Mesh and Algorithm Refinement

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Outline

Numerical simulation of gas flows combining a particle method and a CFD solver.

- Why use particle methods?
- Direct simulation Monte Carlo (DSMC)
- Mesh and Algorithm Refinement (MAR)
- Numerical examples
- Future directions

Particle Methods

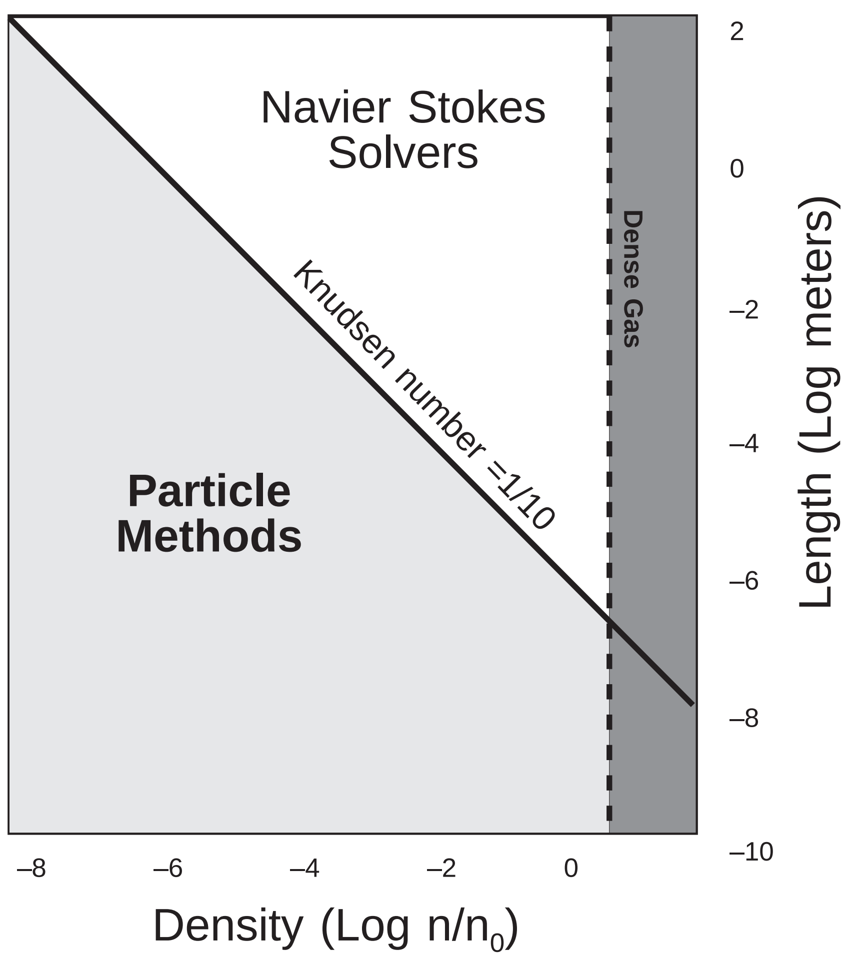
Hierarchy

- Molecular dynamics
- Boltzmann methods
- Lattice gases
- Pseudo-particle methods

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
- Thermal fluctuations and light scattering
- Shock waves and interfaces

Direct Simulation Monte Carlo

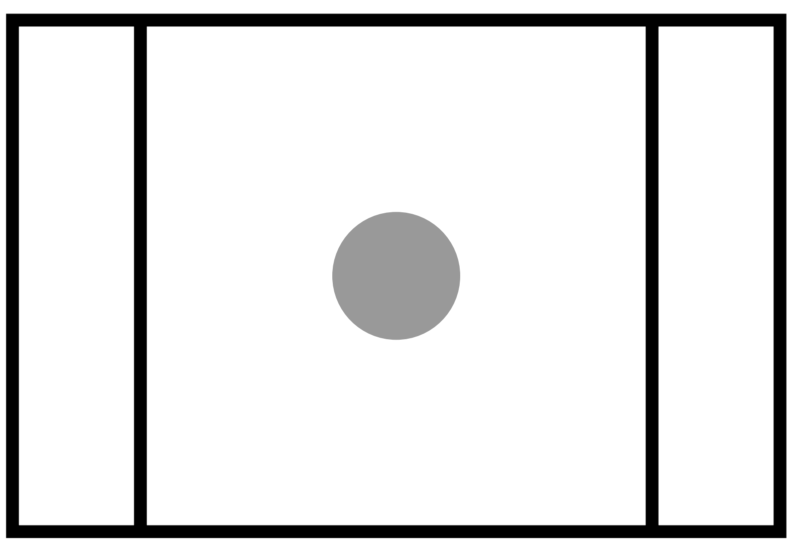
DSMC is a particle-based algorithm for simulating a dilute gas. Particle collisions are evaluated as a stochastic process.

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

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)

DSMC vs CFD

Advantages:

- Correct at high Kn
- Unconditionally stable
- Boundary conditions are simple
- Correct fluctuation spectrum
- Contains microscopic physics

Disadvantage: EXPENSIVE

Solution:

