Towards a Kinetic Code for Astrophysical Simulations

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Kinetic Theory & Transport Models

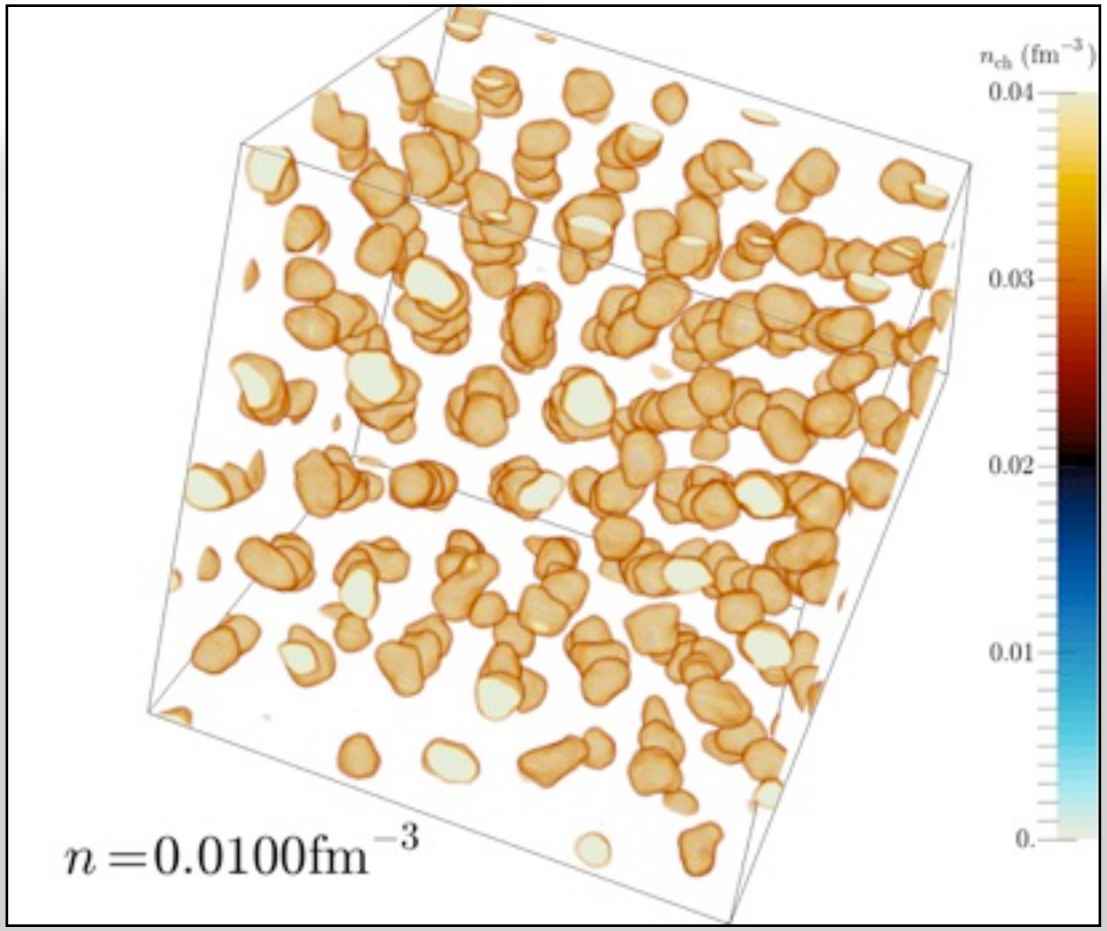
- Solve system's transport equations, e.g.

$$\boxed{\frac{\partial f_i(\vec{r},\vec{p},t)}{\partial t} + \frac{\vec{p}}{m_i}\cdot\nabla f_i(\vec{r},\vec{p},t) + \vec{F}\cdot\frac{\partial f_i(\vec{r},\vec{p},t)}{\partial \vec{p}} = I_{i,\mathrm{coll}}}$$

- Heavy-ion collisions, aerospace research, nano-scale devices, astrophysical N-body simulations
- Numerical methods: Molecular Dynamics, Direct Simulation Monte Carlo, ...
- DSMC: Occupied phase space via delta-functions (test-particles)

$$\boxed{f(\vec{r},\vec{p},t) = \sum \delta^3\left(\vec{r}-\vec{r}_i(t)\right)\delta^3\left(\vec{p}-\vec{p}_i(t)\right)}$$

