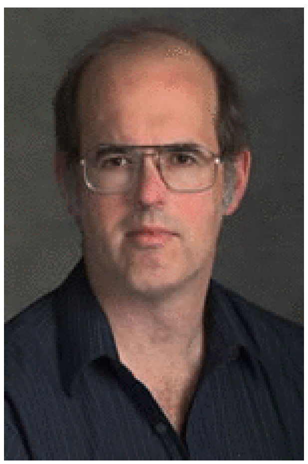
Hydrodynamic Fluctuations and Algorithm Refinement



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Novel Simulation Approaches to Soft Matter Systems
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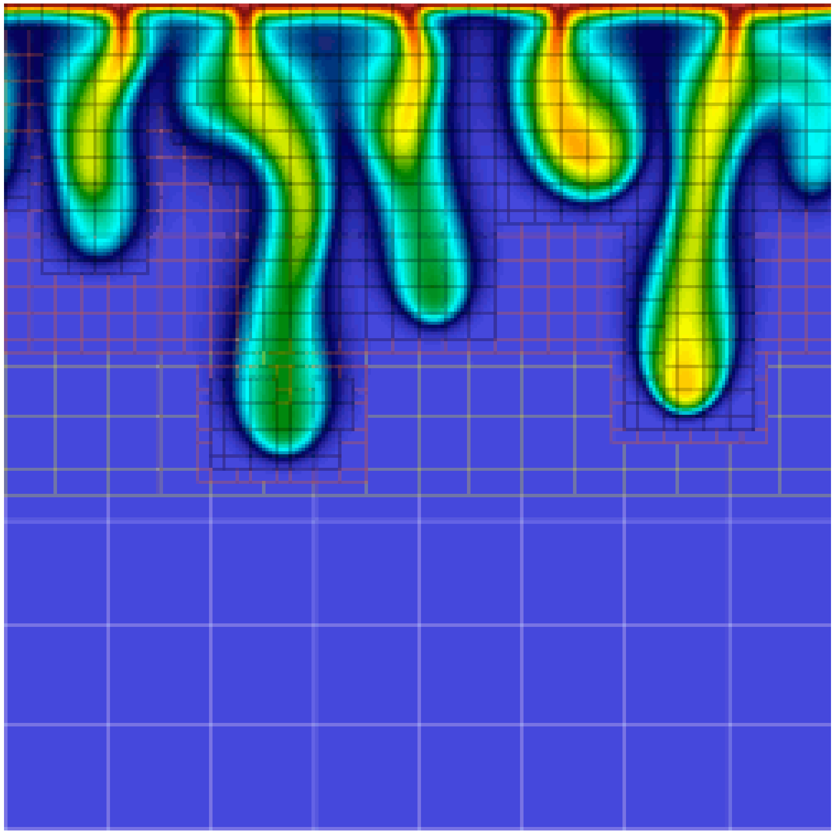
Algorithm Refinement

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.

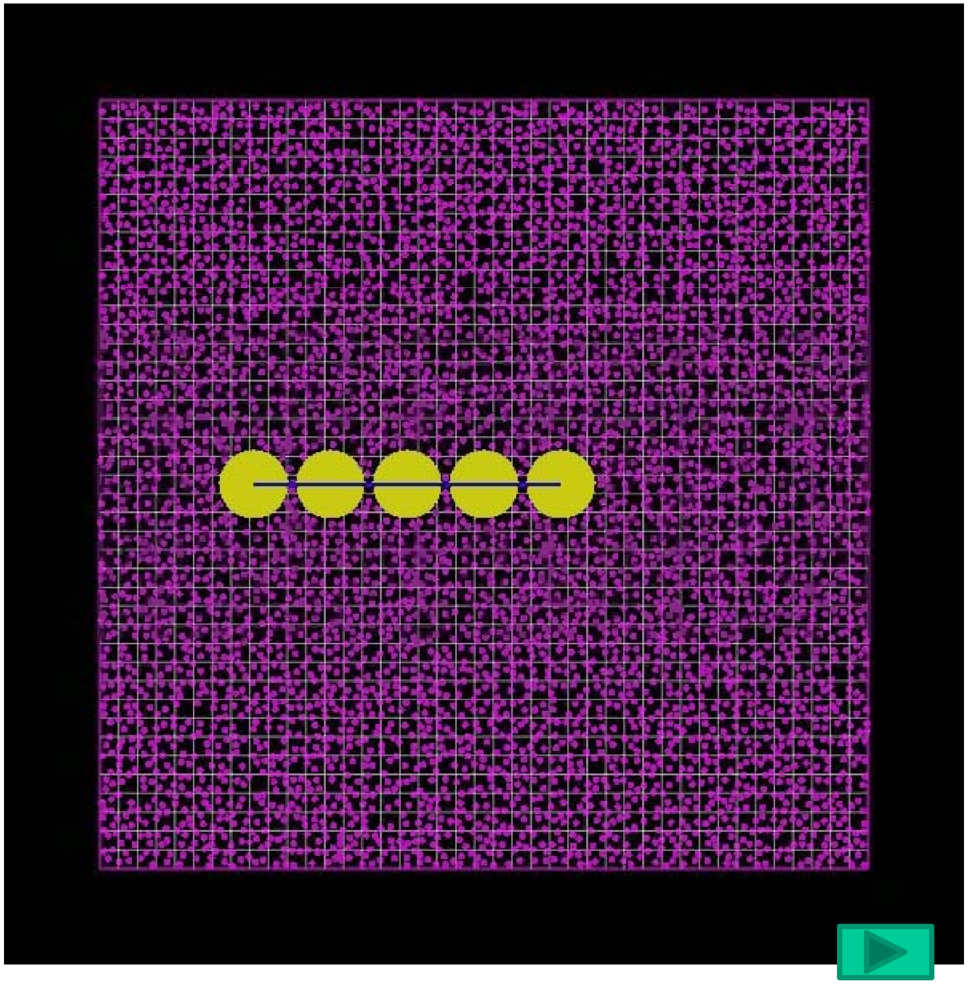


Example: Single Algorithm

Deterministic hard disk MD simulation of polymer in solution.

Small disks (red) are solvent and large disks (yellow) mimic the polymer.

Most of the computational effort spent on solvent far from the polymer.



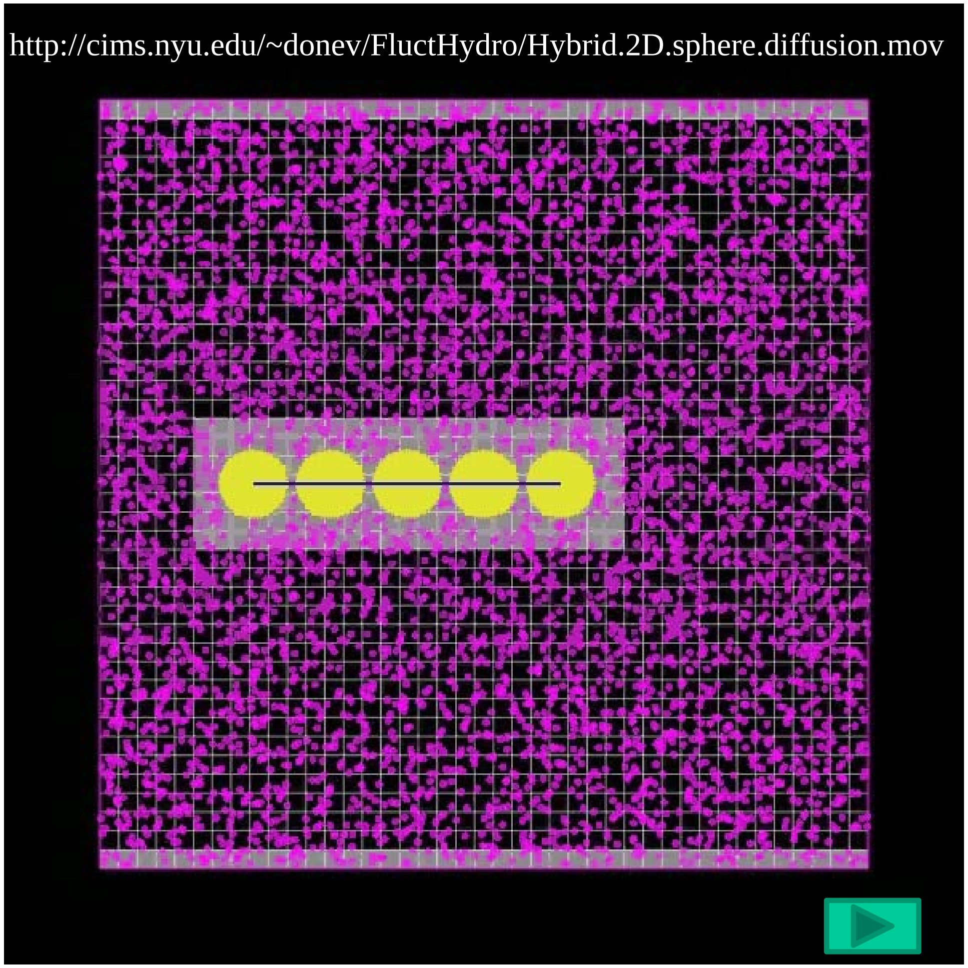
http://cims.nyu.edu/~donev/DSMC/PolymerFlow.2D.MD.mov

Example: Multi-Algorithm

Deterministic hard disk MD algorithm used near the polymer.

An efficient stochastic collision algorithm used for particles far from the polymer.

Important hydrodynamic features are captured without full expense of single algorithm code.



A. Donev, ALG, and B. J. Alder, J. Comp. Phys., 227(4):2644-2665, 2008

Particle/PDE Algorithm Refinement

The most common type of Algorithm Refinement for hydrodynamics is the coupling of a particle scheme (e.g., MD, DSMC) with a continuum PDE scheme.

In AR the continuum/particle interaction is *exactly the same* as between different mesh refinement levels.

* To the PDE solver the particle scheme appears to be a fine mesh patch.
* To the particle scheme, the PDE solver appears to be a (dynamic) boundary condition.

ALG, J. Bell, Wm. Y. Crutchfield and B. Alder, J. Comp. Phys. **154** 134-55 (1999).
S. Wijesinghe, R. Hornung, ALG, and N. Hadjiconstantinou, J. Fluids Eng. **126** 768- 77 (2004).