Only use DSMC where it is needed

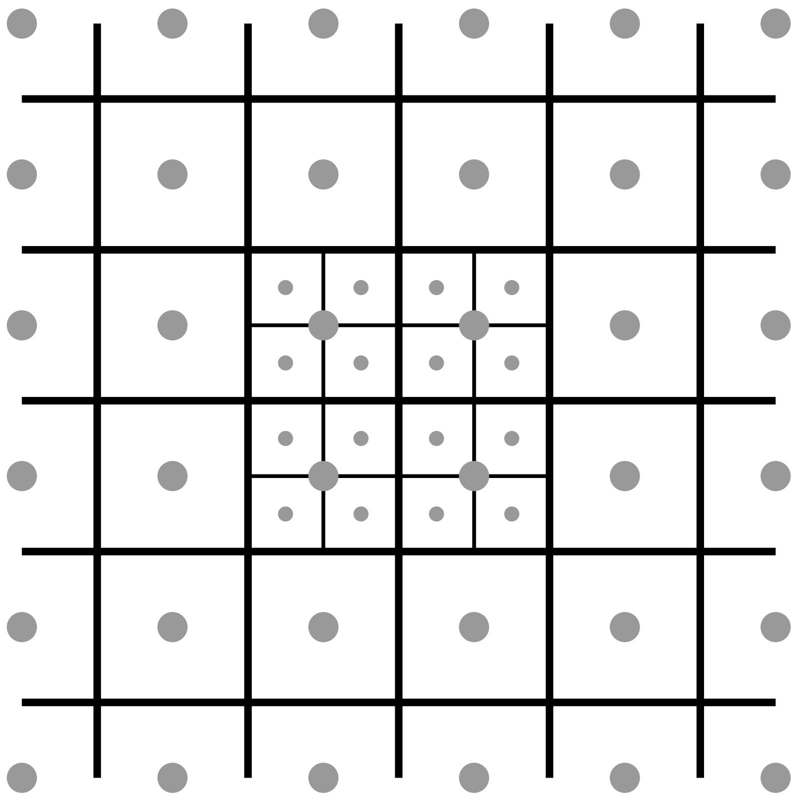
Continuum Mesh Refinement

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

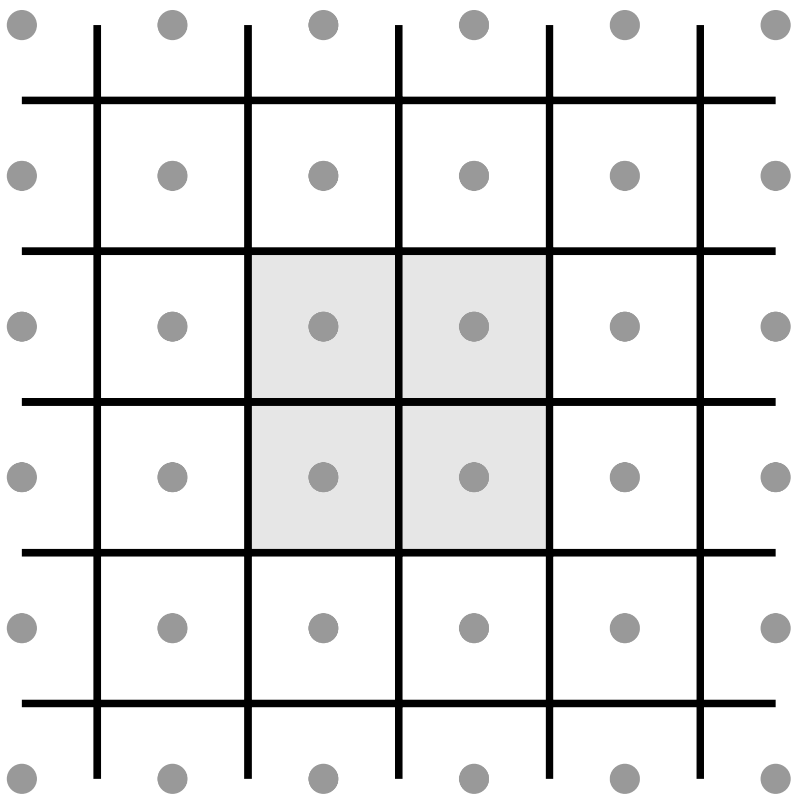


Mesh and Algorithm Refinement

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
- Implicit correction (viscous solver only)
- Backfill overlying coarse cells

MAR Illustration

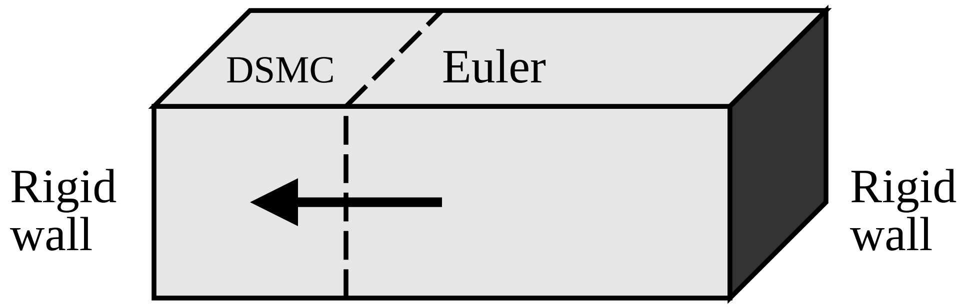


Numerical Examples

Parameters

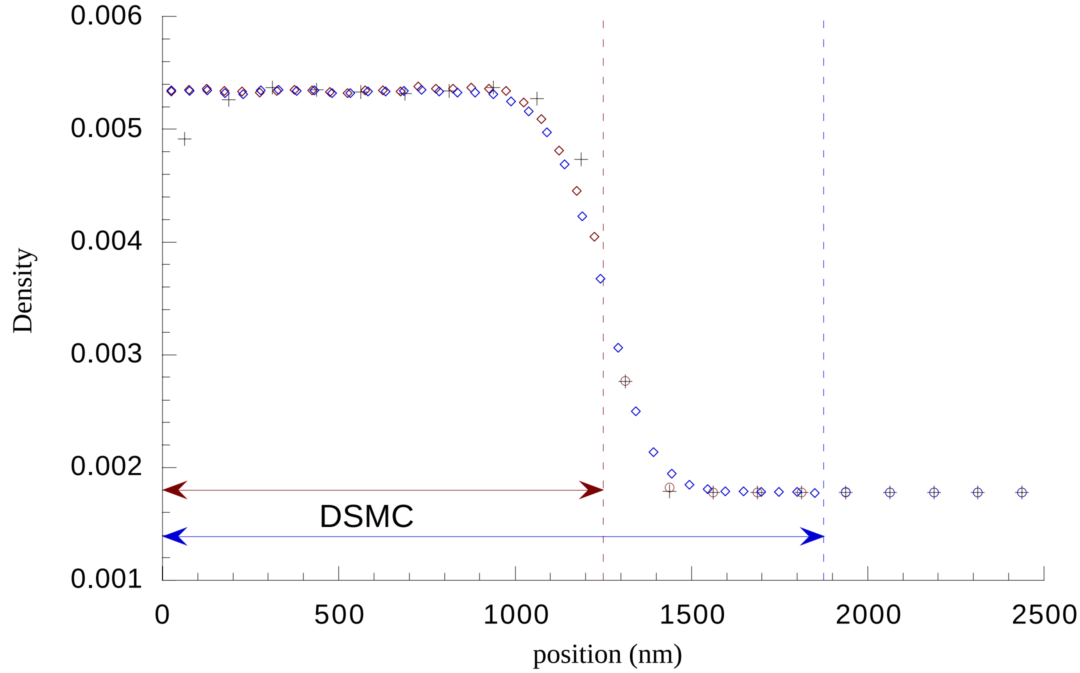
- Hard sphere gas (Argon)
- STP conditions upwind
- Mean free path $\lambda = 62.5$ nm
- 100 DSMC particles per λ^3
- All computations in full 3D
- Grid size = 2λ
- CFL number = 1/4
- Explicit Godunov Euler **or**
- Ex/implicit Godunov Navier–Stokes

