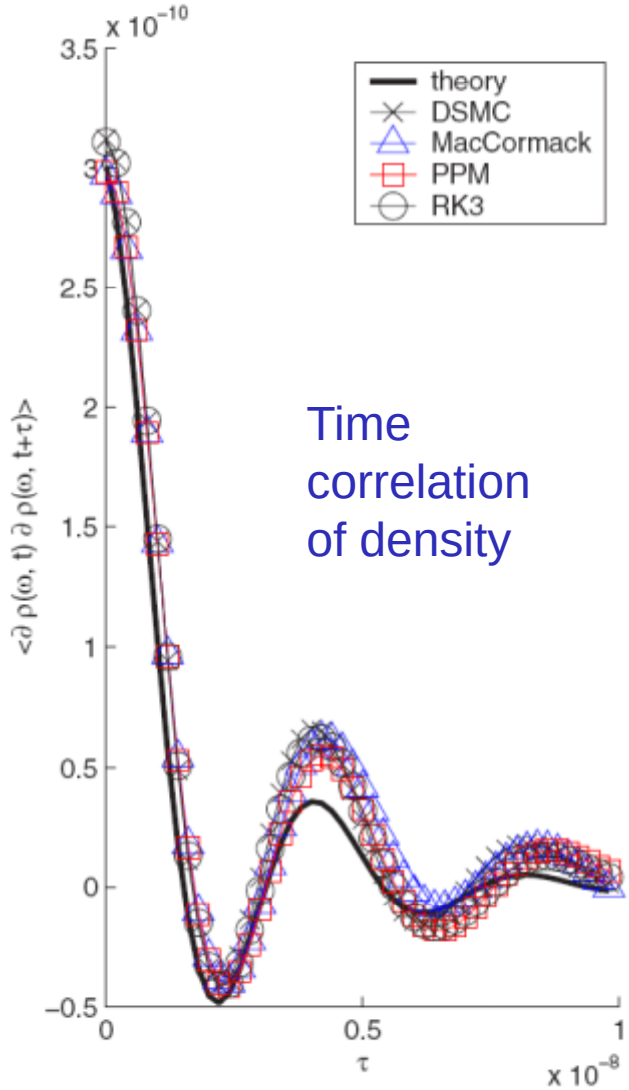
$$
\Delta \boldsymbol{U}_j(\boldsymbol{U}, \boldsymbol{W}) = -\frac{\Delta t}{\Delta x}\left[\boldsymbol{F}_{j+\frac{1}{2}}(\boldsymbol{U}) - \boldsymbol{F}_{j-\frac{1}{2}}(\boldsymbol{U})\right] + \frac{\Delta t^{1/2}}{\Delta x^{3/2}}\left(\boldsymbol{Z}_{j+\frac{1}{2}} - \boldsymbol{Z}_{j-\frac{1}{2}}\right).
$$

J.B. Bell, ALG, and S. Williams, Physical Review E 76 016708 (2007)
A. Donev, E. Vanden-Eijnden, ALG, and J. B. Bell, CAMCOS, 5(2):149-197, (2010)

Comparison with DSMC

DSMC used in testing the numerical schemes for stochastic Navier-Stokes



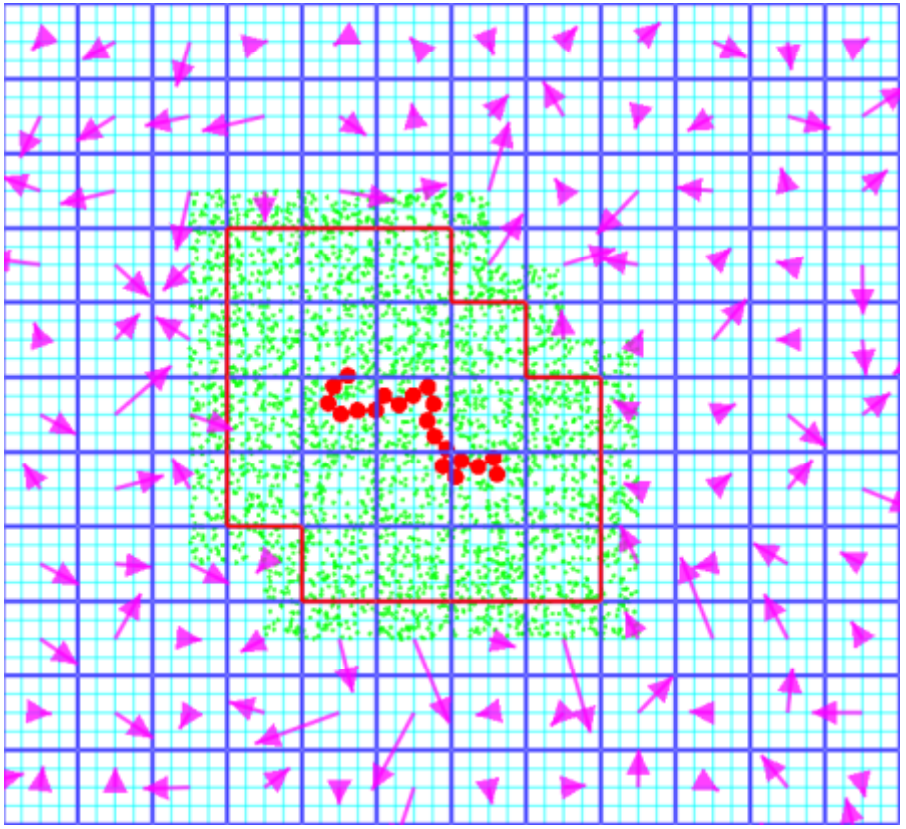


Stochastic vs. Deterministic PDEs?

Question:

Is it necessary to use stochastic PDEs in the continuum region given that the particle region has fluctuations?

Answer: YES!