- Many test-particles can represent one physical particle/object or one test-particle can represent many physical particles/object



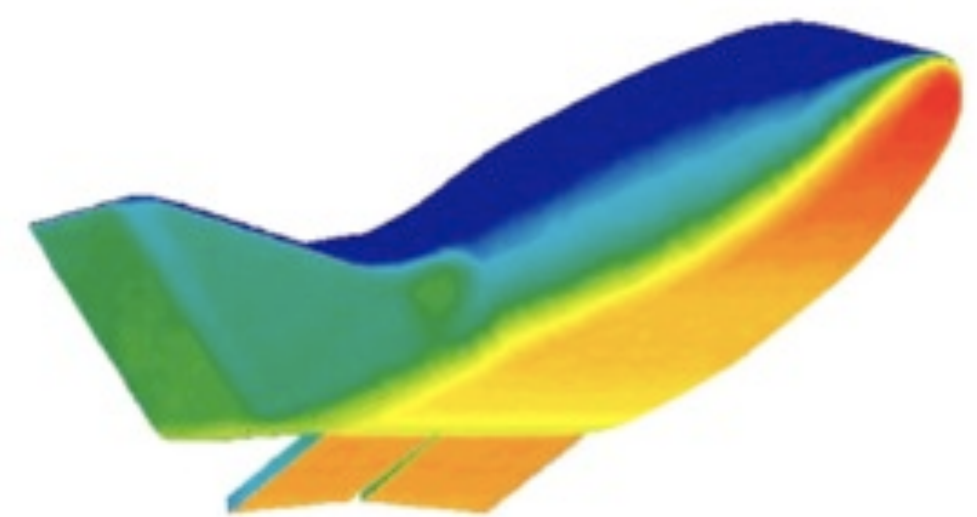
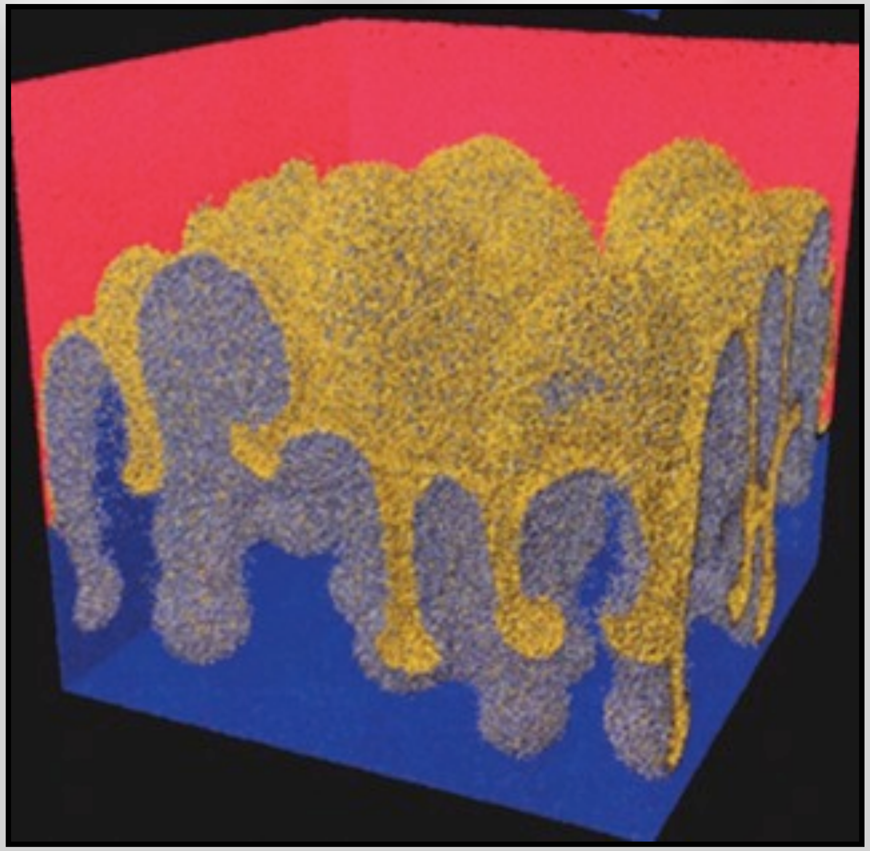
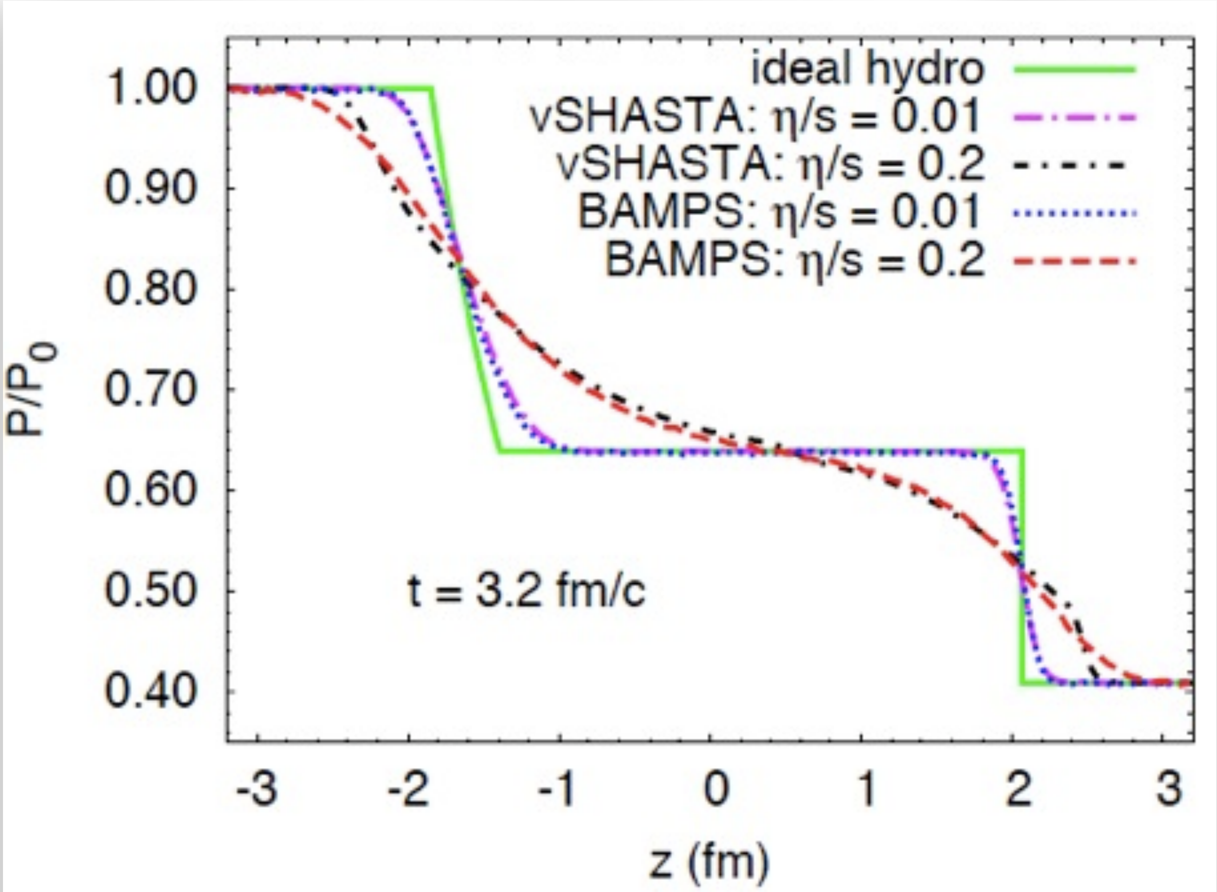


