Stochastic Particle Algorithms From DSMC to CUBA

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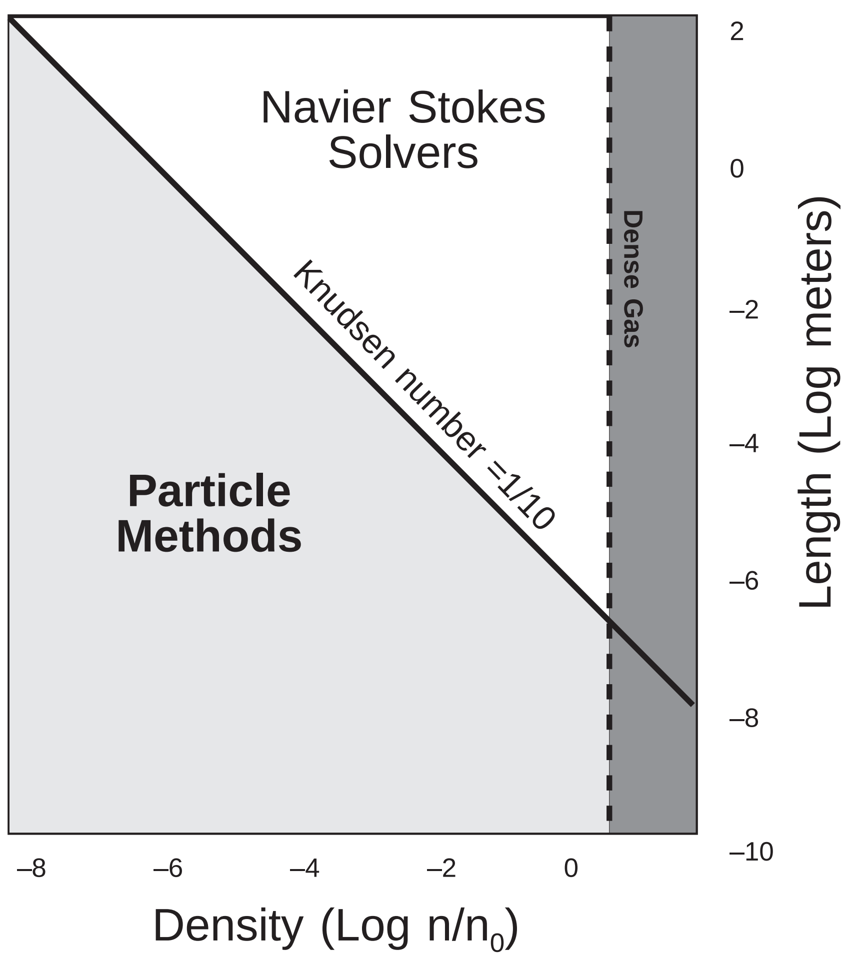
Outline

- Why use stochastic particle methods?
- Direct simulation Monte Carlo (DSMC)
- Selected DSMC applications
- Particle/continuum hybrids
- Dense gases and liquids (CBA & CUBA)
- Future directions

Continuum vs. Particle

When is the continuum description of a gas not accurate?

$$\text{Knudsen number} \equiv \frac{\text{Mean free path}}{\text{Characteristic length}} = \frac{\lambda}{L}$$



High Kn scenarios

- Aerospace flows
- Micromechanical devices
- Fluctuations (e.g., light scattering)
- Shock waves and interfaces

Direct Simulation Monte Carlo

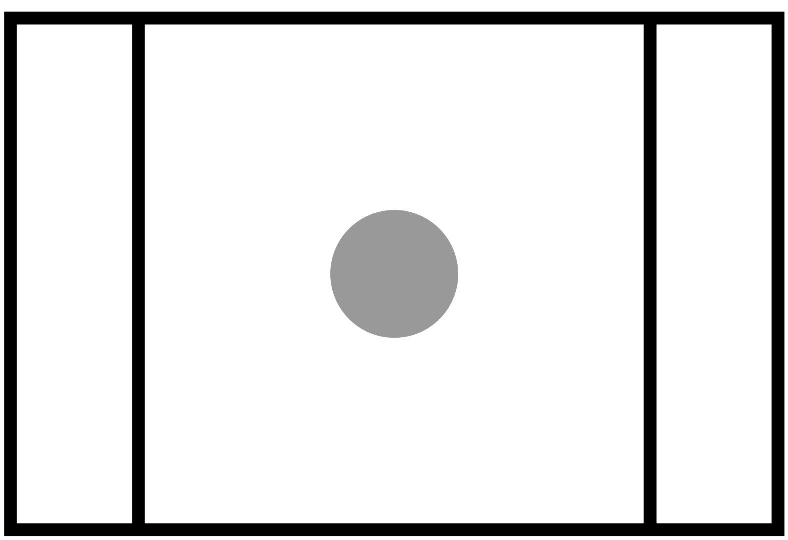
DSMC is a particle-based algorithm for simulating a dilute gas. Particle collisions are evaluated as a stochastic process.

History

- DSMC developed by G.A. Bird (late 60's)
- Popular in aerospace engineering (70's)
- Variants & improvements (early 80's)
- Applications in physics & chemistry (late 80's)
- Used for microscopic flows (early 90's)
- Extended to dense gases & liquids (mid 90's)

