Boltmann Particle Hydrodynamics

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NPO Einstein

Summary

- We develop an unconditionally stable explicit particle CFD scheme:
- Boltzmann Particle Hydrodynamics (BPH)

Steps in BPH

- Space is divided into Cartesian cells
- Finite number of particles ~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 chatacteristics

- 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 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

Classifiction of Computational Fluid Dynamics

Three levels in the description of fluids

Level	Governing equation	Variables
1. Molecules	Newton equation	Position and velocity
2. Distribution function	Boltzman equation BGK eqaution	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: $m, mc_j, mc^2/2$

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

Time splitting of BGK equation

- Distribution function: f; time step: Δt

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

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

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

$$[J]\,nf(\mathbf{c}, t) \equiv n^2\,\mathrm{F}_{\mathrm{coll}}$$

Stochastic time integration

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

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

$$P = \frac{\Delta t}{\tau} = \frac{\Delta t}{bt_c} = \frac{\overline{C}}{b\lambda}\Delta t = \frac{\overline{C}}{ba\Delta x}\alpha\Delta x = \frac{\alpha}{ab}\overline{C}$$

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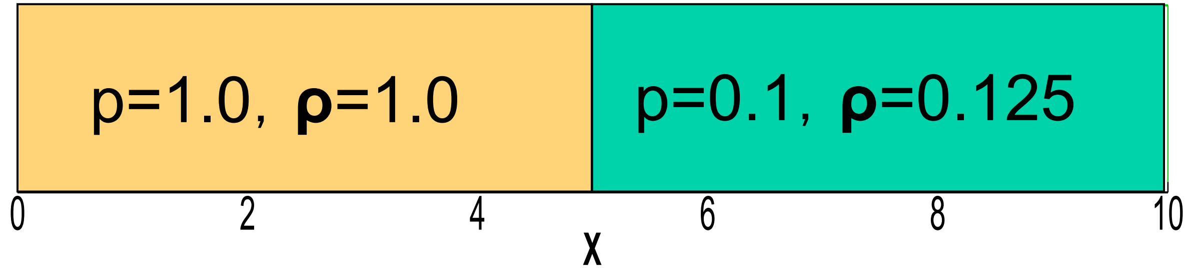
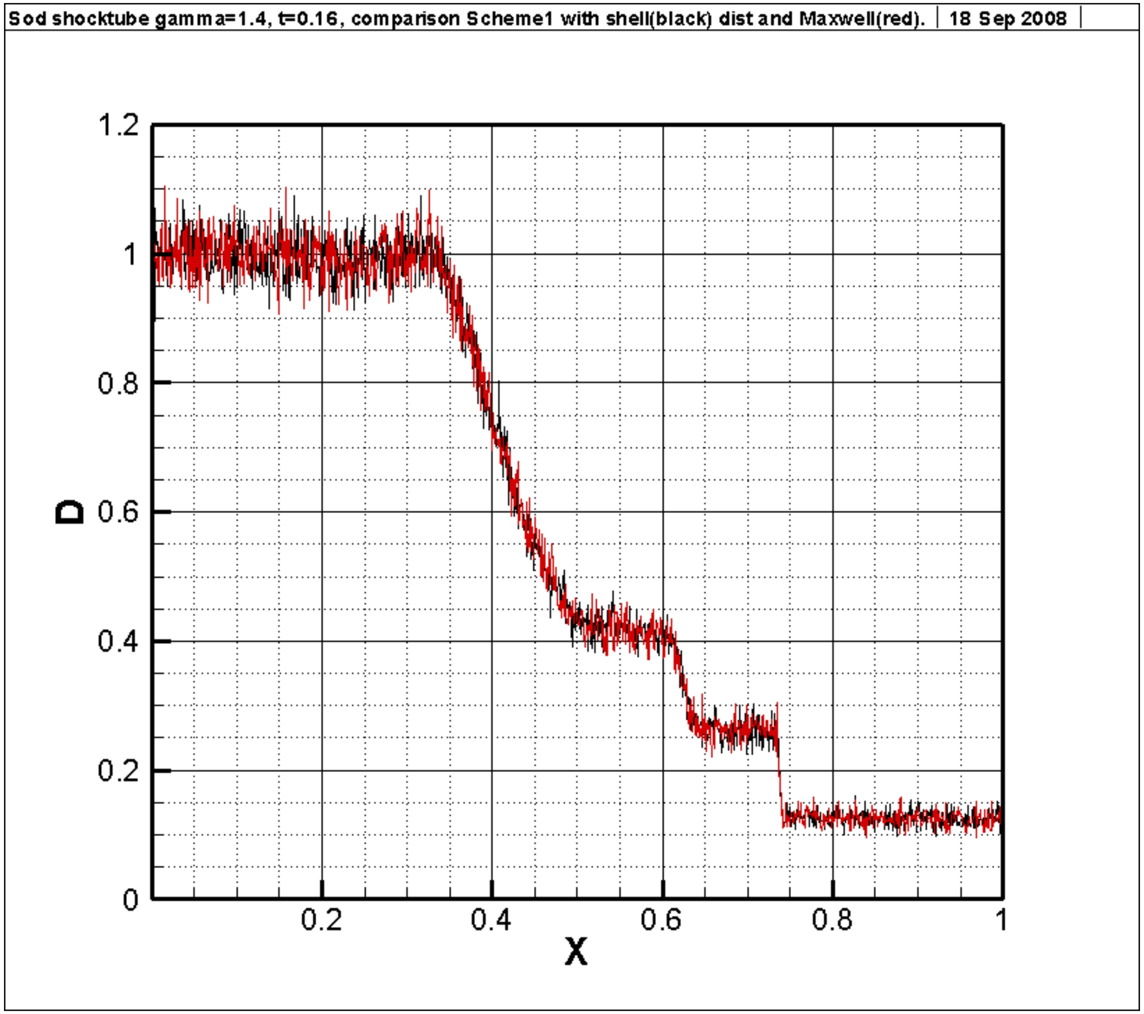
Numerical tests

Shock tube problem (Sod)