Particle/PDE AR Hybrid

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

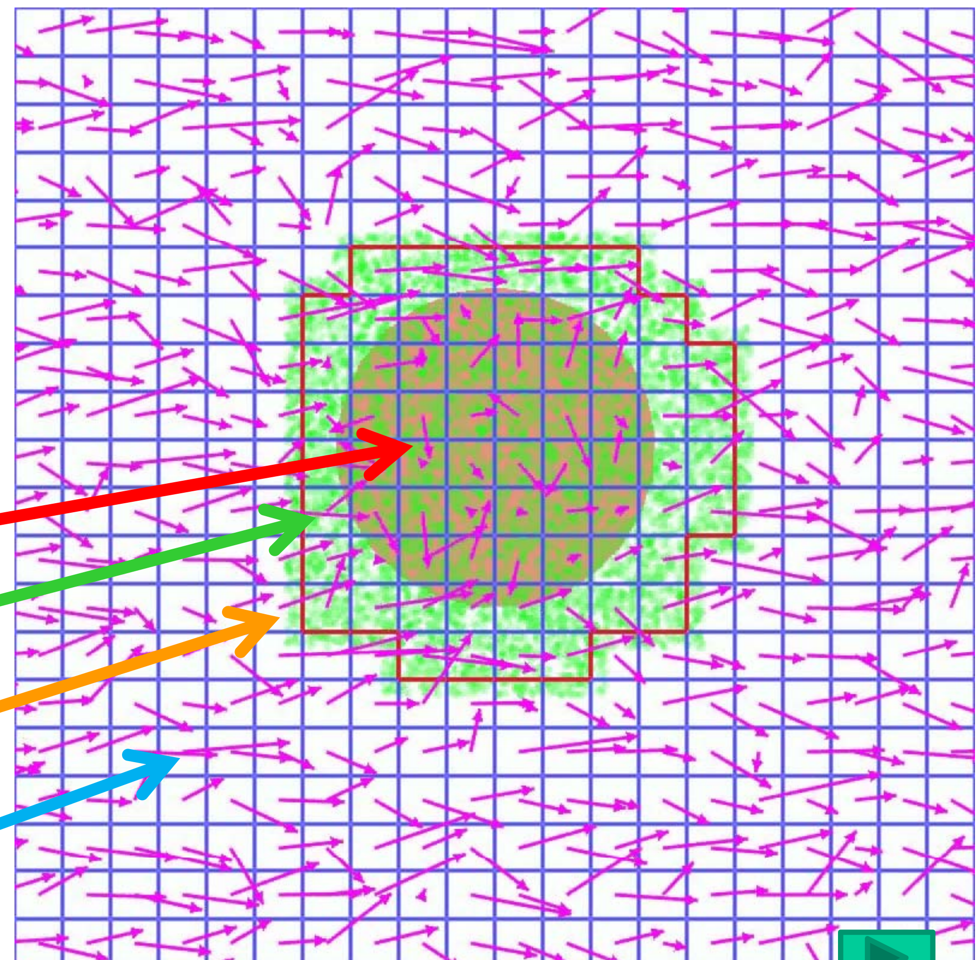
Particle/PDE Algorithm Refinement for flow past a sphere.

Stationary particle

Molecular simulation of solvent fluid

Interface

Continuum simulation of solvent fluid

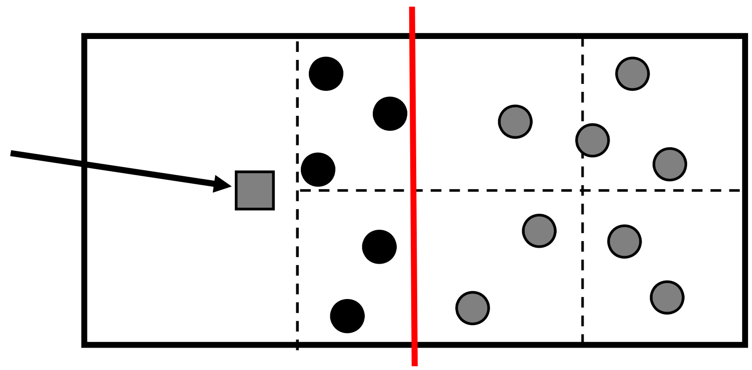


Note: Continuum calculation done everywhere

Coupling continuum → particles

Continuum → particles interface is modeled using a reservoir boundary set with continuum values.

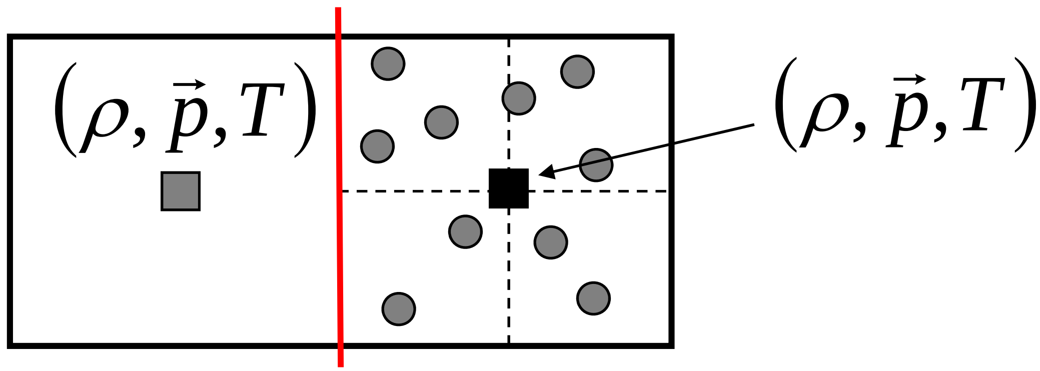
$$\left(\rho, \vec{p}, T\right)$$



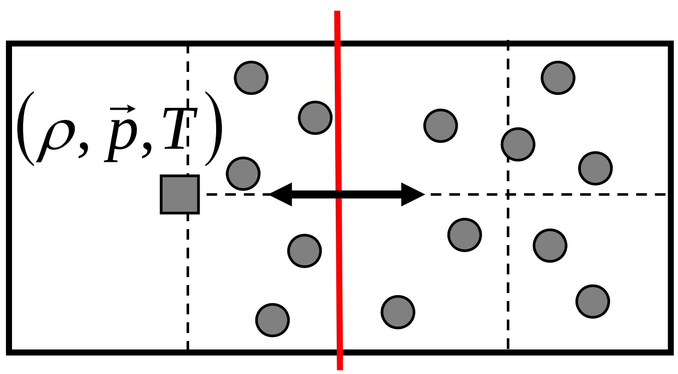
Reservoir particles generated from the Maxwell-Boltzmann or the Chapman-Enskog distribution (which includes velocity and temperature gradient).

Coupling continuum ← particle

- “State-based” coupling: Continuum grid is extended into the particle region



- “Flux-based” coupling: Continuum fluxes are determined from particles crossing the interface

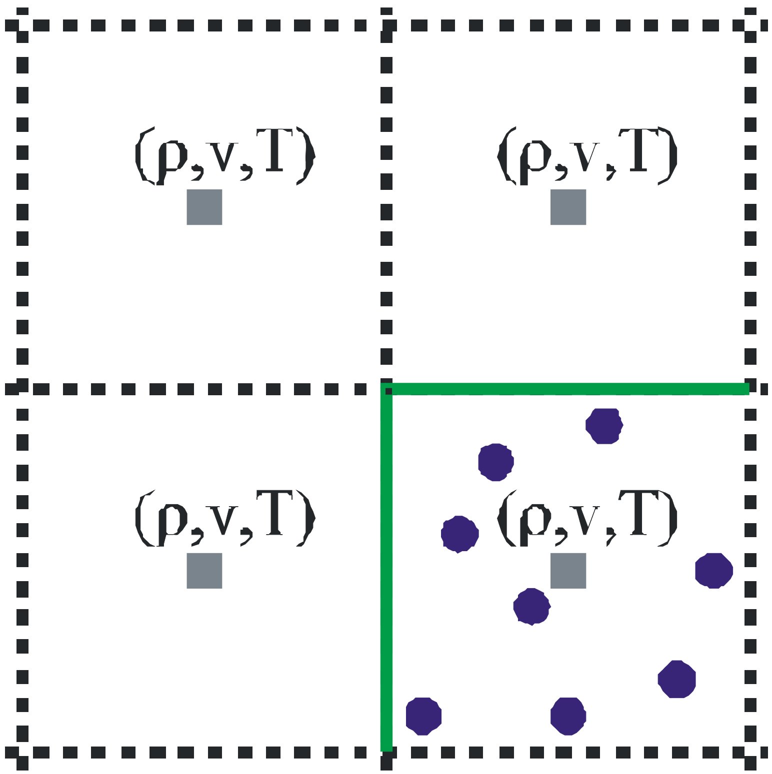


Advancing in Time (1)

Start of a time step

Continuum grid data and particle data are currently synchronized at time *t*.

Mass, momentum and energy densities given by hydrodynamic values ρ, **v** and *T* (or vice versa)

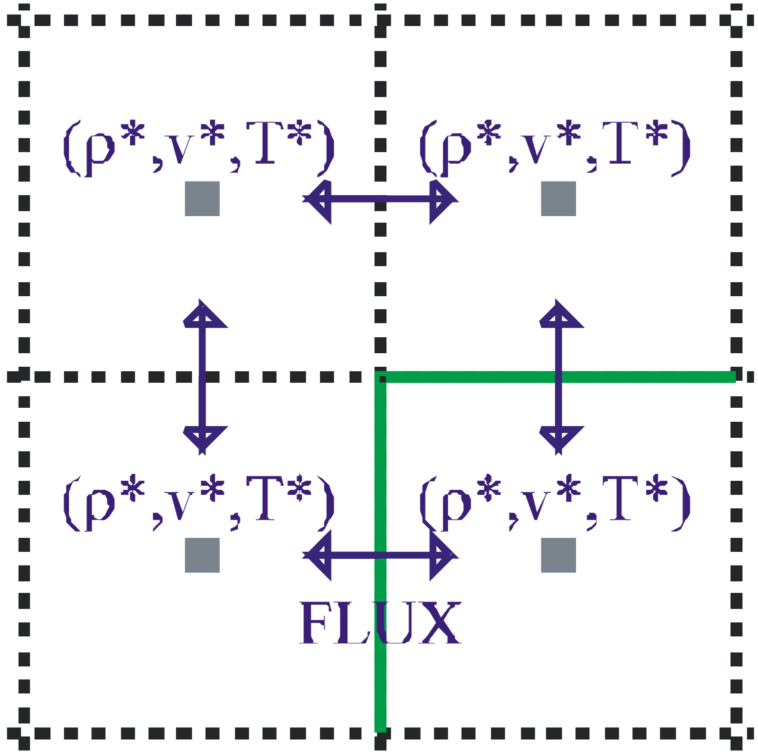


Advancing in Time (2)

Advance continuum

Evaluate the fluxes between grid points to compute new values of ρ*, **v***, and *T** at time *t*+τ*.

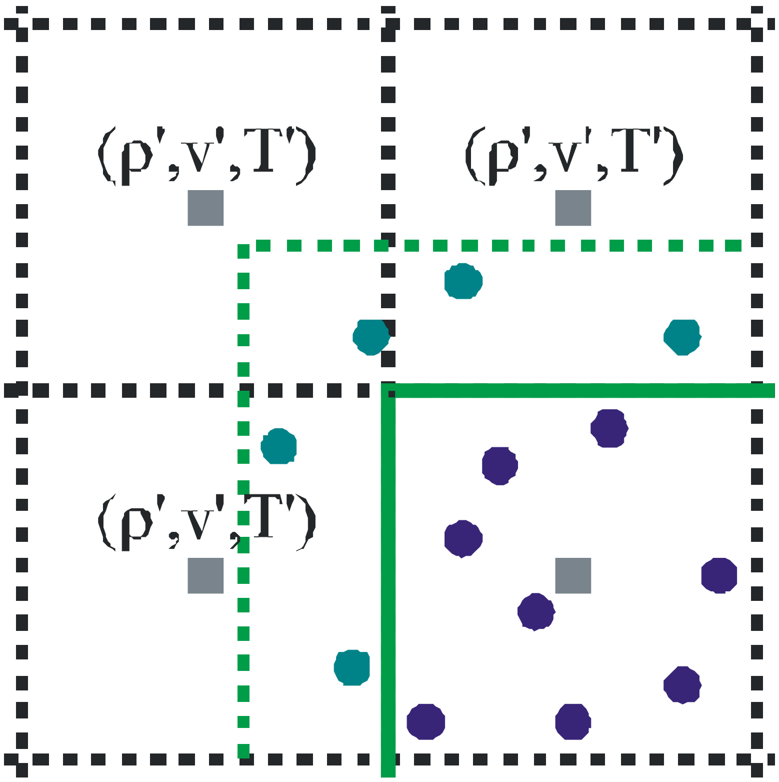
Store both new and old grid point values.