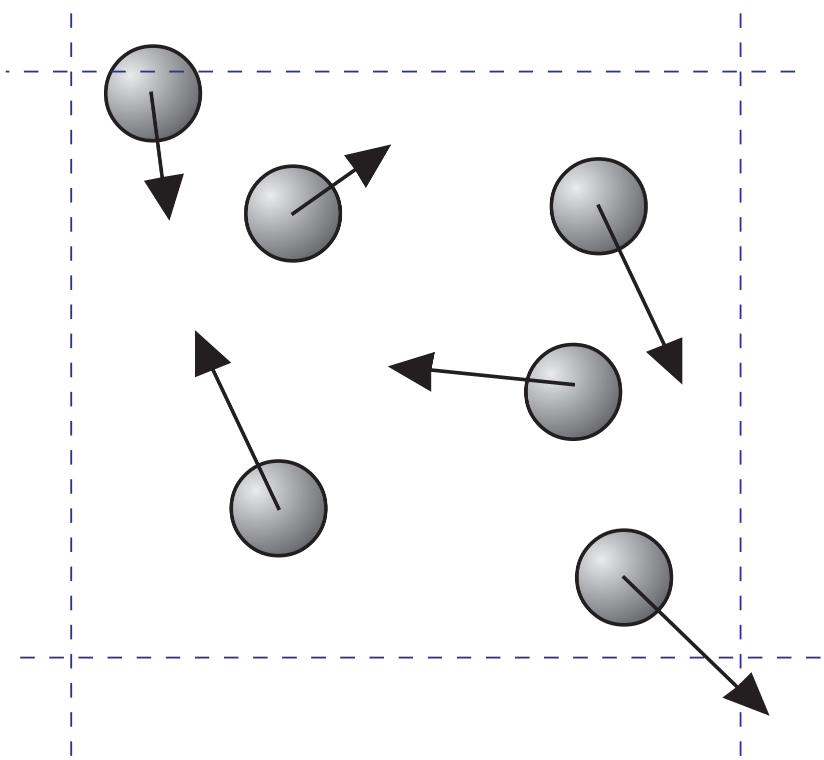
DSMC Algorithm

- Initialize system with particles
- Loop over desired number of time steps
  - Create particles at open boundaries
  - Move all the particles
  - Process particle/boundary interactions
  - Select and execute random collisions



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

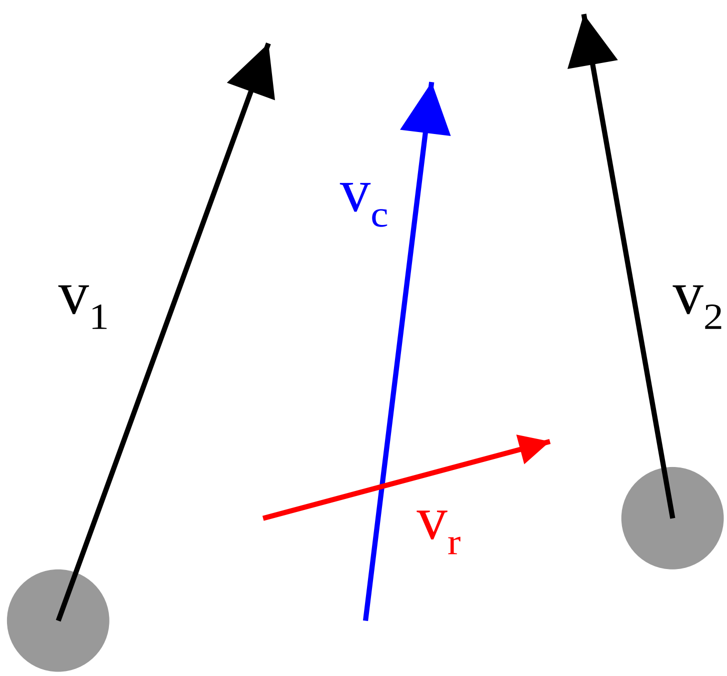


Collisions (cont.)

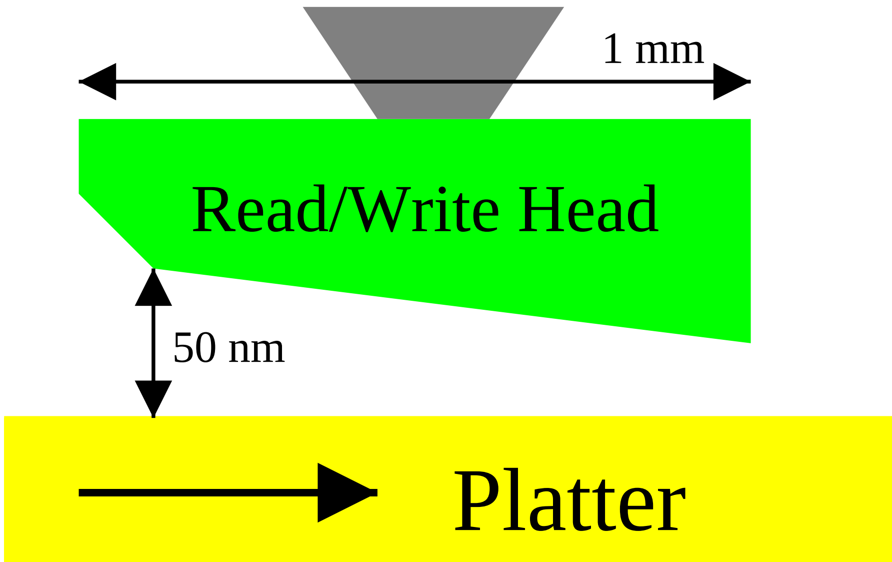
Probability that a pair collides only depends on their relative velocity.

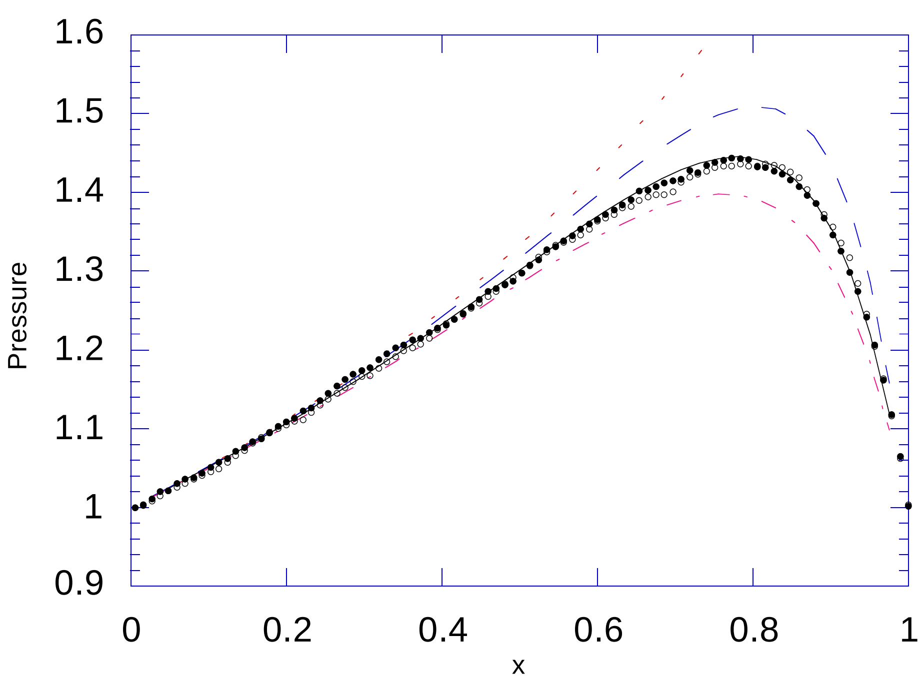
Post-collision velocities (6 variables) given by:

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

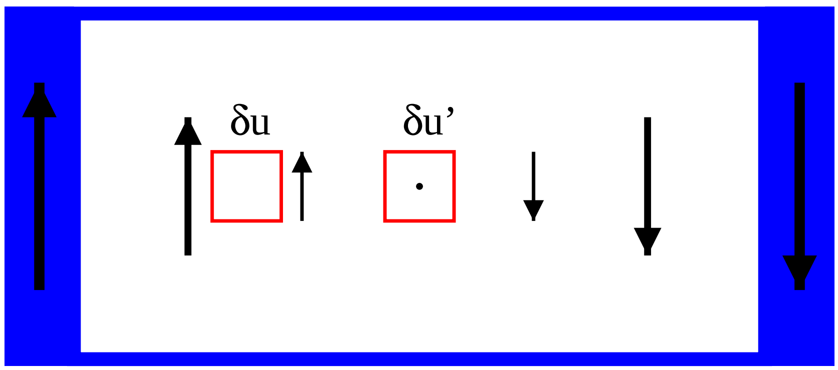


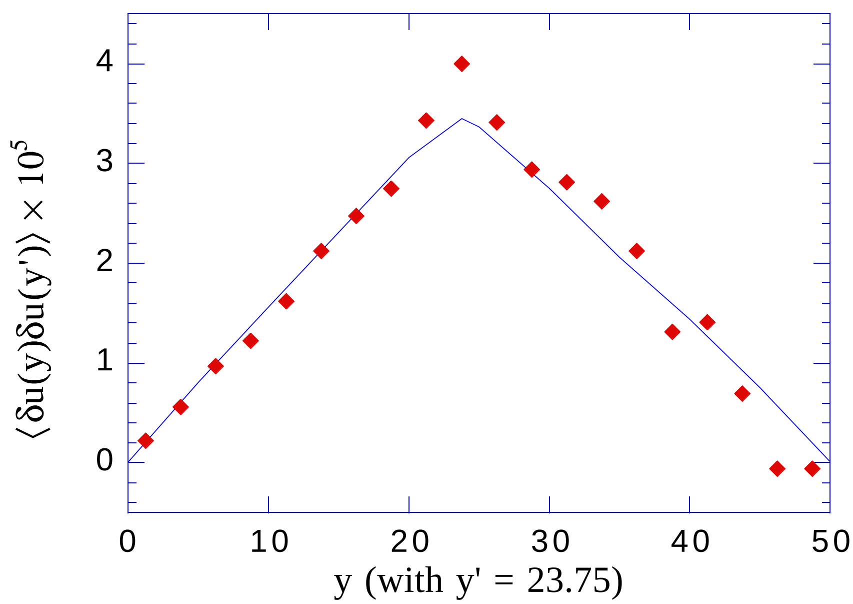
Application: Microchannel Flows





Application: Fluctuations





Continuum/DSMC Hybrids

Problem:

DSMC is computationally expensive

Solution:

Only use DSMC where it is needed

Similar to the idea of mesh refinement

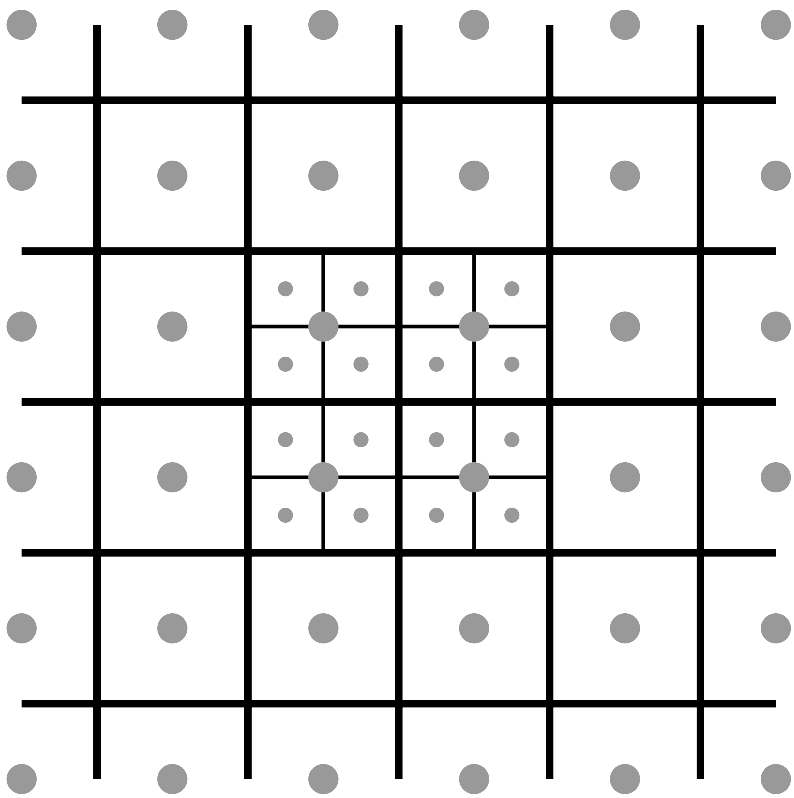
Ordinary Mesh Refinement

Solve equations of the form $\partial_t A = -\nabla \cdot F(A)$ using an explicit PDE solver (e.g., Godunov).

Coarse/Fine Grid Coupling

- Advance coarse grid
- Fill fine/coarse boundary data
  - Advance fine grid
  - Record fluxes at coarse/fine interface
  - Repeat fine grid calculation
- "Reflux" boundary coarse cells
- Backfill overlying coarse cells

