

Monte Carlo
Particle Hydrodynamics
and its application to astrophysics

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Summary

- We develop an unconditionally stable explicit CFD schemes:
- Monte Carlo Particle Hydrodynamics (MCPH)
 - Boltzmann Particle Hydrodynamics (BPH)
 - Molecular Hydrodynamics (MH) \leq DSMC
- Cell Boltzmann method (CB)
- Boltzmann SPH (BSPH)
 - Tsuribe, Imaeda, Inutsuka

Steps in BPH

- Space is divided into Cartesian cells
- Finite number of particles $\sim 10^6$ - 10^7
- **Particles fly freely** between t^n and t^{n+1}
 - Mass, momentum and total energy are conserved
- **Relax** into a (LTE) state **stochastically** at t^{n+1}
 - Not necessarily Maxwellian
 - A class of **Monte Carlo method**
- A particle has internal degrees of freedom
 - Any value of ratio of specific heats

Most prominent character

- **Unconditional stability**
 - Time step is not restricted by the CFL condition, although explicit.
 - Seems to contradict with CFD wisdom
 - In N-S and Euler equation, time steps should be restricted by the CFL condition.
- **Why ?**
 - Lagrangean nature
 - Particles may fly beyond as many cells as like.
 - (Numerical) viscosity is proportional to Δt

Other characteristics

- **Positivity**
 - Pressure and density do not become negative
 - It may happen in conventional CFD schemes
- **Viscosity** has a **physical origin**
 - Can handle N-S equation
- **Gas of zero temperature** can be handled easily
 - Infinite Mach number
- Accuracy is increased by an ensemble average
 - **100% Parallelization**
- Dynamic range of density can be large
 - Density does not proportional to number of particles
 - Contrast to MH and SPH

Disadvantage

- Statistical fluctuation
 - Need large number of particles
 - Restricted by memory size
 - $\sim 10^7$ particles /2GB
- Particle number may be increased by using parallel computers
 - Cray XT at NAO

Theoretical background

Three levels in the description of fluids

Level	Governing equation	Variables
1. Molecules	Newton equation	Position and velocity
2. Distribution function	Boltzman equation BGK equation	Distribution function
3. Continuum fluid	Hydrodynamic equation	Density, velocity, pressure

Classification of CFD methods

	Cell/grid	Particle method
Kinetic approach	Cell-Boltzmann Lattice Boltzmann	Molecular hydrodynamics Boltzmann particle hydrodynamics
Continuum approach	Finite difference Finite volume Finite element	SPH BSPH

BGK equation

$$\frac{\partial(nf)}{\partial t} + \mathbf{c} \cdot \nabla(nf) + \mathbf{F} \cdot \nabla_{\mathbf{c}}(nf) = \frac{n(f_0 - f)}{\tau}$$

- Collision term is approximated by a relaxation
 - linear
- f_0 : Maxwellian distribution function
- τ : Relaxation time

Generalized BGK equation

- f_0 is not necessary Maxwellian
- Condition
 - Spherically symmetric in velocity space
 - Conservation law
 - f_M : Maxwellian
 - Q : $m, mc_j, mc^2/2$

$$\int n f_0 Q dV_c = \int n f_M Q dV_c = \bar{Q}$$

Time splitting of BGK equation

- Distribution function: f ; time step: Δt

$$\frac{\partial(nf)}{\partial t} = -\mathbf{c} \cdot \nabla(nf) - \mathbf{F} \cdot \nabla_{\mathbf{c}}(nf) + n^2 F_{\text{coll}}(t)$$

$$\begin{aligned} nf(\mathbf{c}, t + \Delta t) - nf(\mathbf{c}, t) \\ = \Delta t \left[-\mathbf{c} \cdot \nabla(nf) - \mathbf{F} \cdot \nabla_{\mathbf{c}}(nf) + n^2 F_{\text{coll}}(t) \right] + O(\Delta t^2) \end{aligned}$$

$$\begin{aligned} nf(\mathbf{c}, t + \Delta t) &= [1 - \Delta t \mathbf{c} \cdot \nabla - \Delta t \mathbf{F} \cdot \nabla_{\mathbf{c}} + \Delta t J] nf(\mathbf{c}, t) \\ &\cong [1 + \Delta t J] [1 - \Delta t \mathbf{c} \cdot \nabla - \Delta t \mathbf{F} \cdot \nabla_{\mathbf{c}}] nf(\mathbf{c}, t) \end{aligned}$$

$$[J]nf(\mathbf{c}, t) \equiv n^2 F_{\text{coll}}$$

Stochastic time integration

$$\frac{\partial nf}{\partial t} = \frac{(nf)_0 - nf}{\tau}$$

$$(nf)^{n+1} = \frac{\Delta t}{\tau} (nf)_0 + \left(1 - \frac{\Delta t}{\tau}\right) (nf)^n$$

$$P = \frac{\Delta t}{\tau} = \frac{\Delta t}{t_c} = \frac{\bar{C}}{\lambda} \Delta t = \frac{\bar{C}}{a \Delta x} \alpha \Delta x = \frac{\alpha}{a} \bar{C}$$

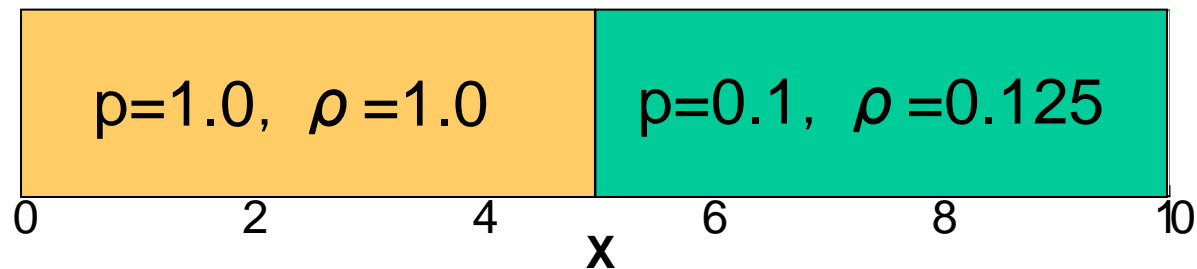
Steps in BPH

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Numerical tests

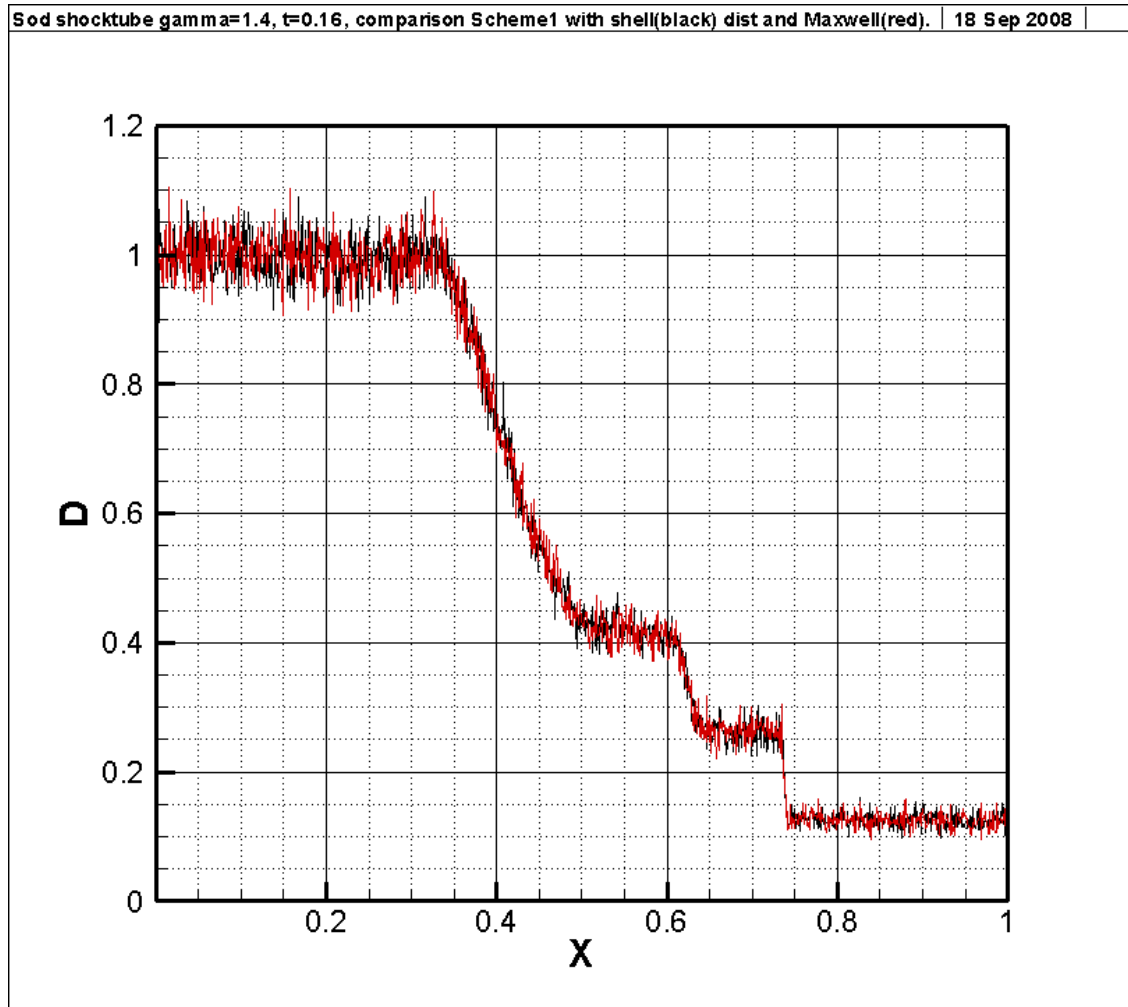
Shock tube problem (Sod)