Advancing in Time (3)

Create buffer particles

Generate particles in the zone surrounding the particle region with time-interpolated values of density, velocity, temperature, and their gradients from continuum grid.



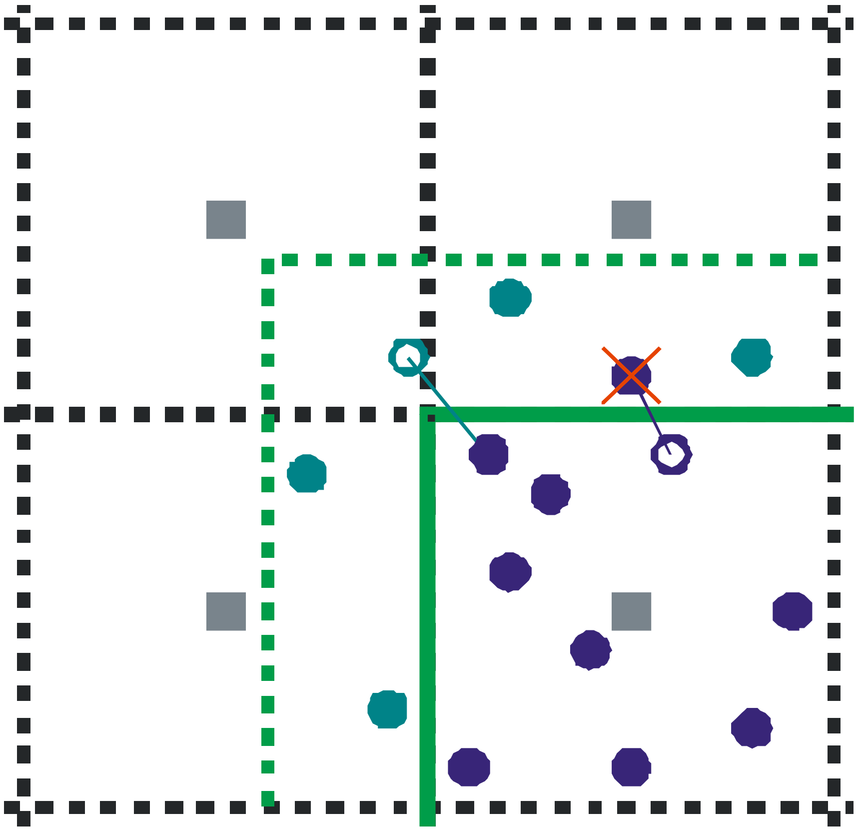
Advancing in Time (4)

Advance particle region

Particles enter and leave the system; discard all finishing outside.

Record fluxes

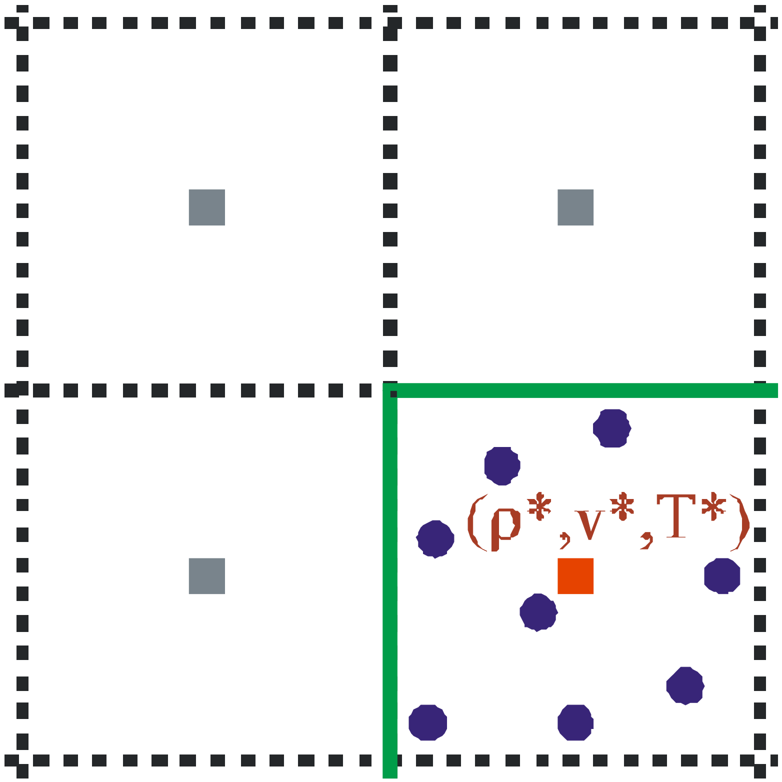
Mass, momentum and energy fluxes due to particles crossing the interface are recorded.



Synchronization (1)

Reset overlaying grid

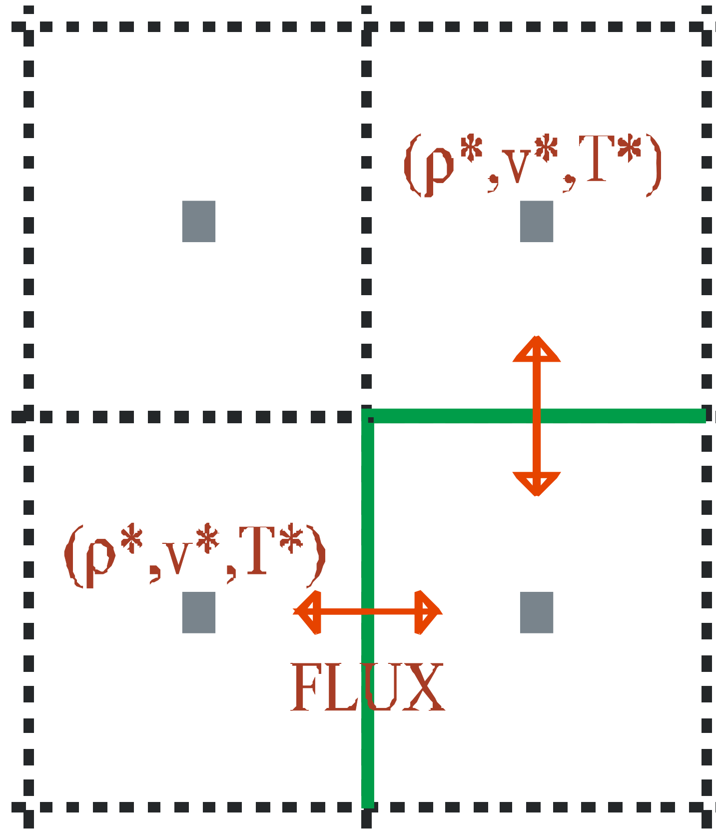
- Compute total mass, momentum, and energy for particles in continuum grid cells. Set hydrodynamic variables in these cells by these values.
- This is a projection of particle data into continnum values.



Synchronization (2)

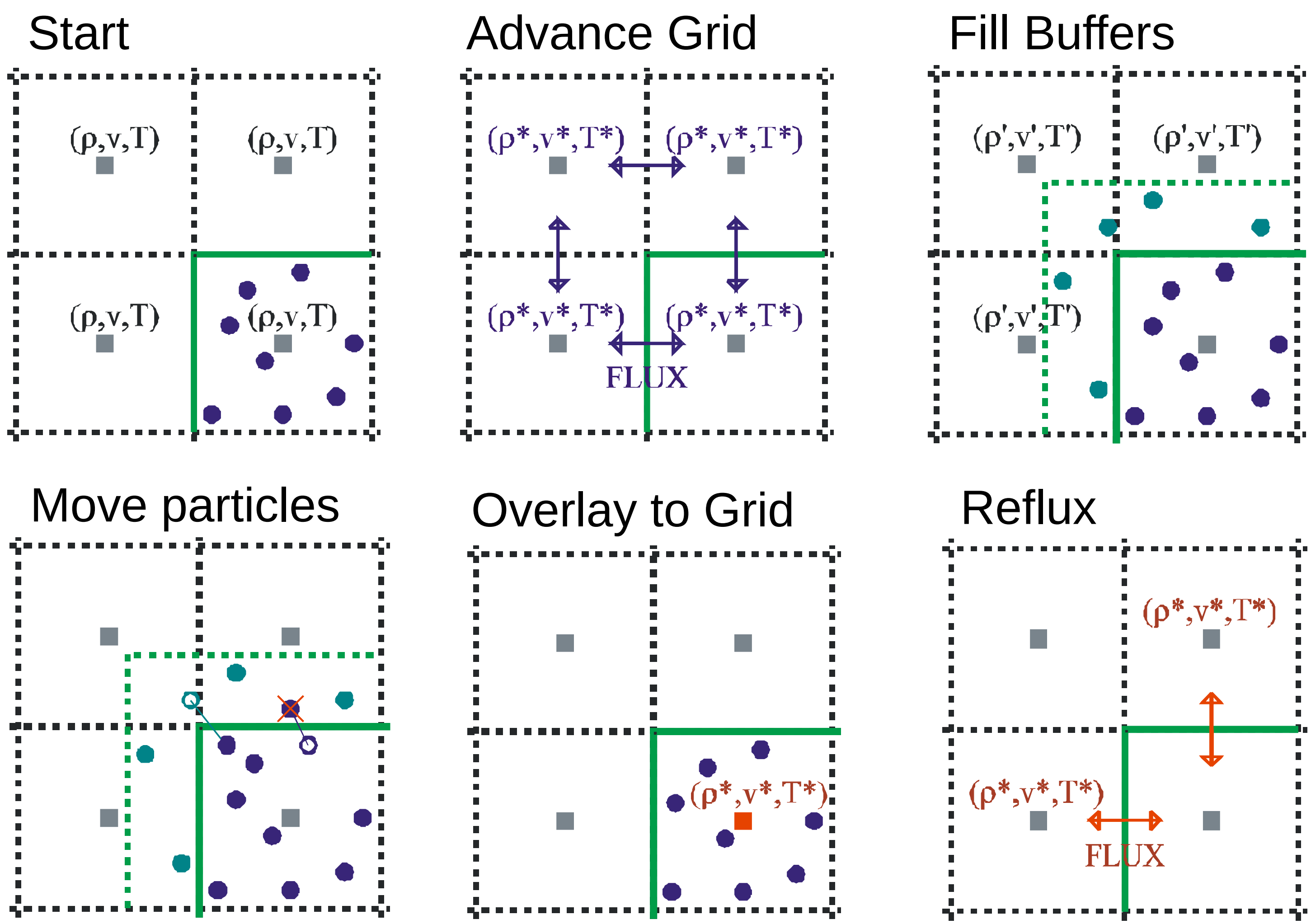
Refluxing

Reset the mass, momentum, & energy density in grid points bordering particle region by difference between the continuum fluxes and the particle fluxes.



Preserves exact conservation.

Summary of the Coupling



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.

