Mesh and Algorithm Refinement using DSMC

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Introduction

Mesh and Algorithm Refinement (MAR) implements DSMC at the finest level of a CFD mesh refinement calculation.

Typical application is flow past a microscopic object.

Outline

- MAR algorithm
- Numerical examples
- Concluding remarks

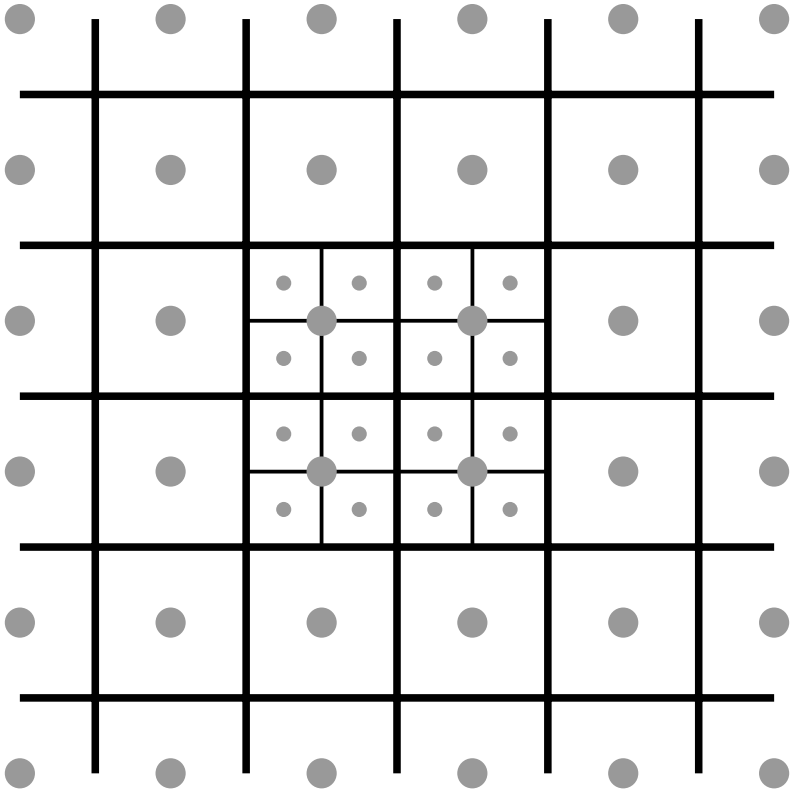
Ordinary Mesh Refinement

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