- Domain: $0 < x < 10$
- Number of cells: 1000
- $\gamma = 1.4$
- $t = 0.16$



Test 1

Choice of velocity distribution f_0



Black: Spherical shell
Red: Maxwellian

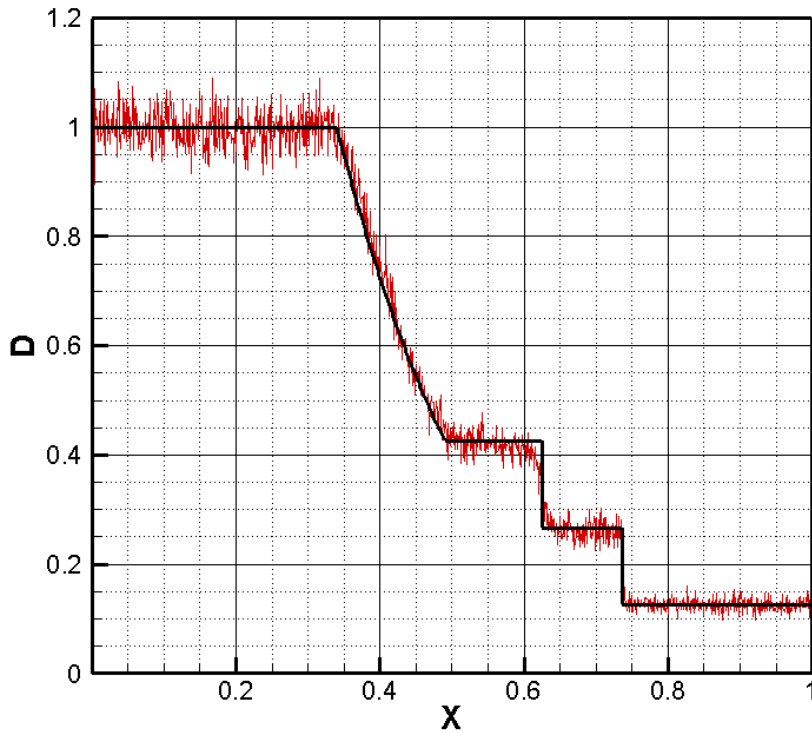
No difference

Test 1: density profile

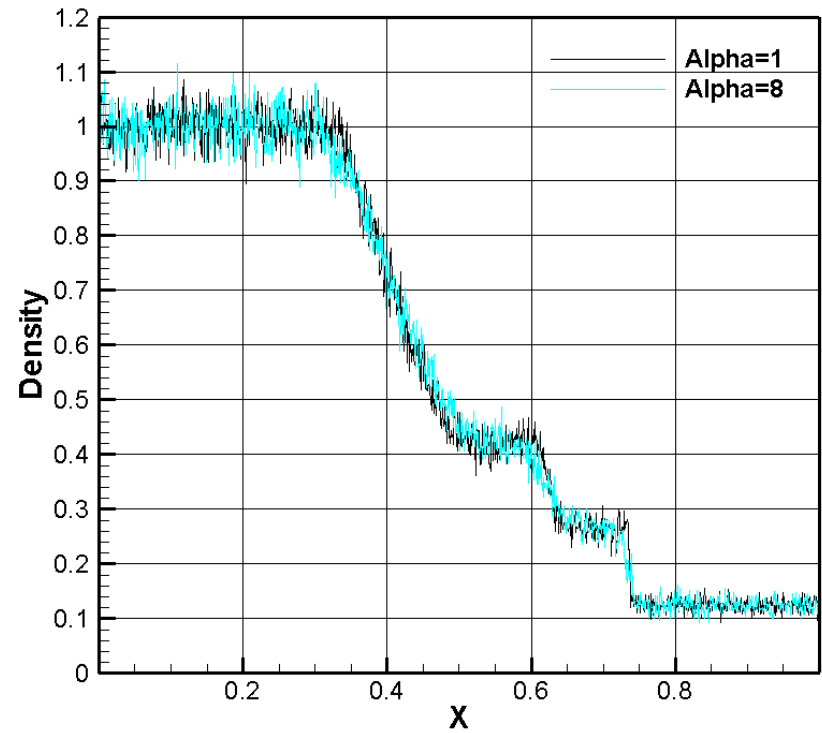
Numerical solution vs analytic one

Courant condition can be violated

Sod shocktube gamma=1.4, t=0.16, comparison Scheme1 with shell dist and analytic sol. | 18 Sep 2008 |



Time step: Black: alpha=1, Blue: alpha=8, nc=1000, np=100 | 15 Nov 2008 |



Number of particles 100/low density section
800/high density section

CFL number $\sim 2\alpha$
 $\Delta t = \alpha \Delta x$

Test 3

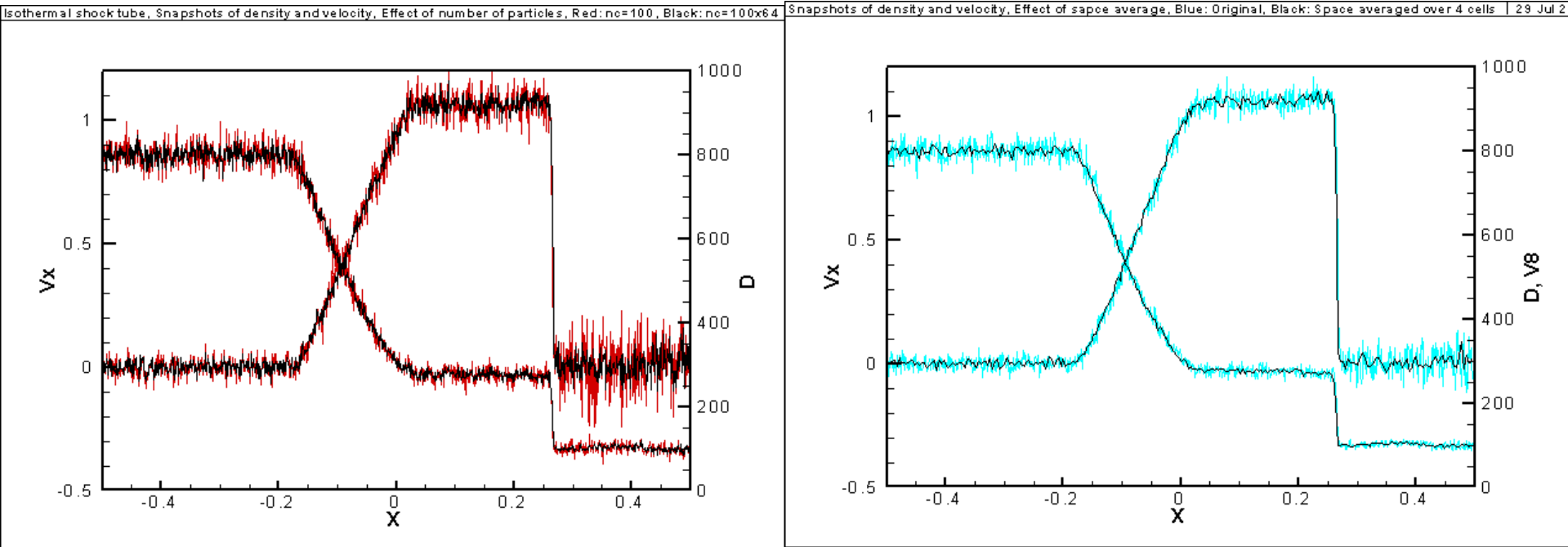
Extreme density ratio

Density ratio $1:10^{-3}$



Test 4: Isothermal shock

Averaging reduces statistical fluctuation
of solution: Density and velocity

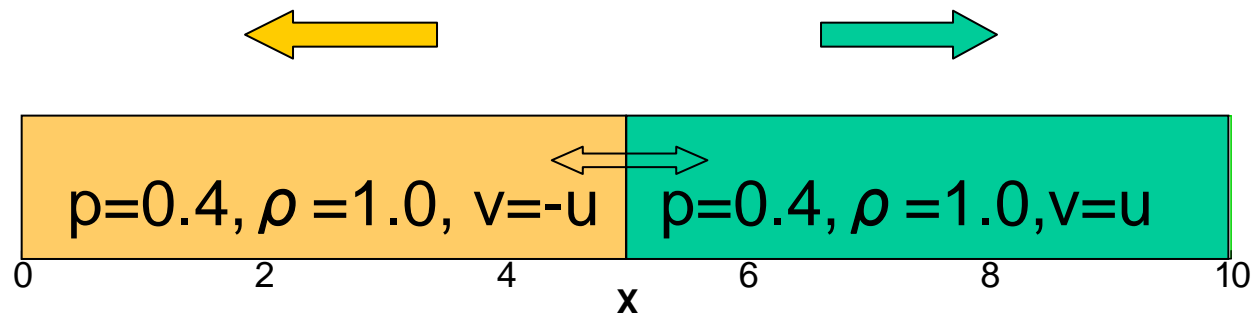


Ensemble average over 64 cases

Space average over 4 cells

Strong rarefaction: Sjögreen test

- Domain : $0 < x < 1$
- Cell number 1000
- $\gamma = 1.4$
- $u = 2.0$ (case 1: No vacuum)
- $u = 5.0$ (case 2: Vacuum)