Mesh Refinement Illustration

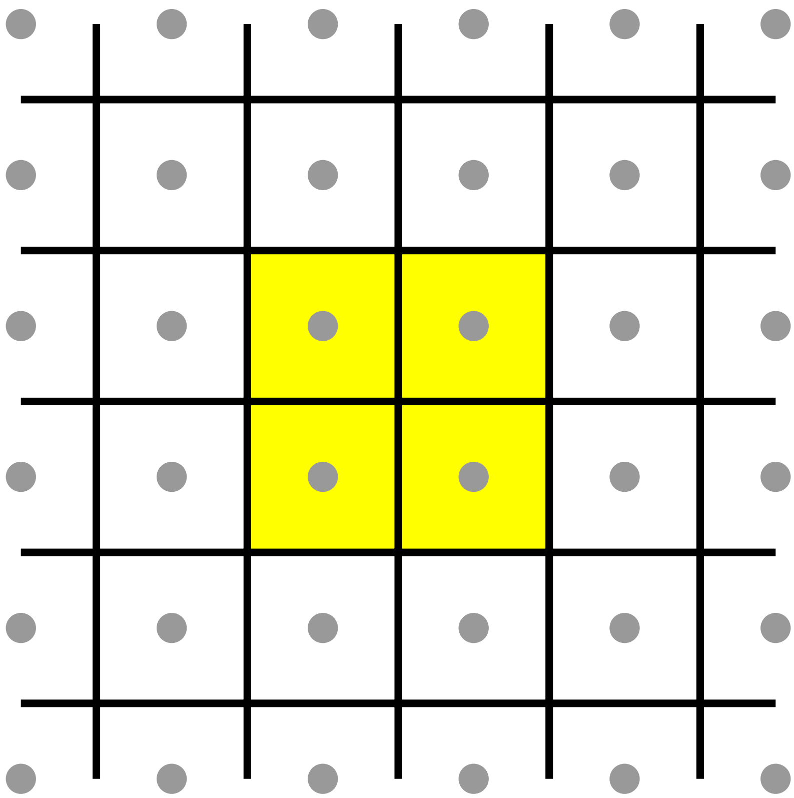


Mesh and Algorithm Refinement

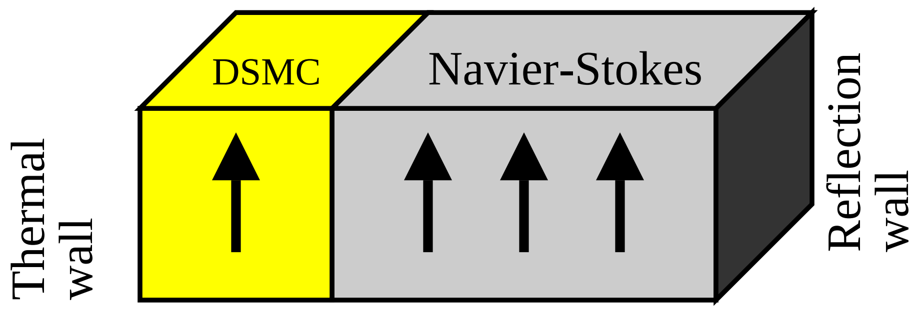
Coarse/DSMC Coupling

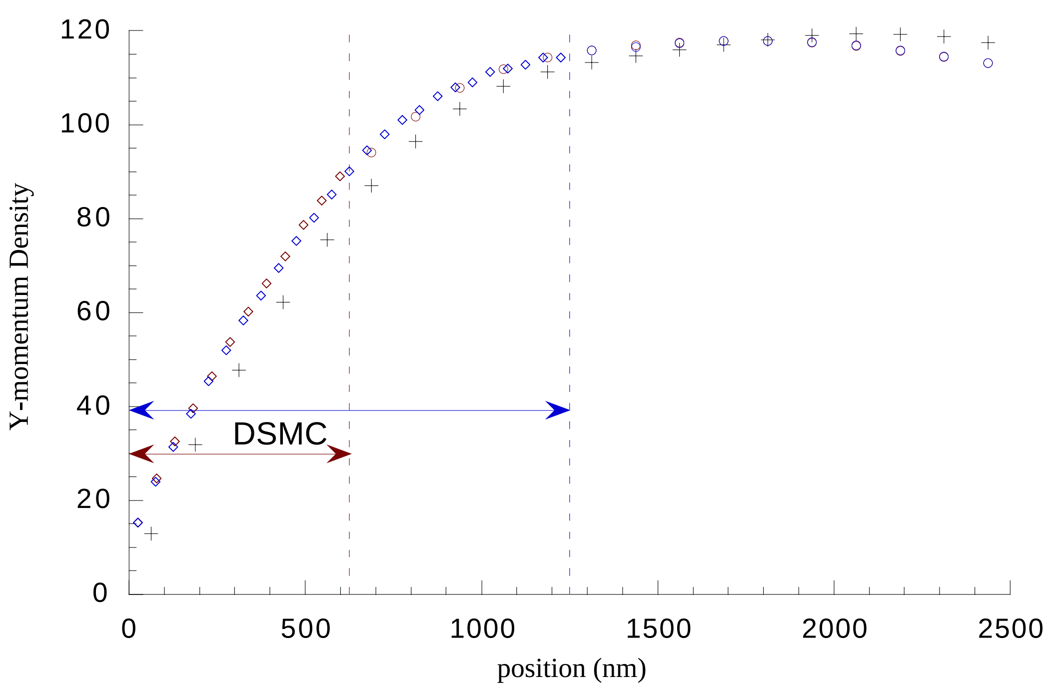
- Advance coarse grid
- Fill DSMC boundary data
  - Create particles in buffer cells
  - Move all particles
  - Record particles crossing interface
  - Discard particles left in buffer region
  - Collide particles within DSMC region
  - Repeat DSMC calculation
- "Reflux" boundary coarse cells
- Backfill overlying coarse cells