- Domain：０＜x＜1
- Number of cells: 1000
- $\gamma=1.4$
- $t=0.16$



Test 1
Choice of velocity distribution f_0

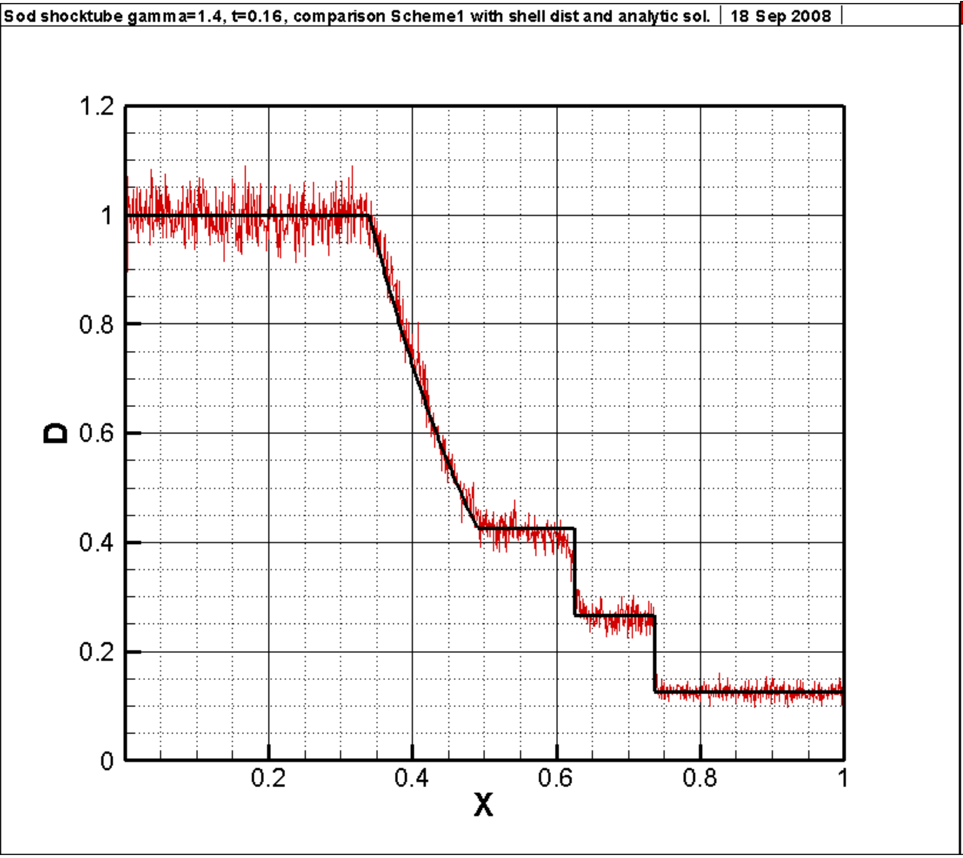


Black: Spherical shell
Red: Maxwellain

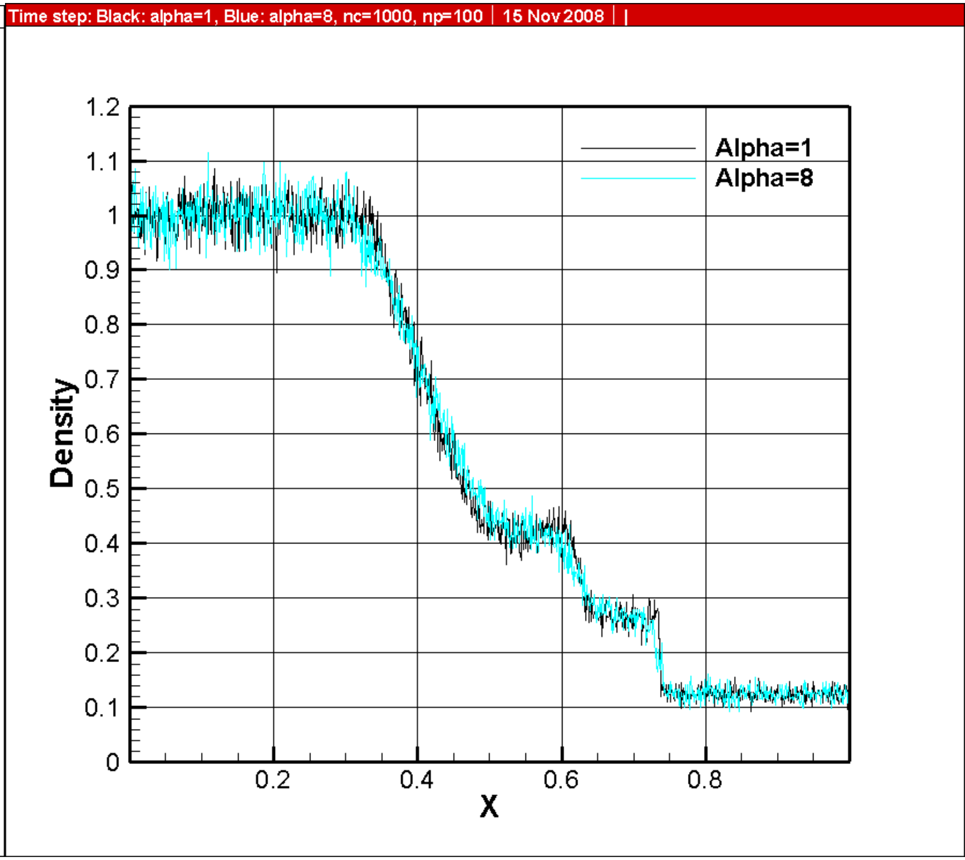
No difference

Test 1: density profile

Numerical solution vs analytic one



Courant condition can be violated



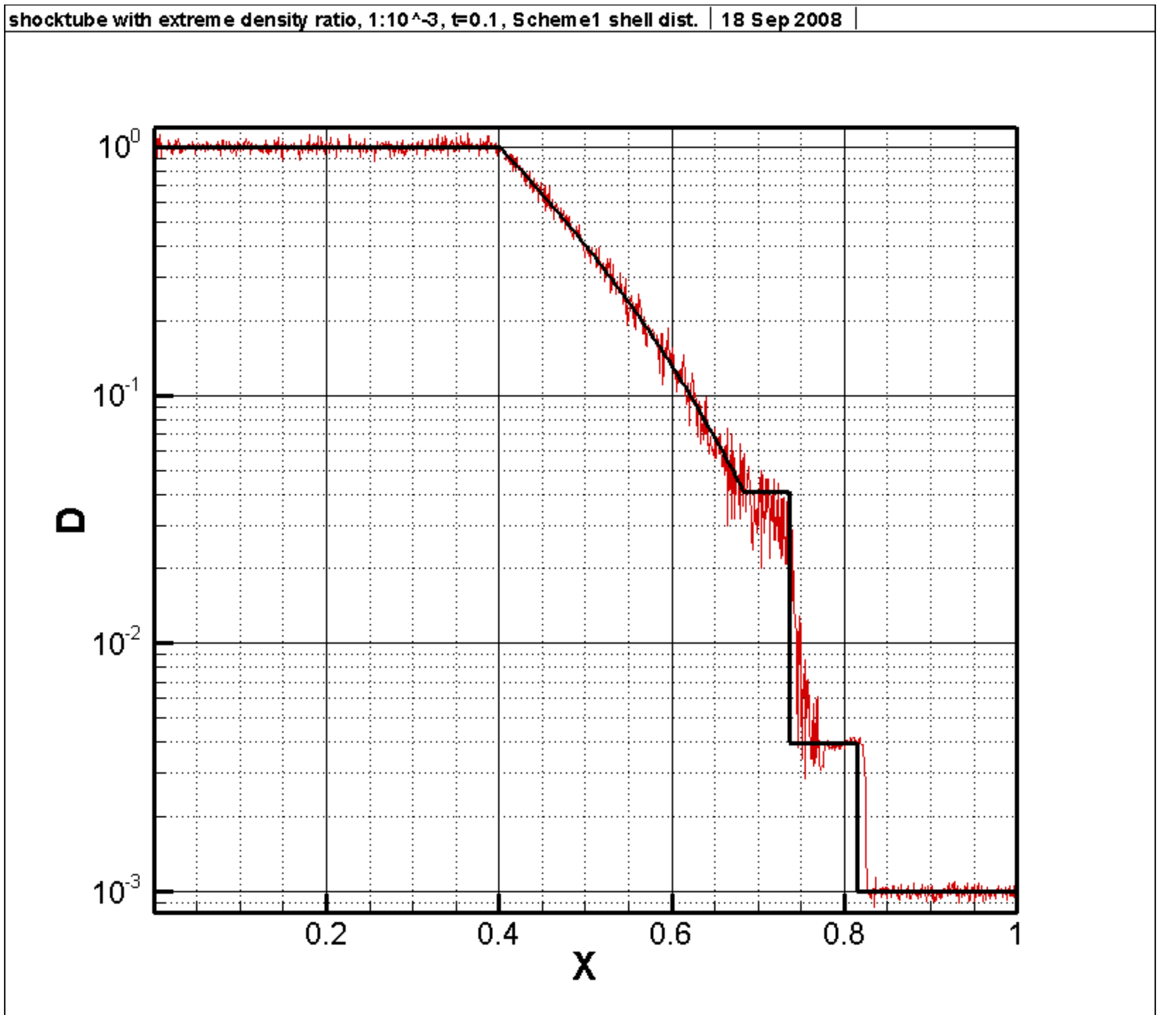
Number of particles 100/low density section