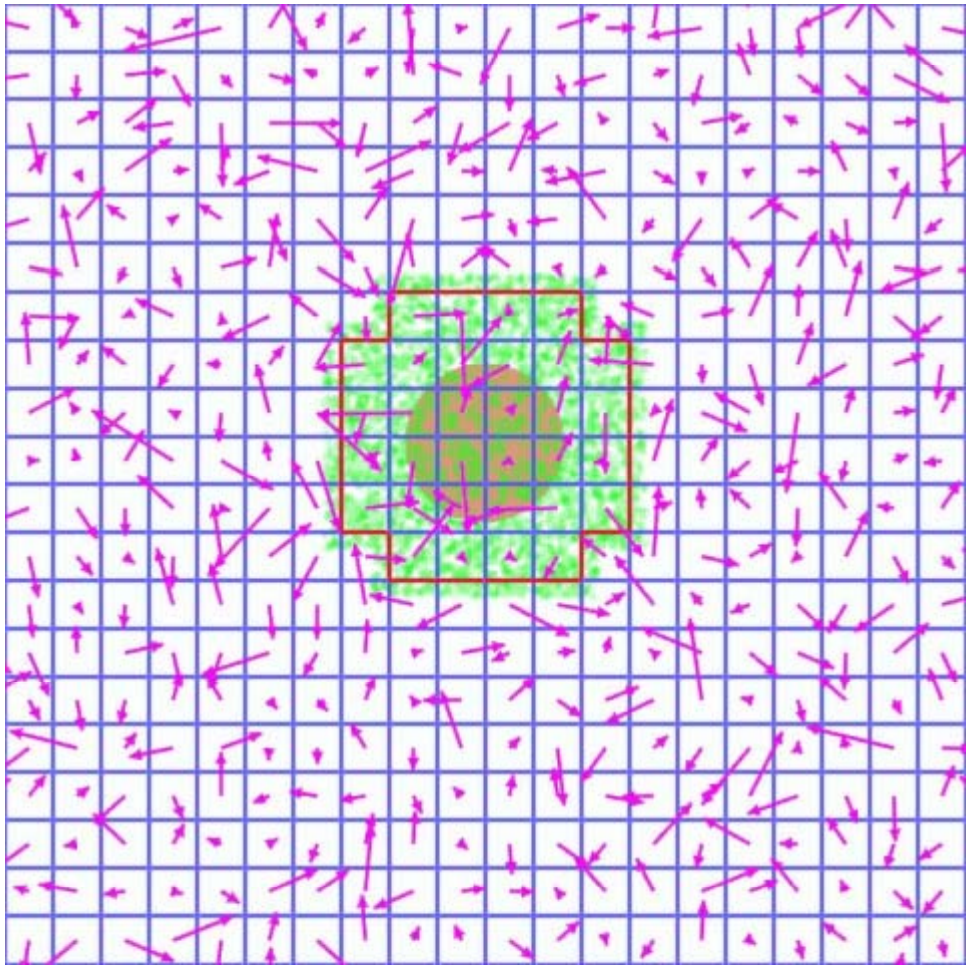


Simple Brownian Motion

First test is the calculation of the Brownian motion of a spherical particle.

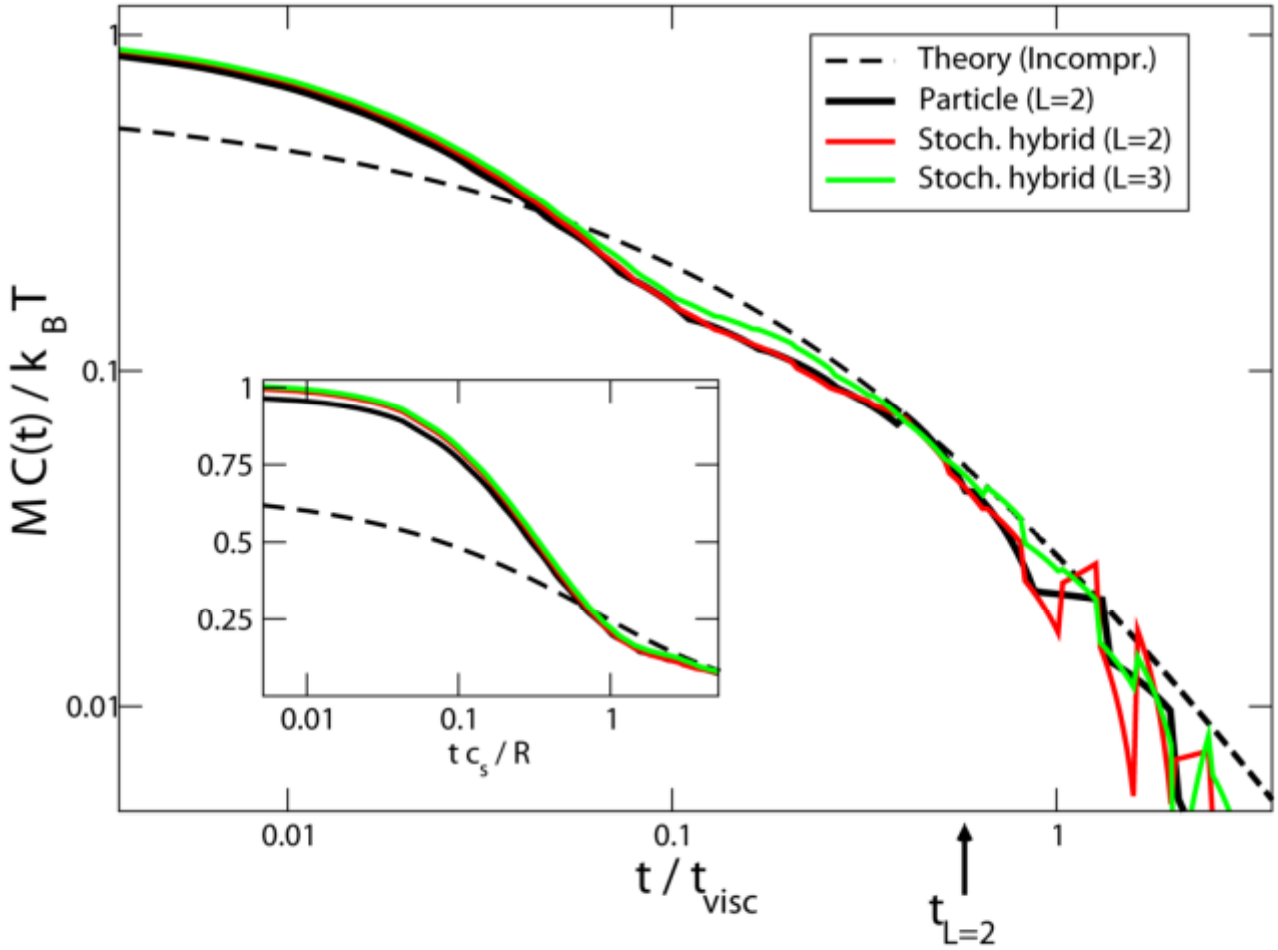
Measure velocity auto-correlation function.