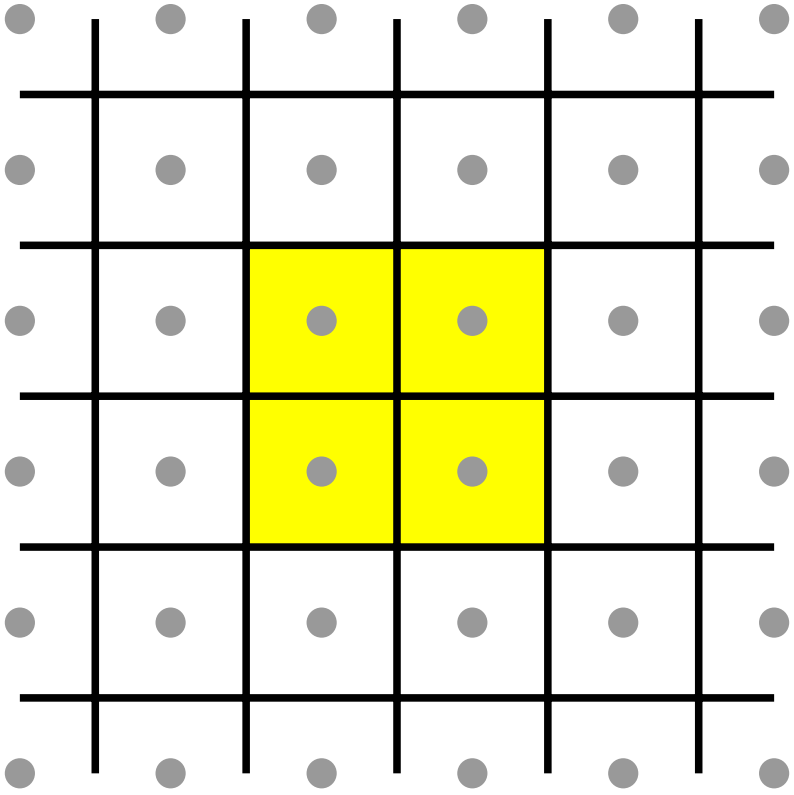


Mesh and Algorithm Refinement

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

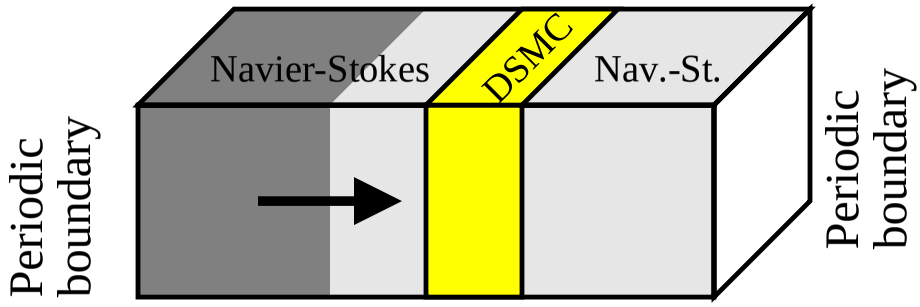


Numerical Examples

Parameters

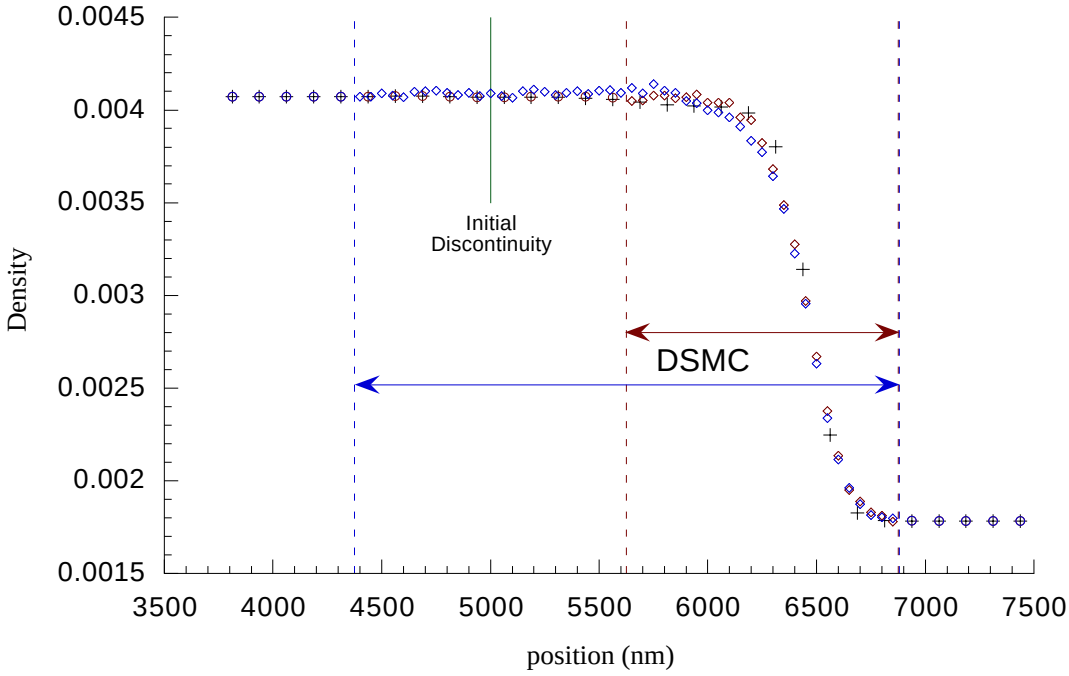
- Hard sphere gas (Argon)
- STP conditions upwind
- Mean free path $\lambda = 62$ nm
- 100 DSMC particles per λ^3
- All computations in full 3D
- Grid size $= 2\lambda$
- CFL number $= 0.25$
- Ex/implicit Godunov Navier–Stokes
- DEC Alpha workstation