800/high density section

CFL number~2α

$\Delta t = \alpha \Delta x$

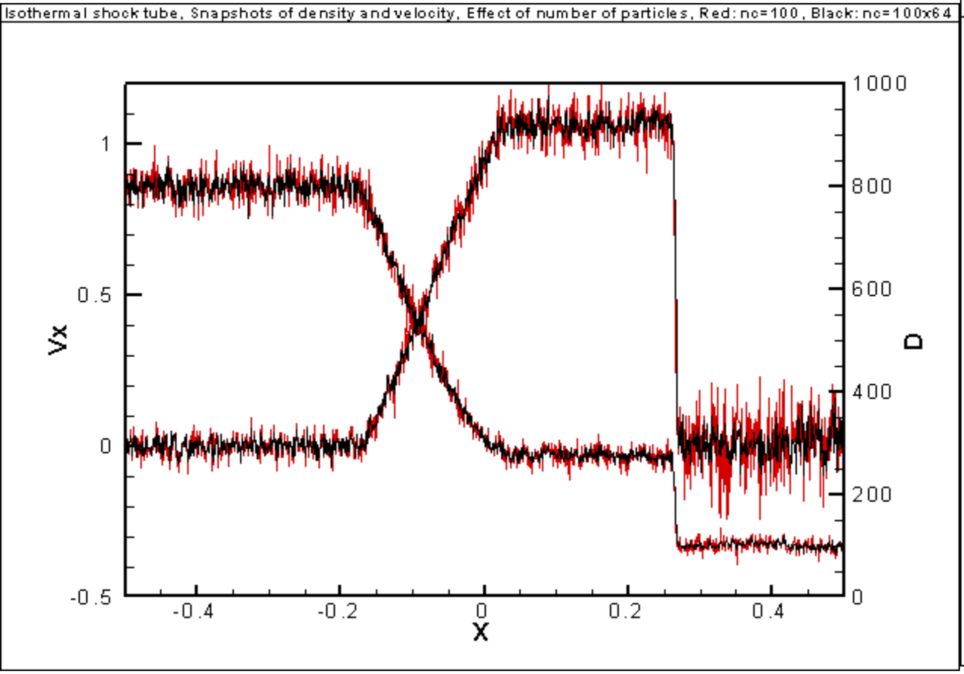
Test 3
Extreme density ratio

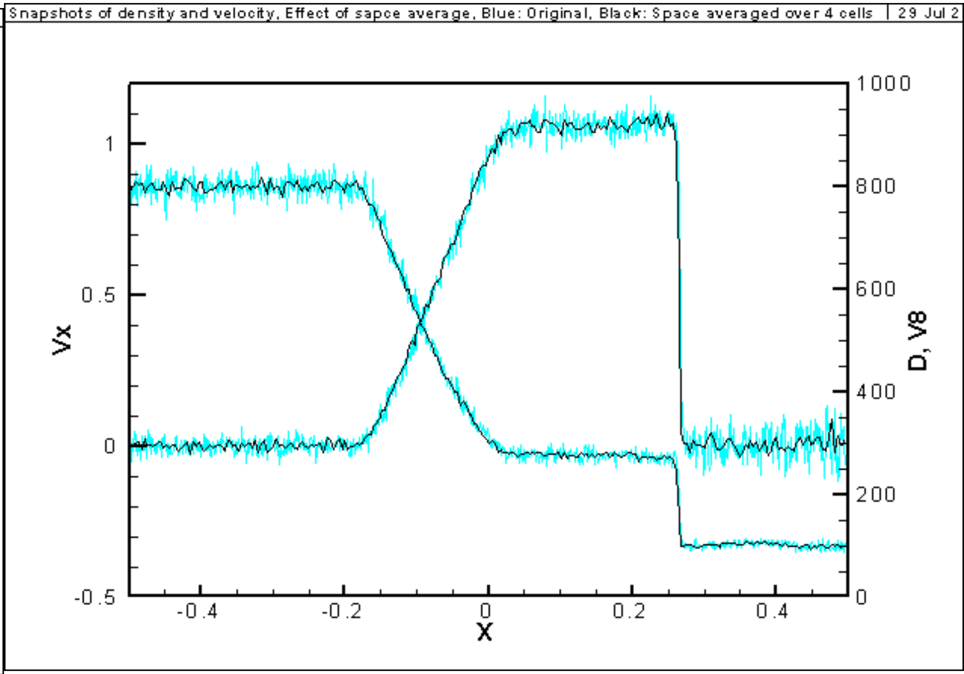


Density ratio 1:10^{-3}

Test 4: Isothermal shock

Averaging reduces statistical fluctuation of solution: Density and velocity



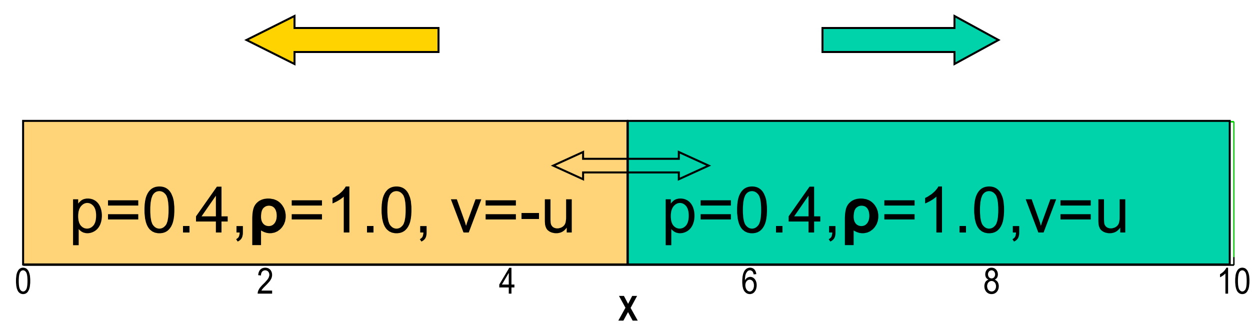


Ensemble average over 64 cases

Space average over 4 cells

Strong rarfaction: Sjögreen test

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

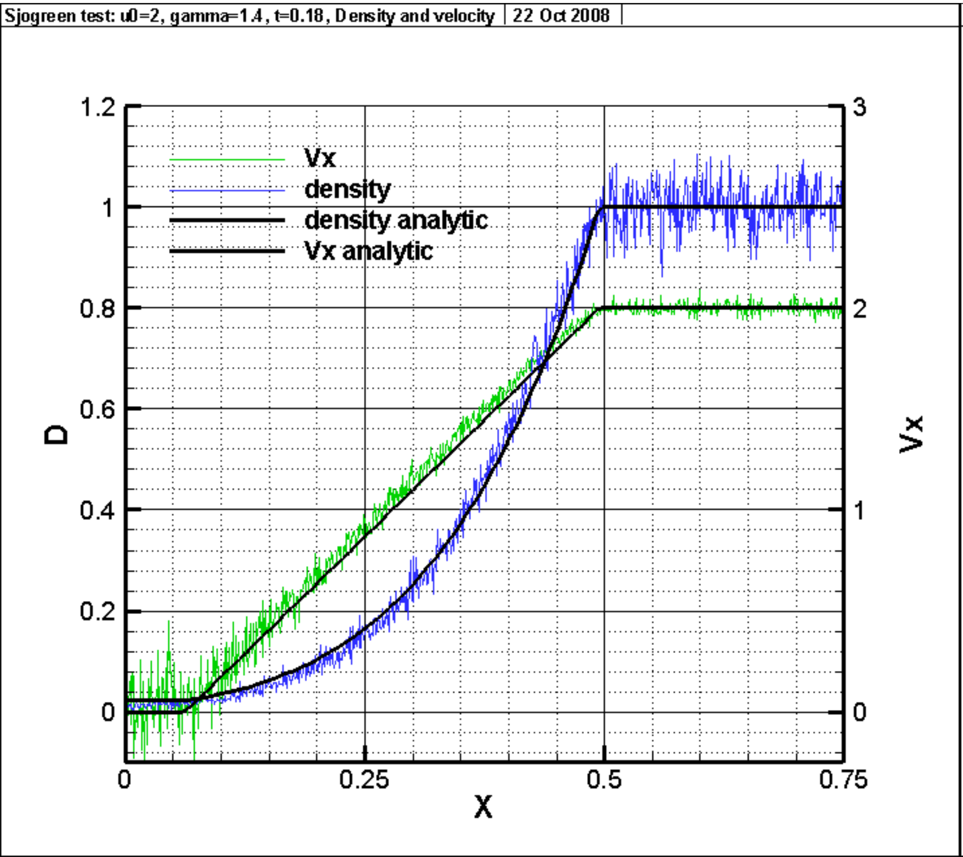