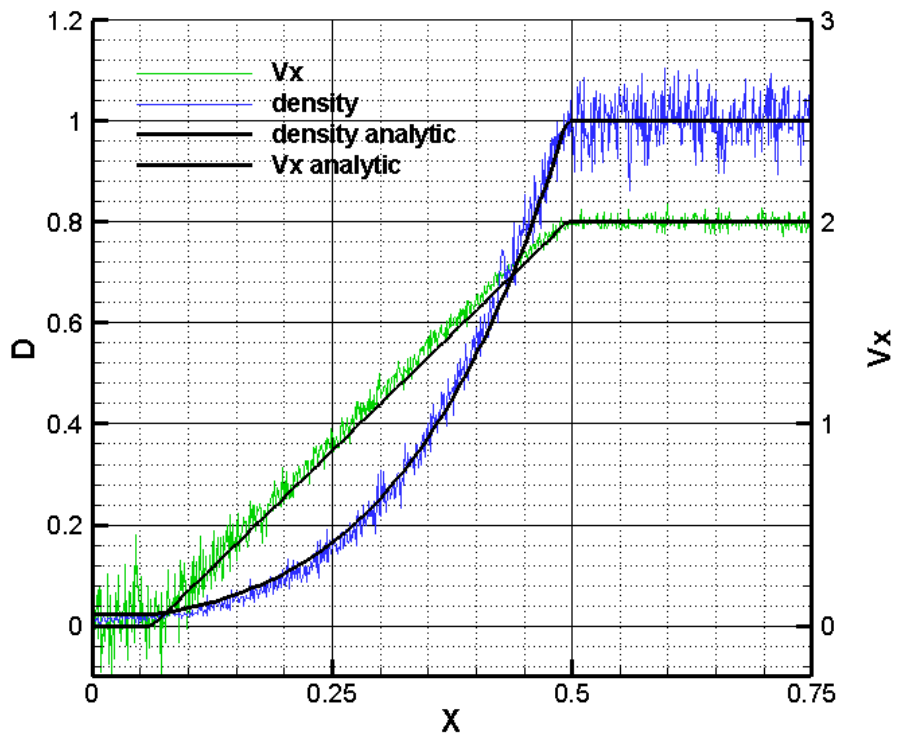


Sjogreen test $u_0=2$ a case without vacuum

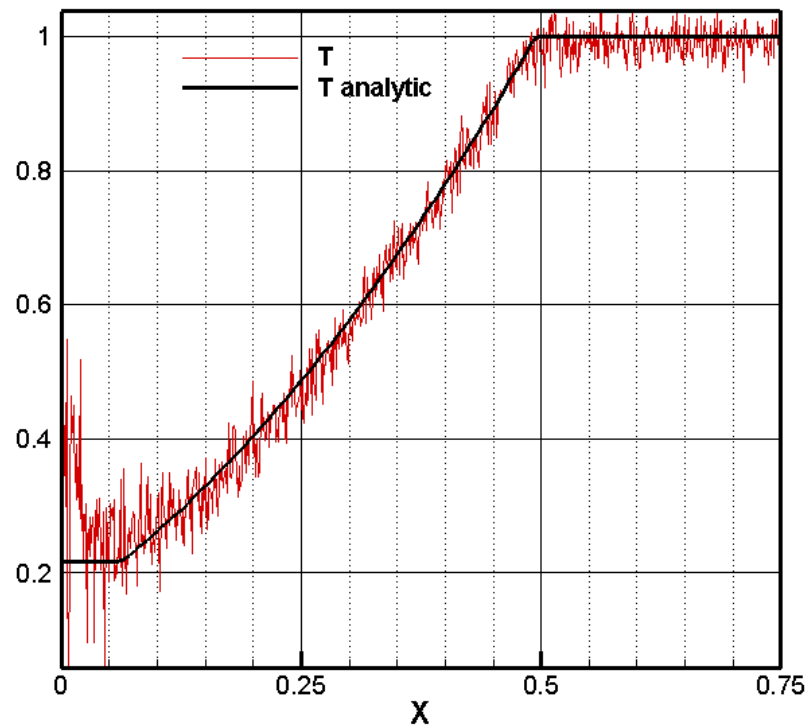
Density and velocity

Temperature

Sjogreen test: $u_0=2$, $\gamma=1.4$, $t=0.18$, Density and velocity | 22 Oct 2008



Sjogreen test: $u_0=2$, $\gamma=1.4$, $t=0.18$, temperature | 22 Oct 2008



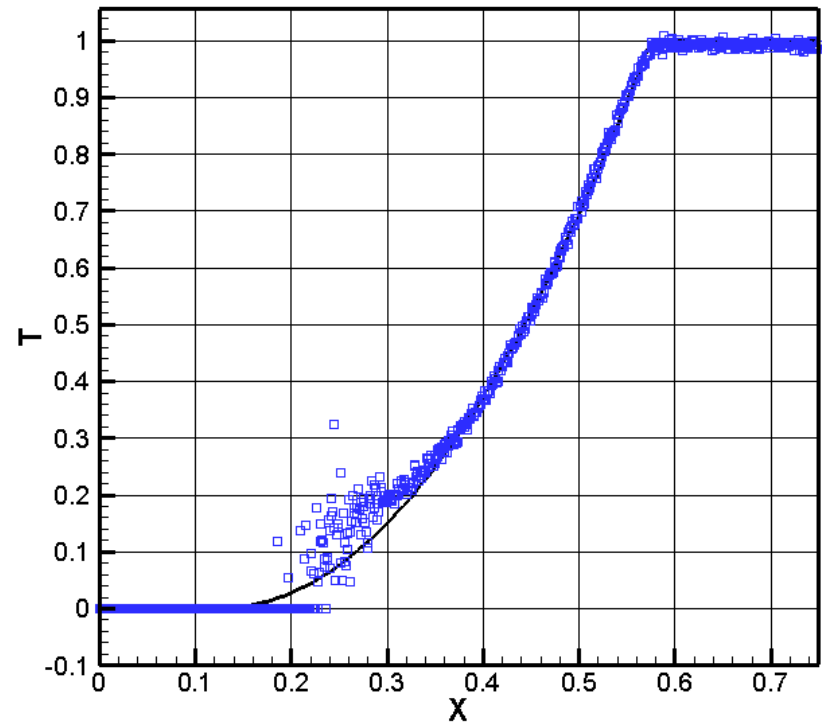
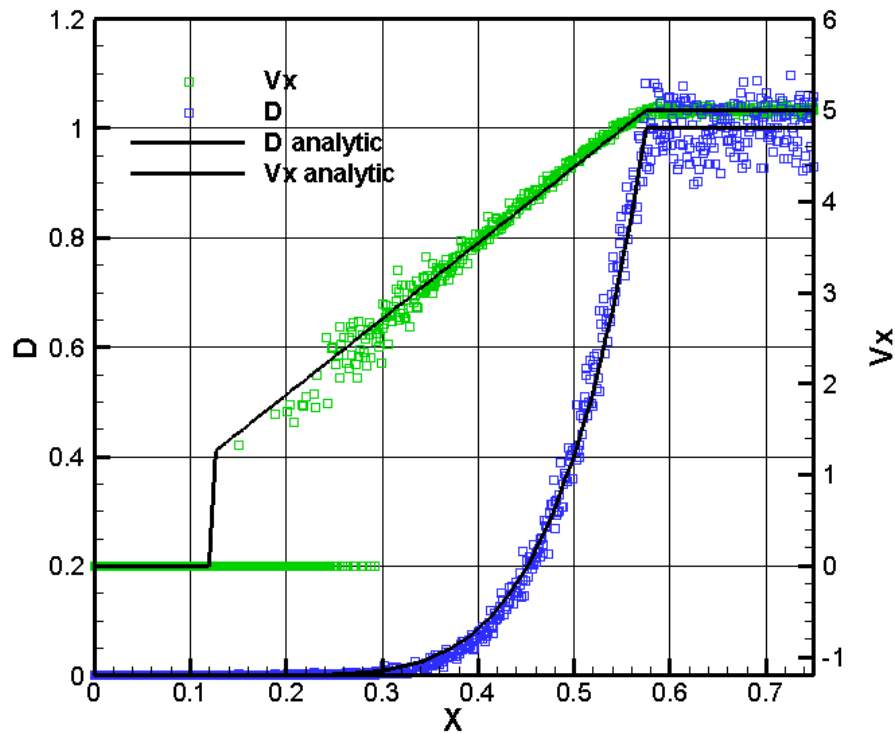
Sjogreen test, $u_0=5$ a case with vacuum