MAR Illustration

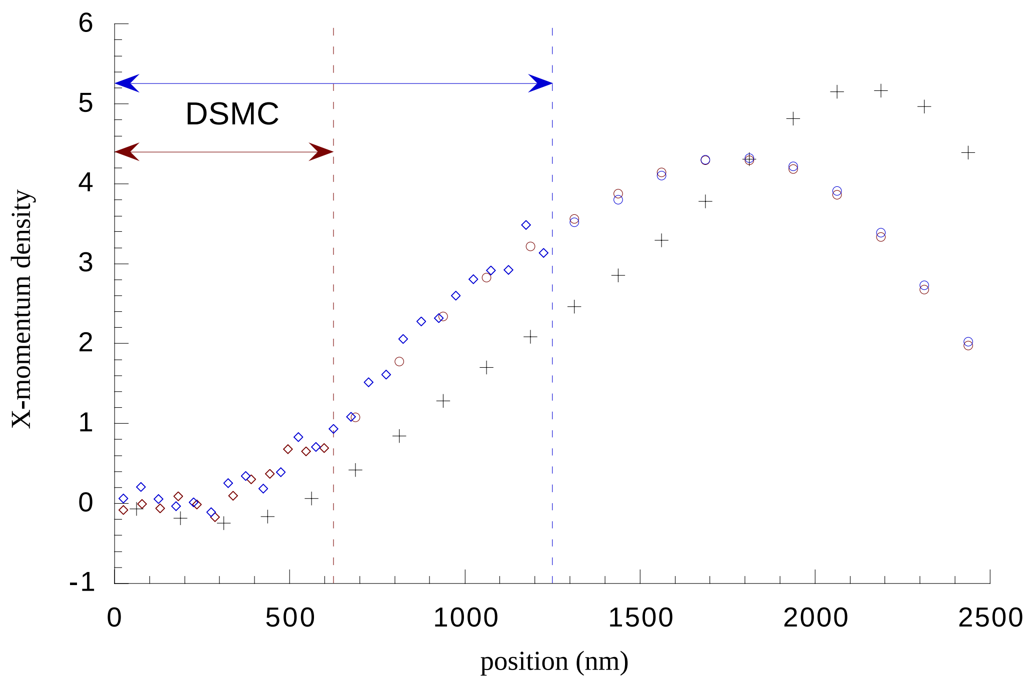


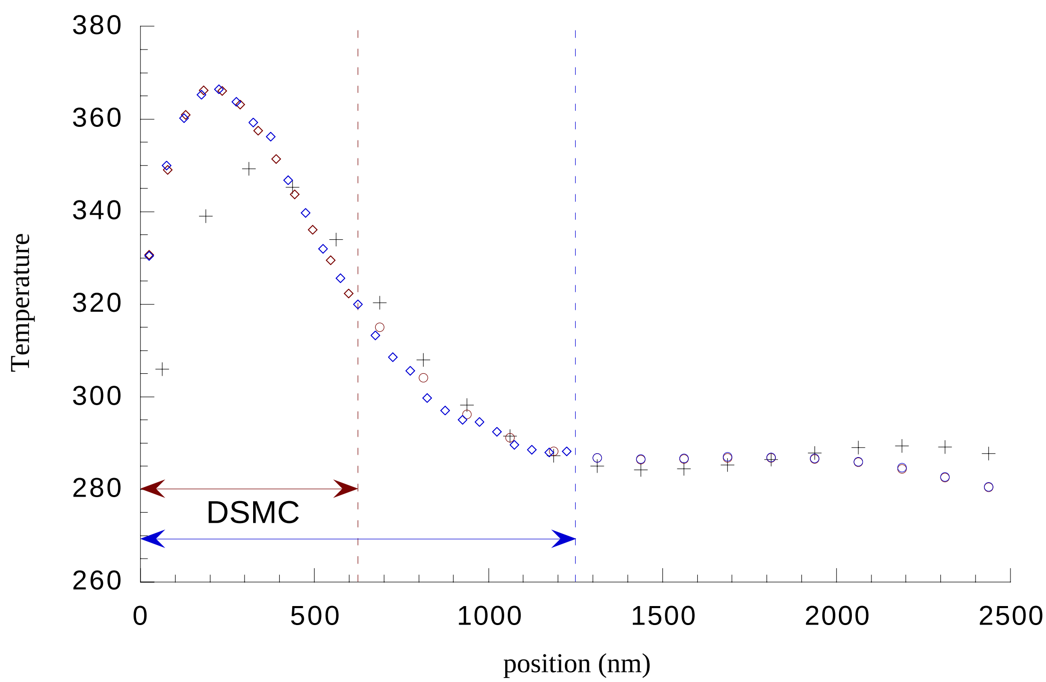
Rayleigh Problem



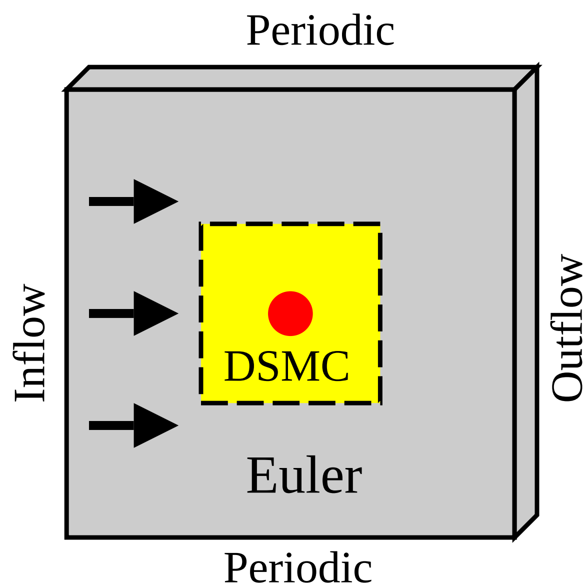


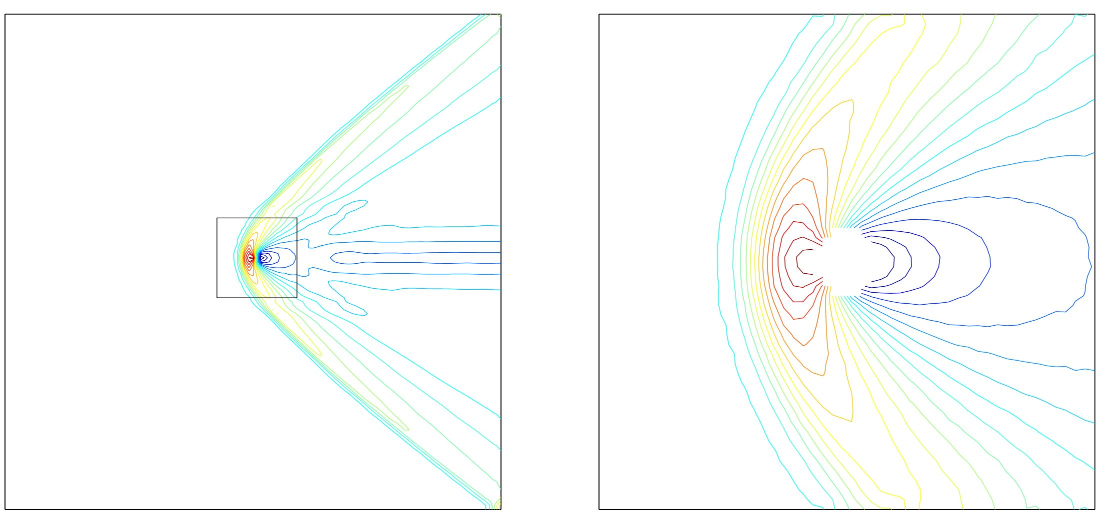
Rayleigh Problem (cont.)