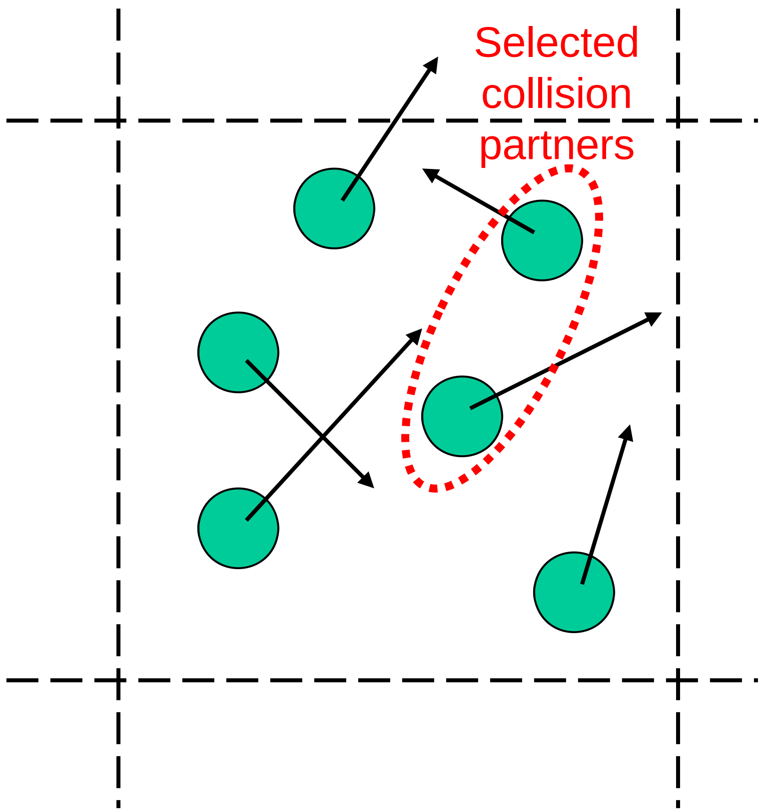
Stochastic Continuum Algorithms – Our original AR method used a deterministic, explicit scheme for the full Navier-Stokes equations. Have developed stochastic PDE schemes to capture hydrodynamic fluctuations.

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

Direct Simulation Monte Carlo

DSMC is a stochastic particle scheme for the Boltzmann equation developed in the early 1960's.

- Sort particles into cells
- Loop over cells
  - Compute collision frequency in a cell
  - Select random collision partners within cell
  - Accept/reject collision based on relative speed
  - Process each collision conserving momentum and energy with random collision angles



MPCD is simplified version of DSMC

Non-ideal DSMC

Modifying the collision process allows you to introduce an equation of state that's not ideal gas.

Various schemes including:

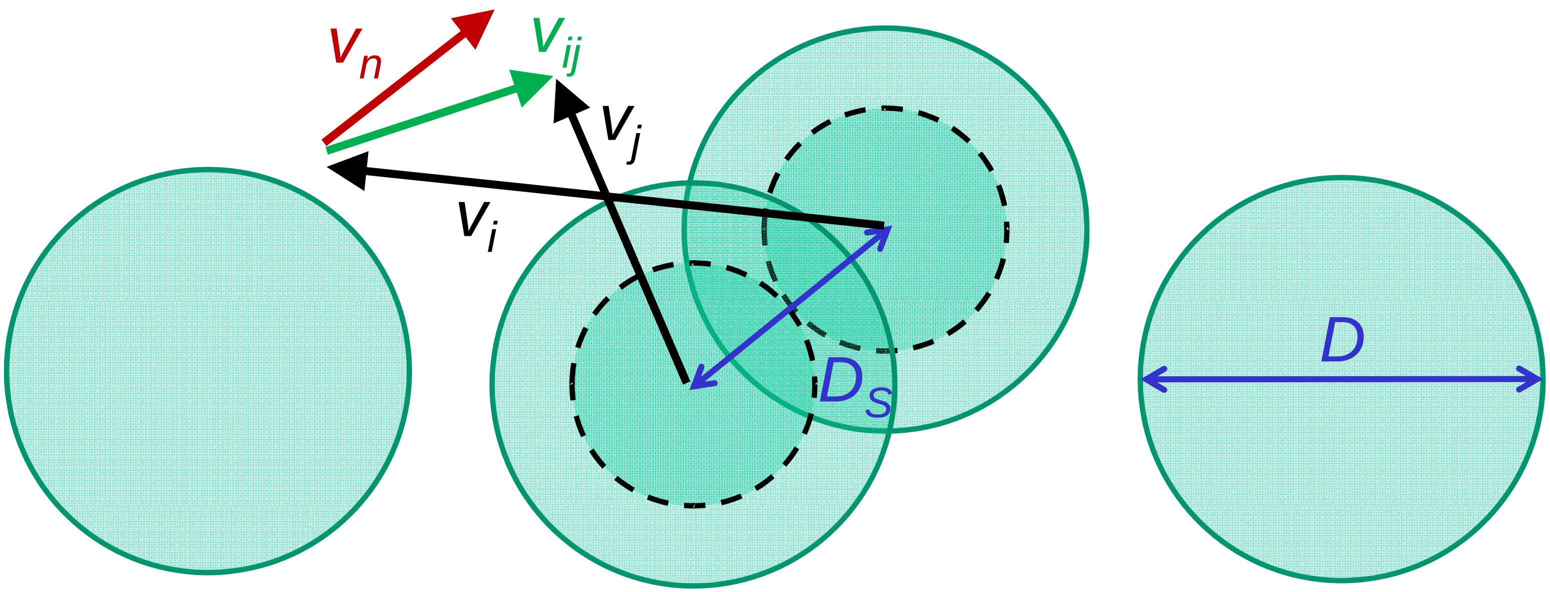
* CBA and Enskog-DSMC for dense hard spheres

* CUBA for a general equation of state

However density fluctuations are wrong (variance not consistent with the compressibility).

F. Alexander, ALG, and B. Alder, Phys. Rev. Lett. **74** 5212 (1995)
N. Hadjiconstantinou, A. Garcia, and B. Alder, Physica A **281** 337-47 (2000)

Stochastic Hard-Sphere Dynamics

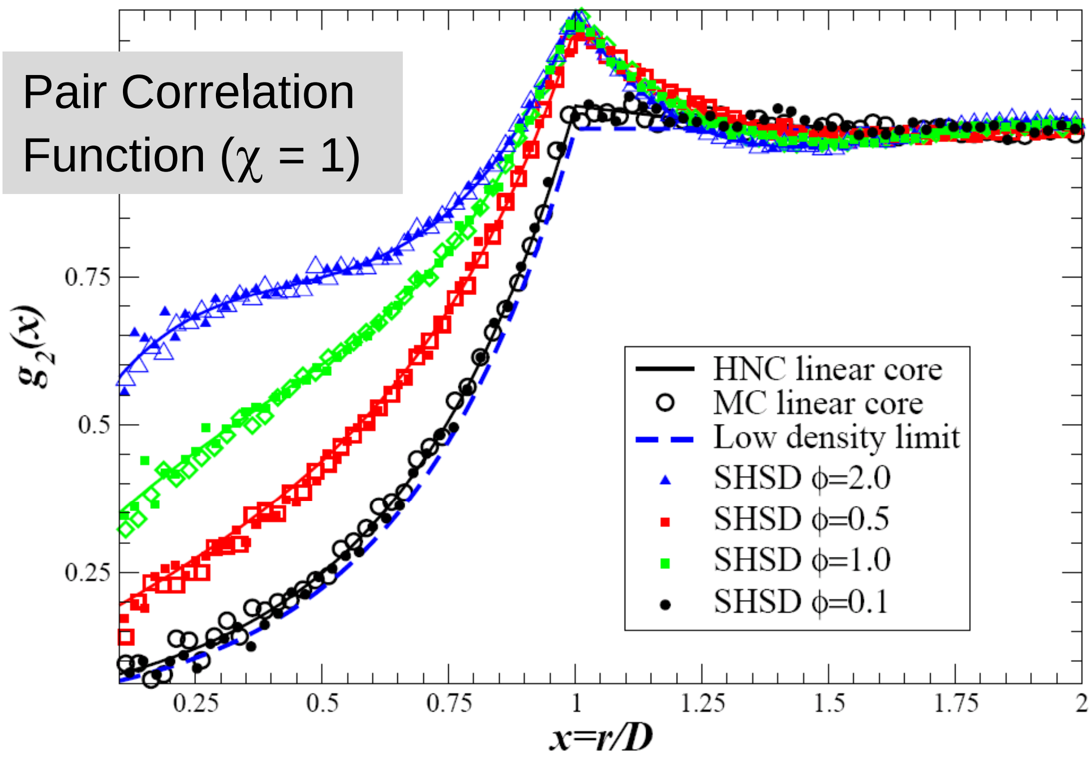


Stochastic Hard-Sphere Dynamics: Particles move ballistically in-between collisions. When two particles i and j are less than a diameter apart, $r_{ij} \leq D$, there is a probability rate $(3\chi/D)v_n\Theta(v_n)$ for them to collide as if they were elastic hard spheres with a variable diameter $D_S = r_{ij}$, where $v_n = -\mathbf{v}_{ij} \cdot \hat{\mathbf{r}}_{ij} > 0$.

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).

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, Parabolic Fluxes, Stochastic Fluxes

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

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

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

Fluctuating Hydrodynamic Solvers

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

$$
\begin{aligned}
U_j^{n+\frac{1}{3}} &= U_j^n + \Delta U_j(U^n, W_1) \text{ (estimate at } t = (n+1)\Delta t \text{)} \\
U_j^{n+\frac{2}{3}} &= \frac{3}{4}U_j^n + \frac{1}{4}\left[U_j^{n+\frac{1}{3}} + \Delta U_j(U_j^{n+\frac{1}{3}}, W_2)\right] \text{ (estimate at } t = (n+\frac{1}{2})\Delta t \text{)} \\
U_j^{n+1} &= \frac{1}{3}U_j^n + \frac{2}{3}\left[U_j^{n+\frac{2}{3}} + \Delta U_j(U^{n+\frac{2}{3}}, W_3)\right],
\end{aligned}
$$

where

$$
\Delta U_j(U, W) = -\frac{\Delta t}{\Delta x}\left[F_{j+\frac{1}{2}}(U) - F_{j-\frac{1}{2}}(U)\right] + \frac{\Delta t^{1/2}}{\Delta x^{3/2}}\left(Z_{j+\frac{1}{2}} - Z_{j-\frac{1}{2}}\right).
$$

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)

Hydrodynamic Instabilities

One application for these new stochastic PDE solvers is the study of hydrodynamic instabilities in the presence of thermal fluctuations.

http://cims.nyu.edu/~donev/RT/RT.DSMC.2D.g_7.8E-6.dx_6.8.stoch.rho1.mov

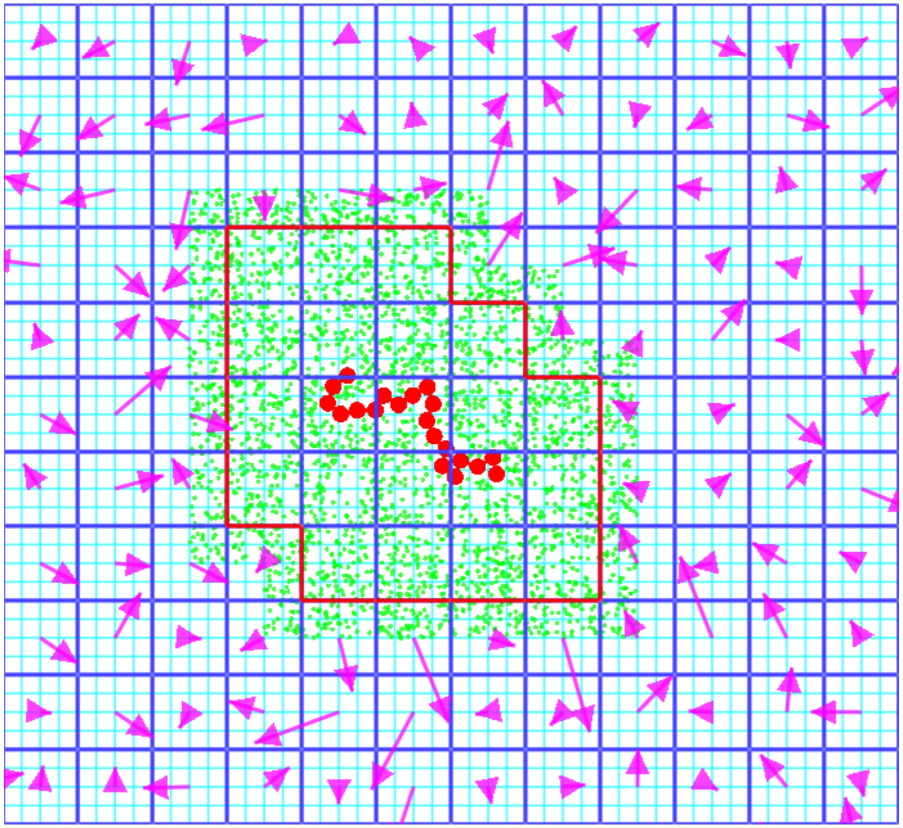
Heavy fluid falling and mixing with light fluid below it (Rayleigh-Taylor instability).