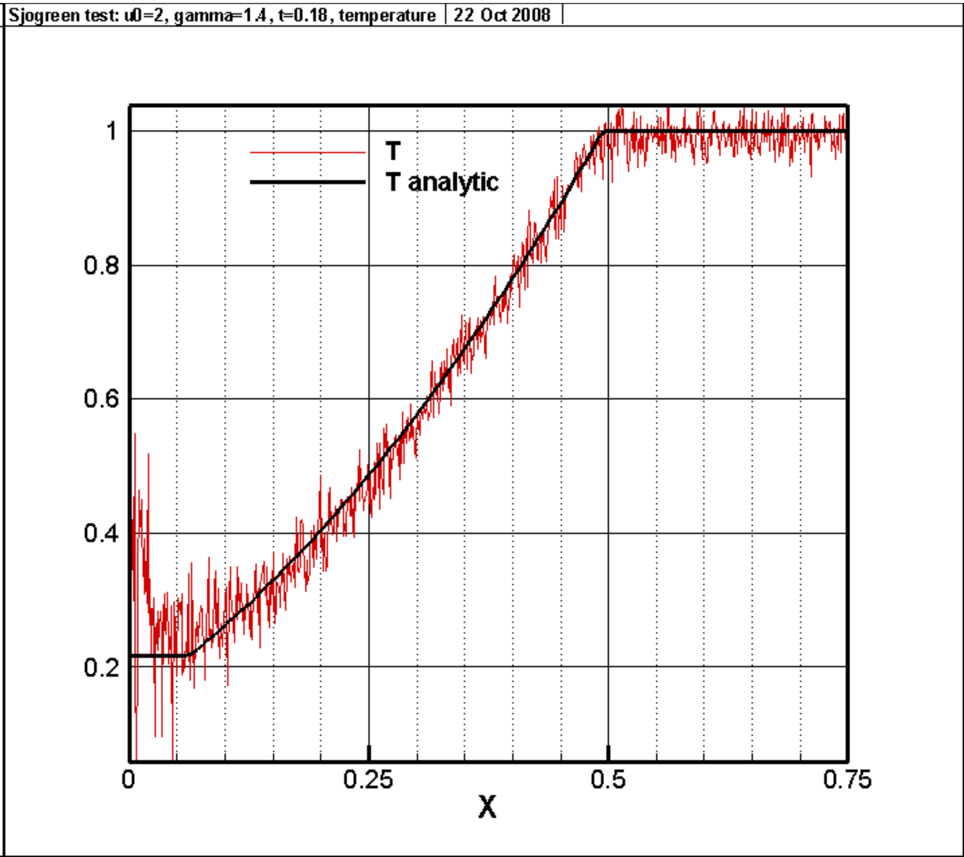
Sjogreen test u_0=2

a case without vacuum

Density and velocity

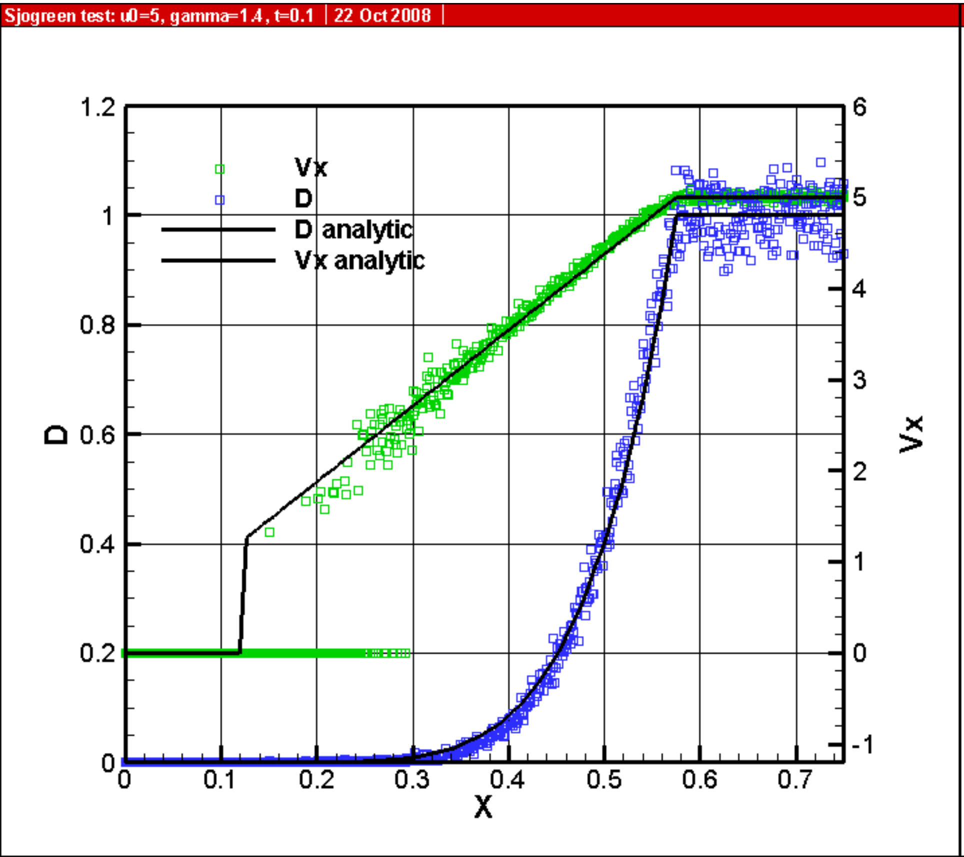
Temperature



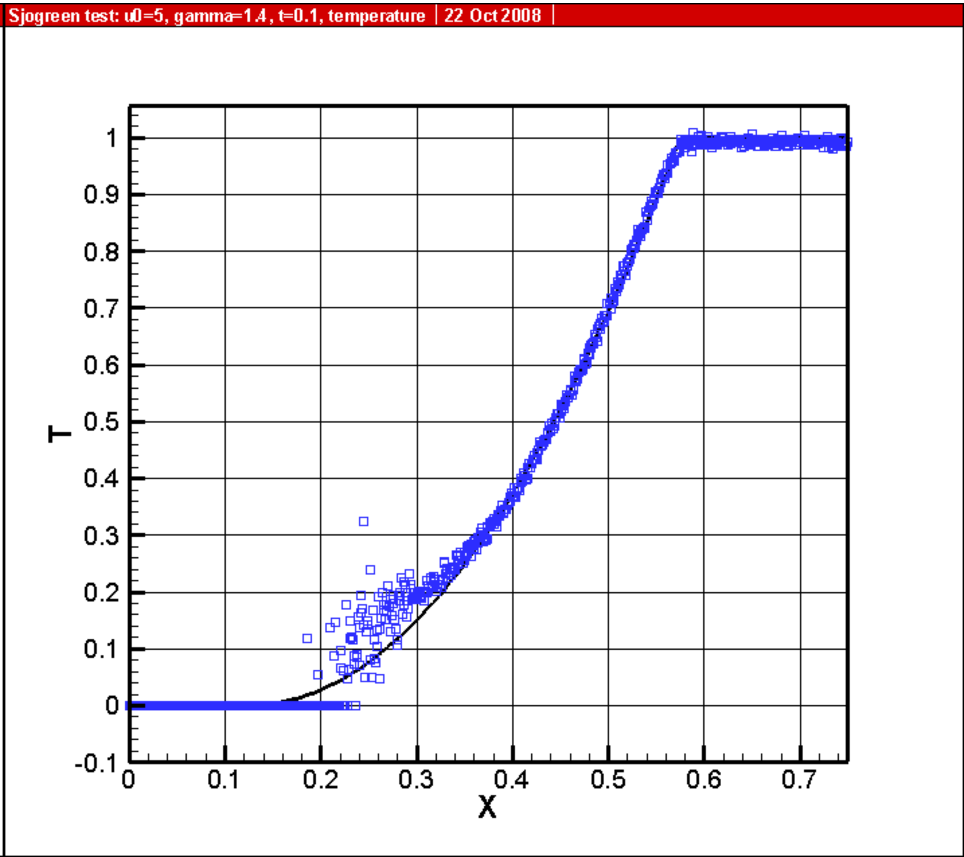


Sjogreen test, u_0=5
a case with vacuum

Density and velocity

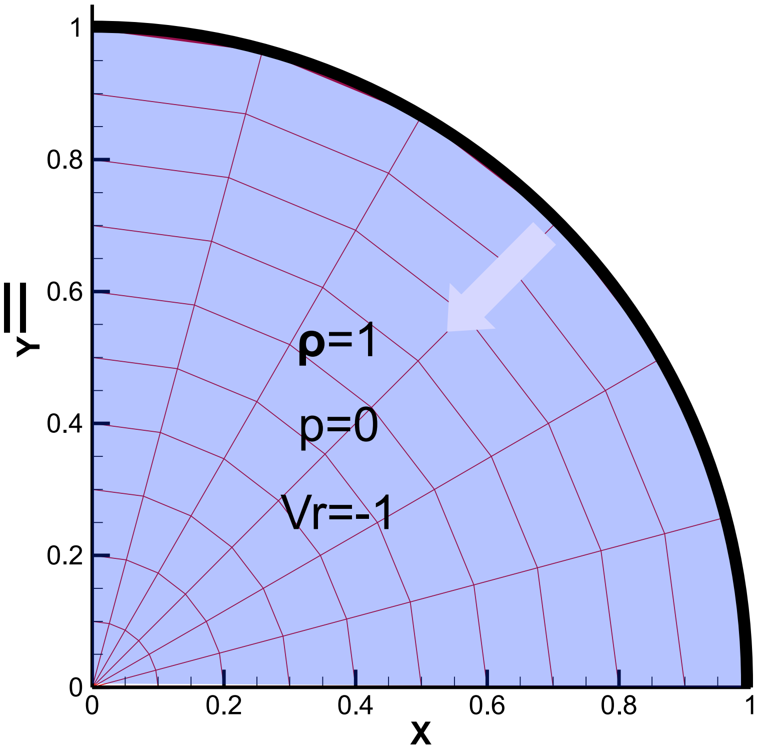


Temperature



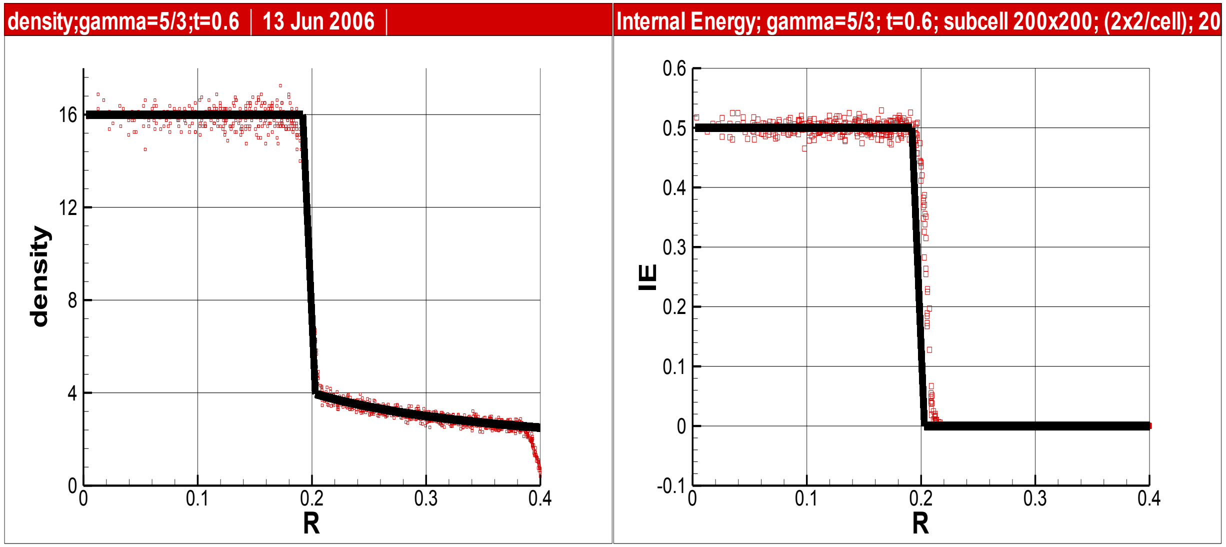
Noh problem

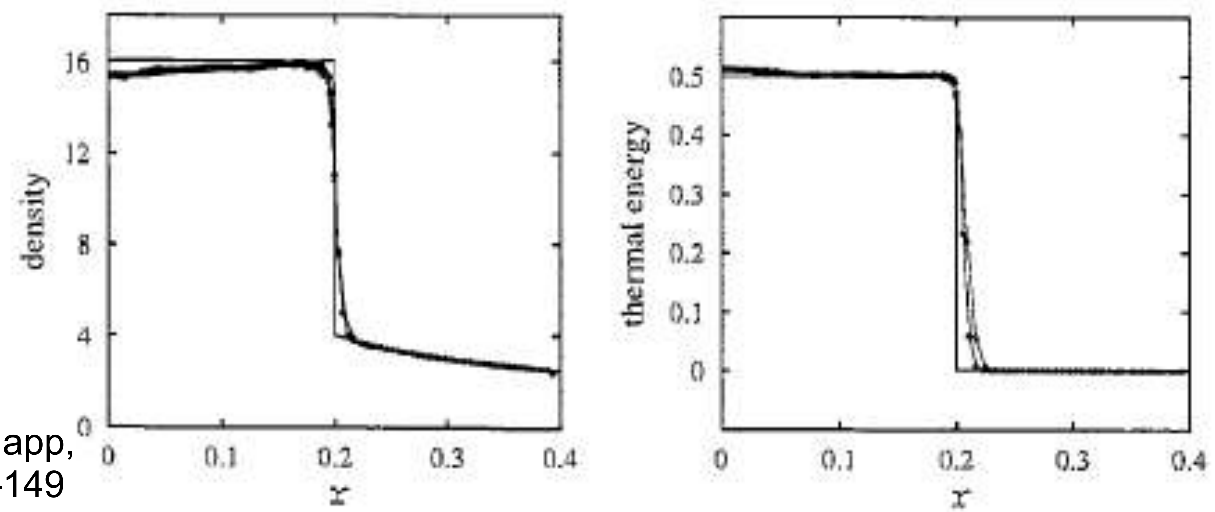
- Computational domain :
  r<1, 0<θ<π/2
- cells 200x200 :
  2x2 cells/ macro-cell
- γ =5/3
- t=0.6