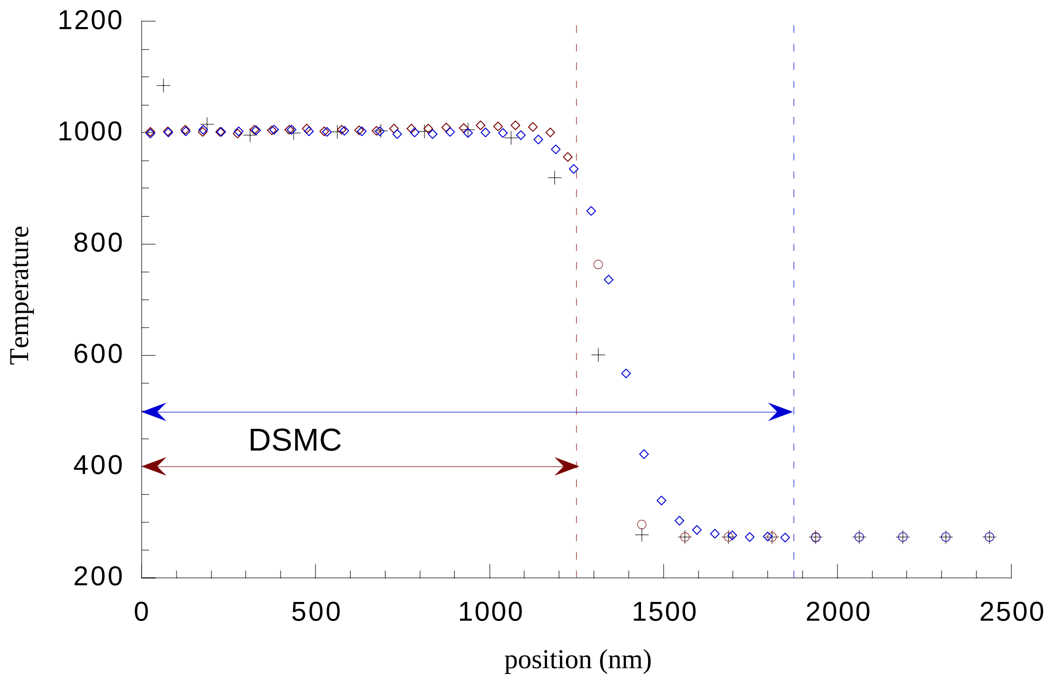
Impulsive Piston



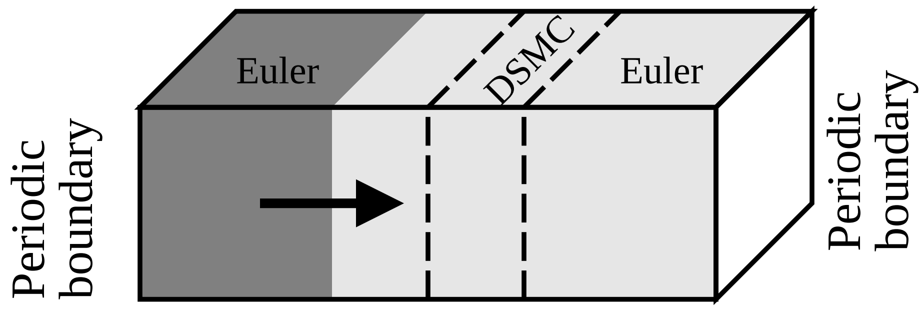
- Piston's reference frame
- Mach 2 piston
- Time-dependent flow
- $100 \times 16 \times 16$ grid
- Run times: 5 min (Euler), 13 hr (MAR)
- 2 to 7 million DSMC particles
- Nearly 200 million collisions