http://cims.nyu.edu/~donev/FluctHydro/Hybrid.2D.sphere.diffusion.mov



AR with Stochastic PDEs

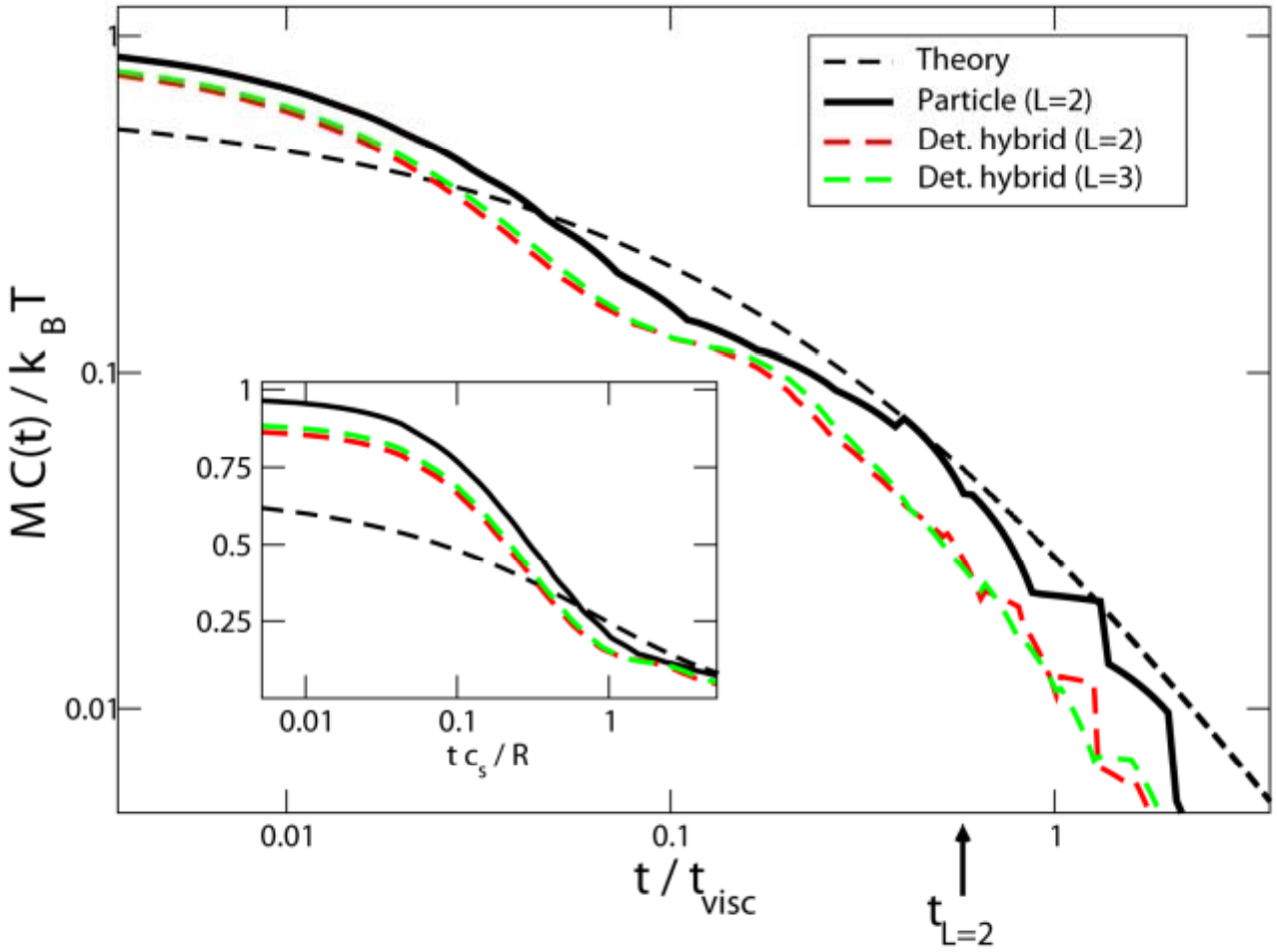
Excellent agreement between a hybrid using stochastic PDE solver and an (expensive) pure particle calculation.



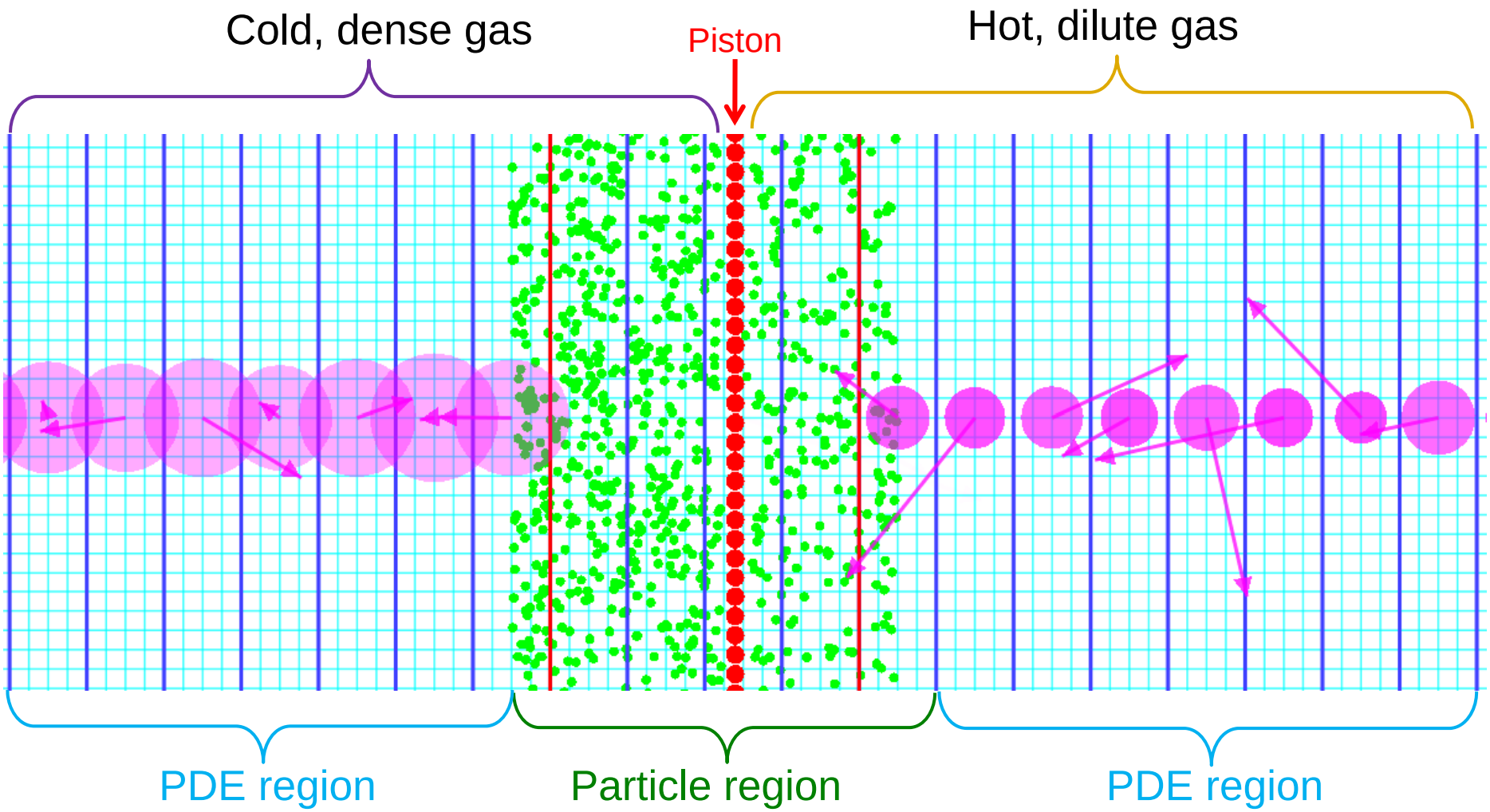
A. Donev, J.B. Bell, ALG, and B. Alder, *SIAM Multiscale Mod. Sim.* **8** 871-911 (2010).