Fig. 7. Surface pressure distribution on X-38 vehicle at 400 kft predicted by DAC.

Top Fig.: Schneider, Horowitz, Hughto, Berry, arXiv:1307.1678

Hydrodynamic Limit





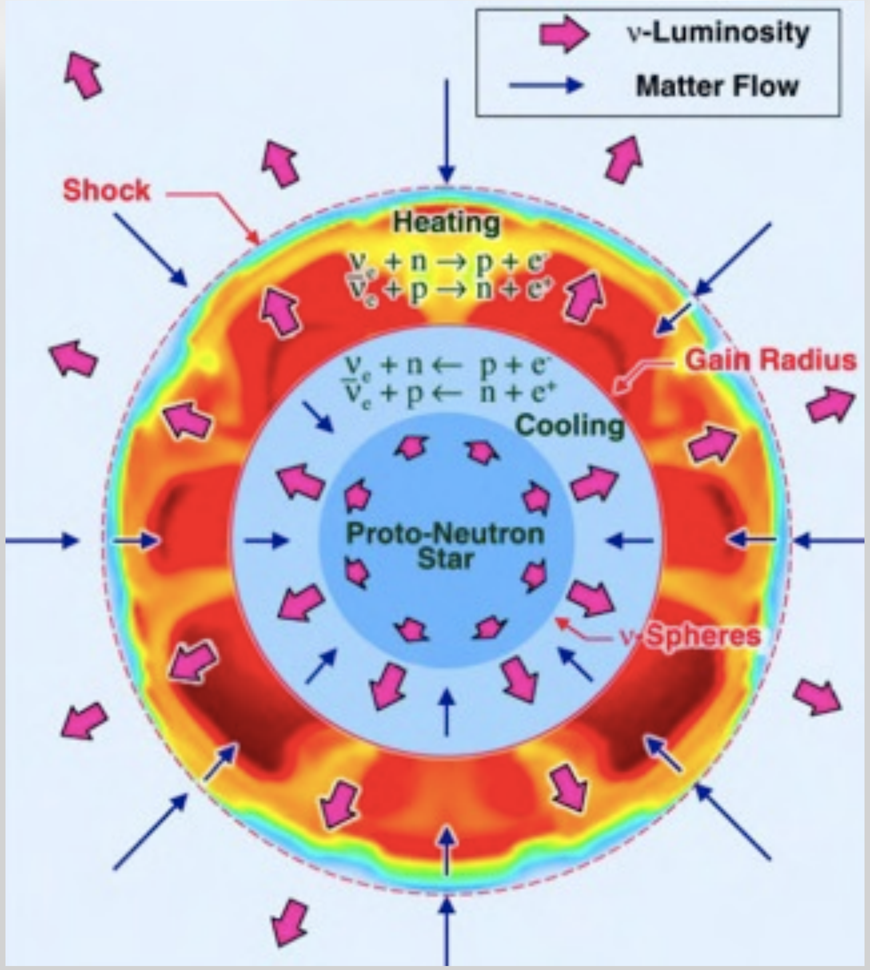
- In the limit of small Knudsen number: $K = \lambda/L$ (mean-free-path/length scale)
- Transport models can reproduce (viscous) hydrodynamic behavior, e.g.:
  - Hydrodynamic shocks
  - Fluid instabilities

Figs: Bouras et al., PRL 103 (2009), Kadau et al. PNAS 101, 16 (2004)

Application areas of interest

Core-collapse supernovae

- Death of massive stars ($M > 8M_{sun}$), triggered by the gravitational collapse of the star's iron core
- Production site for heavy elements, birth place of neutron stars and black holes
- Important for explosion: Interplay between neutrino transport and fluid instabilities



Inertia confinement fusion (ICF)

- Implosion and ignition of fusion fuel capsule (deuterium, tritium) by lasers (direct) or x-ray radiation (indirect)
- Formation of Rayleigh-Taylor instabilities causes non-uniform heating, premature heating of fusion fuels.
- Non-equilibrium effects