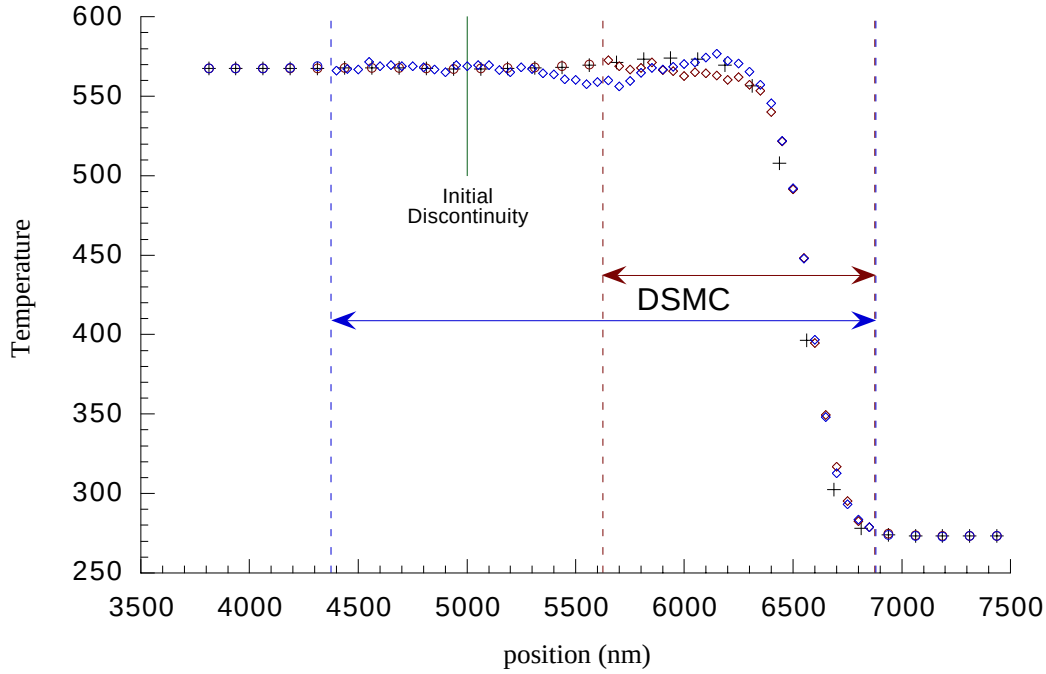
Riemann Problem



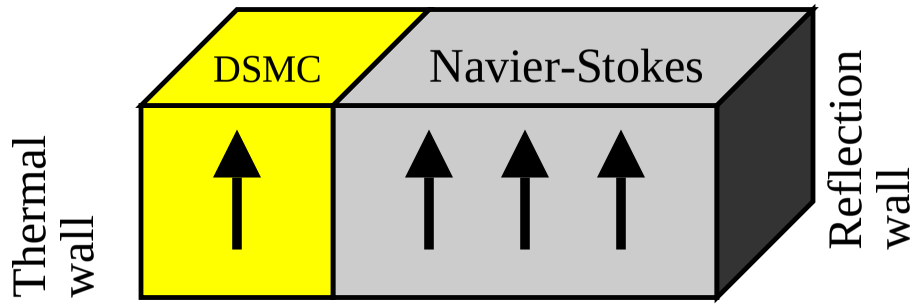
- Mach 2 shock wave jump conditions
- Time-dependent flow
- Initial discontinuity at $x = 5000$ nm
- Coarse grid is $100 \times 16 \times 8$
- DSMC: $(10 - 20) \times 16 \times 8$ grid points
- Run times: 16 min (Navier–Stokes)
  90 to 300 min (MAR)
- 1 to 4 million particles in system
- Over 50 million collisions