AR with Deterministic PDEs

A hybrid using a deterministic PDE solver significantly under-predicts the velocity auto-correlation function.

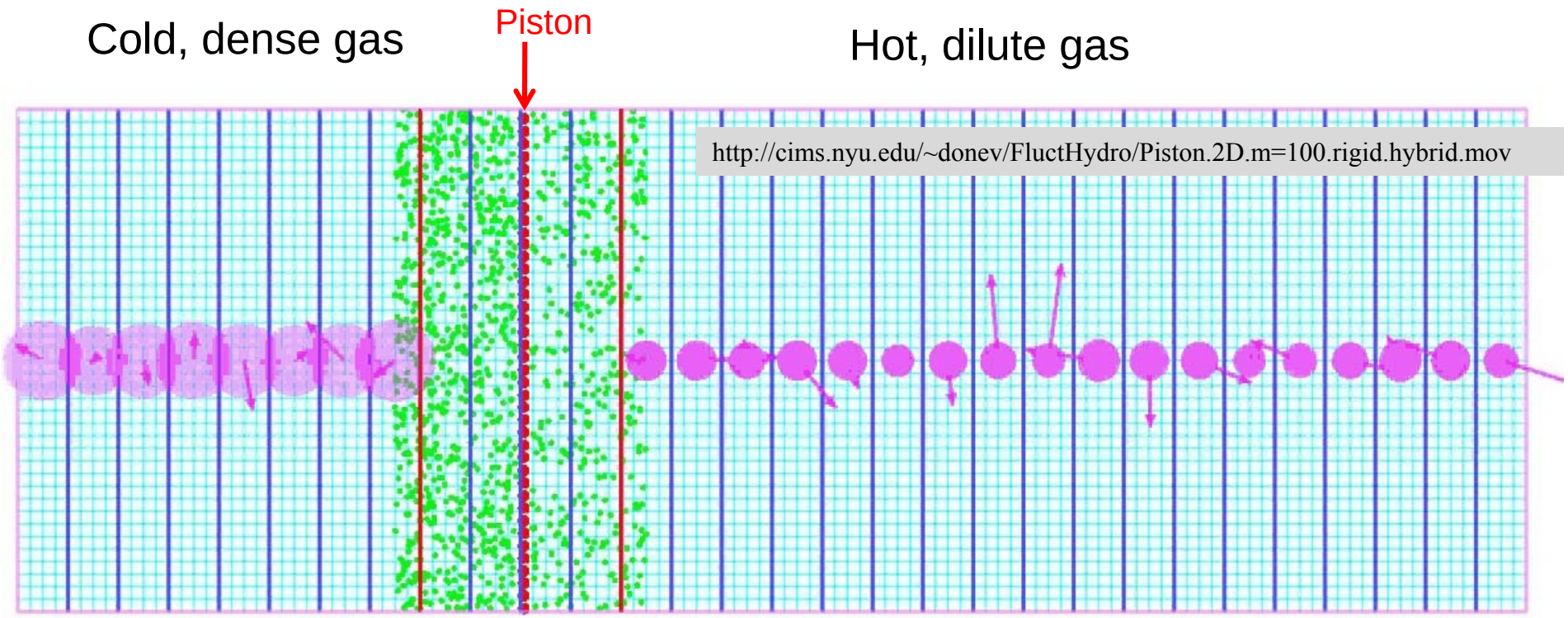


Adiabatic Piston



Initially the gas pressure is equal on both sides of the piston.