A. Donev, J.B. Bell, B.J. Alder, ALG, in progress

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!

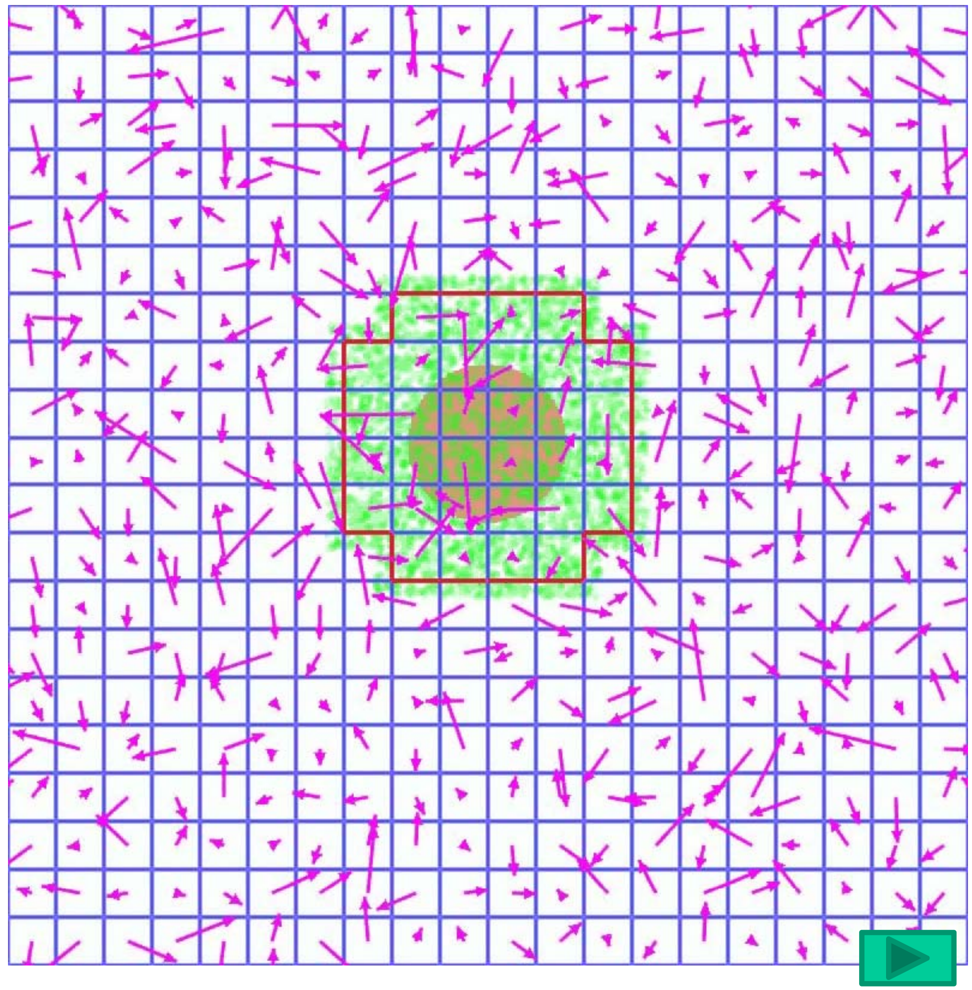


Simple Brownian Motion

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

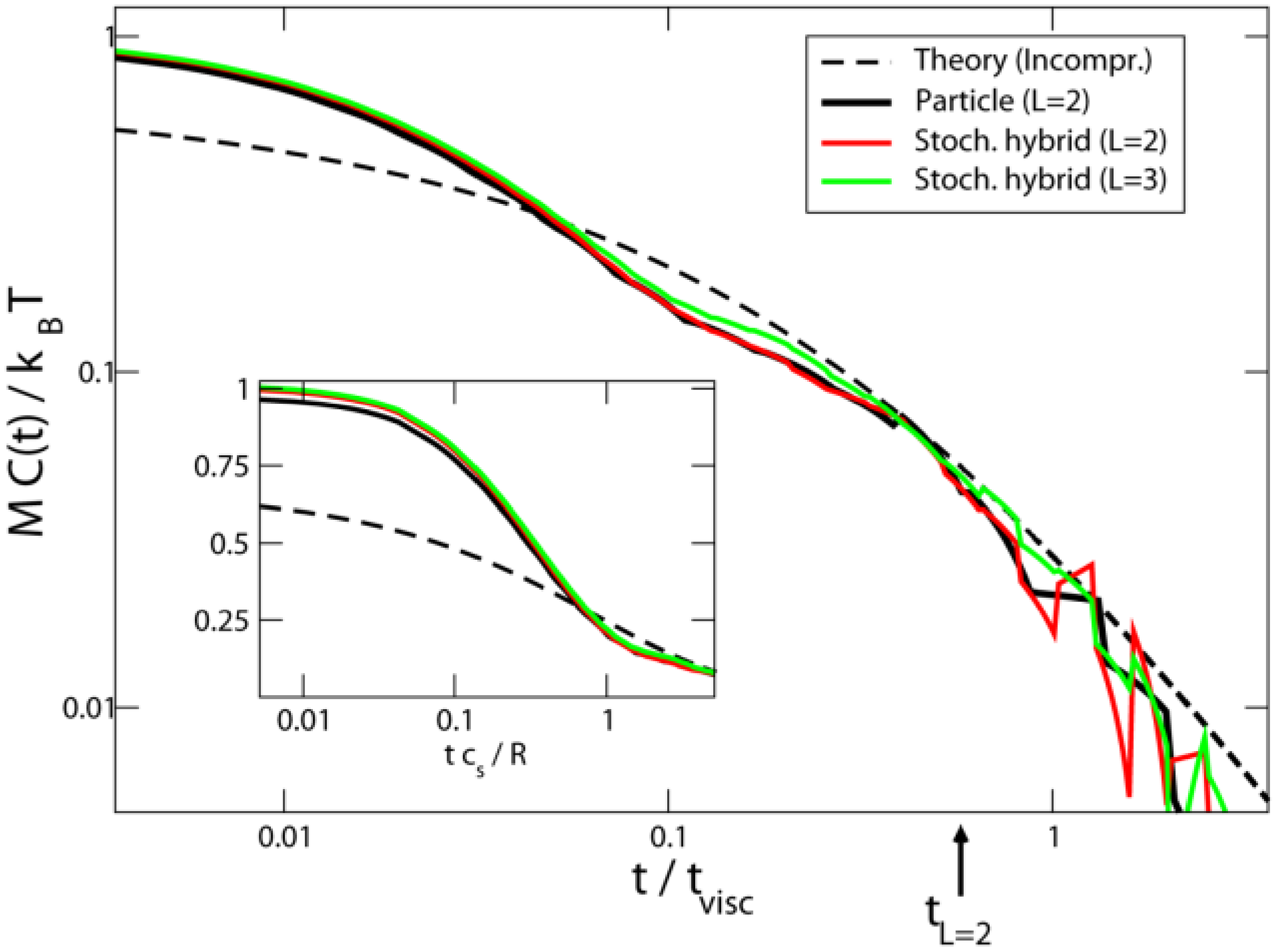
Measure velocity auto-correlation function.

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



AR with Stochastic PDEs

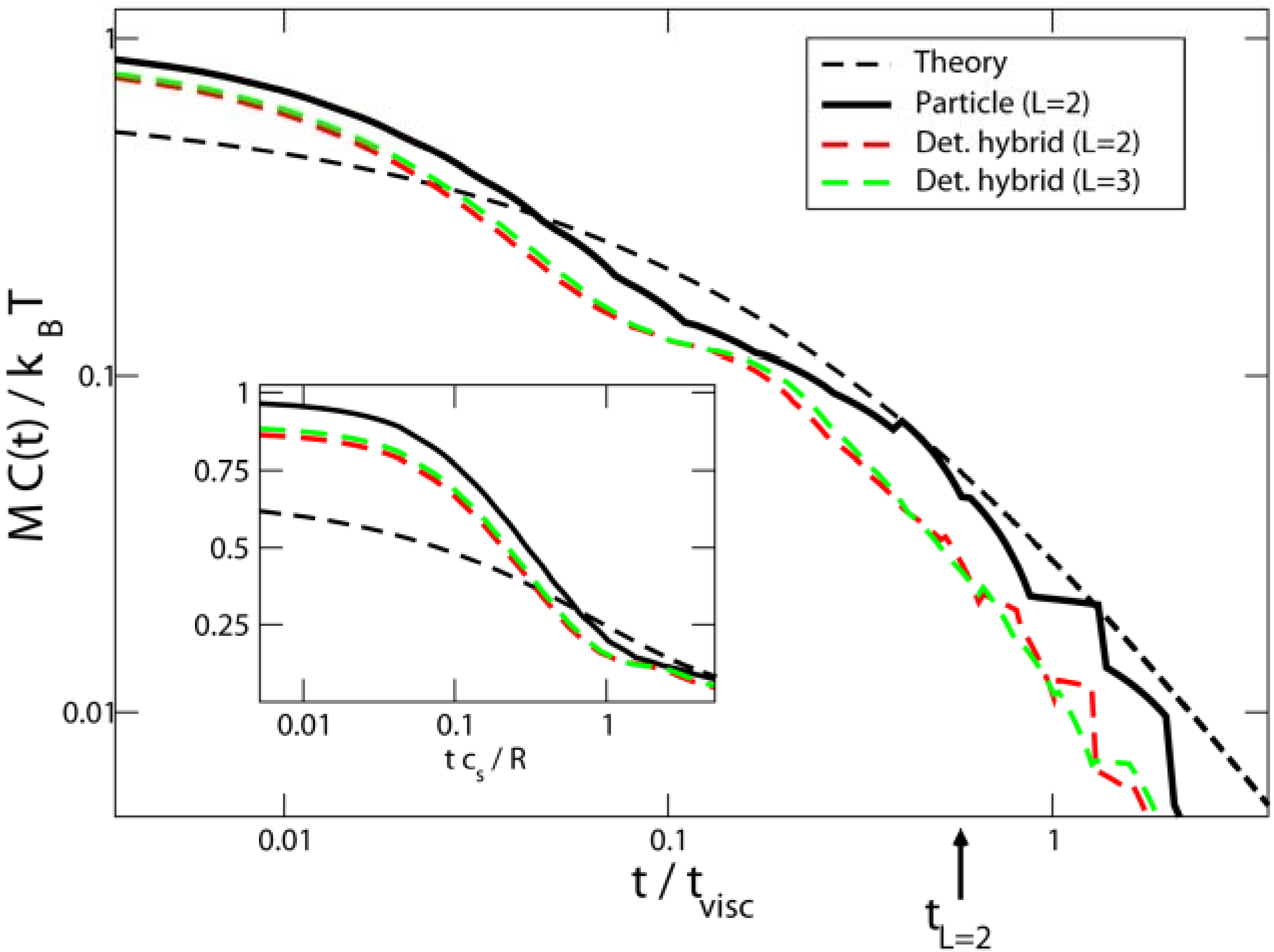
Excellent agreement between a hybrid using stochastic PDE solver and an (expensive) pure particle calculation.