Density & Temperature



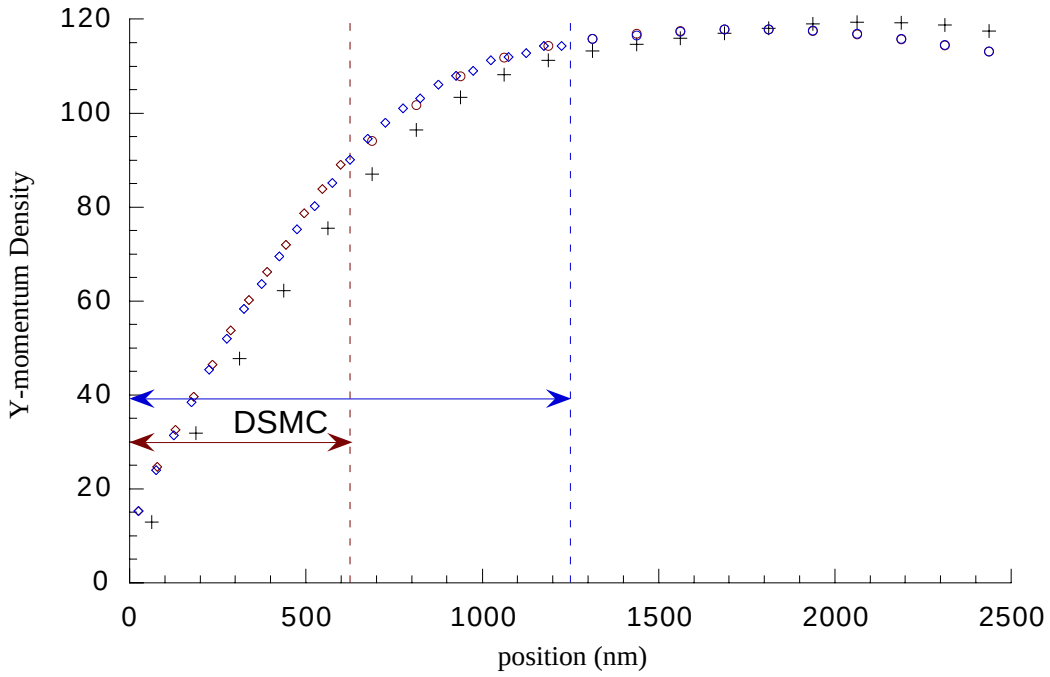


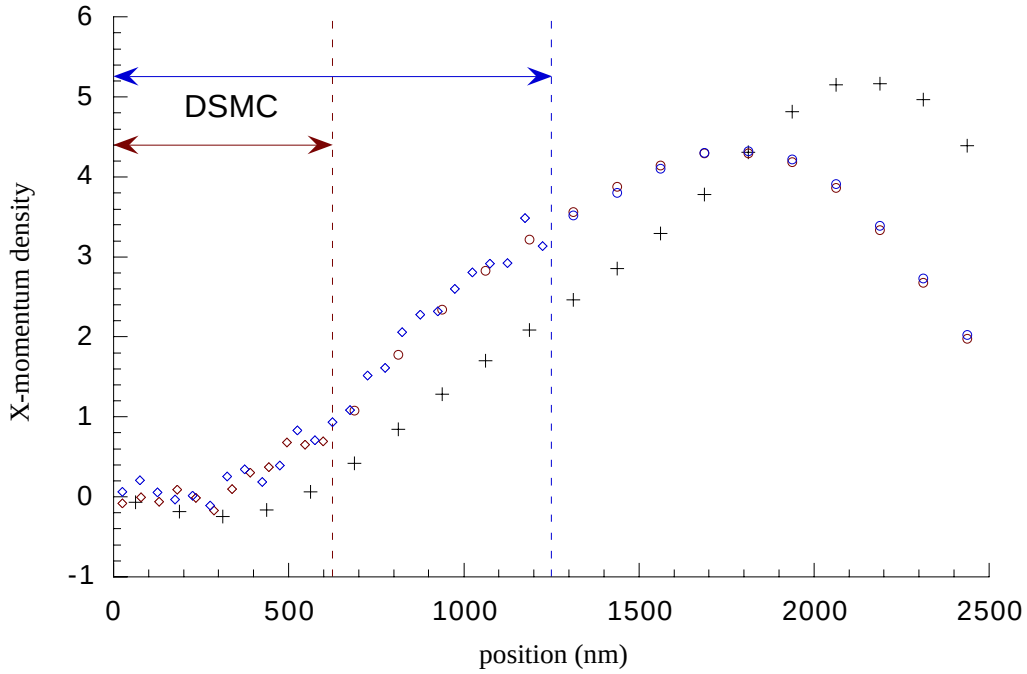
Rayleigh Problem



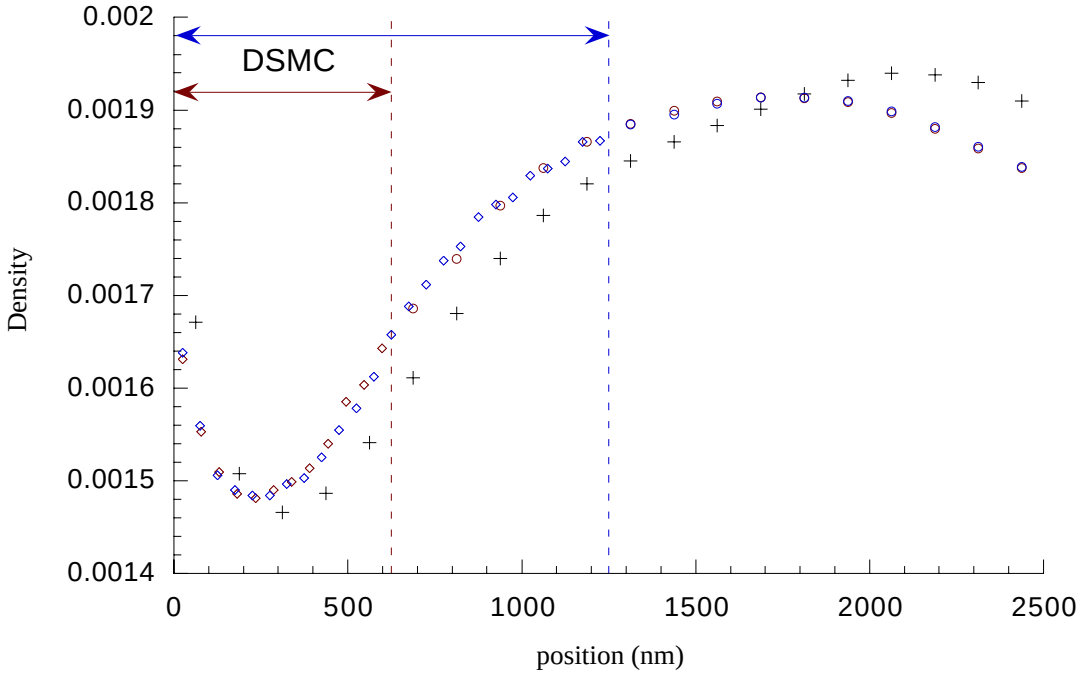
- Moving wall's reference frame
- Mach 2 wall; constant temperature
- Time-dependent flow
- Coarse grid is $100 \times 16 \times 16$
- DSMC: $(5 - 10) \times 16 \times 16$ grid points
- Run times: 45 min (Navier–Stokes)
  3 to 6 hr (MAR)
- 2 to 3 million DSMC particles
- 40 to 70 million collisions