Sample Run of Adiabatic Piston

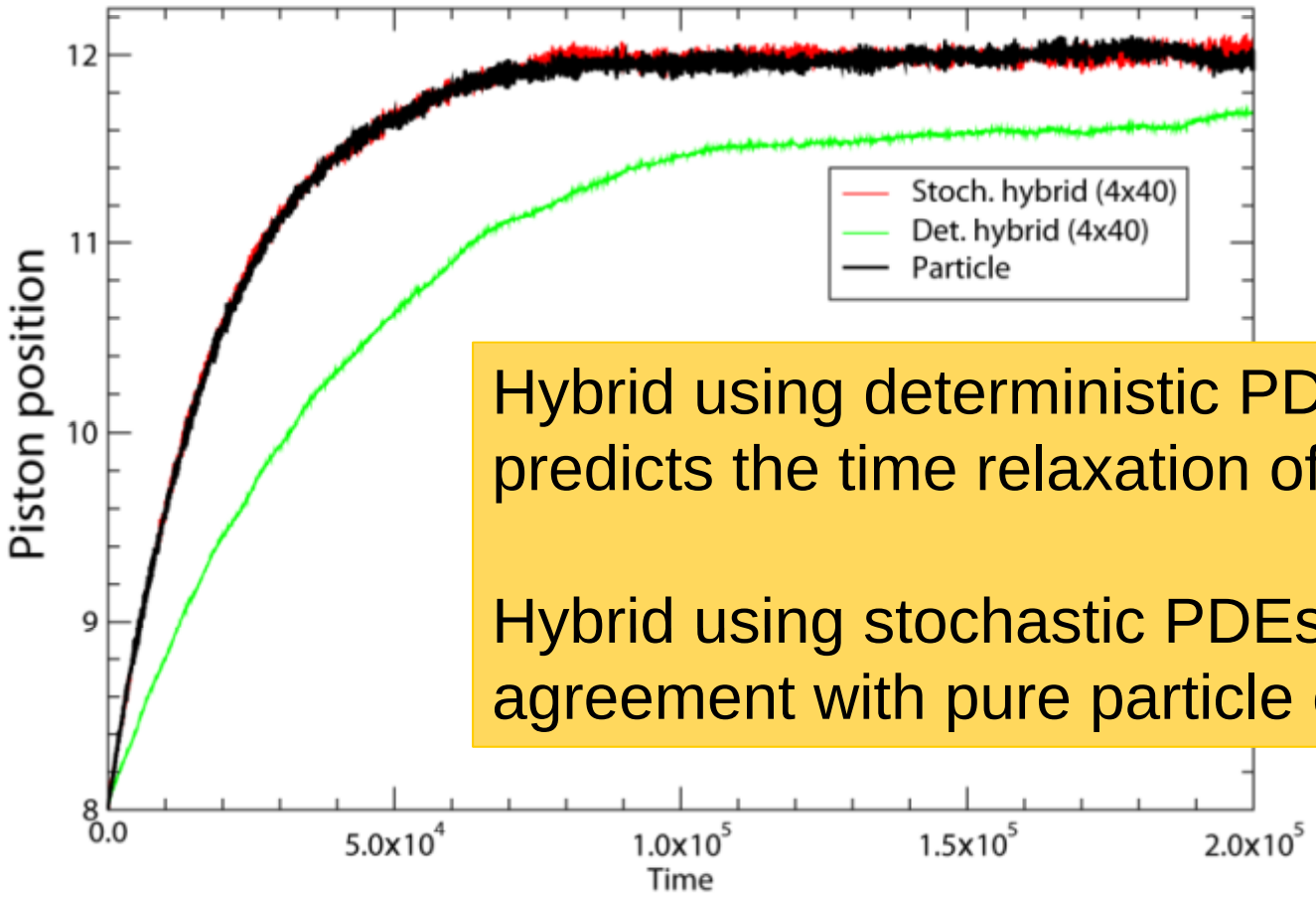


$\rho = {}^{4}/_{3}\ \rho_{eq}$
$T = {}^{3}/_{4}\ T_{eq}$

$\rho = {}^{3}/_{4}\ \rho_{eq}$
$T = {}^{4}/_{3}\ T_{eq}$

Note: Adiabatic Piston is a simple Brownian heat engine

Time Relaxation of the Piston

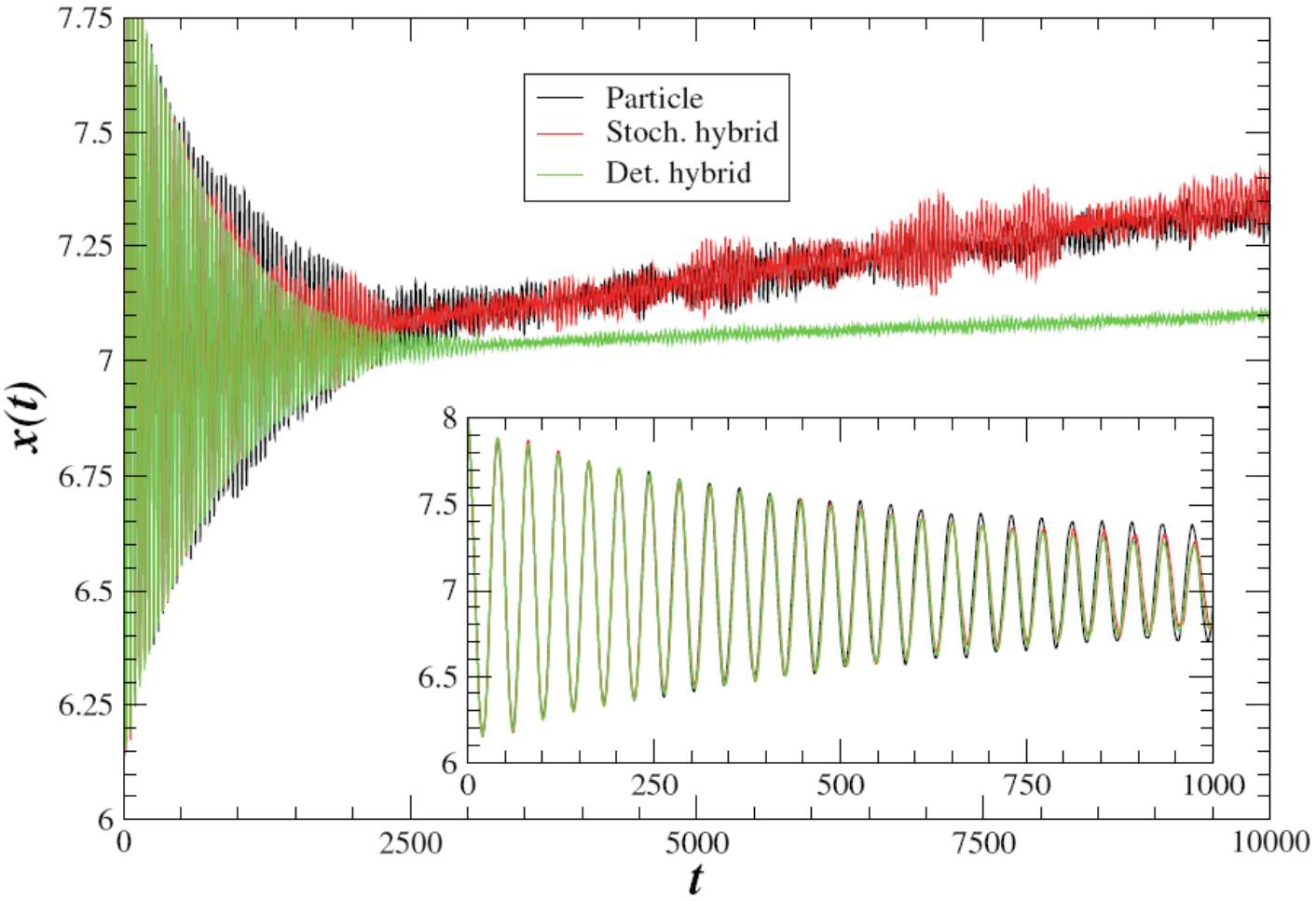


Hybrid using deterministic PDEs under-predicts the time relaxation of the piston.