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

AR with Deterministic PDEs

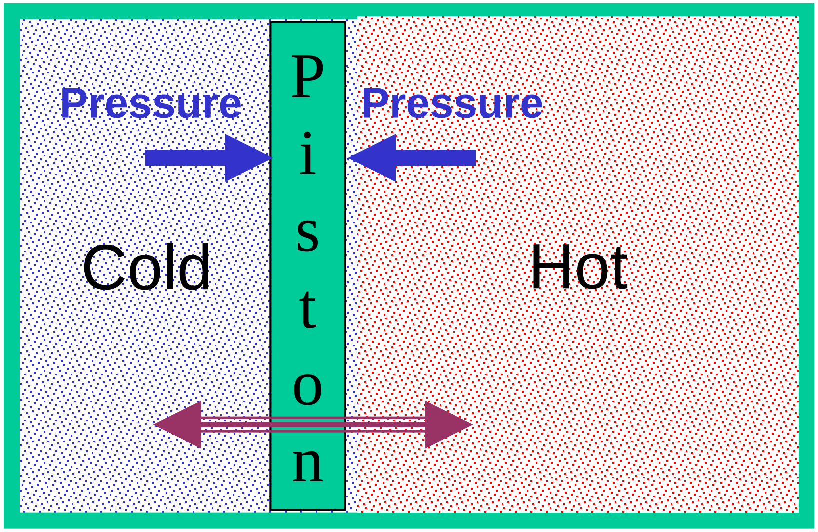
A hybrid using a deterministic PDE solver significantly under-predicts the velocity auto-correlation function.



Adiabatic Piston

Adiabatic piston is a classic problem in statistical mechanics.

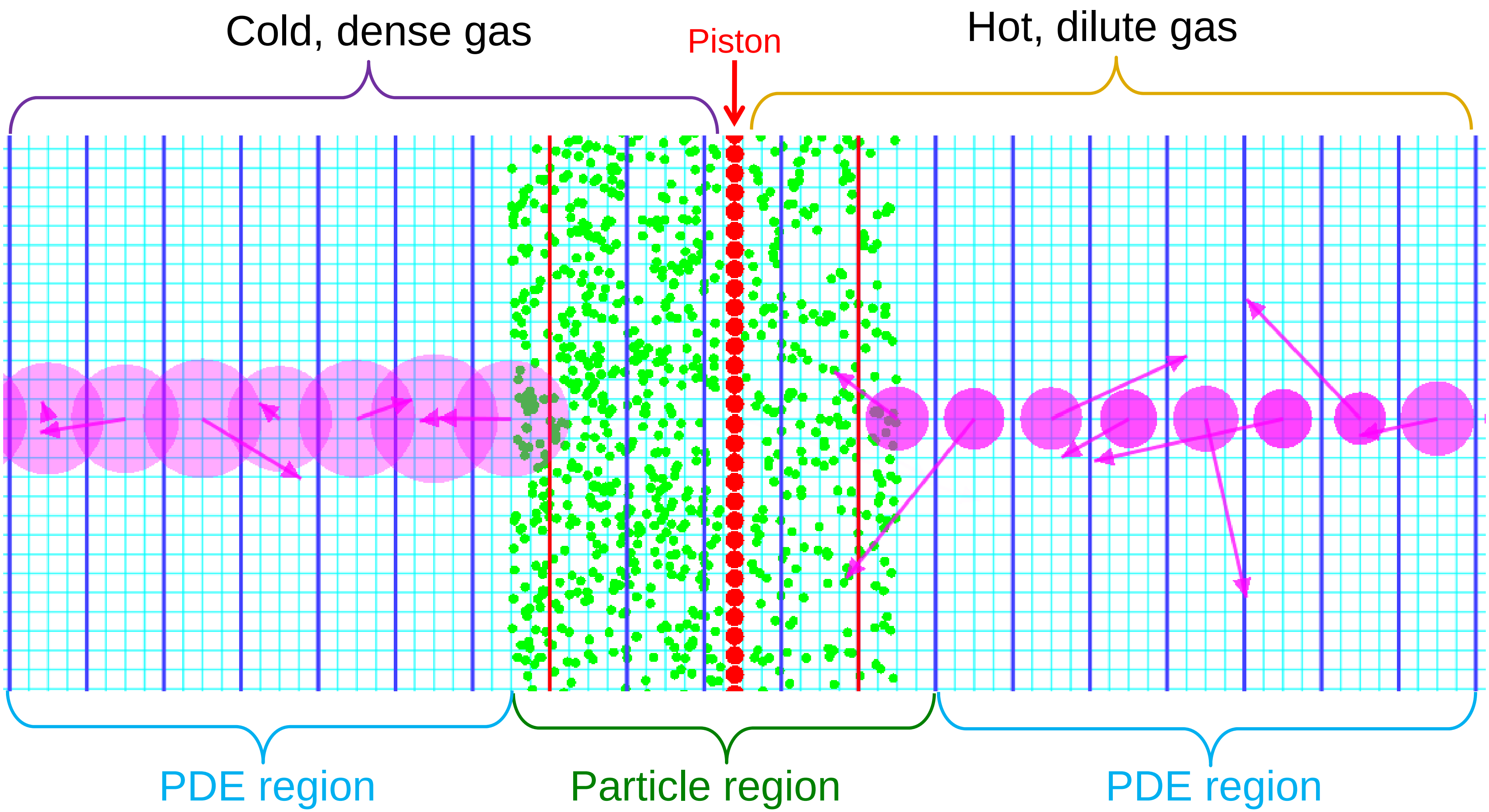
Chambers have gases at different temperatures but equal pressures.



Walls and piston are perfectly elastic to particle collisions yet the gases equilibrate to common temperature.

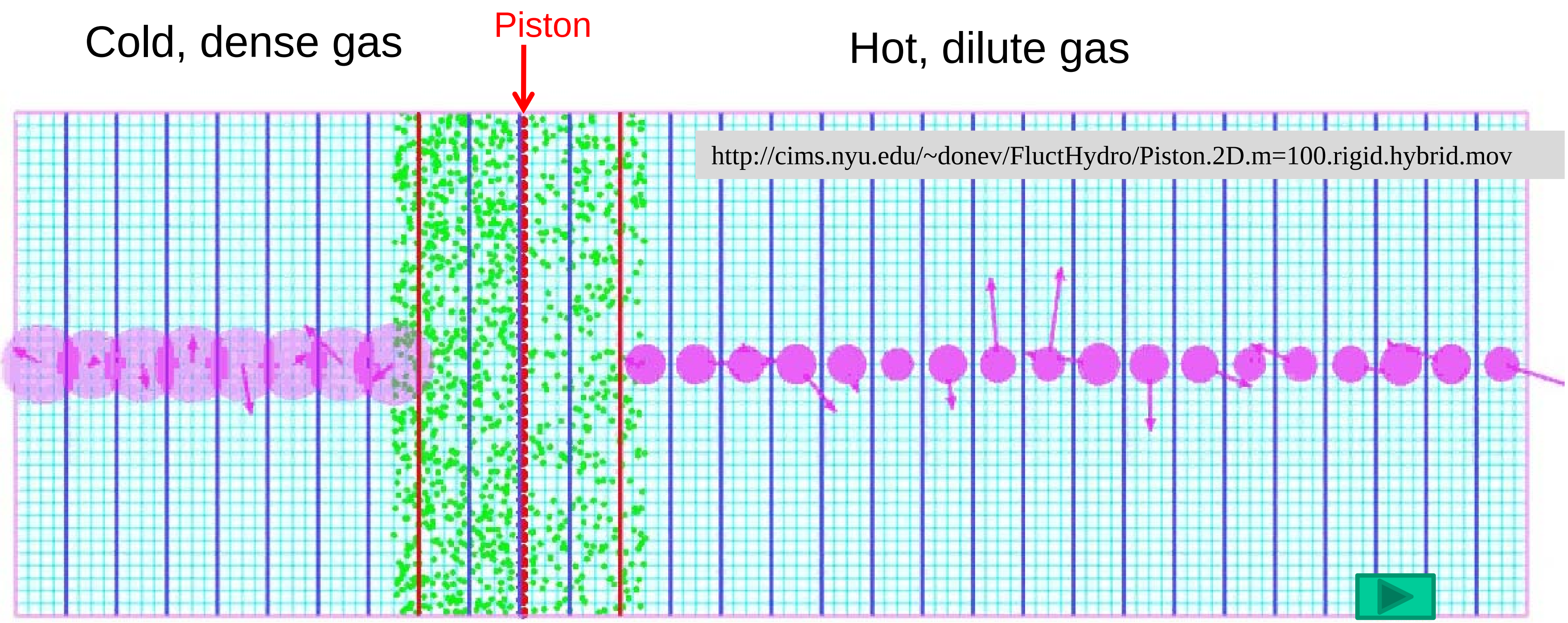
How? Heat is conducted between the chambers by the Brownian motion of the piston.