Result of Noh problem

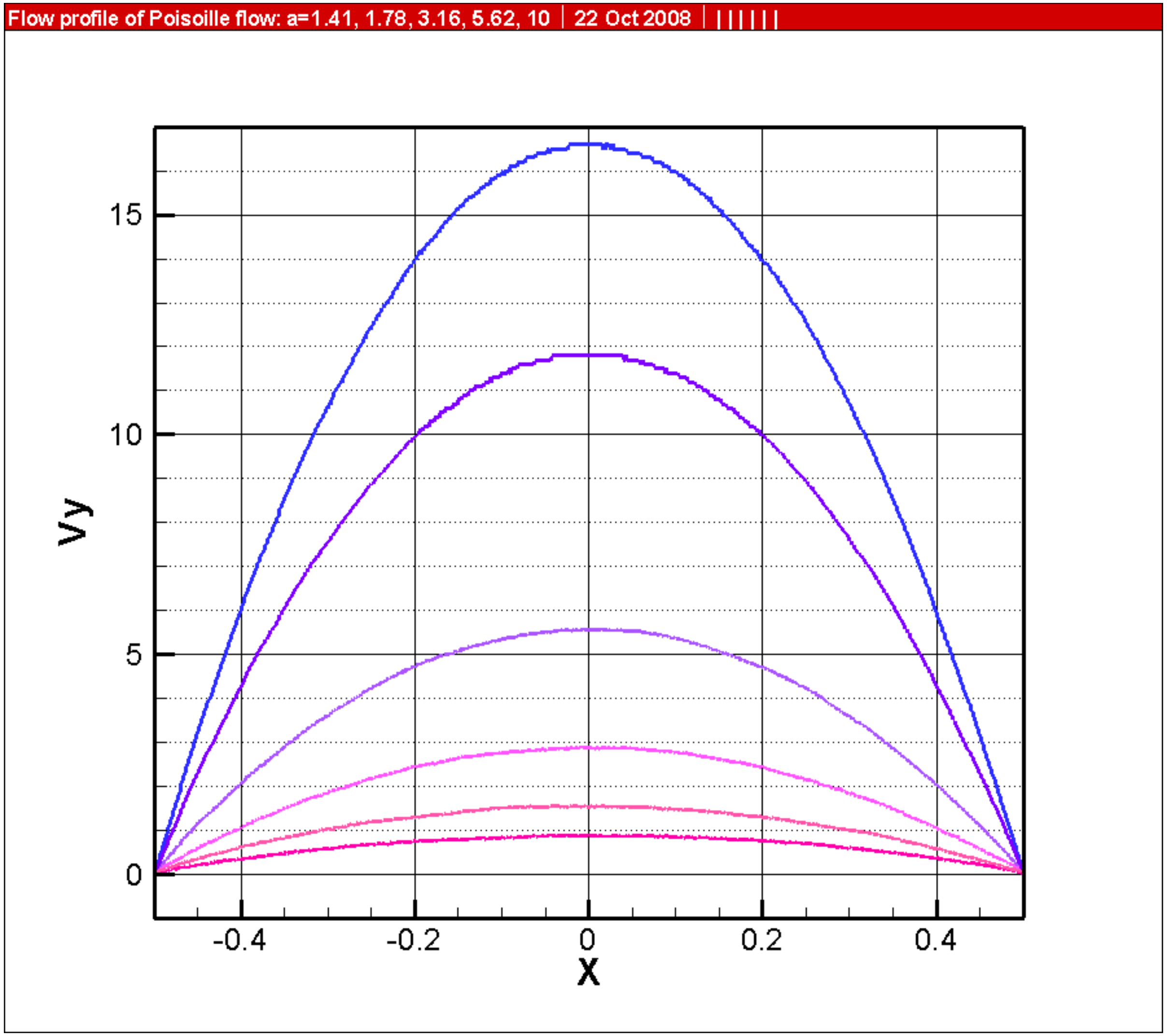
No wall heating



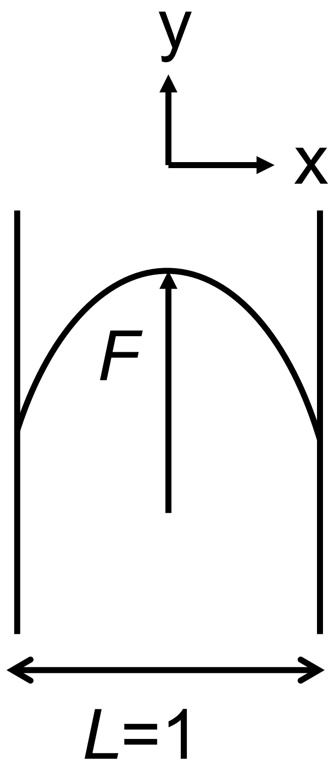


Sigalotti,López,Donoso,Sira and Klapp, J.Compt,Phys. vol.212 (2006) 124-149

Viscous flow
Plane Poiseuille flow



Plane Poiseuille Flow : γ=1.0



Navier-Stokes eqn.