Density and velocity

Temperature

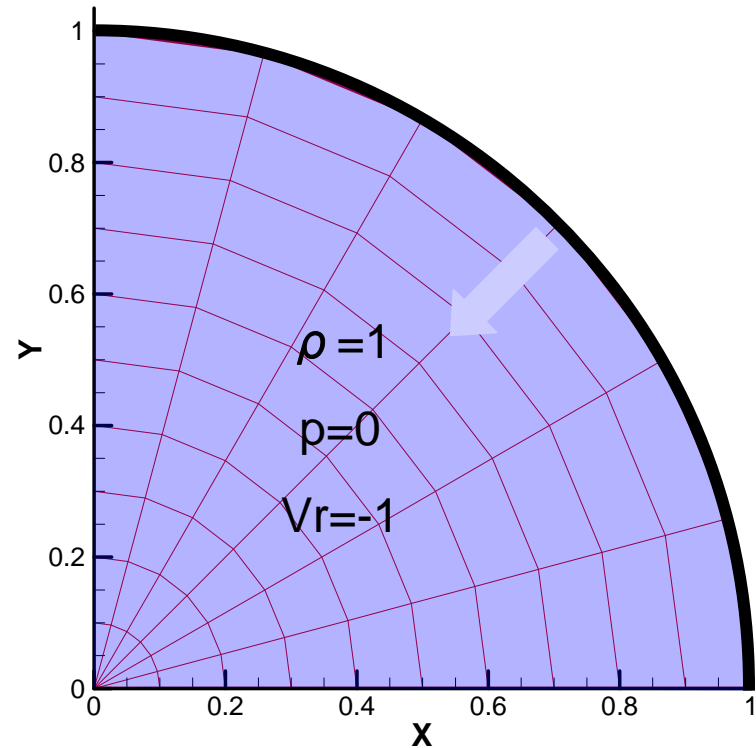
Sjogreen test: $u_0=5$, $\gamma=1.4$, $t=0.1$ | 22 Oct 2008

Sjogreen test: $u_0=5$, $\gamma=1.4$, $t=0.1$, temperature | 22 Oct 2008



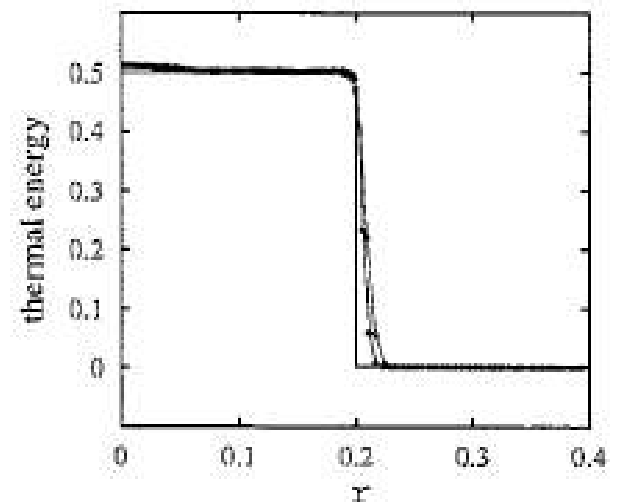
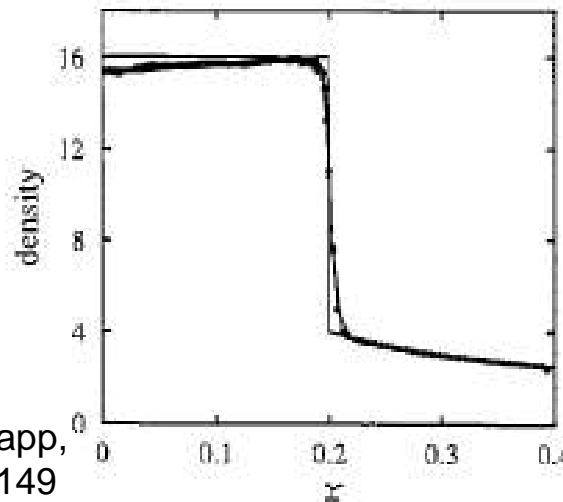
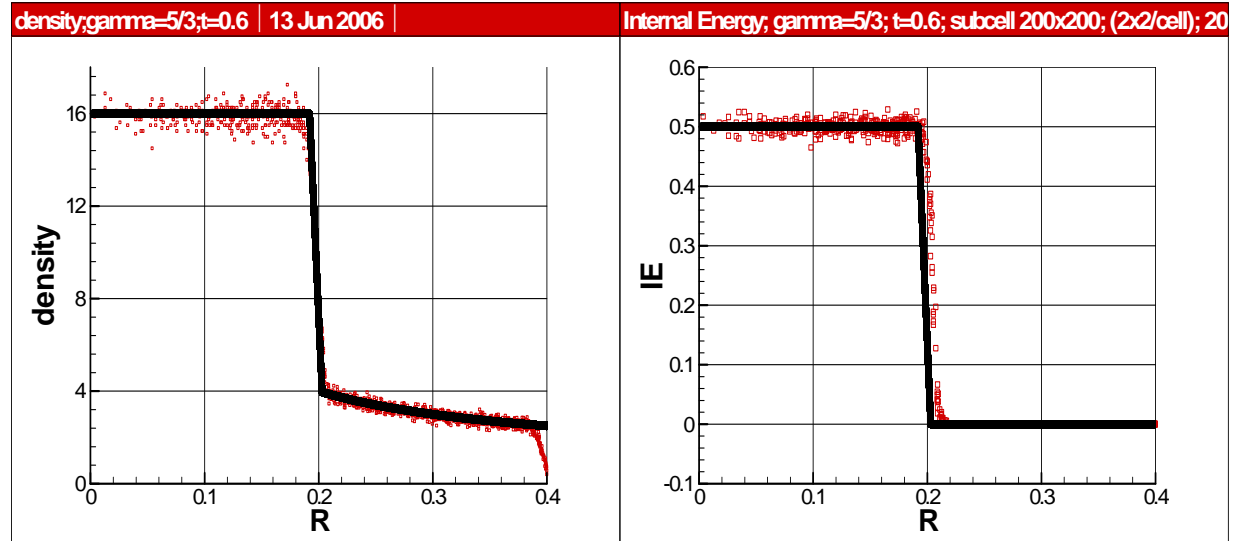
Noh problem

- Computational domain :
 $r < 1, 0 < \theta < \pi / 2$
- cells 200x200:
2x2 cells/ macro-cell
- $\gamma = 5/3$
- $t = 0.6$