Piston Density & Temperature



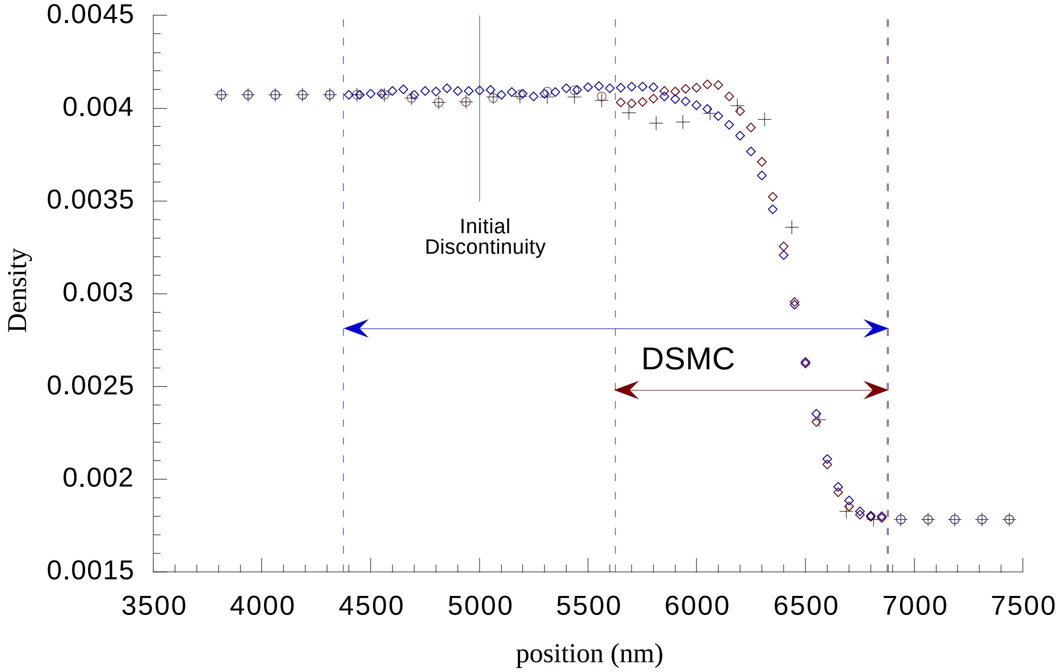


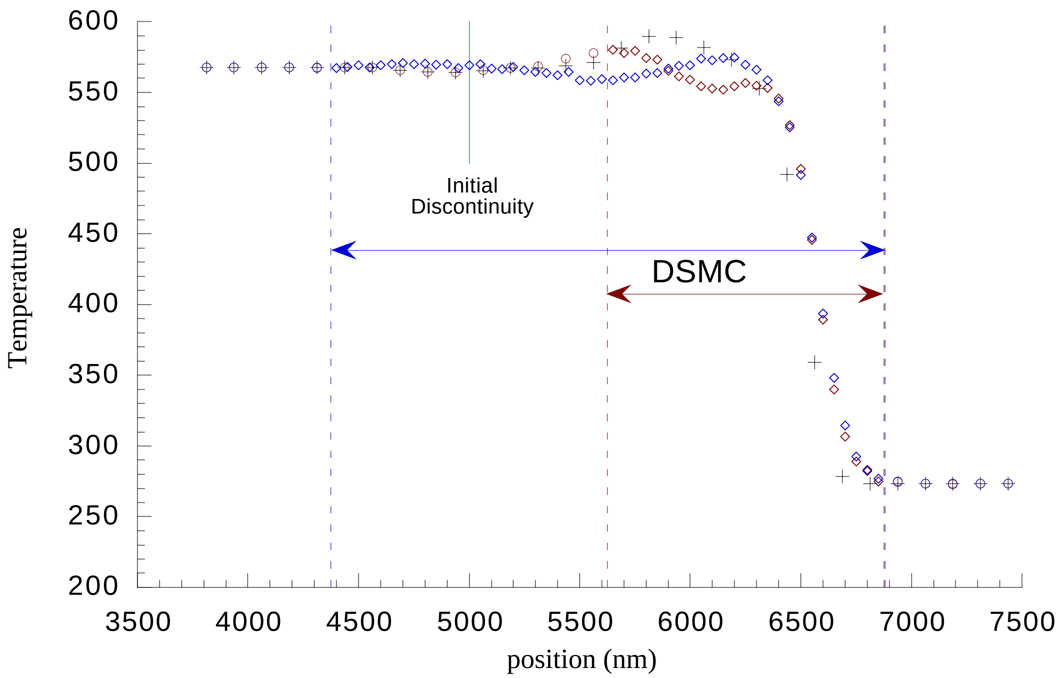
Riemann Problem



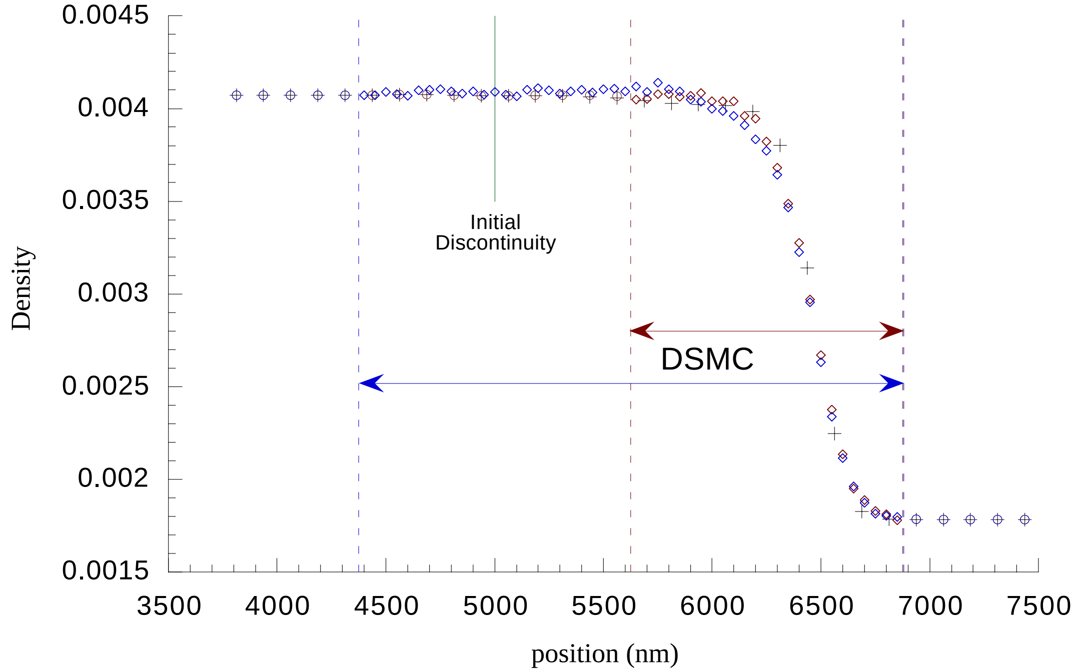
- Mach 2 shock wave jump conditions
- Time-dependent flow
- Initial discontinuity at $x = 5000$ nm
- $100 \times 16 \times (8 \text{ or } 16)$ grid
- Run times: 3 min (Euler), 2 to 8 hr (Euler MAR), 16 min (NS), $1\frac{1}{2}$ to $4\frac{1}{2}$ hr (NS MAR)
- 2 to 8 million particles in system
- Over 100 million collisions