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

Flow field

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

Eq. Motion

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

Computational domain $-0.5<x<0.5$

No. cells : 1000

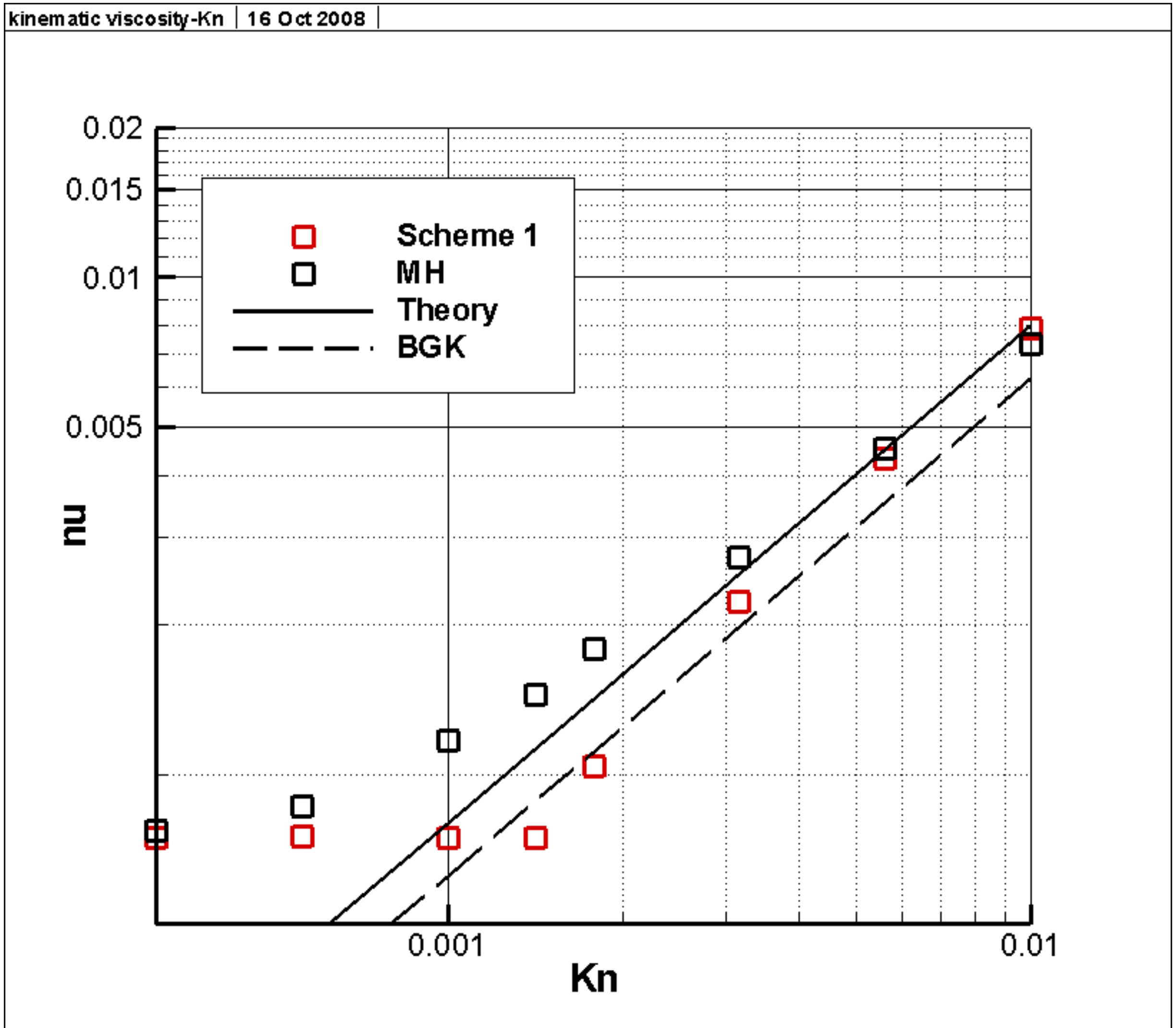
No. Particles : 10/cell

F=0.1

a=1-10, α=1

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

Plane Poiseuille flow
Kinematic viscosity: Knudsen number

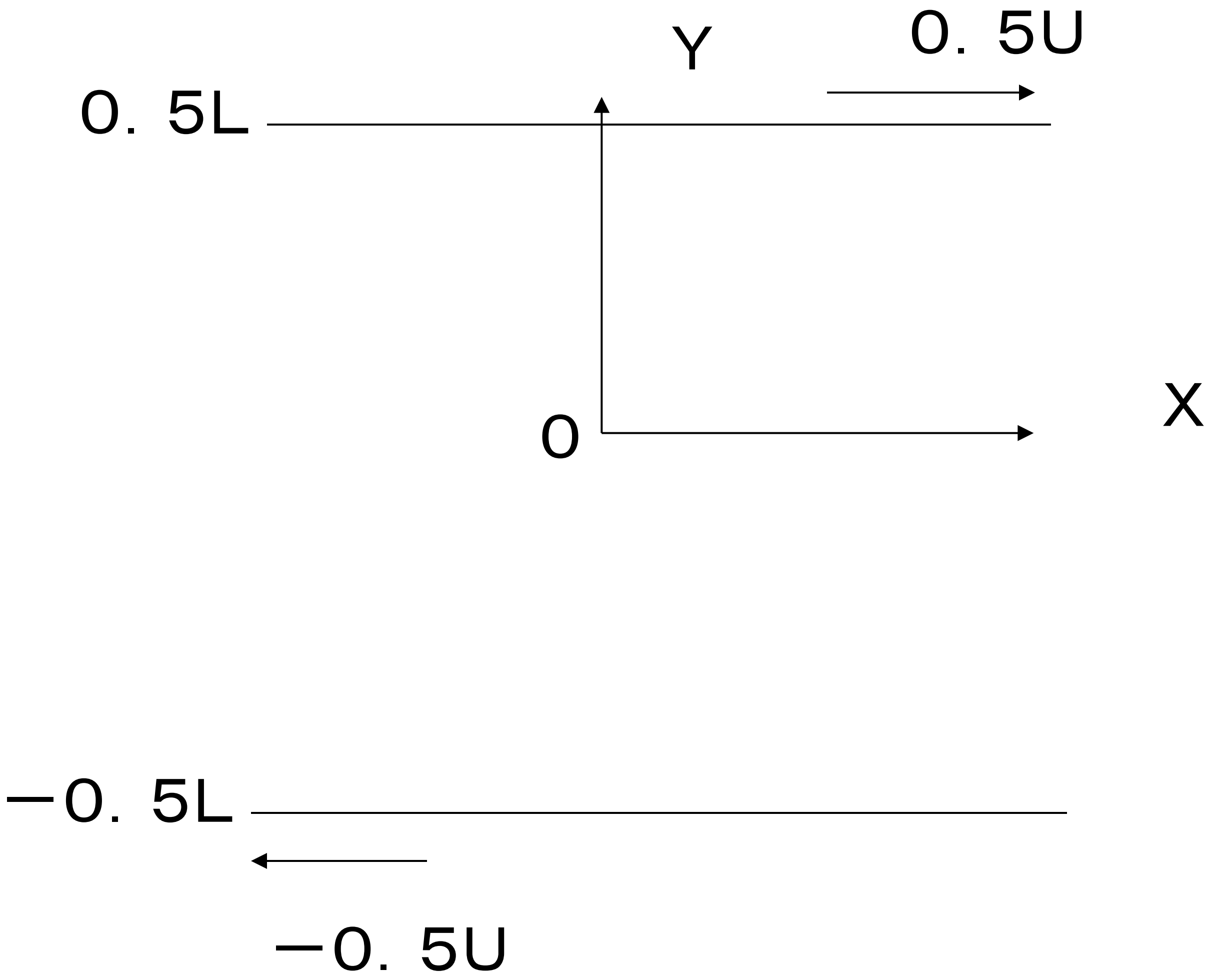


Theoretical curves

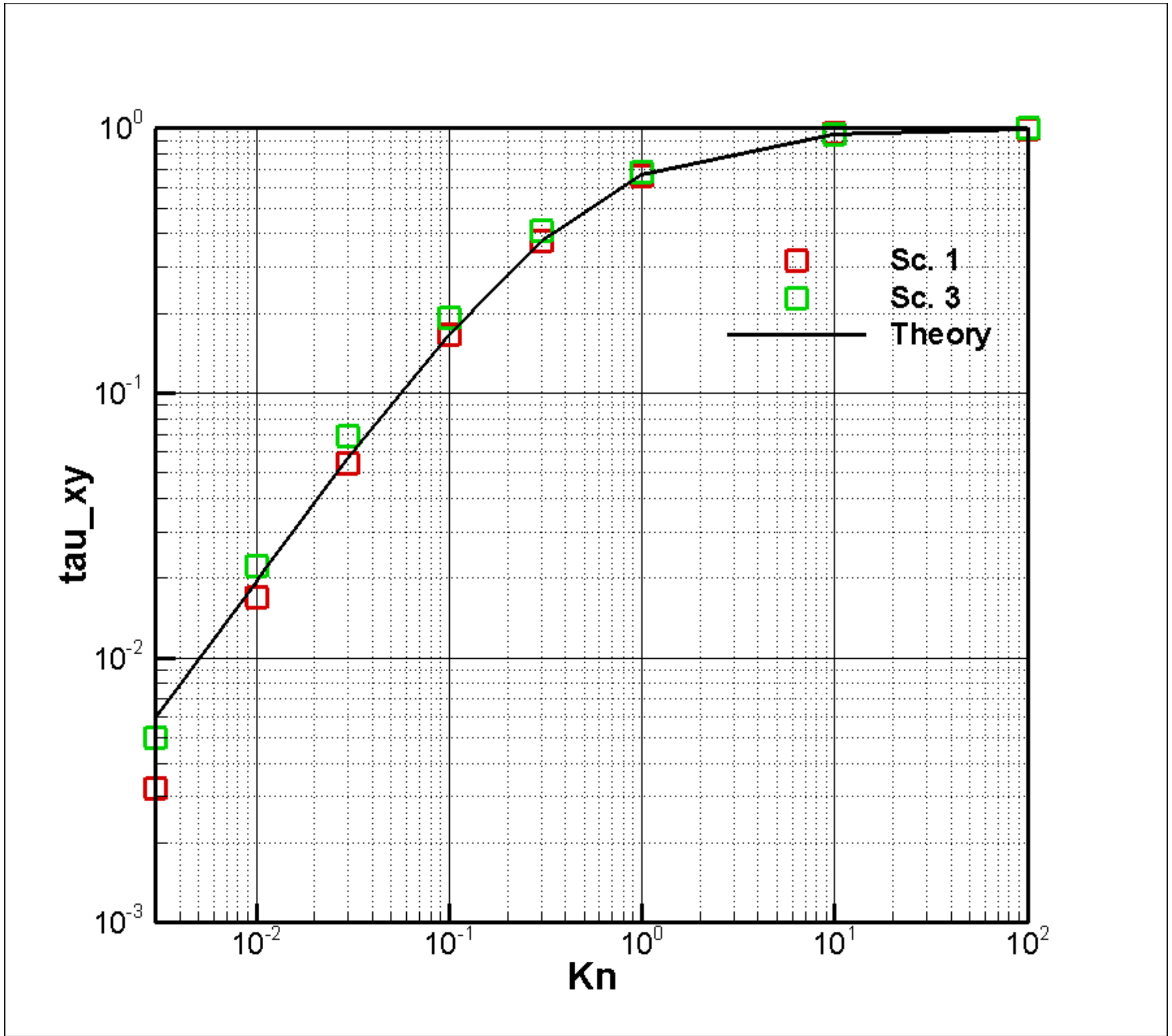
$$\nu = \frac{1}{2}\overline{C}\lambda = 0.798\lambda$$