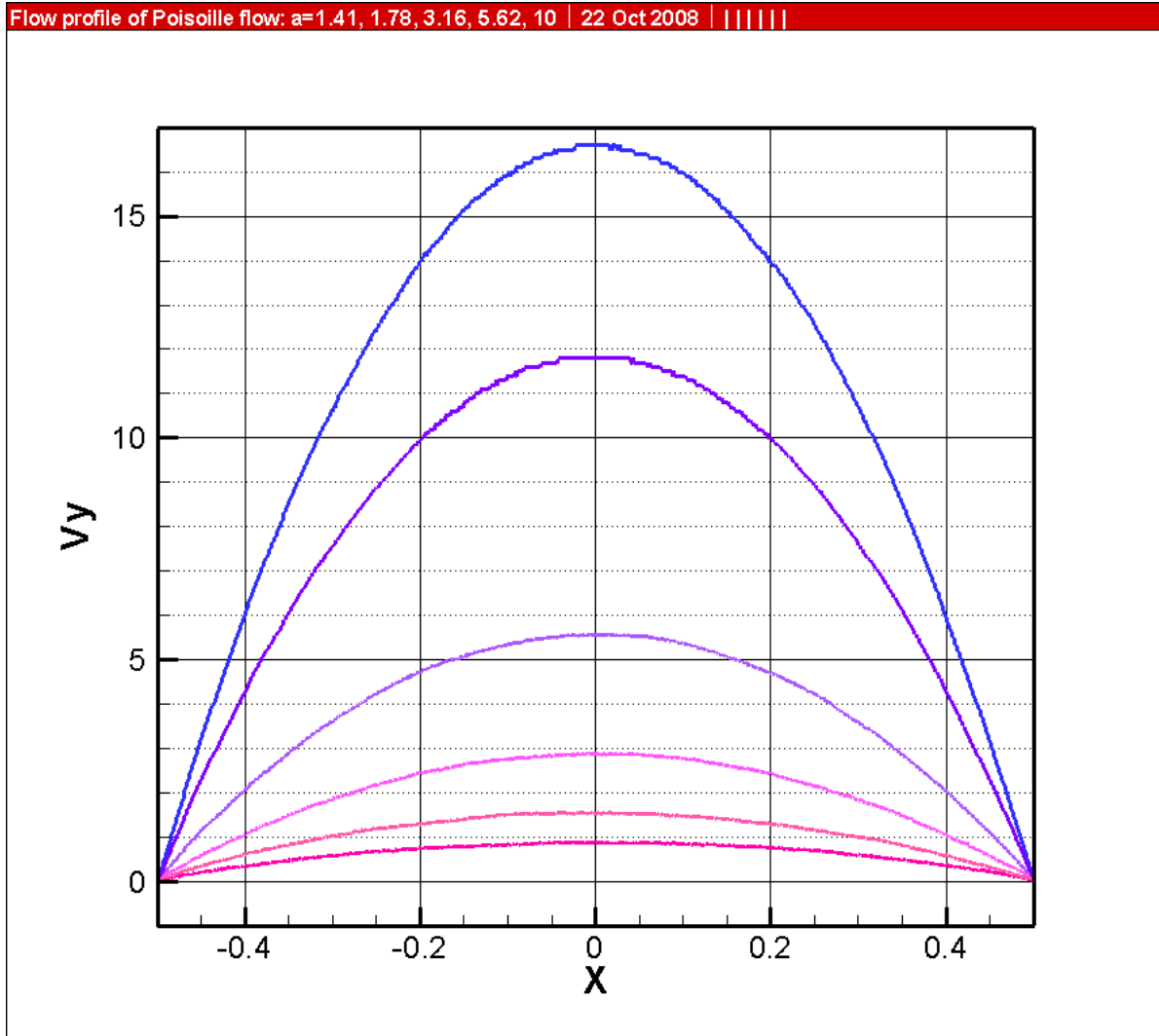
Result of Noh problem

No wall heating

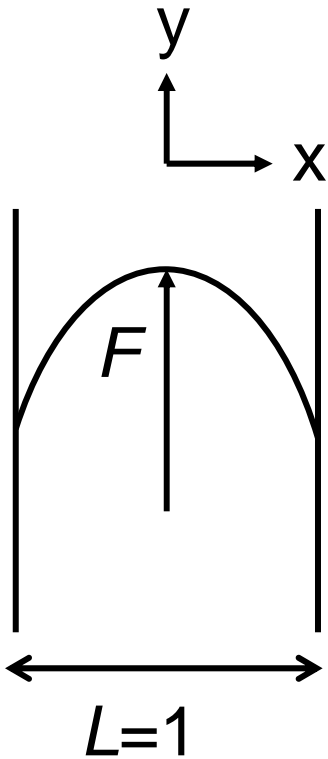


Viscous flow

Plane Poiseuille flow



Plane Poiseuille Flow : $\gamma = 1.0$



Navier-Stokes eqn.