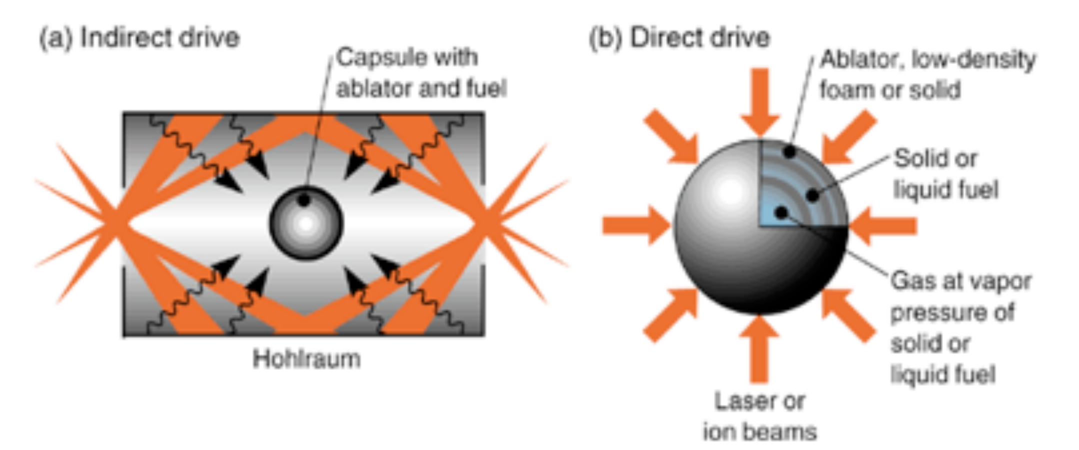
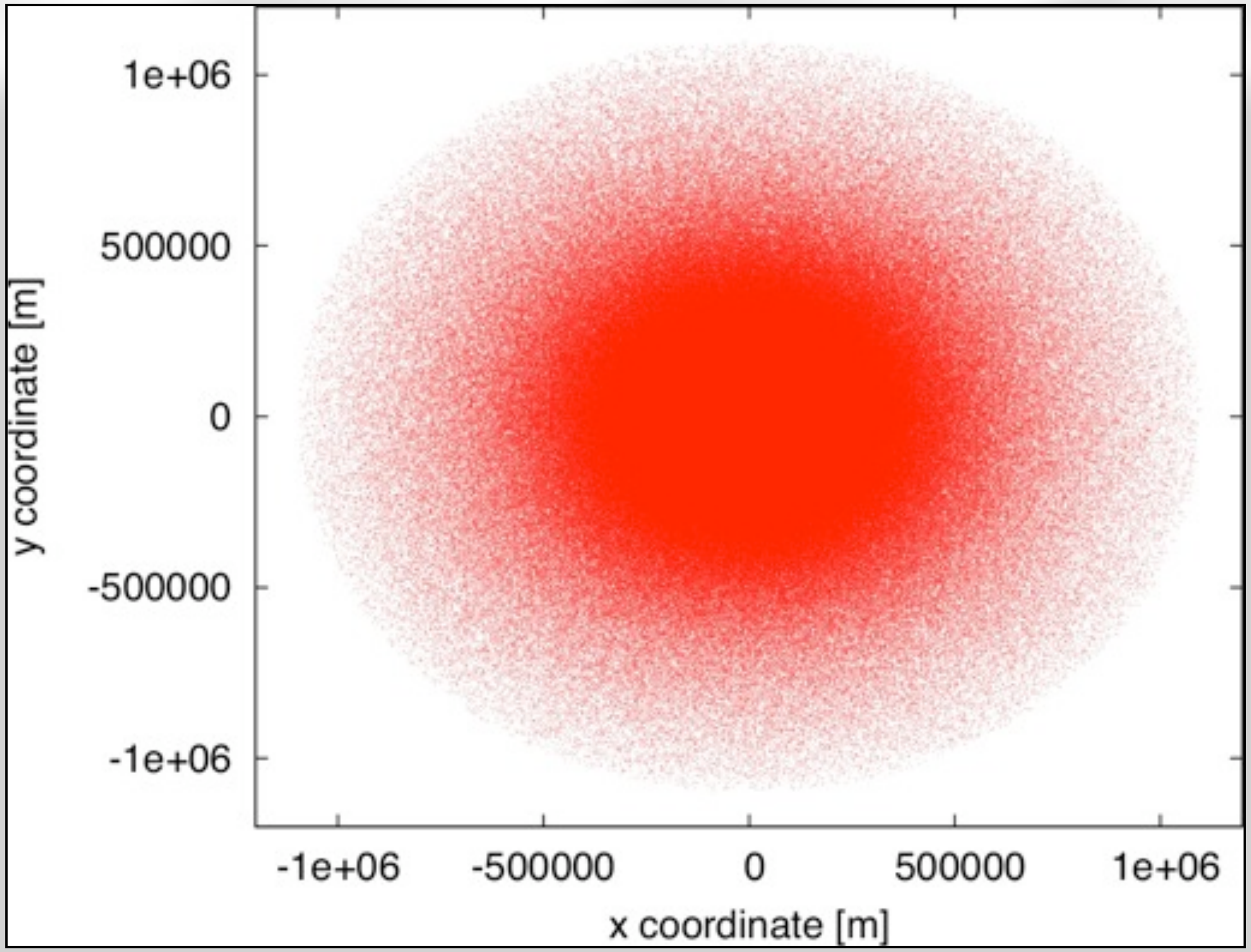


Figure 1. Ignition experiments on NIF will use indirect drive to heat the inside of a cylinder (hohlraum). The incident laser light will enter the cylinder through holes at its end caps and will be converted to x rays that will converge on a 2-millimeter-diameter capsule. NIF also has an option to conduct direct-drive experiments, with the laser light directly incident on a capsule.