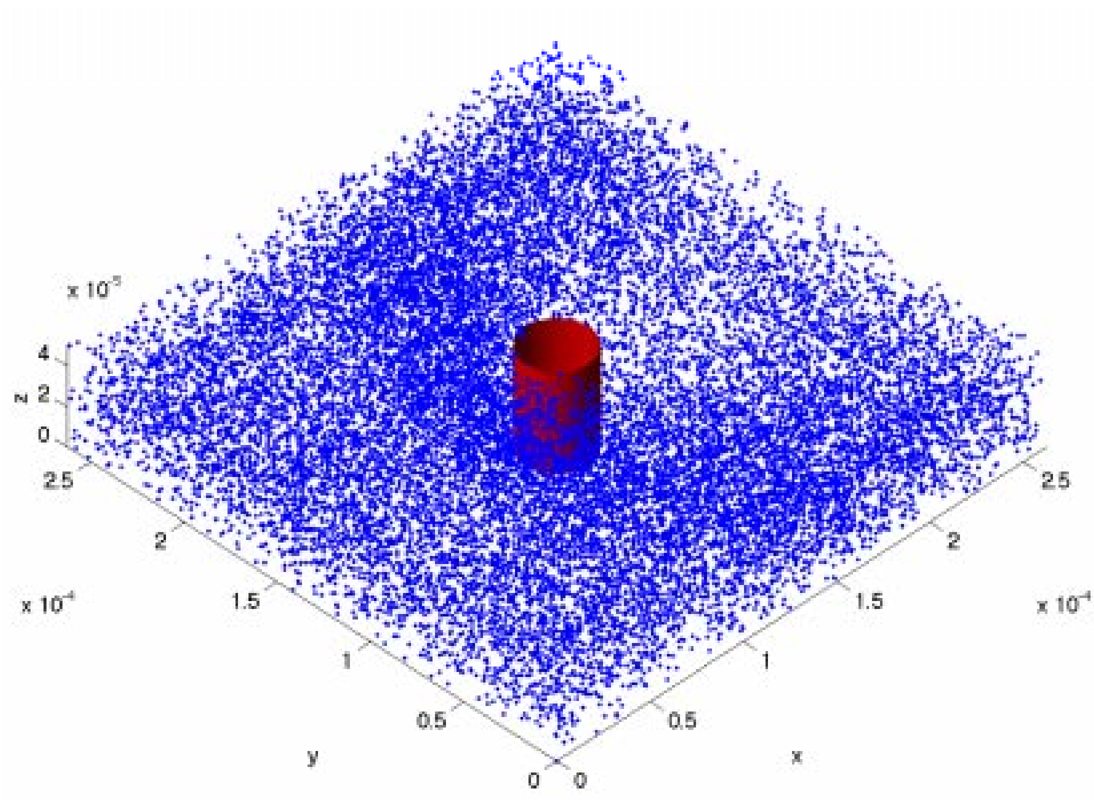
Flow past a Cylinder





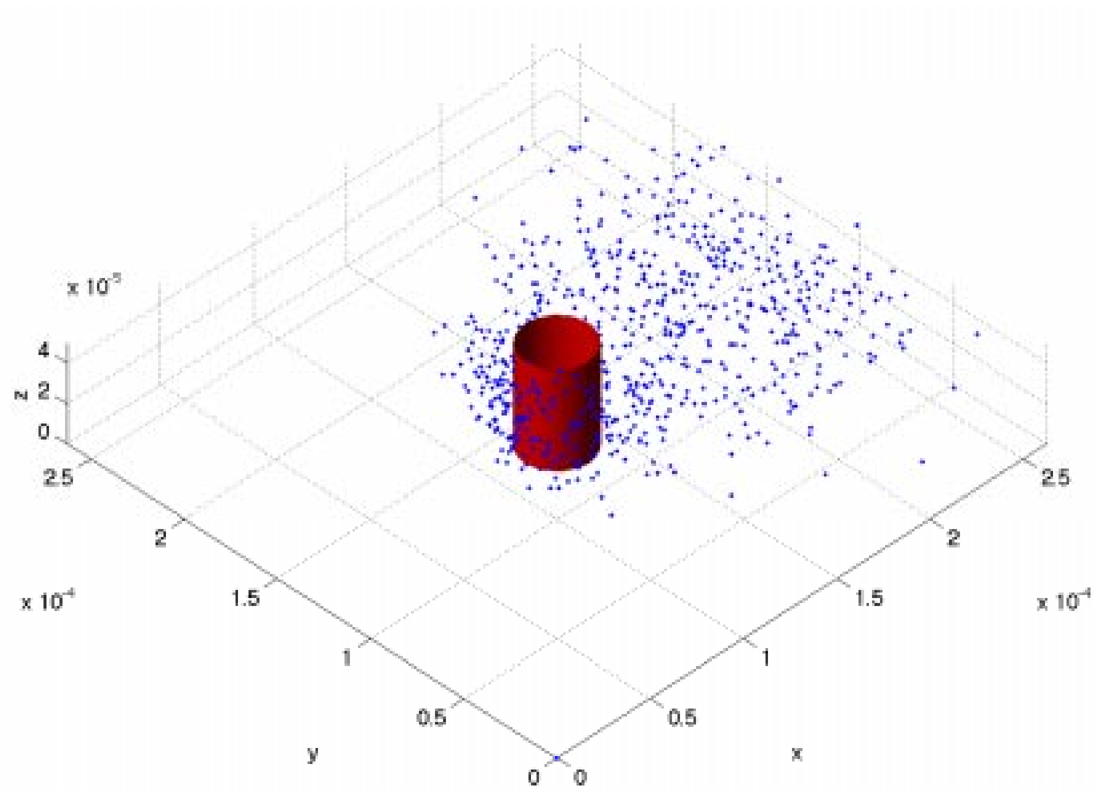
Particles near Cylinder

Sample of particles (1 in 75)



Particles near Cylinder (cont.)