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

Couette flow

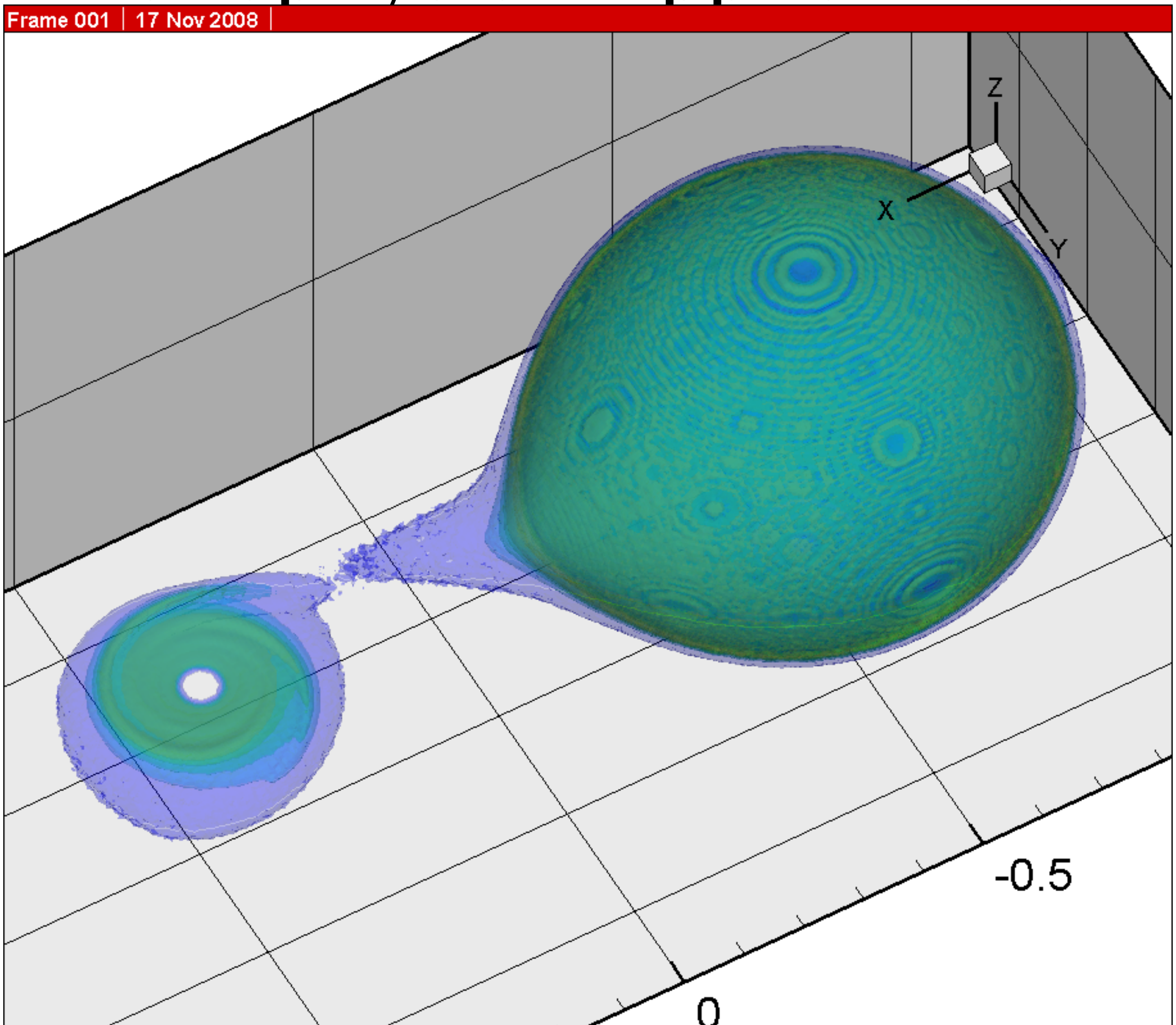


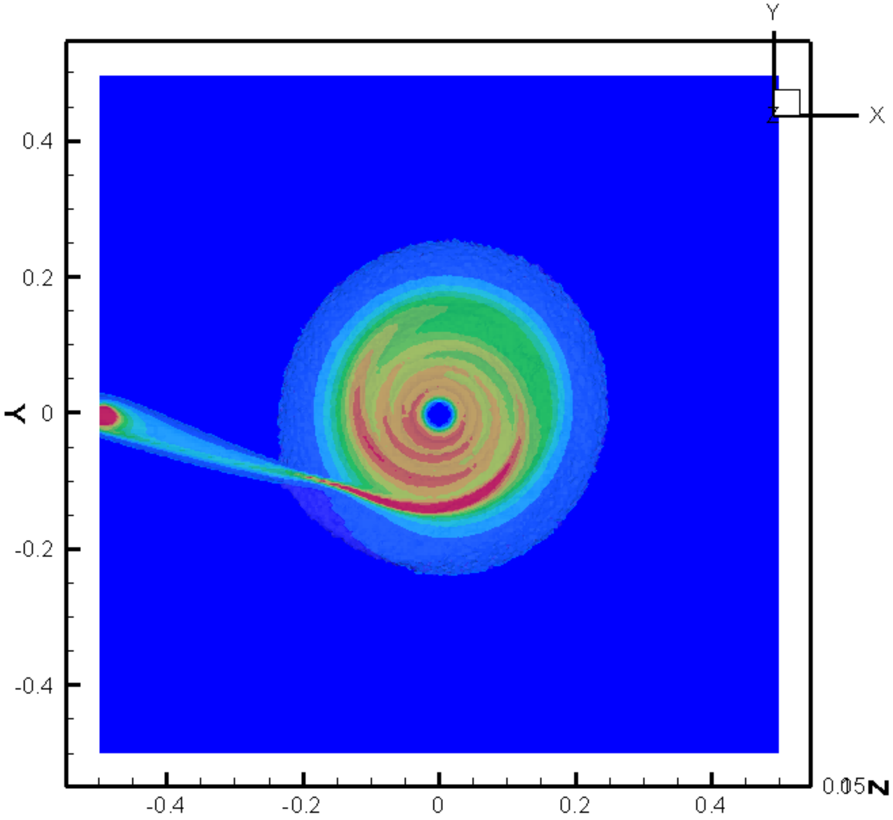
Couette flow
Viscous stress: Knudsen number