$$\nu \frac{\partial^2 V_y}{\partial x^2} = -F$$

Flow field

$$V_y = \frac{F}{8\nu} \left(1 - \left(\frac{x}{1/2} \right)^2 \right)$$

Eq. Motion

$$\frac{dc_{iy}}{dt} = -F$$

Computational domain $-0.5 < x < 0.5$

No. cells: 1000

No. Particles: 10/cell

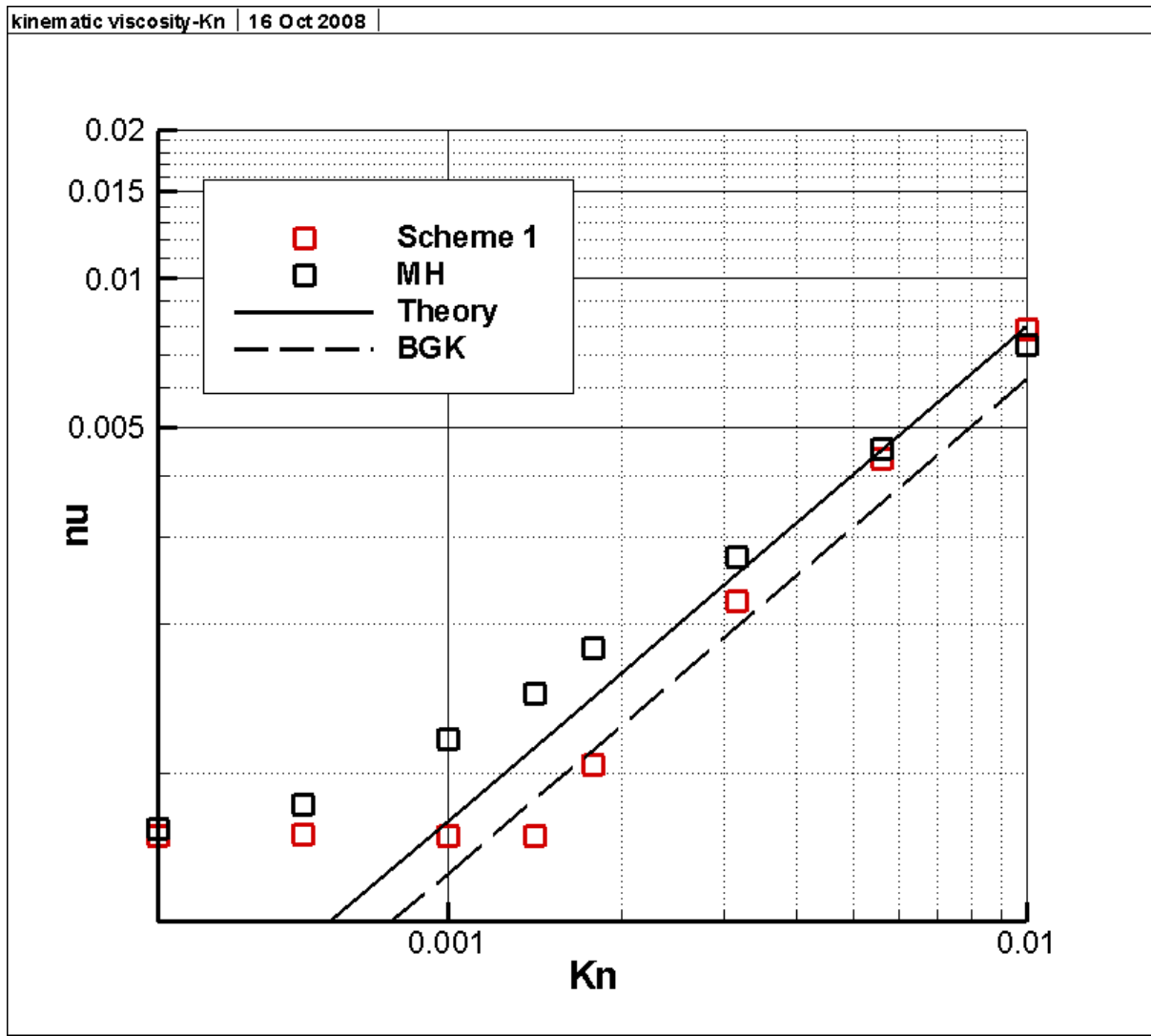
$F=0.1$

$a=1-10, \alpha=1$

$$V_{\text{unit}} = \sqrt{\frac{8}{\pi} RT}$$

Plane Poiseuille flow

Kinematic viscosity: Knudsen number

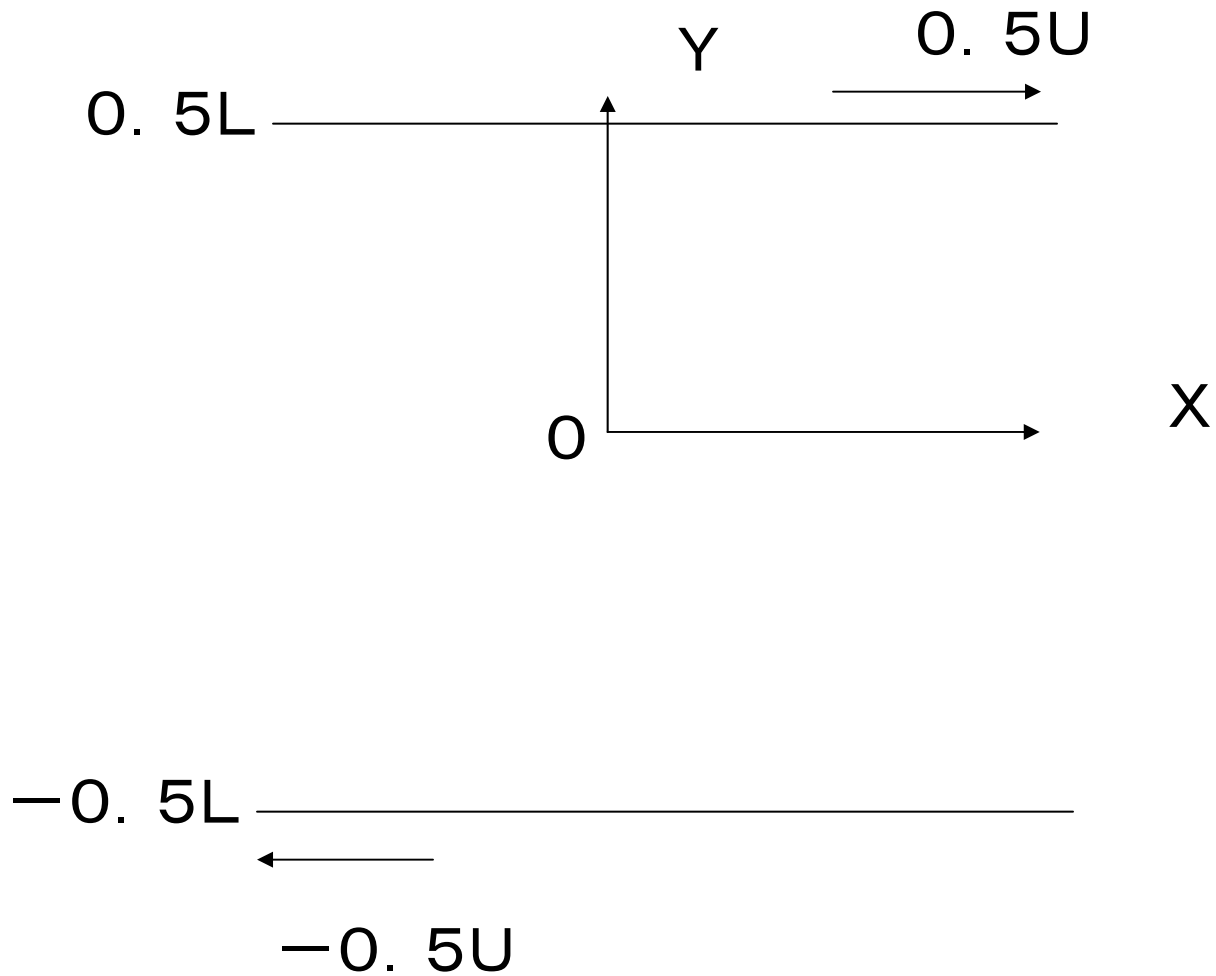


Theoretical curves

$$\nu = \frac{1}{2} \bar{C} \lambda = 0.798 \lambda$$

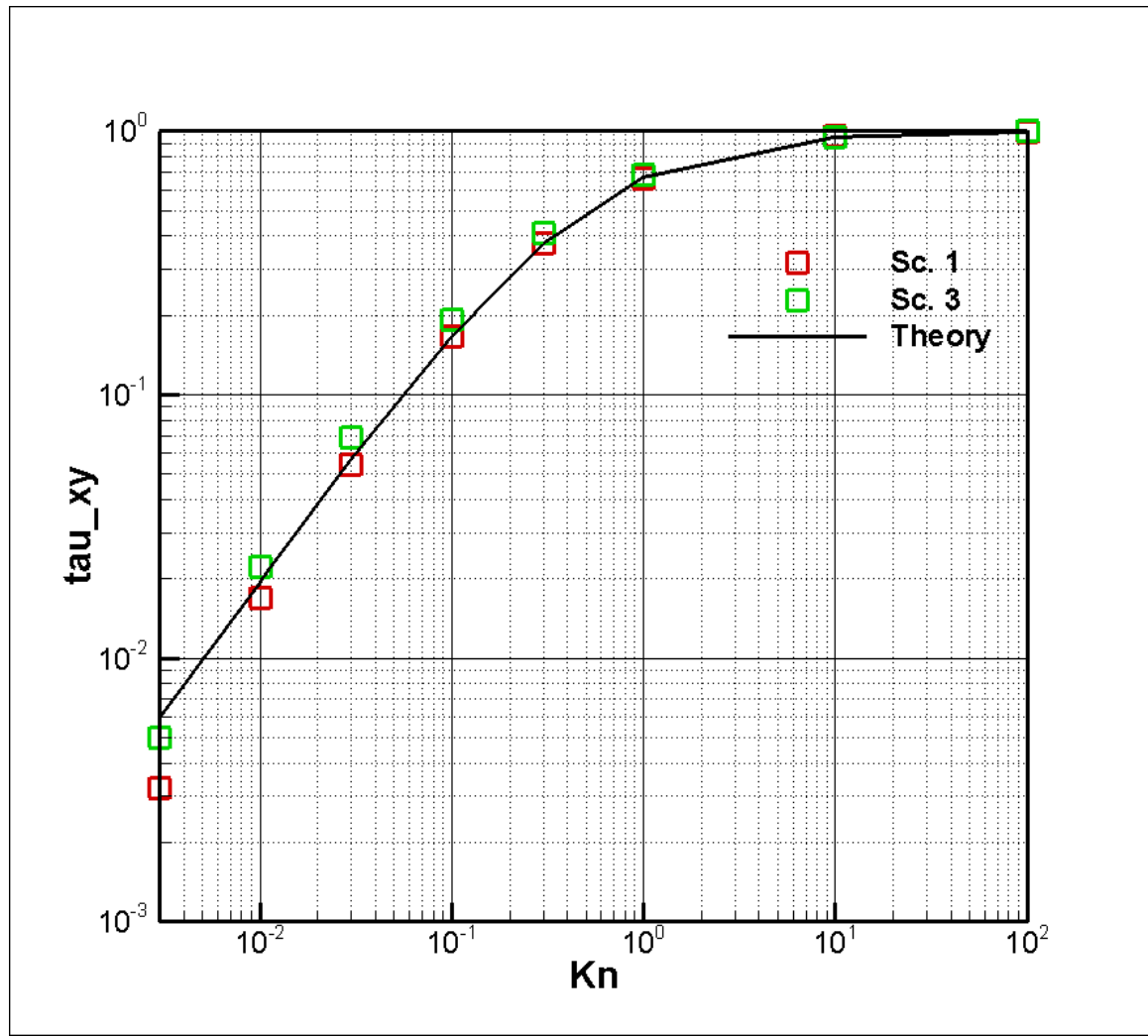
$$\nu = \frac{RT}{\tau} = \frac{RT}{C} \lambda = 0.626 \lambda$$