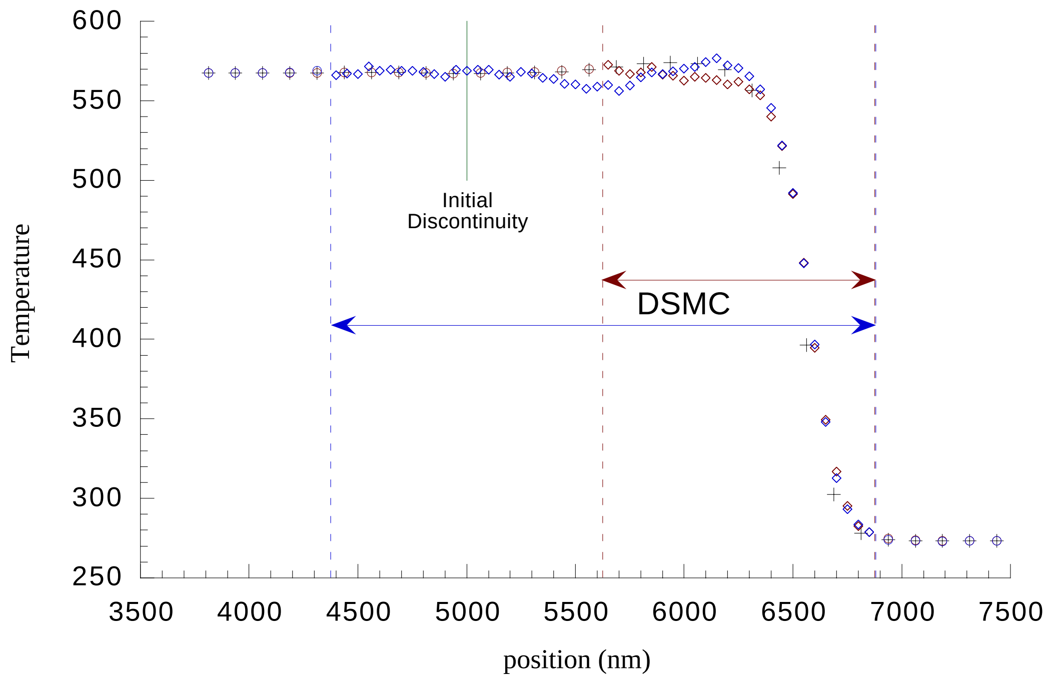
Riemann Problem: Euler



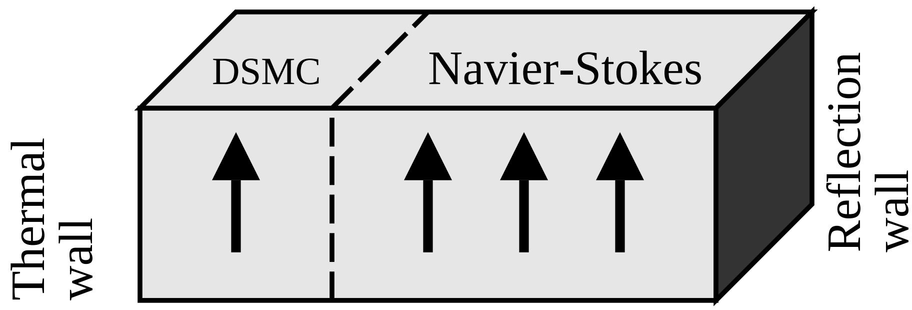


Riemann Problem: Navier–Stokes



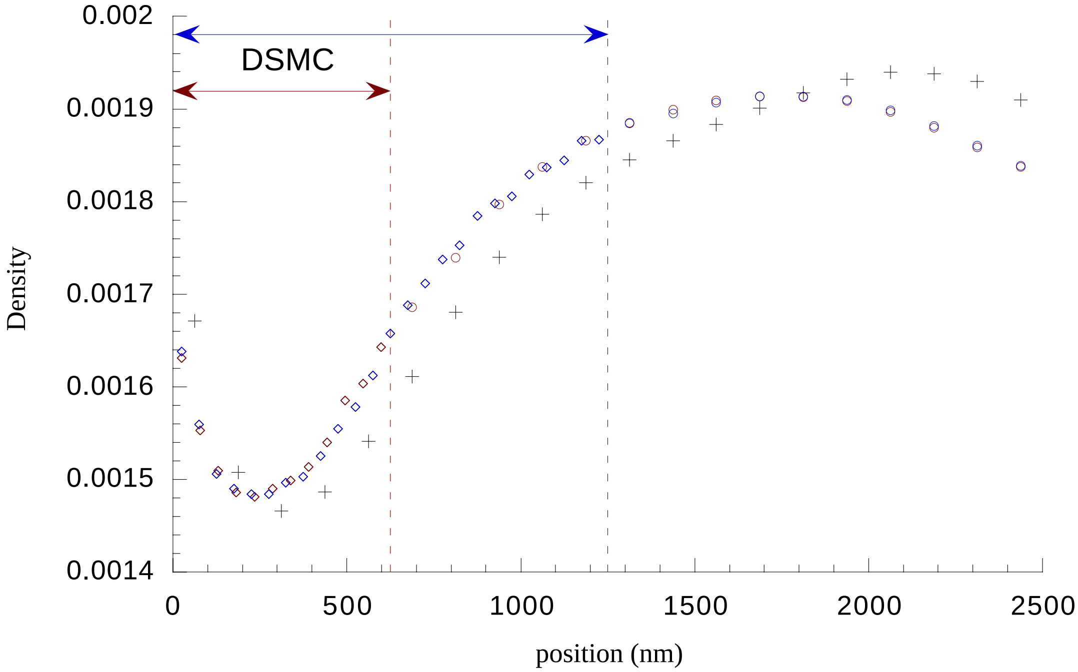


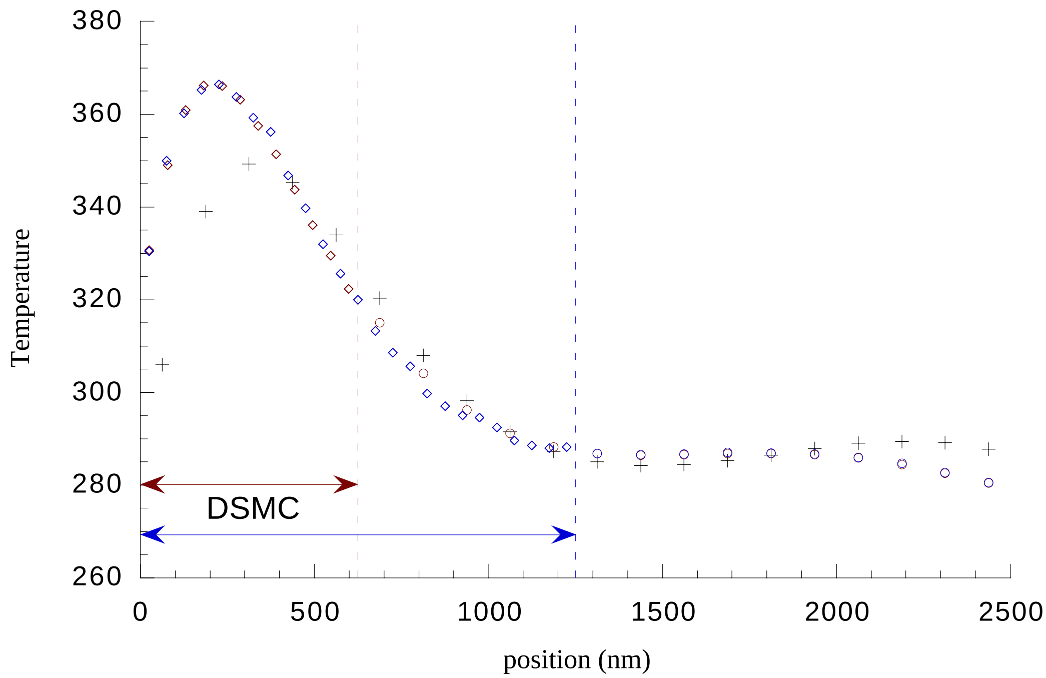
Rayleigh Problem