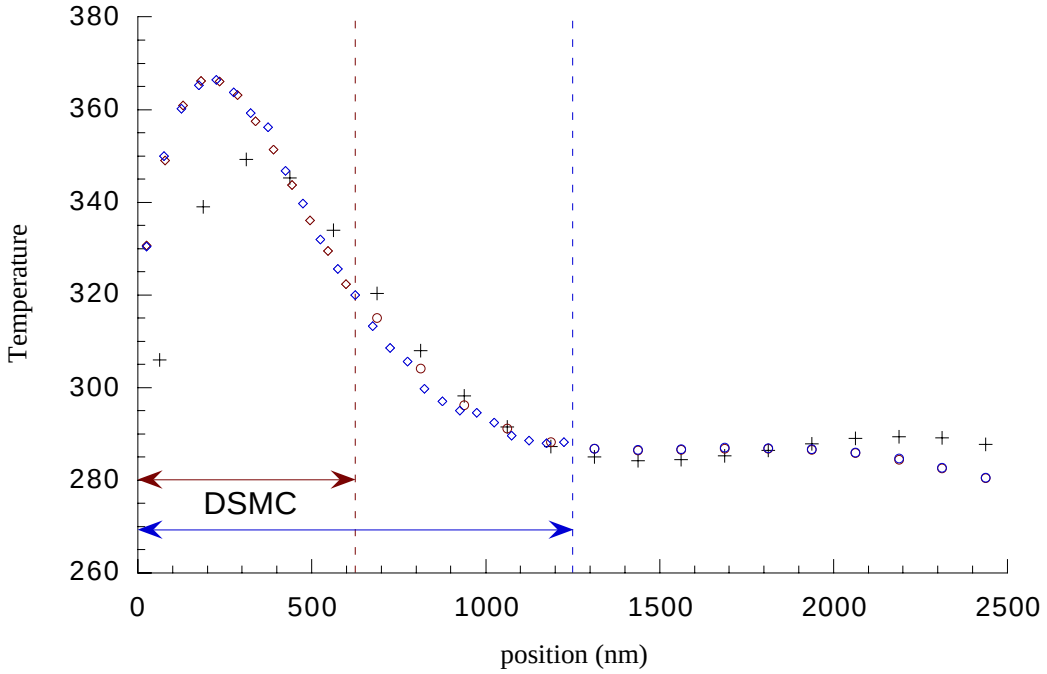
Parallel & Normal Momentum



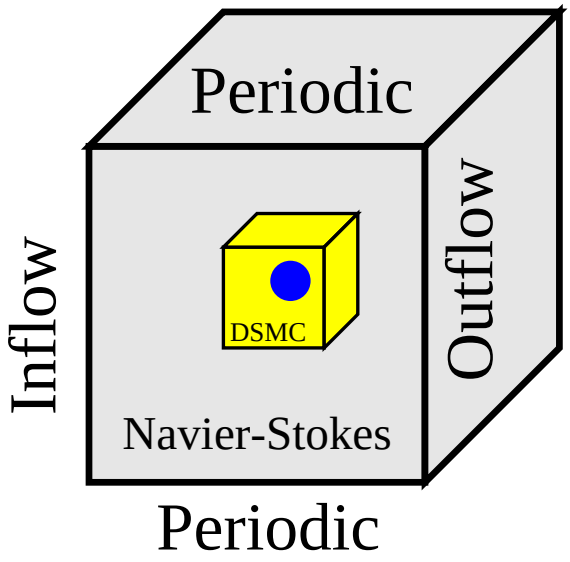


Density & Temperature





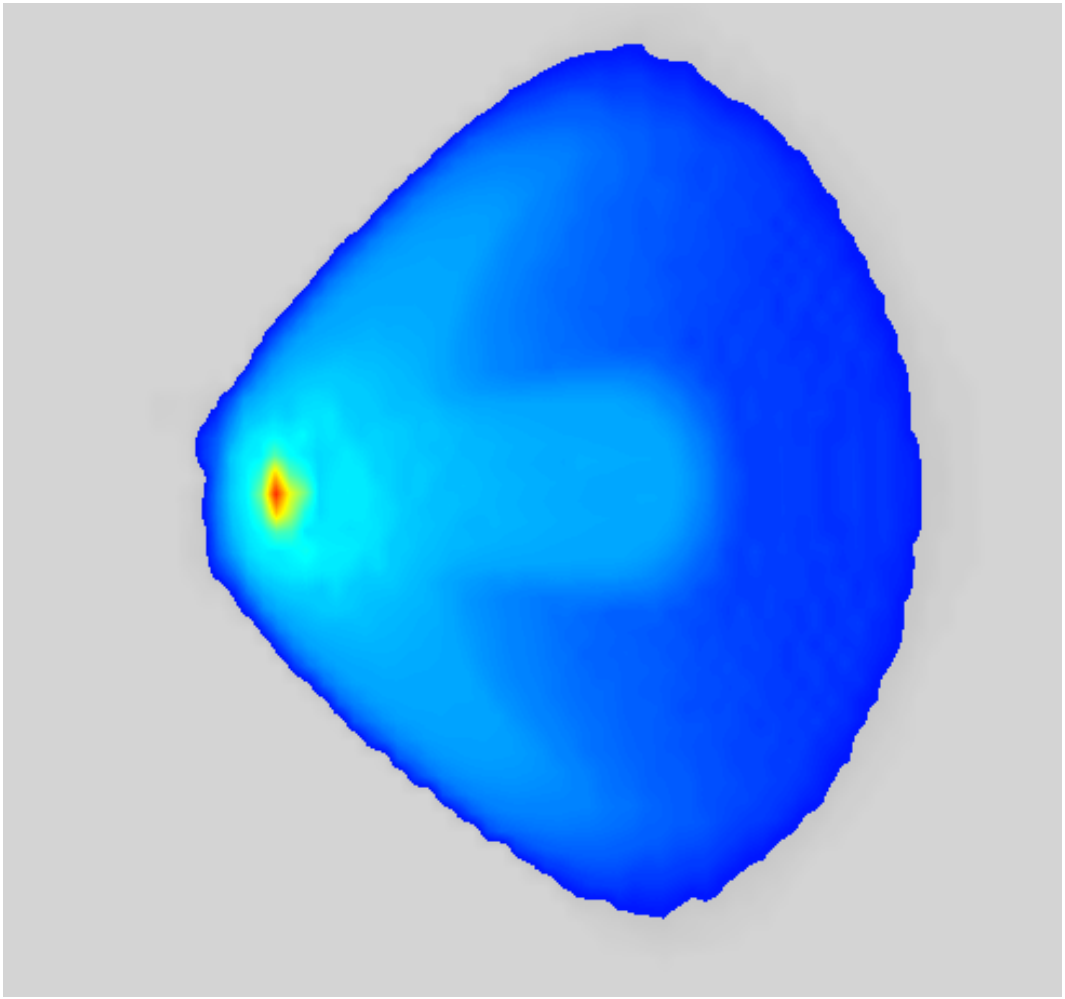
Flow past a Sphere



- Sphere's reference frame
- Diameter = 5 mean free paths
- Mach 2 inflow
- Steady state flow
- Coarse grid is $50 \times 50 \times 50$
- DSMC: $10 \times 10 \times 10$ grid points
- DSMC occupies $< 1\%$ of domain
- Run times: 4 hr per 100 steps
- 800 thousand DSMC particles