Simulation Geometry



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

Sample Run of Adiabatic Piston

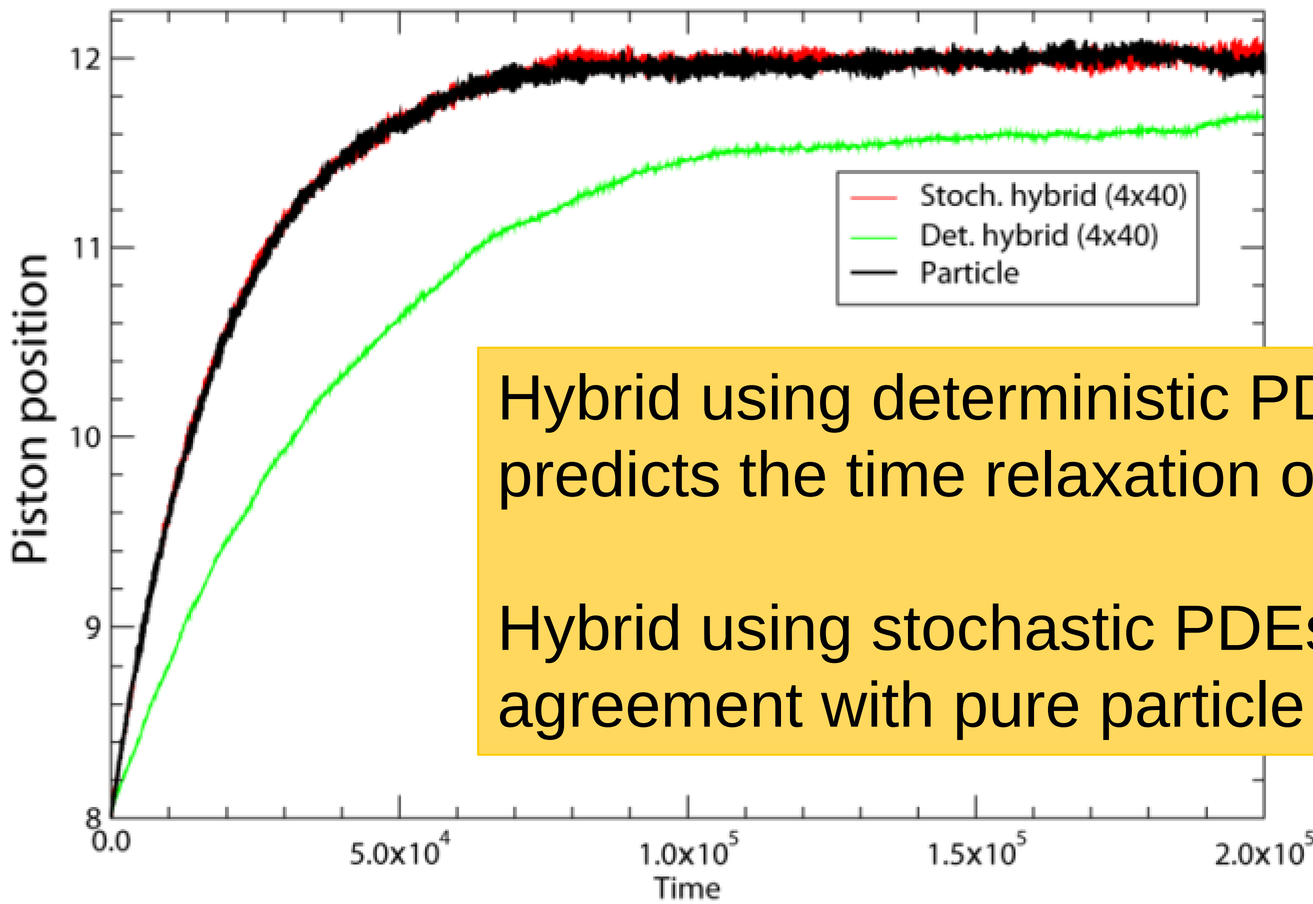


$\rho = {}^{4}/_{3}\ \rho_{eq}$
$T = \frac{3}{4}\ T_{eq}$

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

Note: Adiabatic Piston is a simple Brownian heat engine

Time Relaxation of the Piston

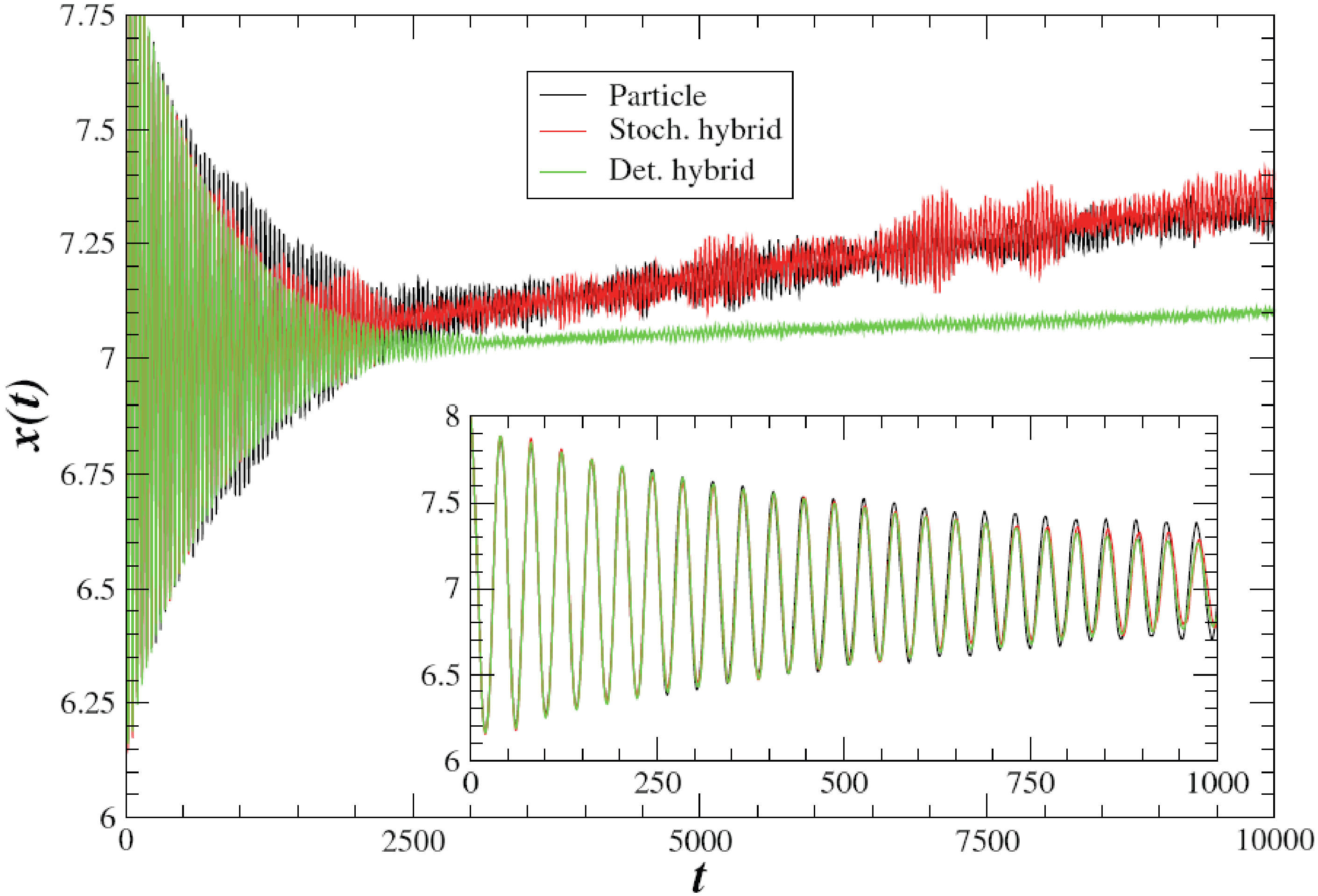


Hybrid using deterministic PDEs under-predicts the time relaxation of the piston.

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

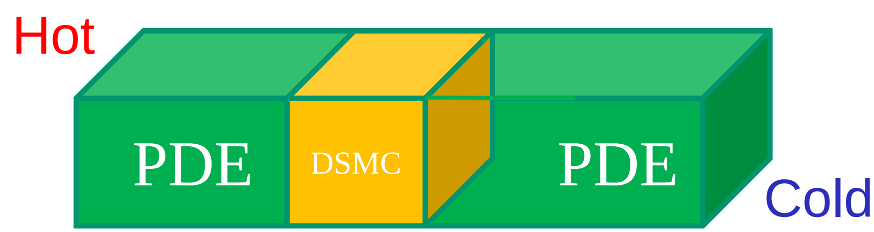
A. Donev, J.B. Bell, ALG, and B. Alder, *SIAM Multiscale Mod. Sim.* **8** 871-911 (2010).

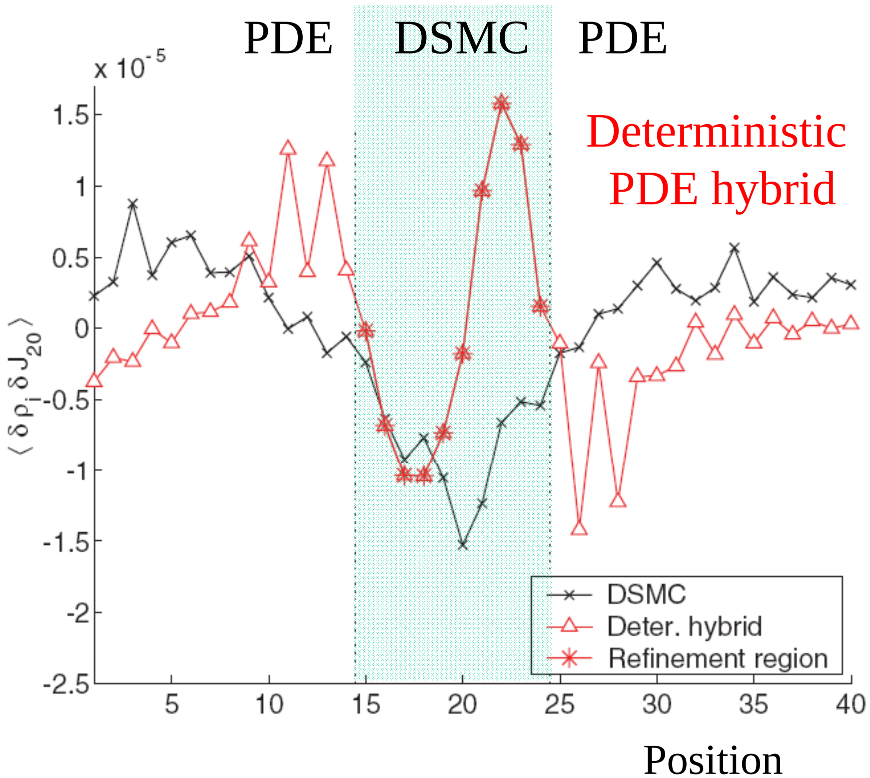
Relaxation from Mechanical Non-Equilibrium

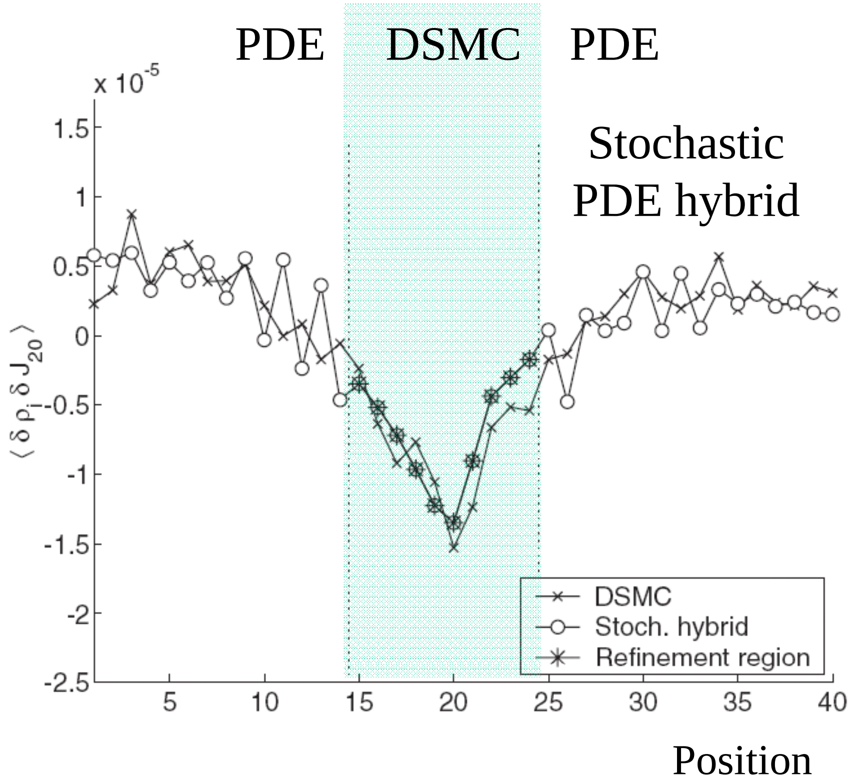


Correlations of Fluctuations

Correlation of density-momentum fluctuations in hybrids, compared with pure DSMC calculation.