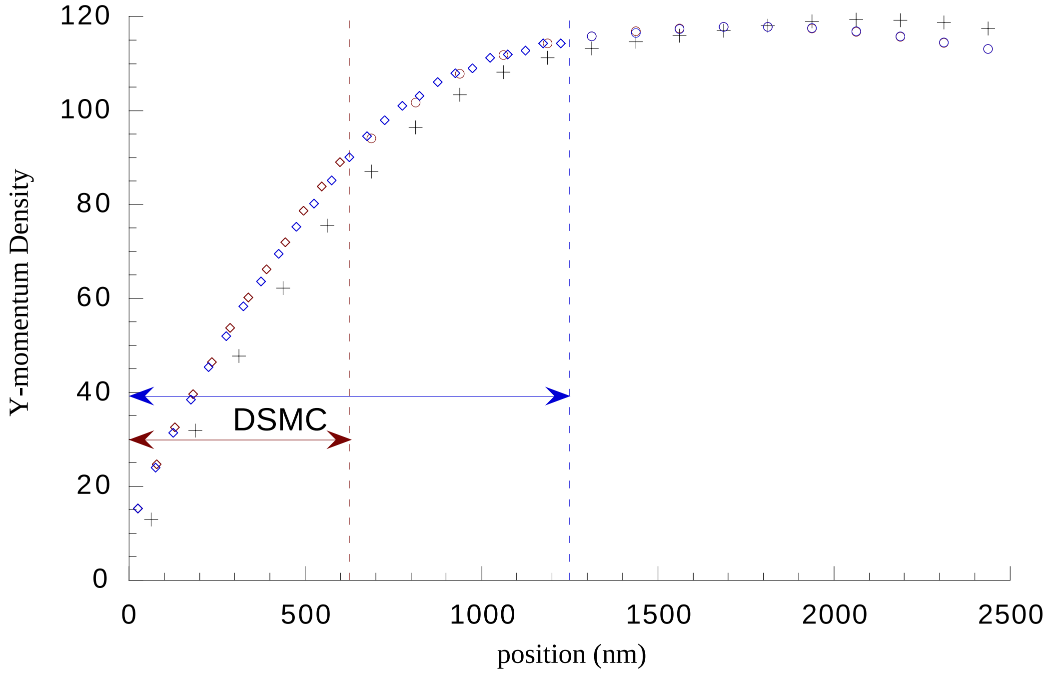
- Moving wall's reference frame
- Mach 2 wall; constant temperature
- Time-dependent flow
- $100 \times 16 \times 16$ grid
- Run times: 45 min (Nav.–St.),
3 to 6 hr (NS MAR)
- 2 to 3 million DSMC particles
- 40 to 70 million collisions