Hybrid using stochastic PDEs in excellent agreement with pure particle calculations.

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

Relaxation from Mechanical Non-Equilibrium



DSMC Variants for Dense Gases

DSMC variants have been developed for dense gases of hard spheres,

* Consistent Boltzmann Algorithm (CBA)
* Enskog-DSMC

and for general potentials,

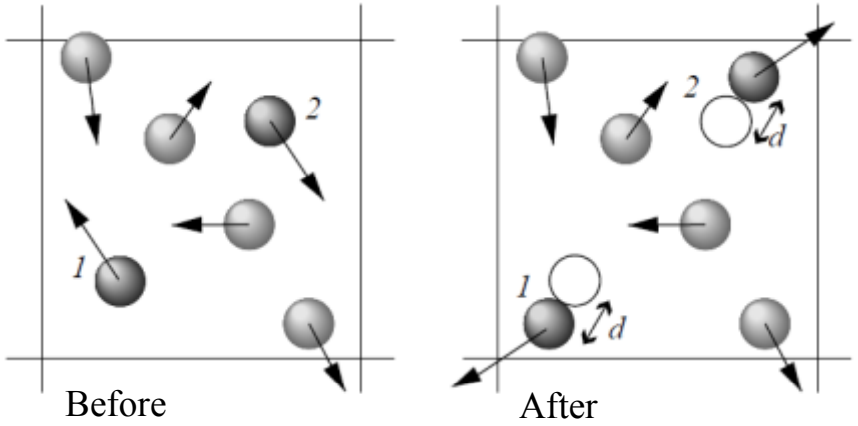
* Consistent Universal Boltzmann Algorithm (CUBA)

Basic idea is to modify the collision process so that the collisional transport produces the desired non-ideal equation of state.

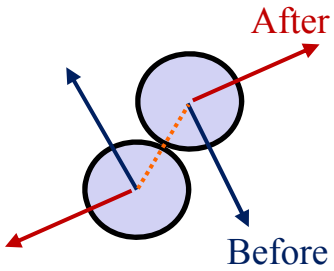
Consistent Boltzmann Algorithm (CBA)

In CBA, a particle's position as well as its velocity changes upon collision.

The displacement of position has magnitude equal to the diameter.



Direction is along the apse line (line between their centers) for a hard sphere collision with the same change in the relative velocity.



Very easy to implement in DSMC (really!).

F. Alexander, A. Garcia and B. Alder, *Physical Review Letters* **74** 5212 (1995)

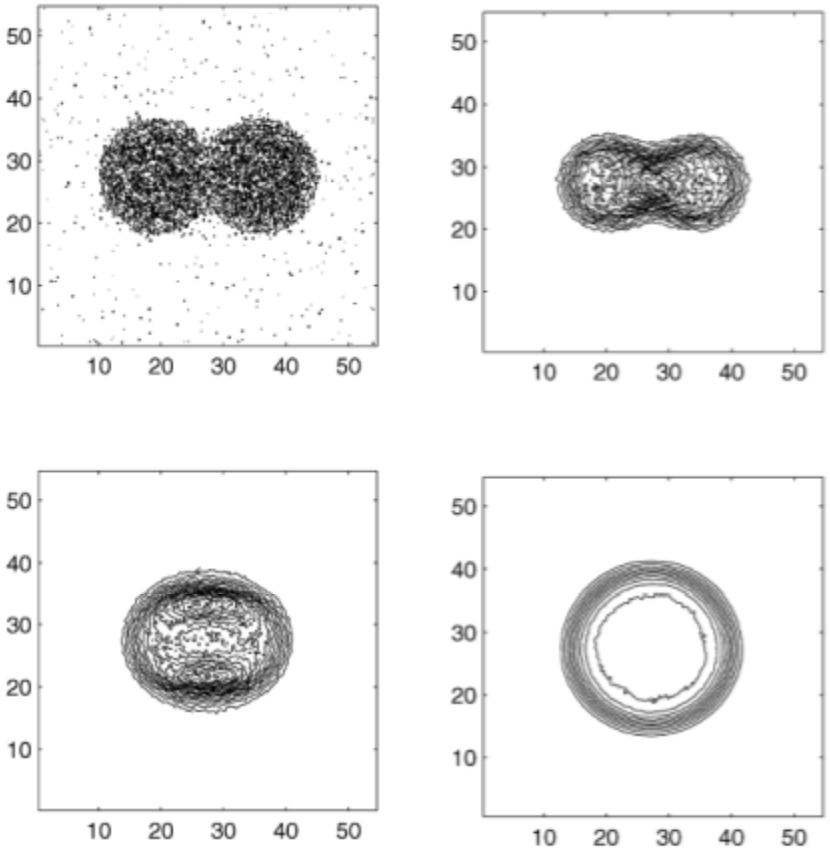
Consistent Universal Boltzmann Algorithm (CUBA)

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

Using van der Waals EOS we can even form condensation into a liquid with DSMC.