Particles that struck cylinder (1 in 75)



Dense Gas Variants

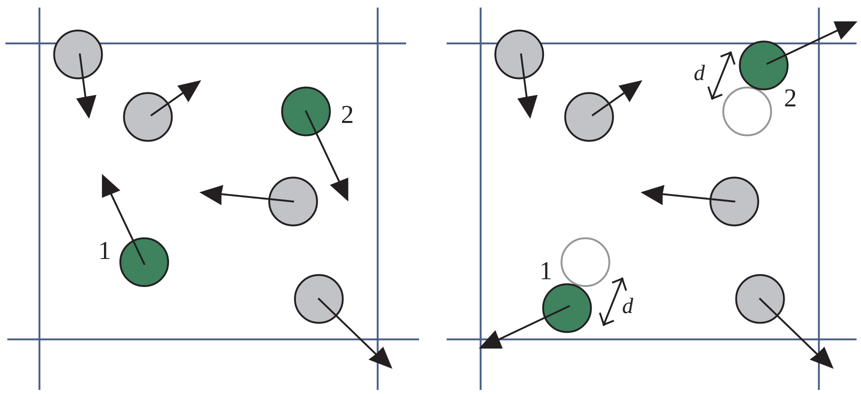
DSMC collisions are statistically equivalent to "point" collisions because particle positions are irrelevant in a collision

Problem:
DSMC gives ideal gas EOS

Solution:
Modify collisions to give non-zero virial

Consistent Boltzmann Algorithm

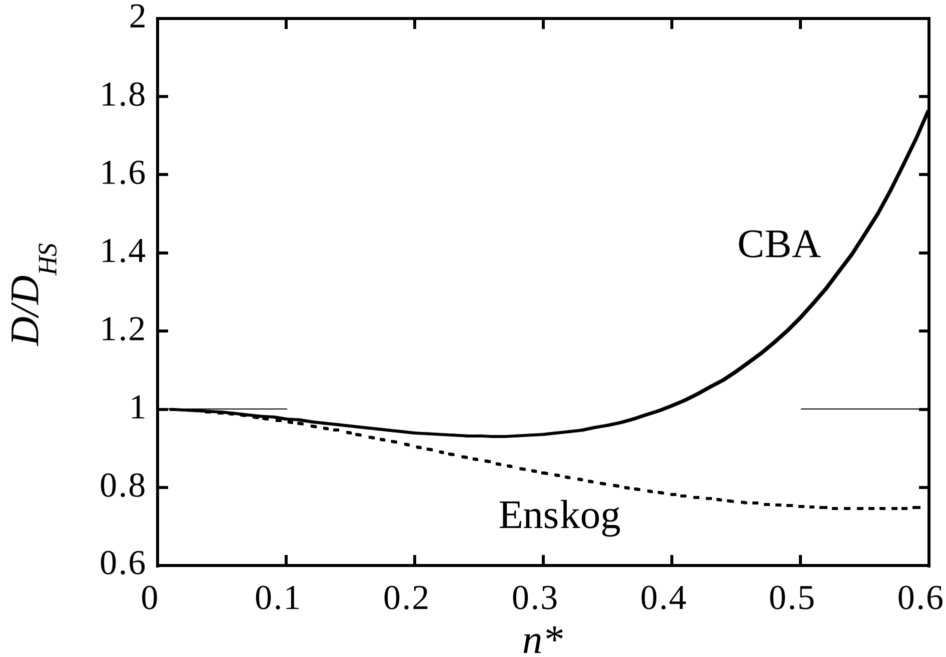
Hard sphere displacement



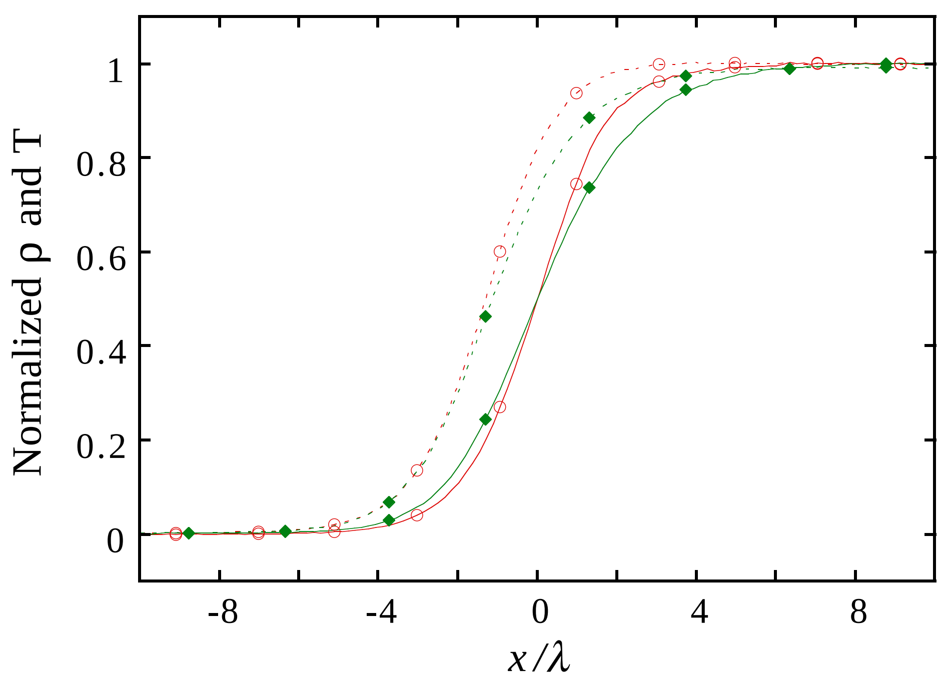
Displacement is parallel to line connecting centers at impact, as determined from pre- and post-collision velocities.

CBA gives *exact* hard sphere equation of state

CBA Results



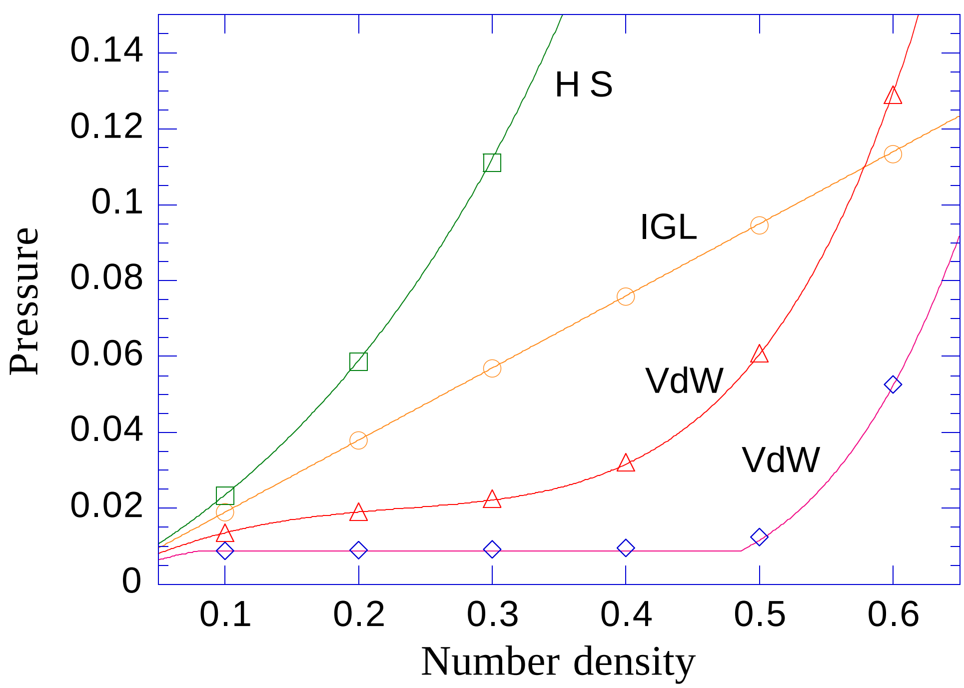
2
1.8
1.6
1.4
1.2
1
0.8
0.6
D/D_{HS}
CBA
Enskog
0
0.1
0.2
0.3
0.4
0.5
0.6
n^*