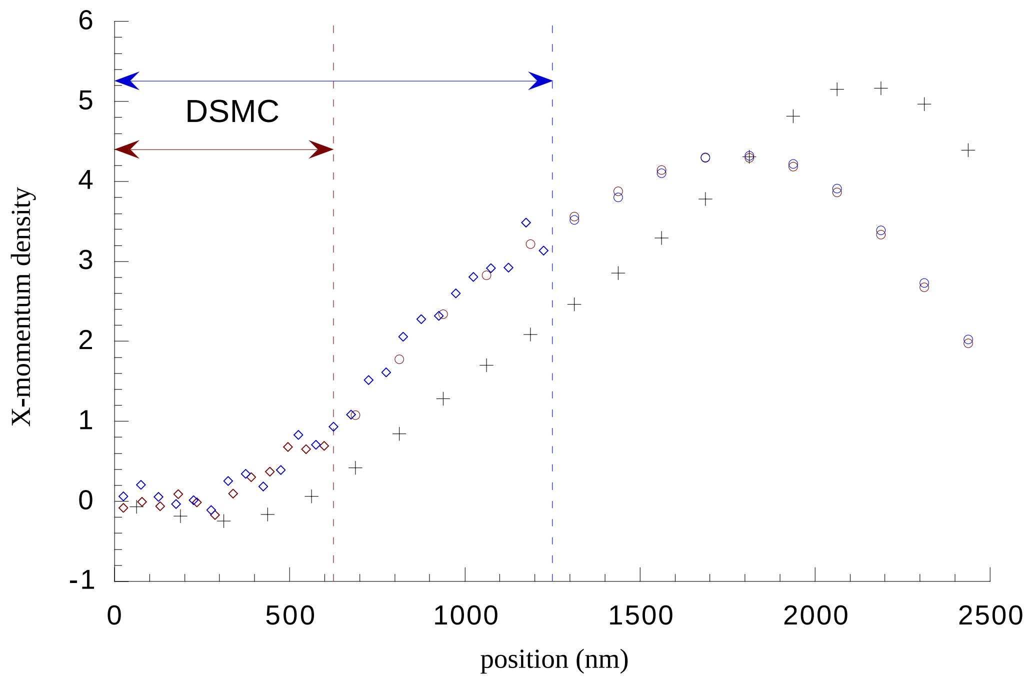
Density & Temperature



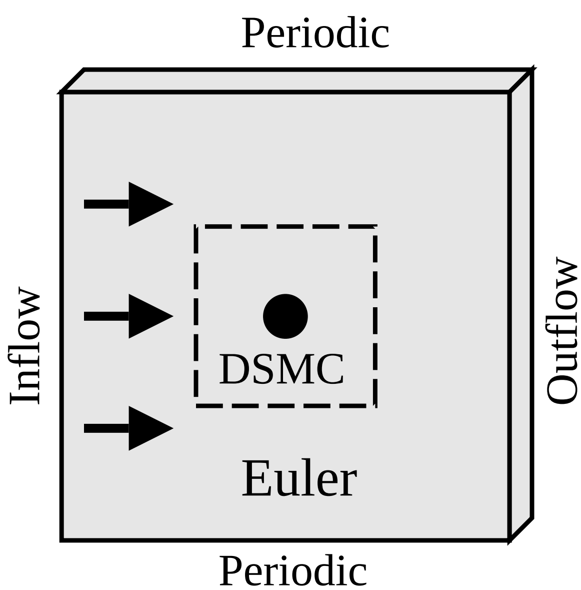


Tangent & Normal Momentum



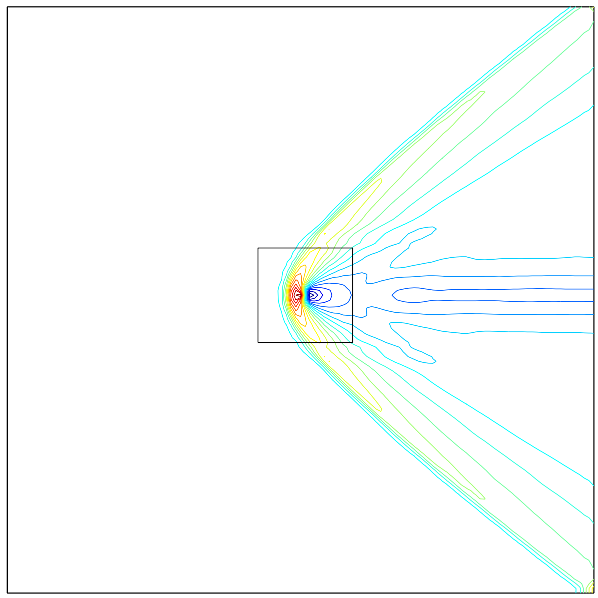


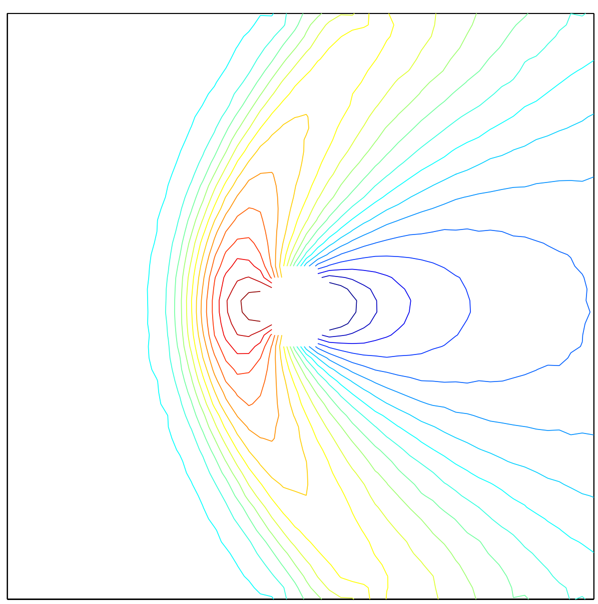
Flow past a Cylinder



- Cylinder's reference frame
- Mach 2 inflow
- Steady state flow
- $125 \times 125 \times 4$ grid
- DSMC region is $< 3\%$ of domain
- Run times: 20 hr per 1000 steps (MAR)
- 1.5 million DSMC particles