Couette flow



Couette flow

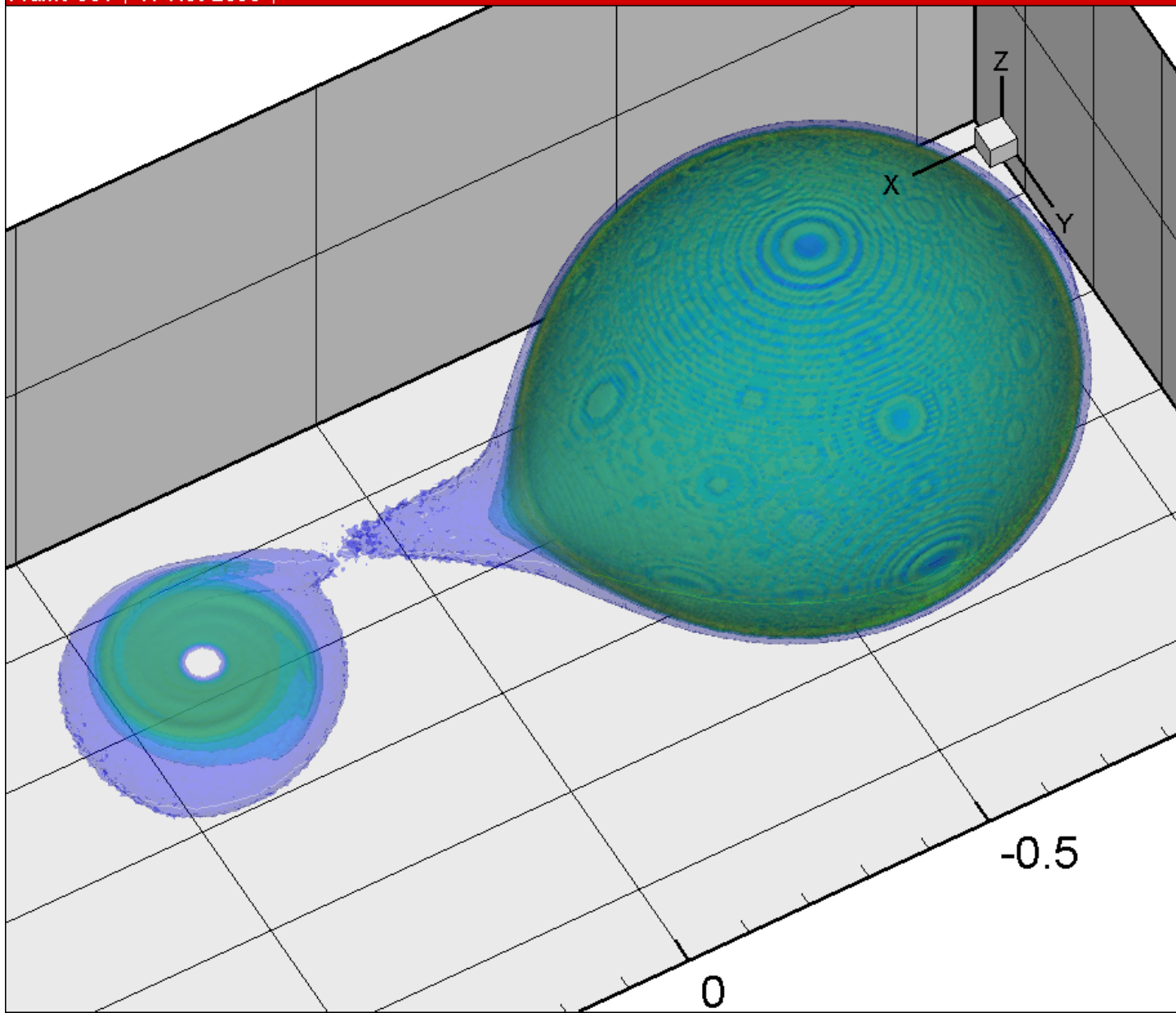
Viscous stress: Knudsen number

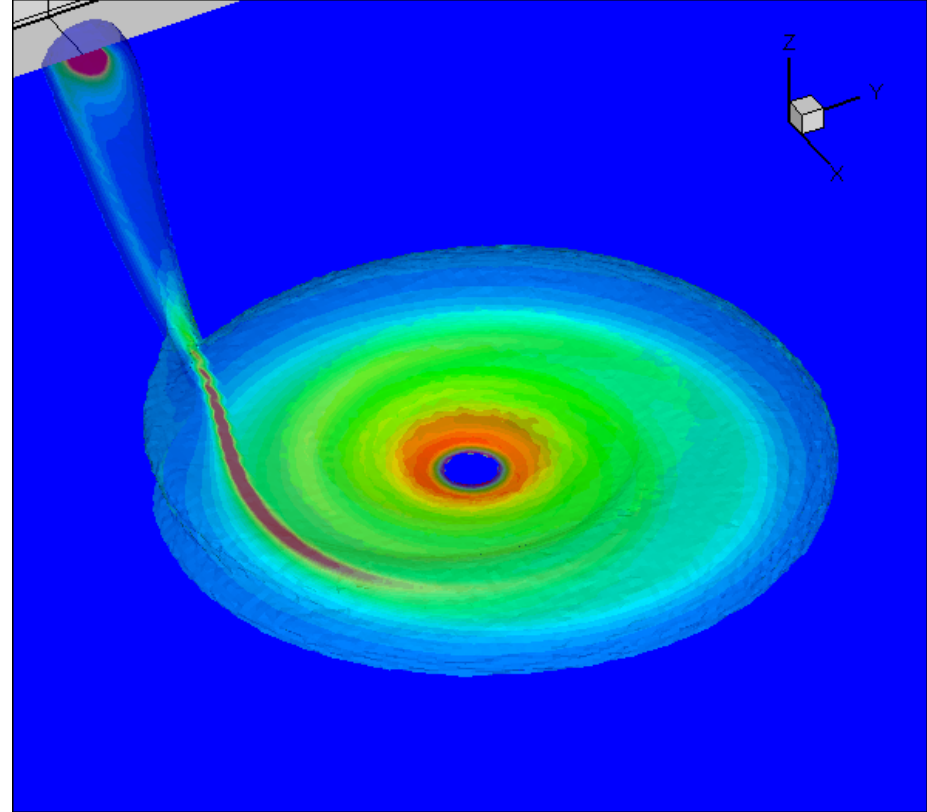
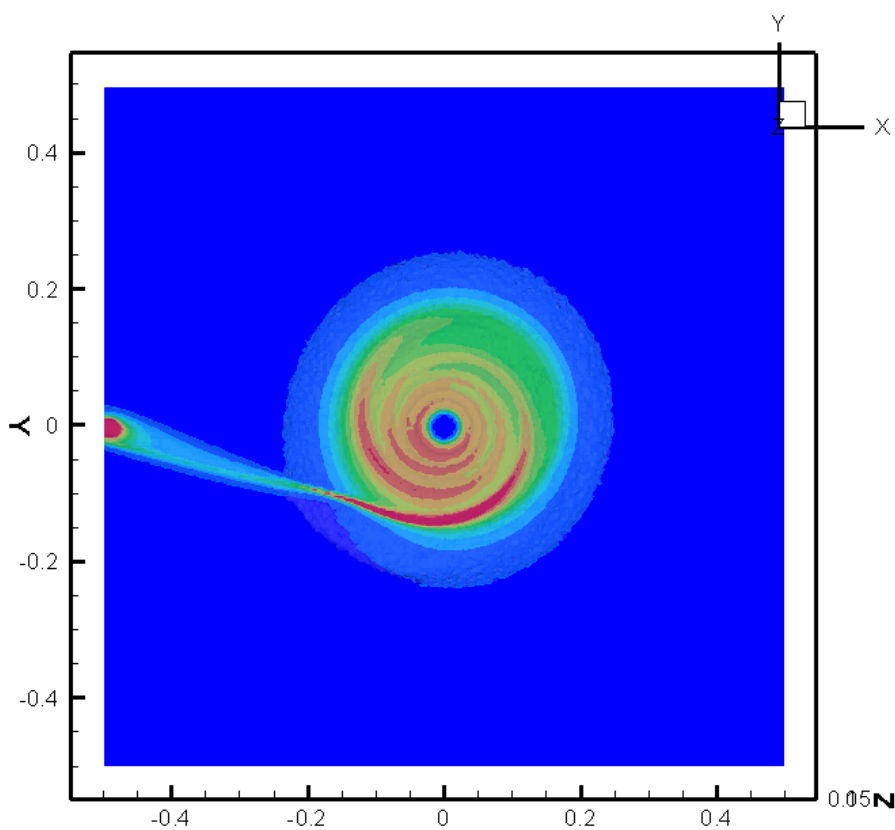