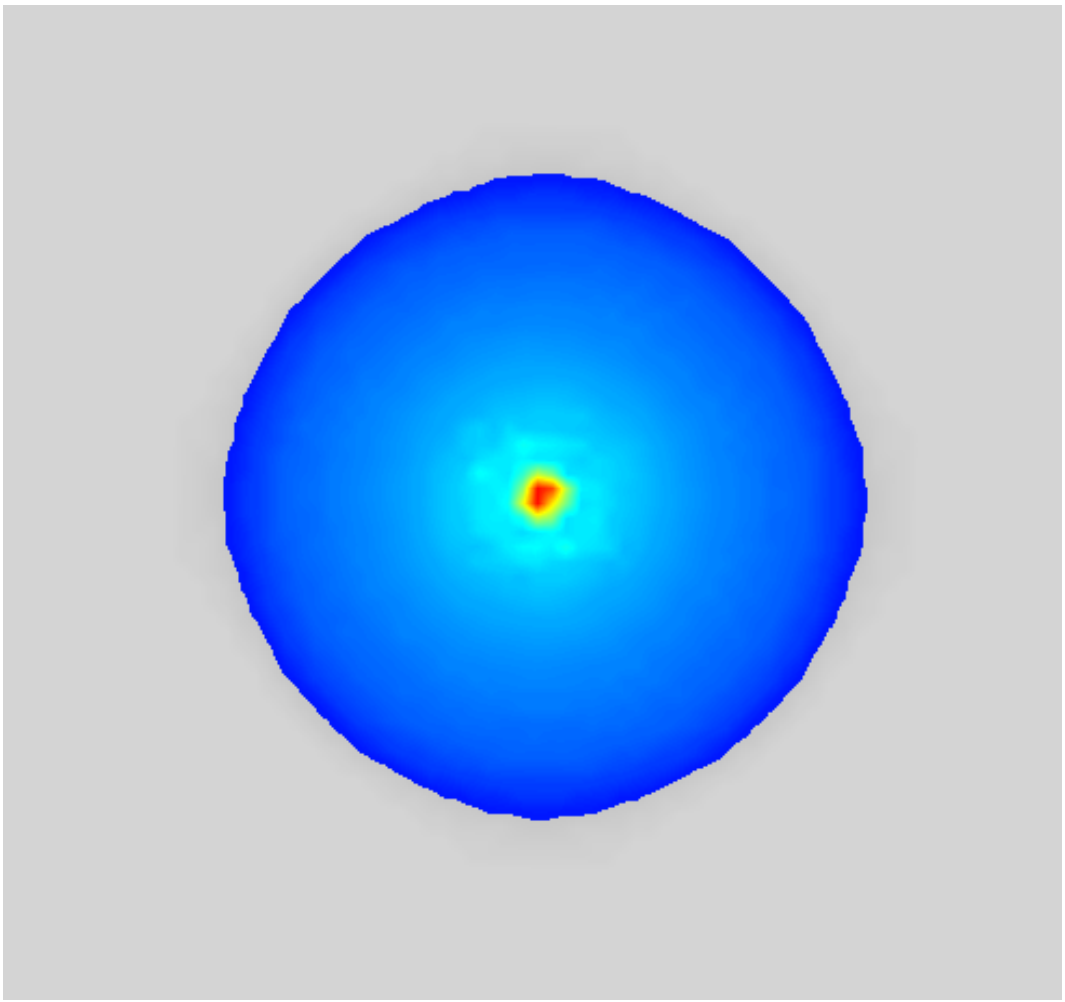
Temperature past Sphere

Full system



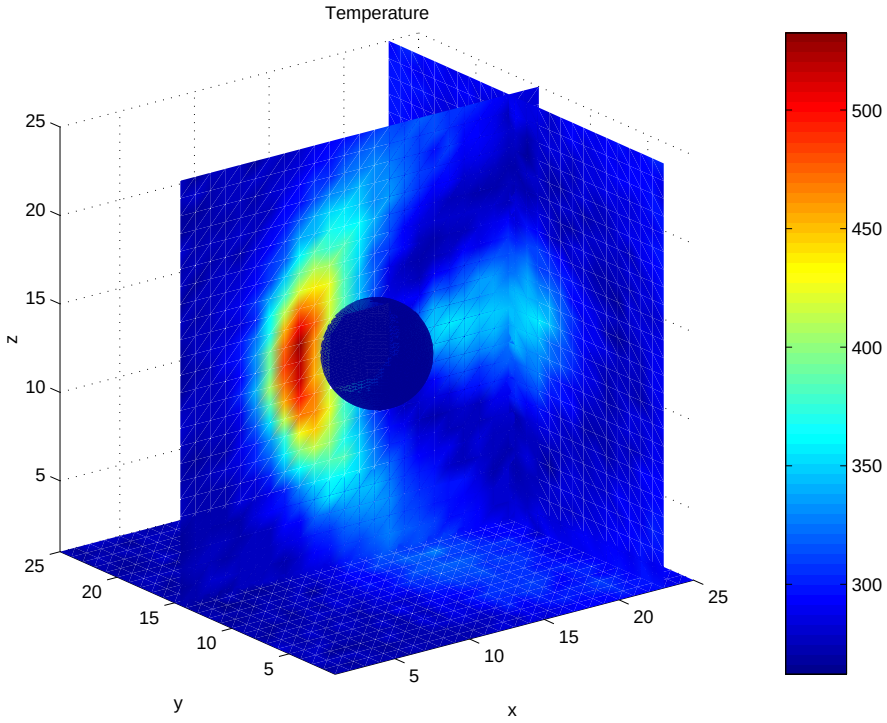
Temperature past Sphere

Front view

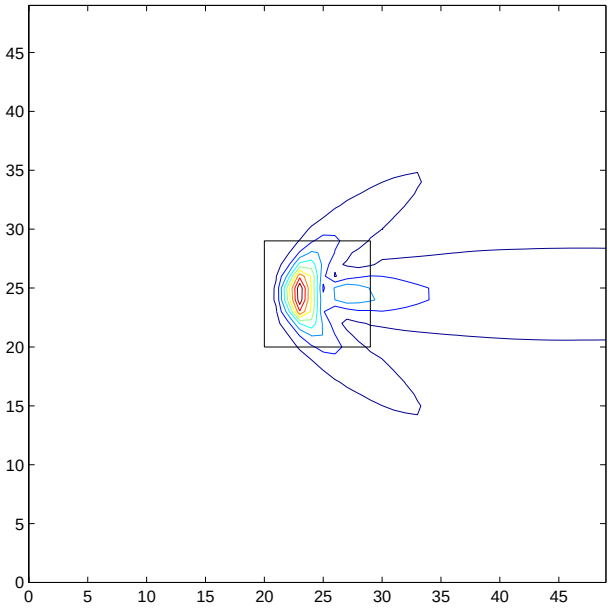


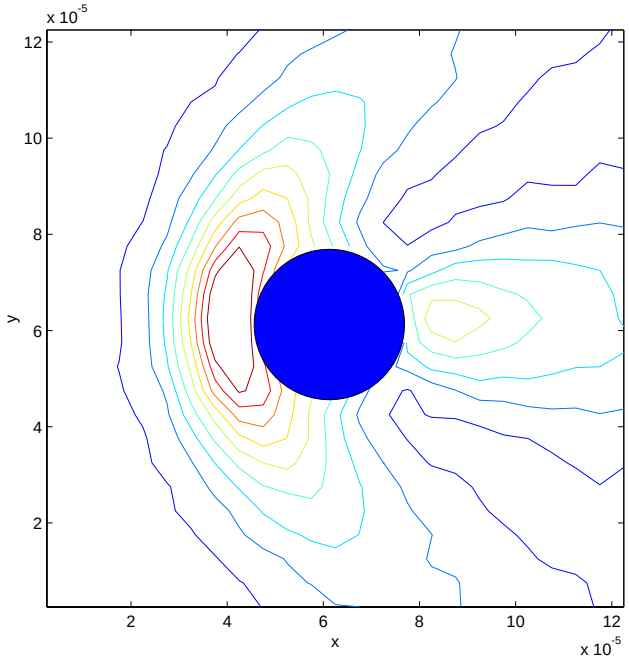
Temperature past Sphere

DSMC region



Temperature past Sphere





MAR Highlights

- Particle description at finest grid level
- DSMC transparent to Navier–Stokes solver
- NS & DSMC grids are independent
- NS & DSMC time steps are independent
- Both steady & time-dependent flows
- Conservation of mass, momentum & energy
- Excellent stability
- No "drift" of solution at steady state
- Fully 3D with no "corner" error
- Can use Euler instead of Navier–Stokes

Future Work

- Parallel version
- Fully adaptive mesh refinement
- Dense gases & liquids (CBA & CUBA)
- Molecular dynamics MAR
- Applications (e.g., MEM devices)