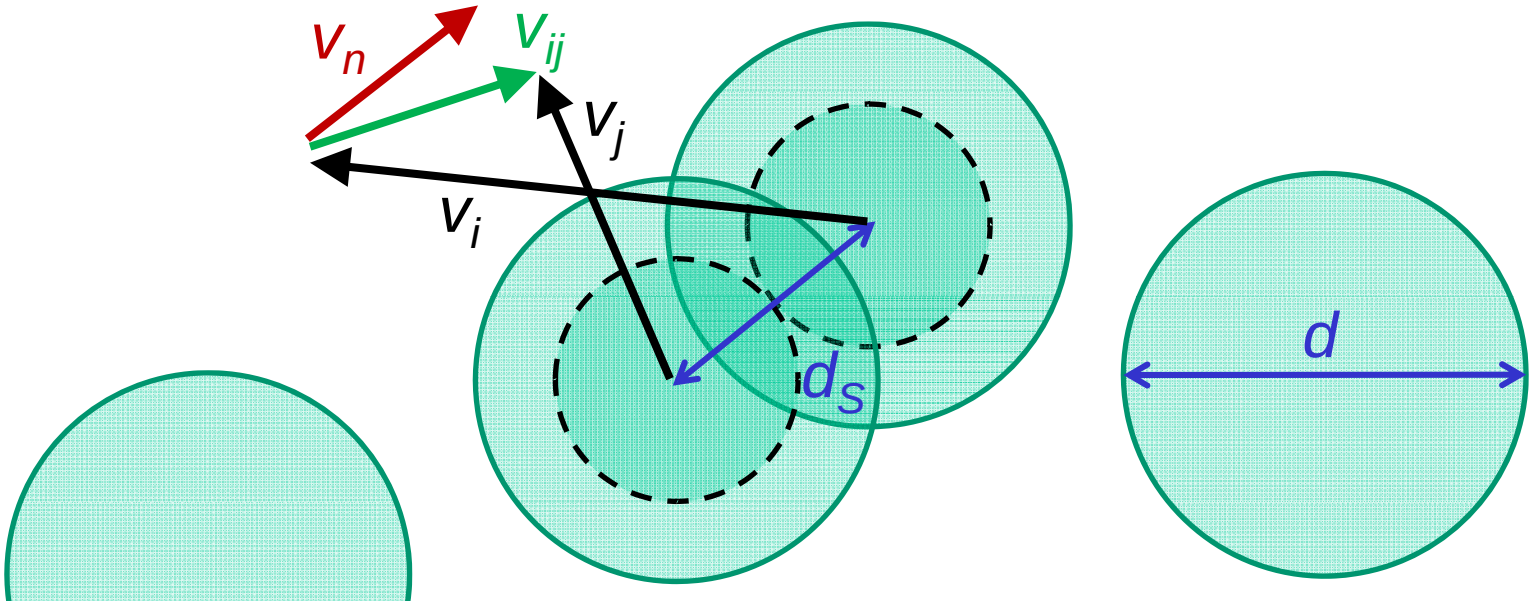
Not computationally efficient versus Molecular Dynamics.

Vapor condensation into droplet
Density contours at t =2,100,300,5000



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

Stochastic Hard-Sphere Dynamics

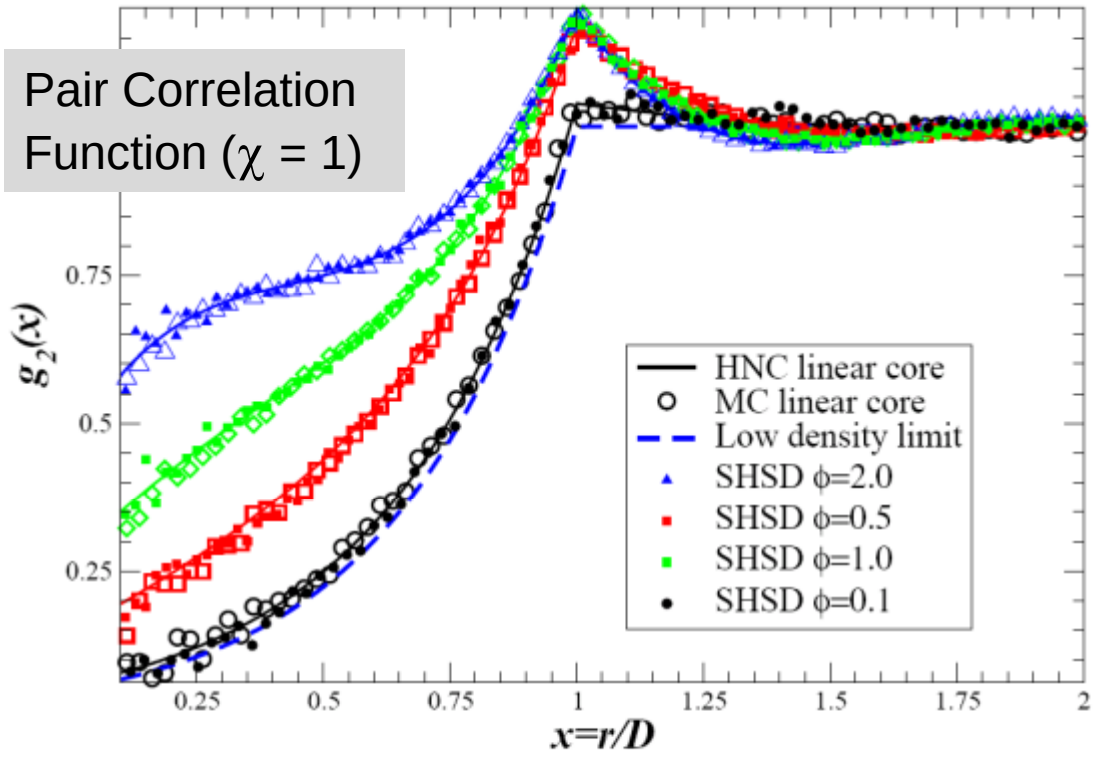


When two particles, i and j, are less than a diameter apart ($|\boldsymbol{r}_{ij}| < d$) there is a probability rate ($3\chi/d$) v_n for them to collide, where $v_n = -\boldsymbol{v}_{ij} \cdot \boldsymbol{r}_{ij}/|\boldsymbol{r}_{ij}|$; particles only collide if they are approaching (i.e., if $v_n > 0$). Accepted collisions are evaluated *deterministically* as if the particles had a hard-sphere diameter of $d_s = |\boldsymbol{r}_{ij}|$.

A. Donev, B.J. Alder, and ALG, *Physical Review Letters* **101**, 075902 (2008).

Properties of SHSD

Stochastic Hard Sphere Dynamics (SHSD) is equivalent to a fluid with a linear core pair potential.