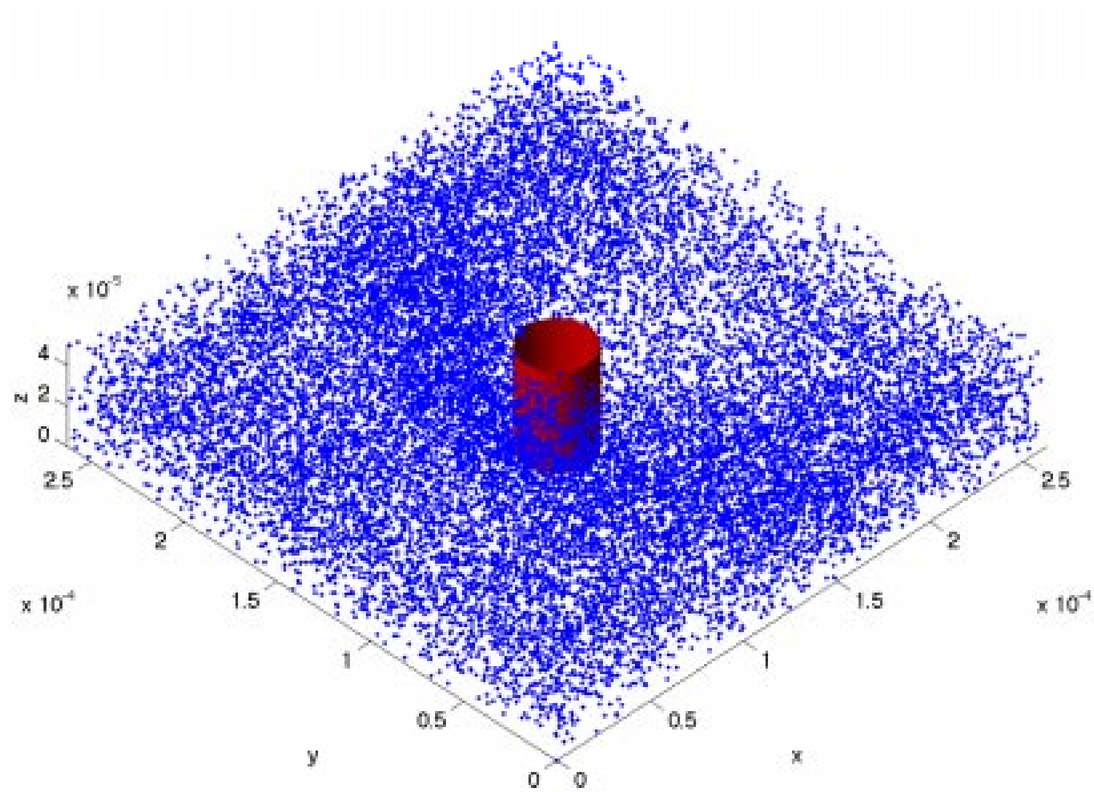
Density past Cylinder





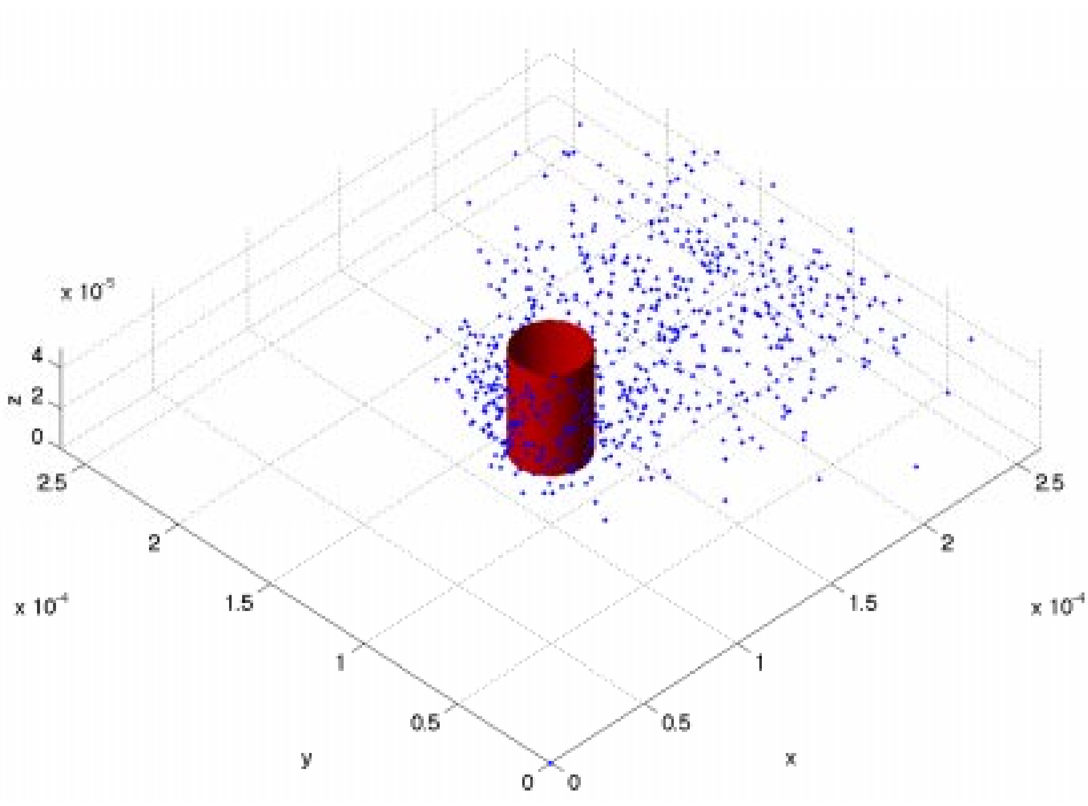
Particles near Cylinder

Sample of particles (1 in 75)



Particles near Cylinder (cont.)

Particles that struck cylinder (1 in 75)



Future Work

- Parallel version
- Fully adaptive mesh refinement
- Dense gases & liquids (CUBA)
- Molecular dynamics MAR
- Applications