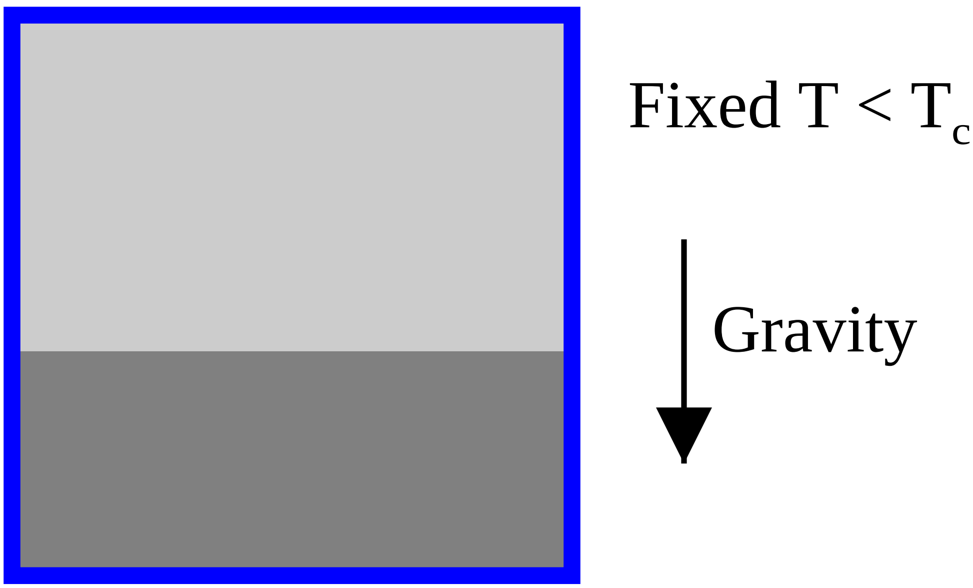
1
0.8
0.6
0.4
0.2
0
Normalized ρ and T
-8
-4
0
4
8
x/λ

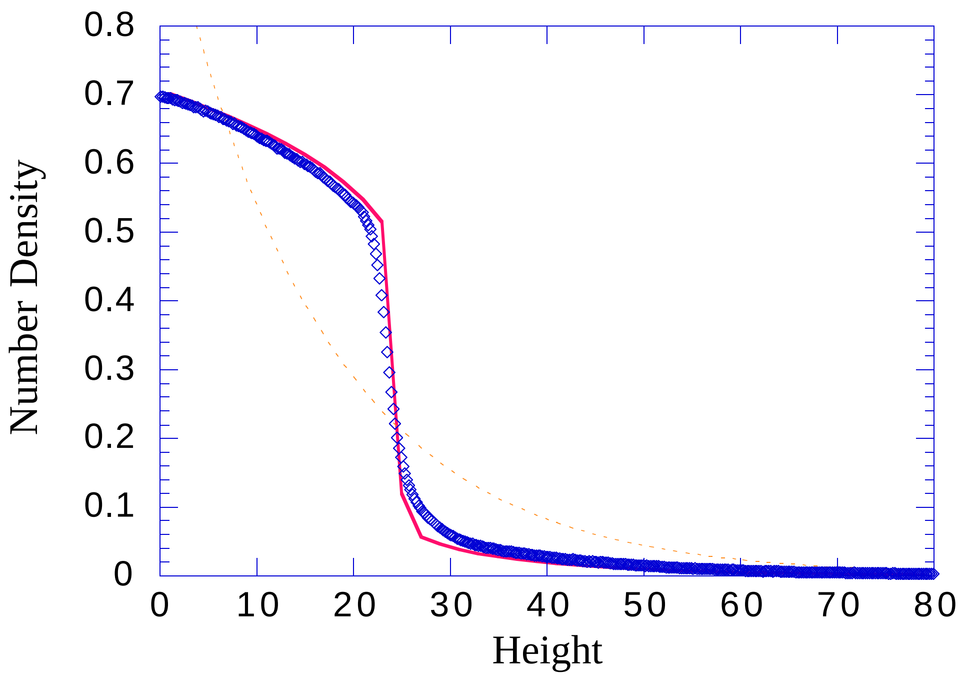
Consistent Universal Boltzmann Algorithm

Magnitude of the displacement varies with density and temperature, according to the desired equation of state.



Van der Waals CUBA





Future Directions

- MAR hybrids using MD, LG or LB

- Particle hybrids (e.g., MD & CBA)

- Statistical mechanics of CUBA models

- Applications (e.g., micromachines)

References

- **DSMC Tutorial**

Alexander & Garcia, Comp. in Phys. **11** 588 (1997)

- **DSMC Book**

Bird, "Molecular Gas Dynamics and the Direct Simulation of Gas Flows", Clarendon, Oxford (1994)

- **DSMC Microflows**

Alexander, Garcia & Alder, Phys. Fluids **6** 3854 (1994)

- **DSMC Fluctuations**

Mansour, Garcia, Lie & Clementi, Phys. Rev. Lett. **58** 874 (1987)

- **Hard sphere CBA**

Alexander, Garcia & Alder, Phys. Rev. Lett. **74** 5212 (1995)

- **Van der Waals CUBA**

Alexander, Garcia & Alder, Physica A **240** 196 (1997)

- **Mesh & Algorithm Refinement**

Garcia, Bell, Crutchfield & Alder, these proceedings