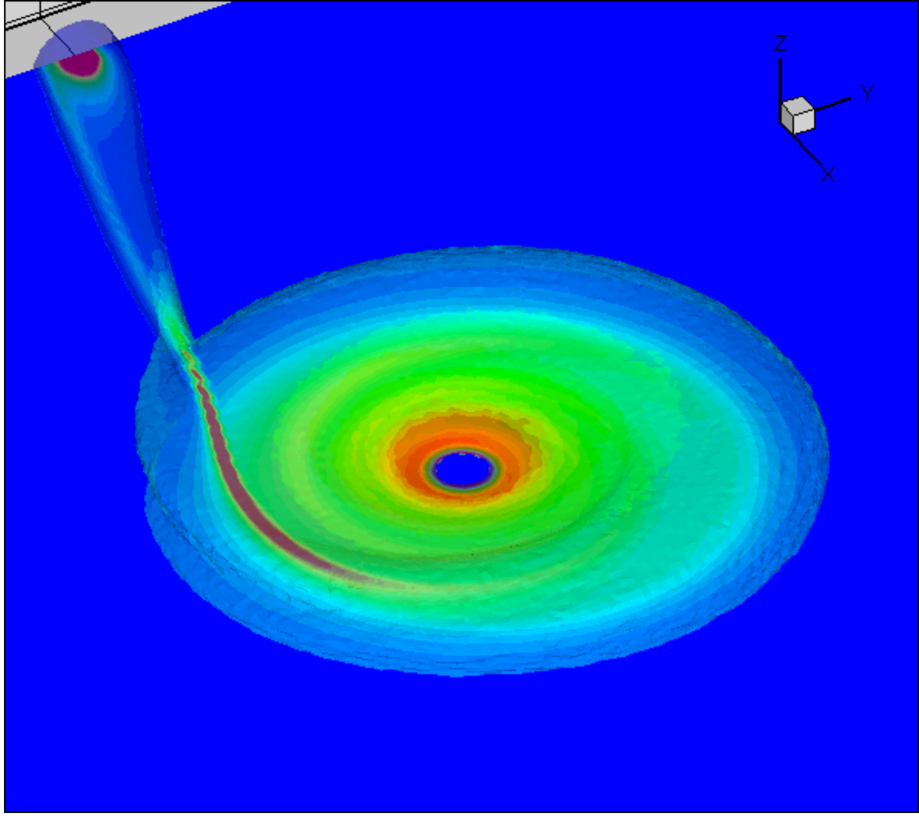


Astrophysical applications

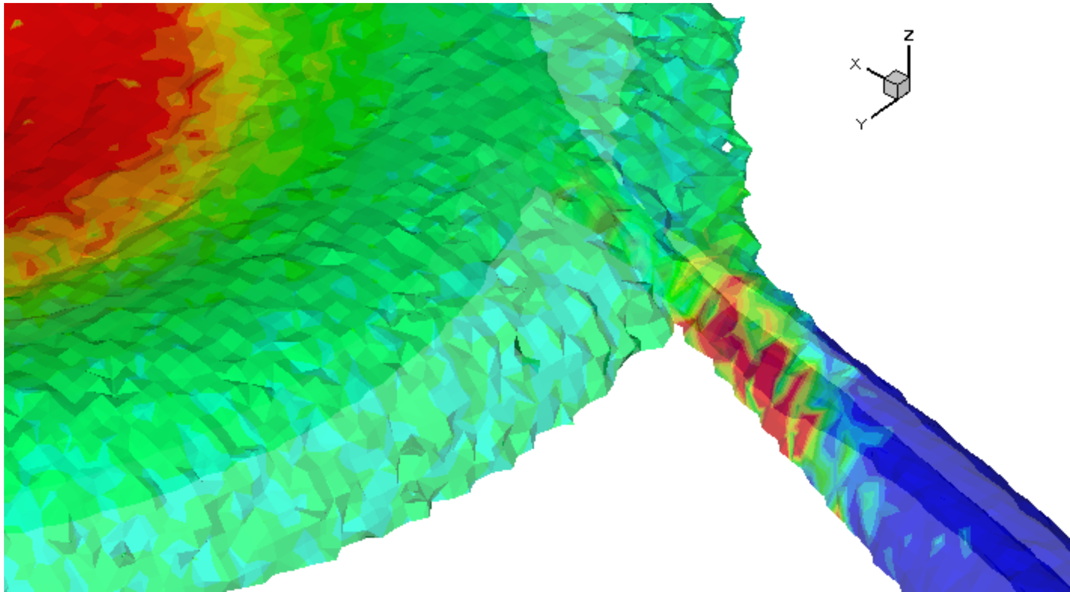
Astrophysical applications



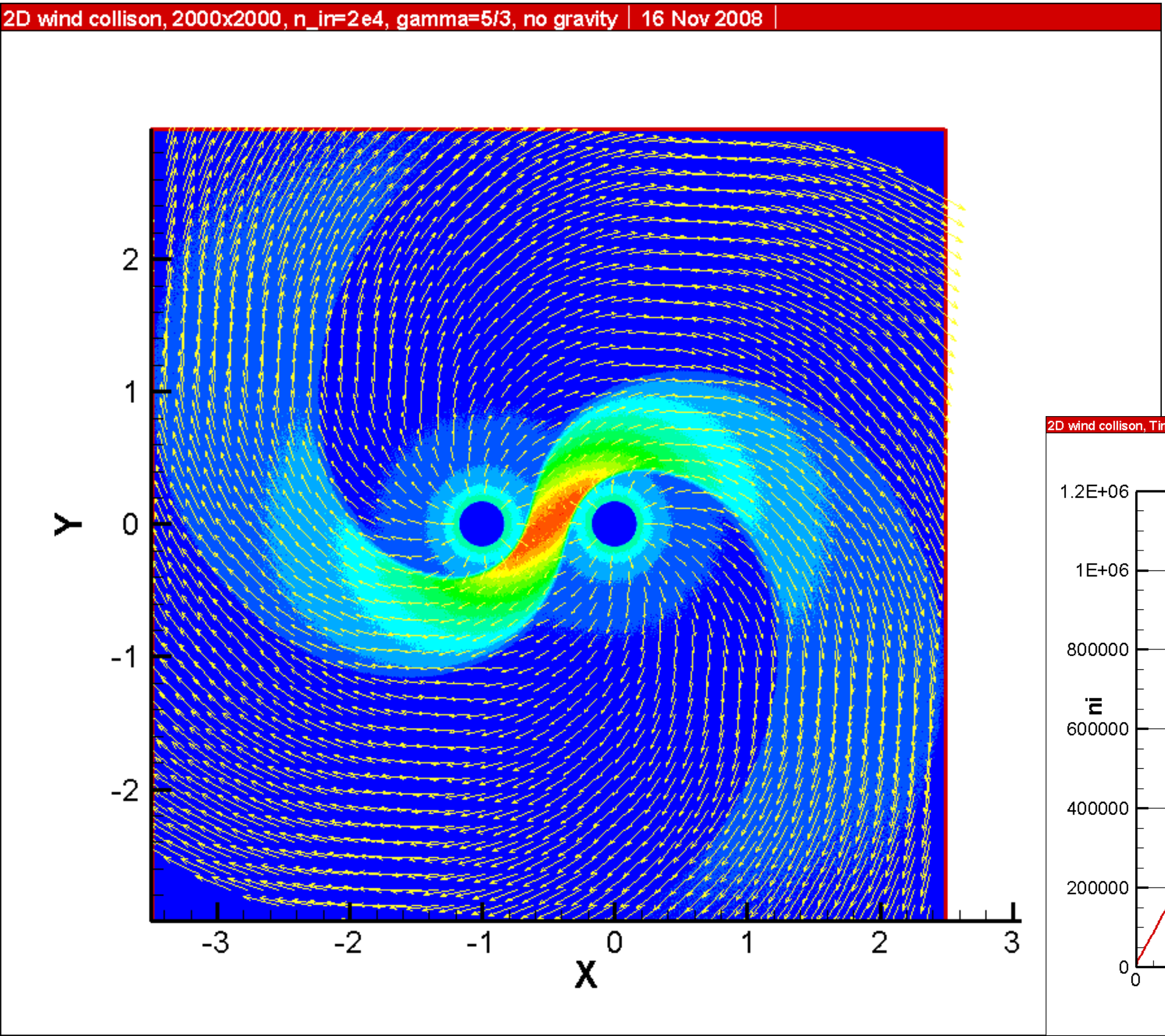




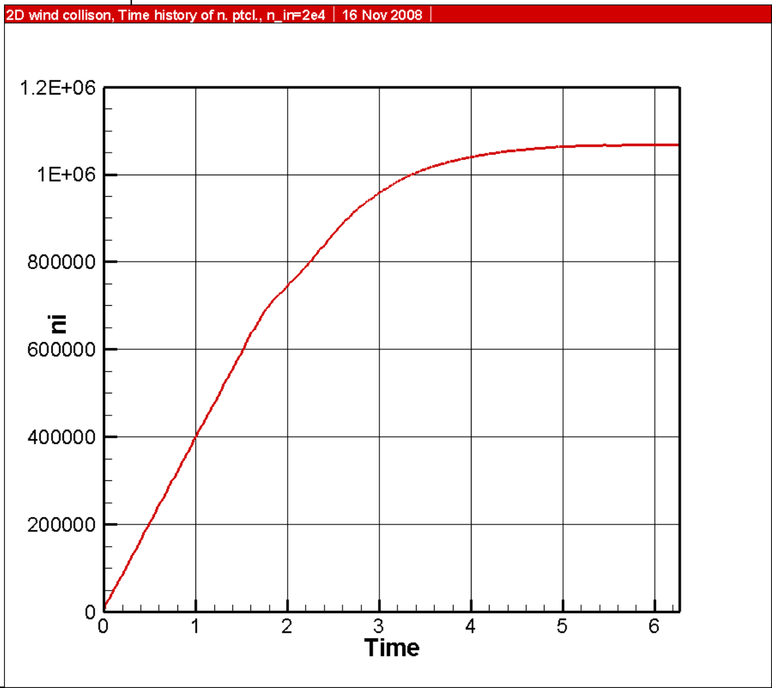
Inflow from L1 point
γ=1.01
Mass ratio=1
T=27



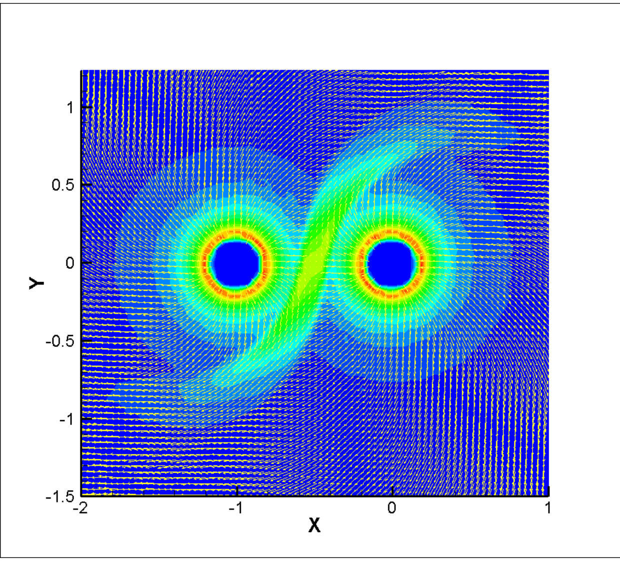
2D wind collision



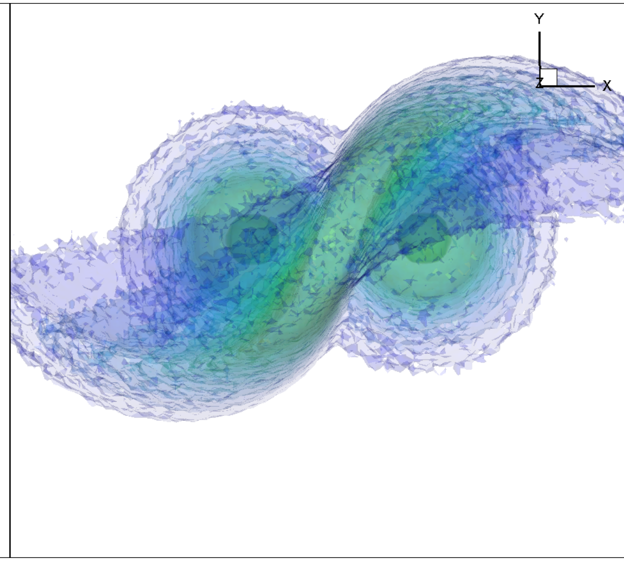
2000×2000
γ=5/3
No gravity
N_in=2e10
Pentium D
45 min



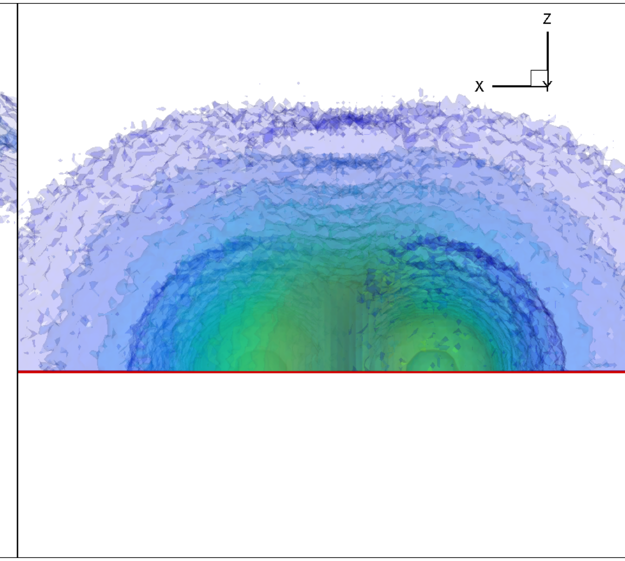
3D wind collision



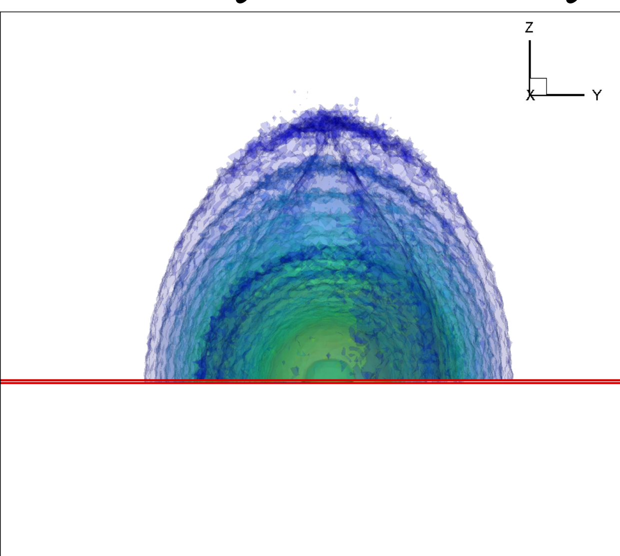
Density and velocity



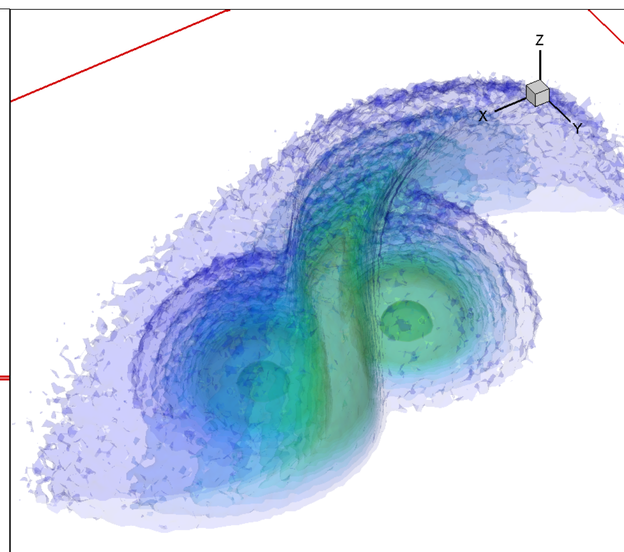
View from z-axis



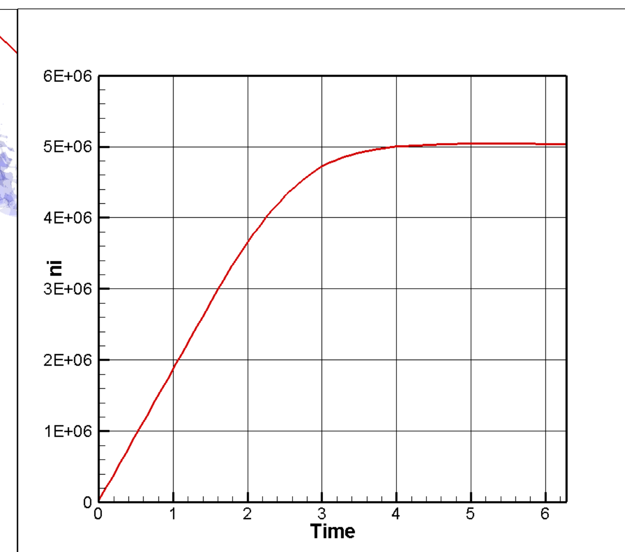
x-axis



y-axis



Bird eye view



Number of particles