Astrophysical applications

Astrophysical applications

Frame 001 | 17 Nov 2008



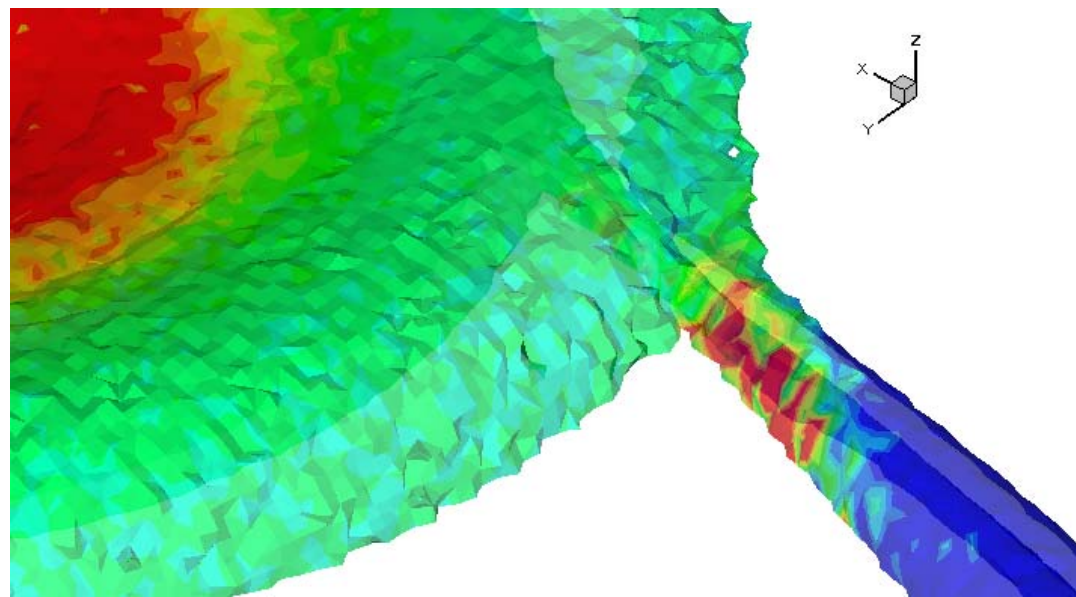


Inflow from L1 point

$$\gamma = 1.01$$

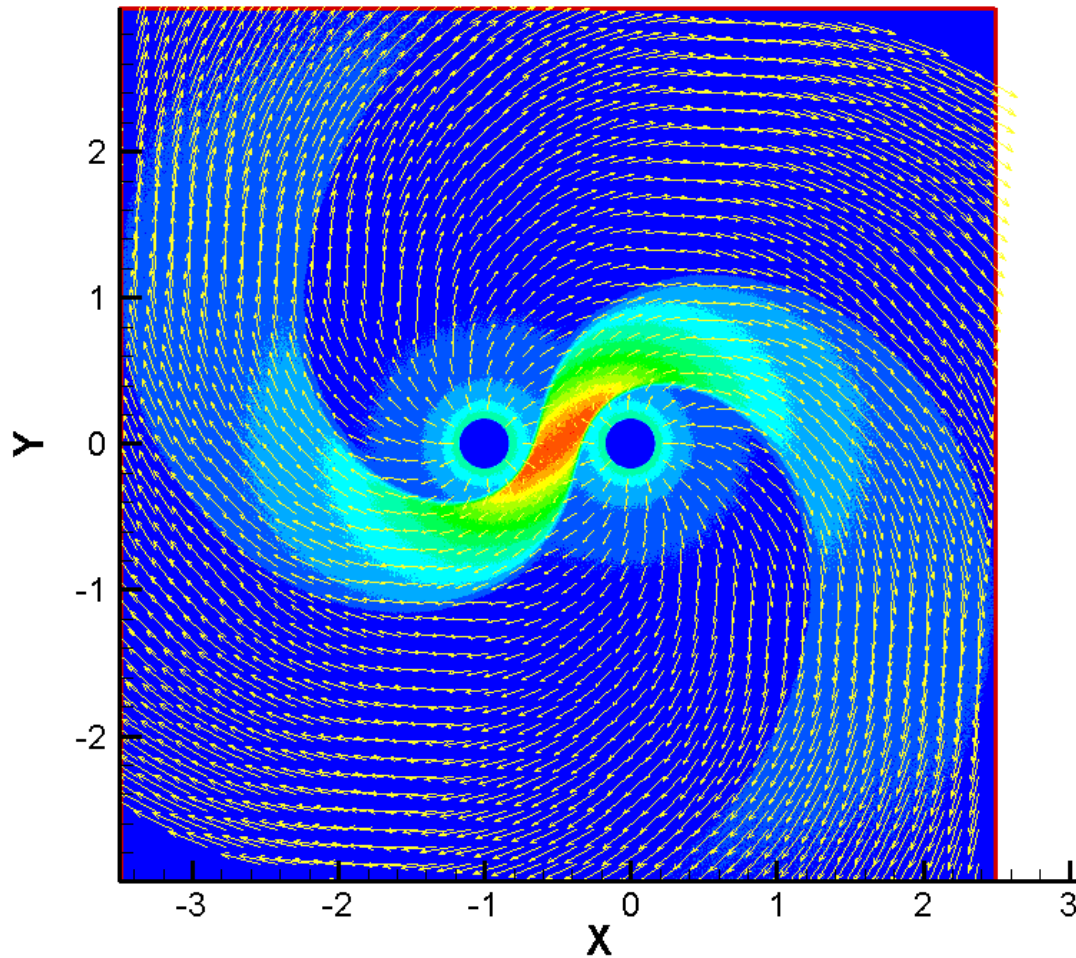
Mass ratio=1

$T=27$



2D wind collision

2D wind collision, 2000x2000, n_in=2e4, gamma=5/3, no gravity | 16 Nov 2008



2000 × 2000

$$\gamma = 5/3$$

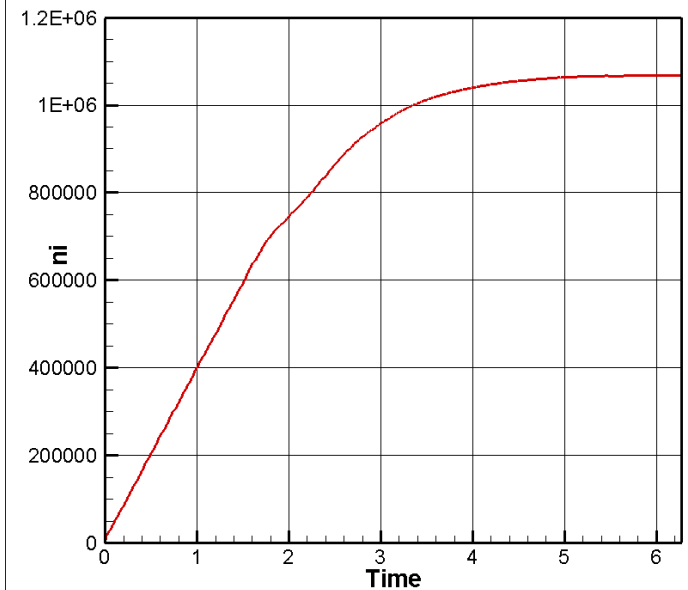
No gravity

$N_{in} = 2e10$

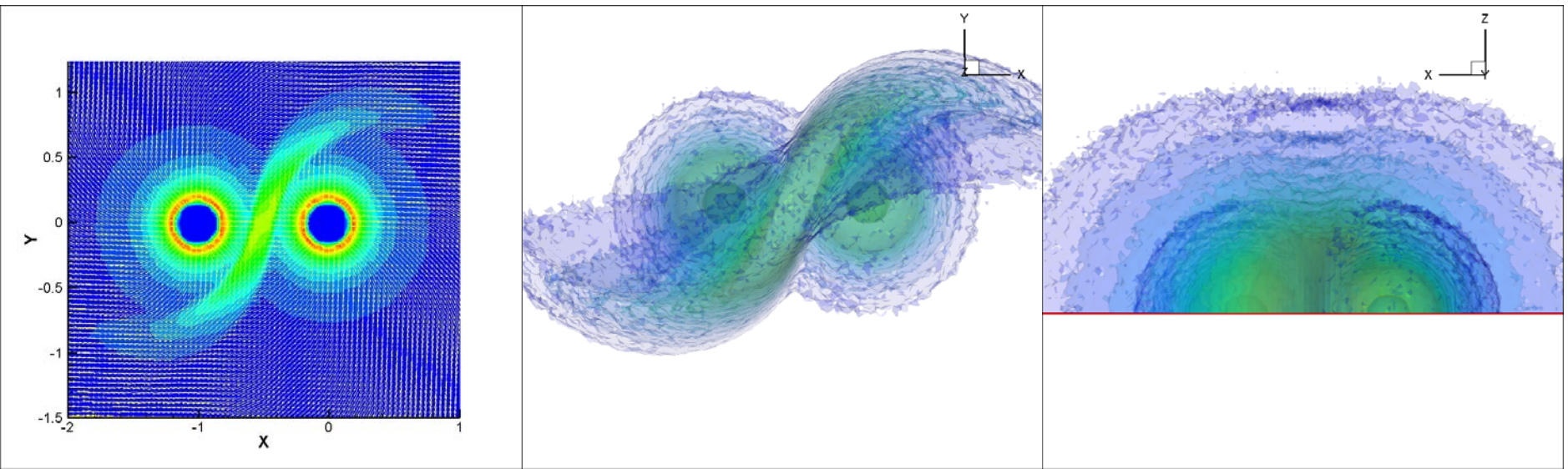
Pentium D

45 min

2D wind collision, Time history of n_ptcl., n_in=2e4 | 16 Nov 2008



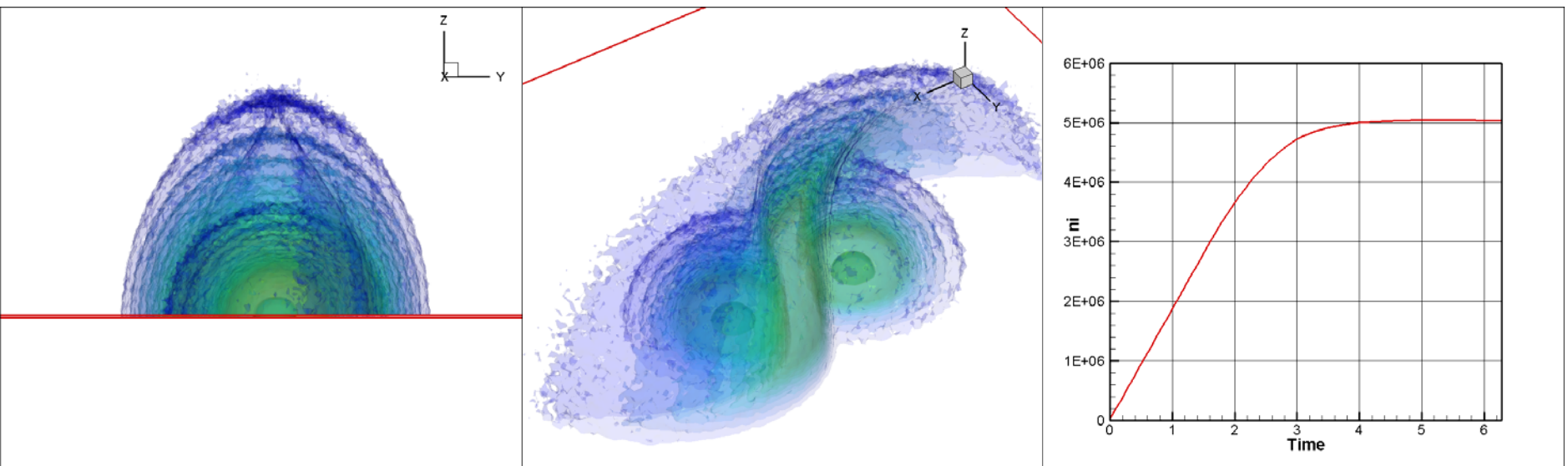
3D wind collision



Density and velocity

View from z-axis

x-axis



y-axis

Bird eye view

Number of particles