Fluctuations of density are consistent with the equation of state (i.e., compressibility)

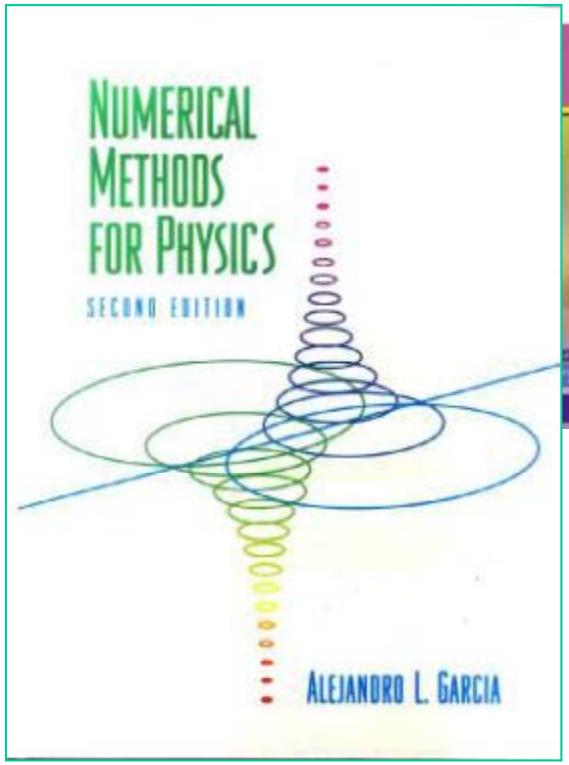
A. Donev, B.J. Alder, and ALG, *J. Statistical Mechanics* P11008 (2009).

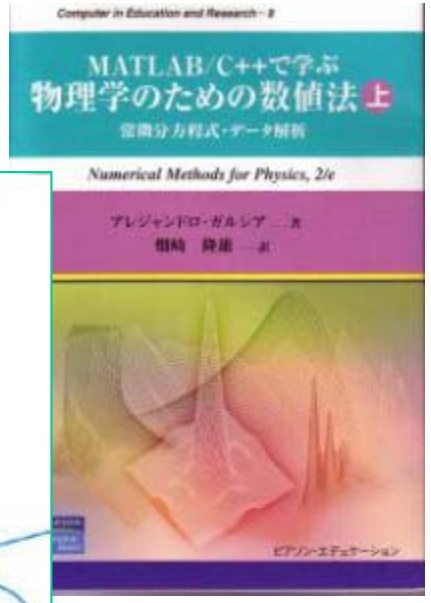
References and Spam

Reprints, pre-prints and slides available:

www.algarcia.org

DSMC tutorial & programs in my textbook.





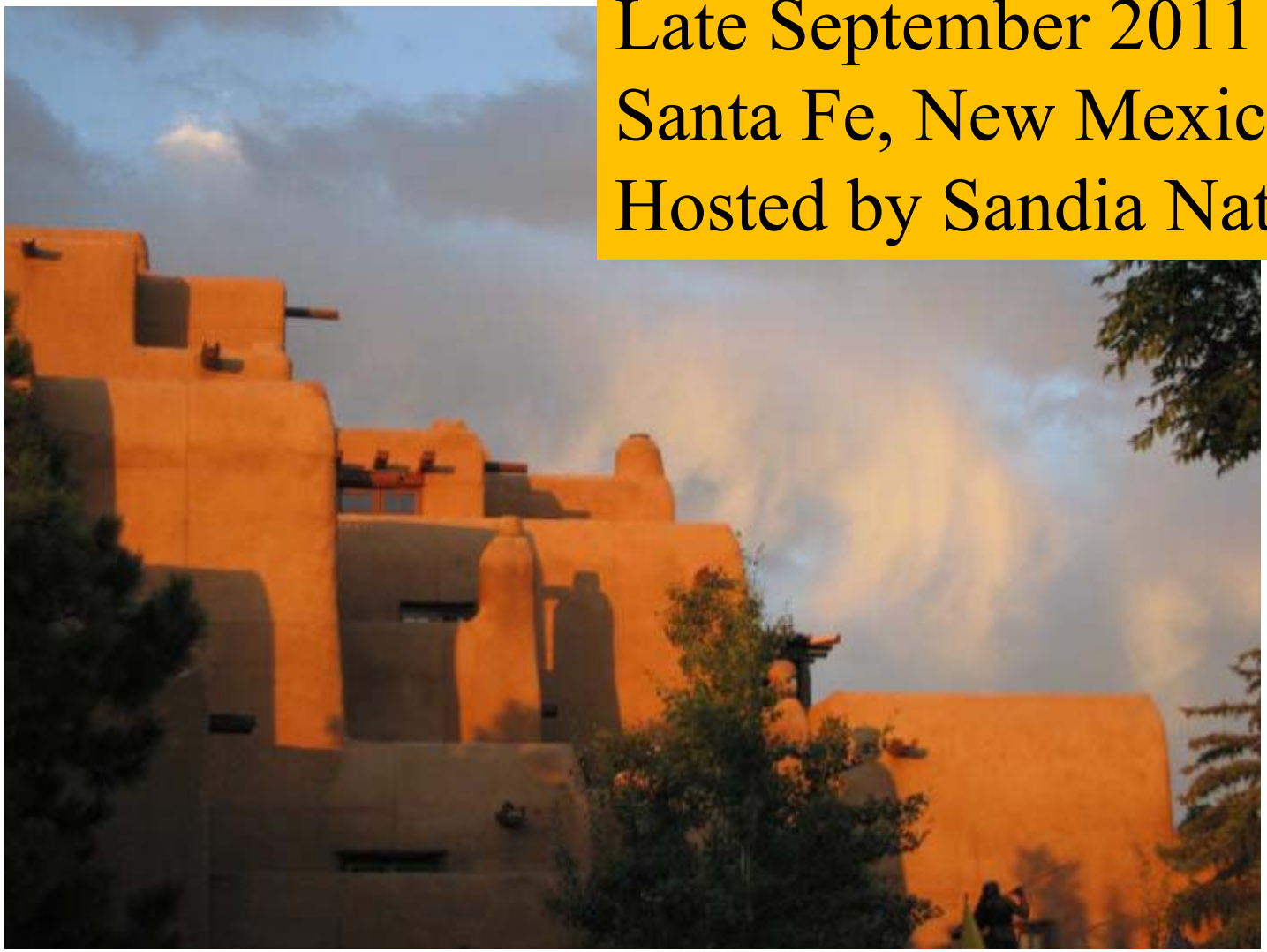
Japanese

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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