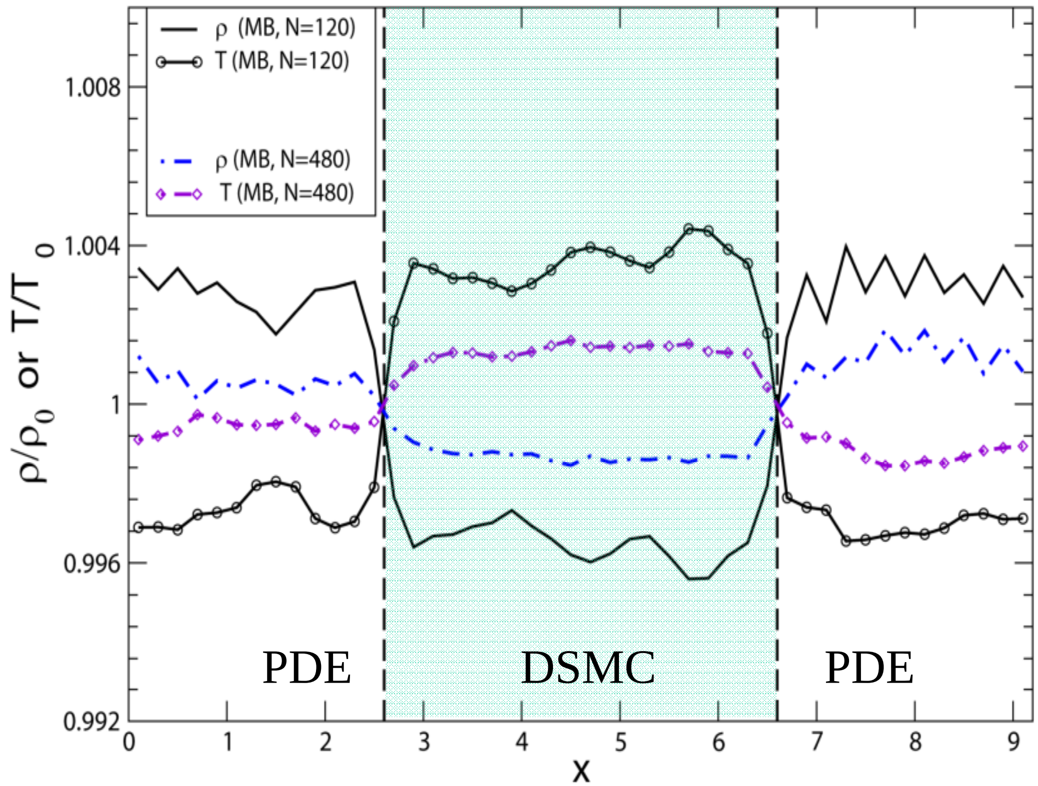
S. Williams, J.B. Bell, and ALG, *SIAM Multiscale Mod. Sim.*, **6** 1256-1280 (2008).

Imperfect Matching at Interface

Algorithm Refinement works well yet matching at interface is still not seamless, even at equilibrium

Error in density and temperature of about ½ % for *N*=100 particles per cell

Error goes as 1/*N* and is due to the use of instantaneous values for the hydrodynamic variables at interface.

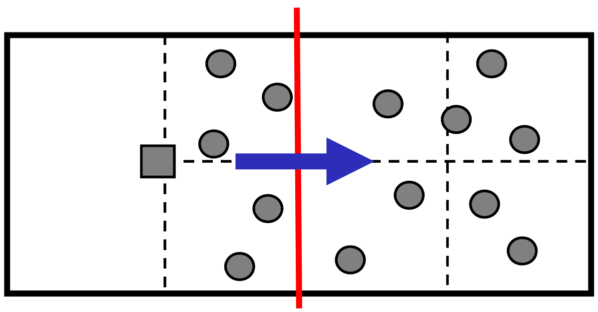


A. Donev, J.B. Bell, ALG, and B. Alder, *SIAM Multiscale Mod. Sim.* **8** 871-911 (2010).

Bias in Fluxes at AR Interfaces

A bias occurs with fluxes due to fluctuations; the one-way mass flux for dilute gas is,

$$F(\rho,T) = \sqrt{\frac{k}{2\pi m}}\,\rho T^{1/2}$$



However

$$\left\langle \rho T^{1/2} \right\rangle \neq \left\langle \rho \right\rangle \left\langle T \right\rangle^{1/2}$$

And thus

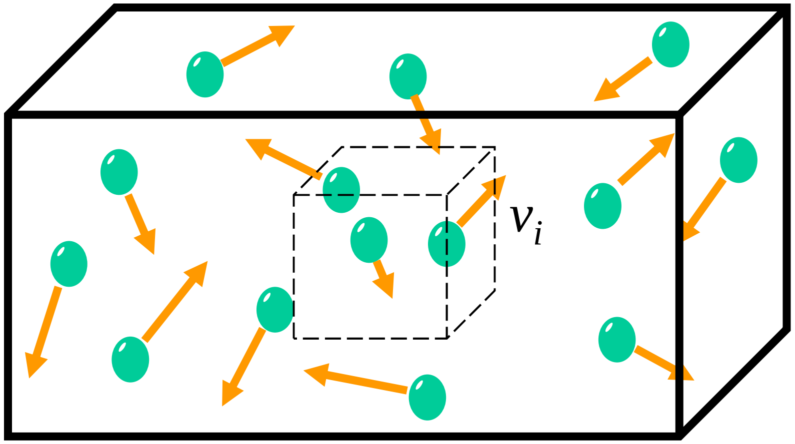
$$\left\langle F(\rho,T) \right\rangle = F(\langle \rho \rangle, \langle T \rangle) \times \left(1 - \frac{1}{12N} \right)$$

So the bias goes as 1/N.

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 $u = \bar{v}$

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:

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

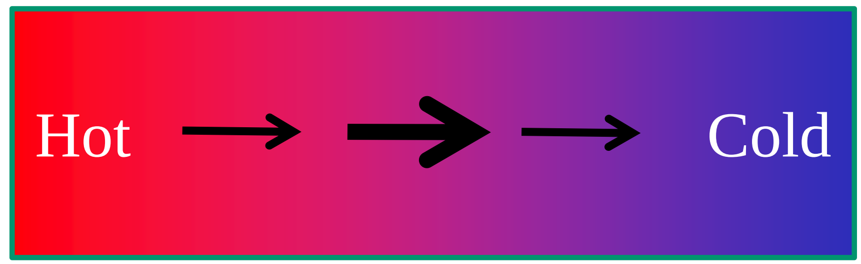
Mean Instantaneous   Mean Cumulative

Which definition gives the correct hydrodynamic fluid velocity?

Anomalous Fluid Velocity

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

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



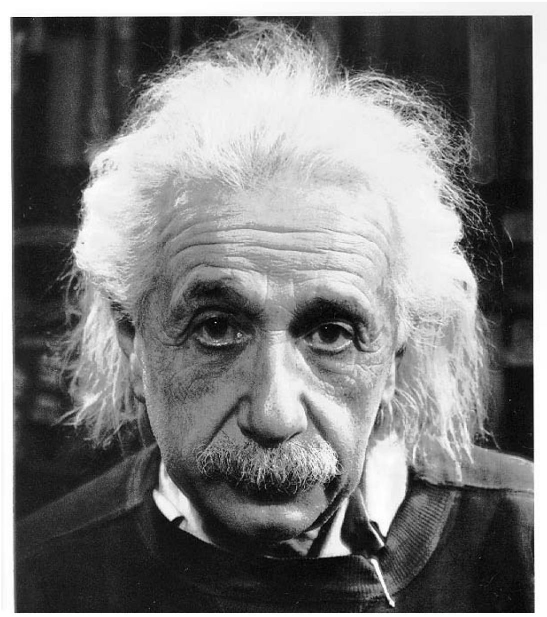
Using the cumulative mean, $\langle u \rangle_*$, gives the expected result of zero fluid velocity.

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

Landau Model for Students

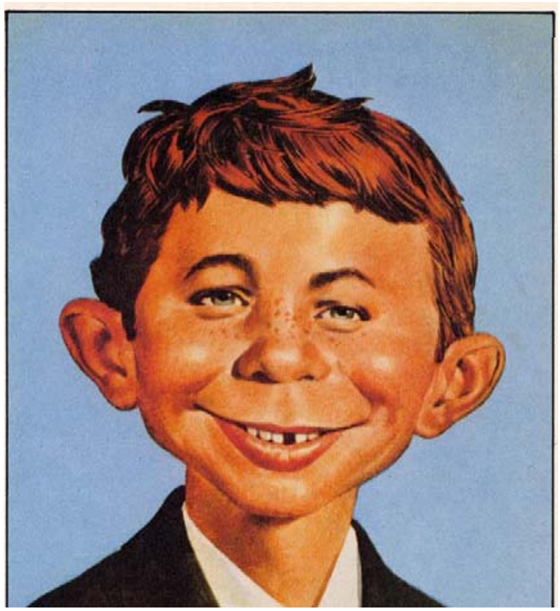
Simplified model for university students:

Genius



Speed = 3

Not Genius



Speed = 1

Three Semesters of Teaching

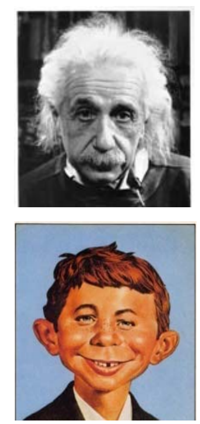
First semester

Average = 3

Second semester

Average = 1

Third semester



Sixteen students in three semesters

Total value is 2x3+14x1 = 20.

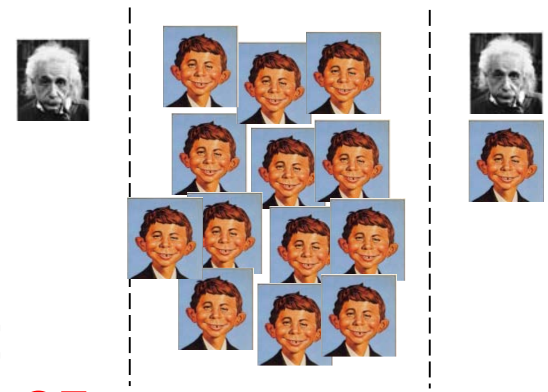
Average = 2

Average Student Speed?

What is the speed of the average student in your courses?

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 when the class size (number of particles) and speed of students in the class is correlated.

Bias in Instantaneous Fluid Velocity

From the definitions,

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

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.

Similar bias occurs with temperature, pressure, etc.

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

Future Work

- Adding further complexity to our stochastic particle schemes (e.g., internal states, chemistry)

- Developing incompressible (low-Mach number) scheme for fluctuating hydrodynamics

- Further exploring coupling issues as well as stability and accuracy in Algorithm Refinement.

For more information, visit:
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