Kinetic approach to supernova simulations

- Evolve collapse and explosion stages of stellar core with transport model
- For ~10^6 matter/baryon test-particles & neutrino test-particles → ~10^{51} baryons/test-particle
- Number of matter/baryon test-particles is conserved; neutrino test-particles can be created and absorbed
- Matter/baryon test-particles can represent neutrons, protons, or nuclei
- Test-particles are subject to nuclear mean-field force, gravitation, and scattering



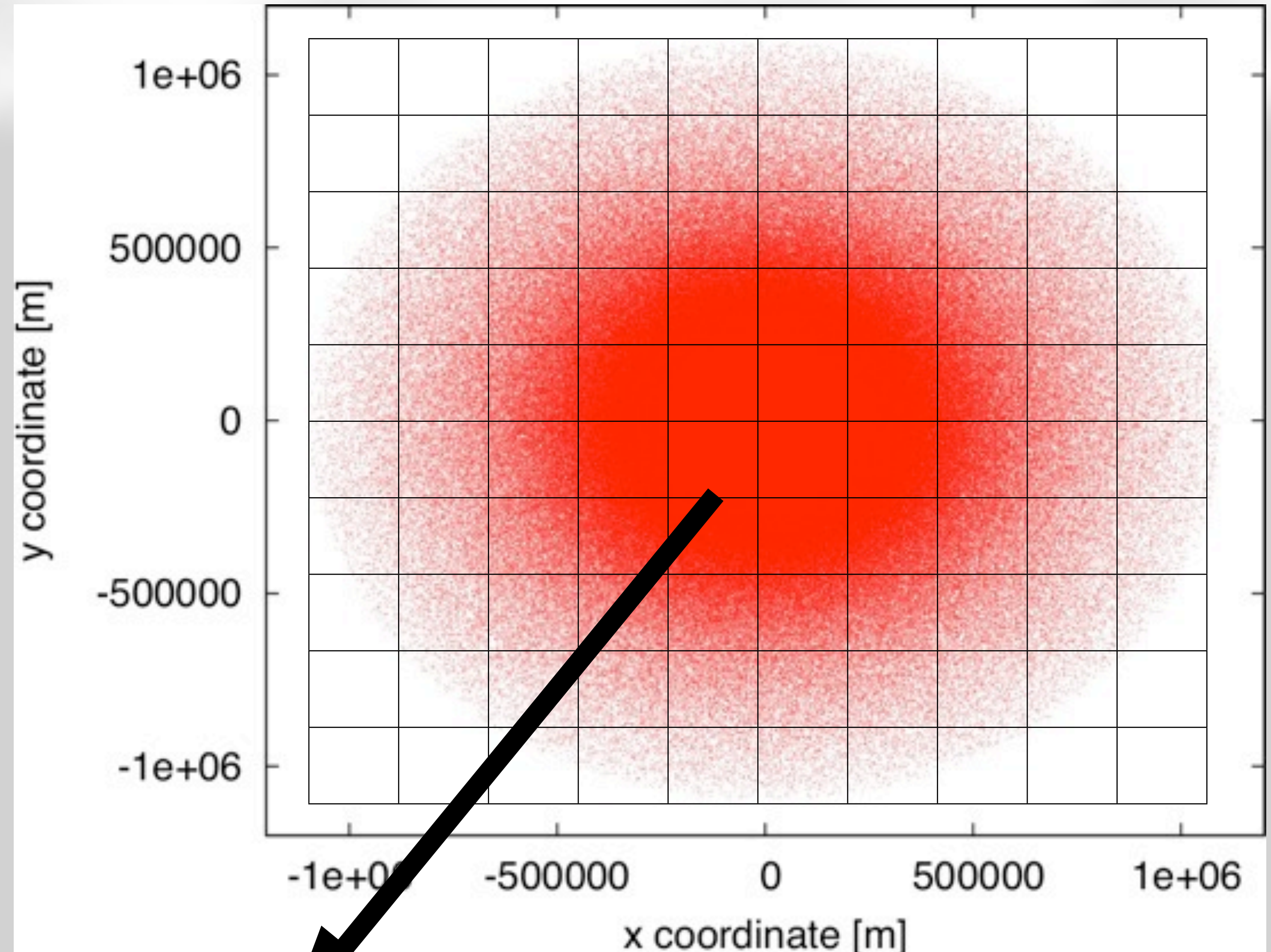
$$\frac{d}{dt}\mathbf{p}_j = -\nabla U_{EoS,e-}(\vec{r}_j) + \mathbf{F}_{Grav(j)} + \mathbf{F}_{Coll}(\mathbf{p}_j)$$

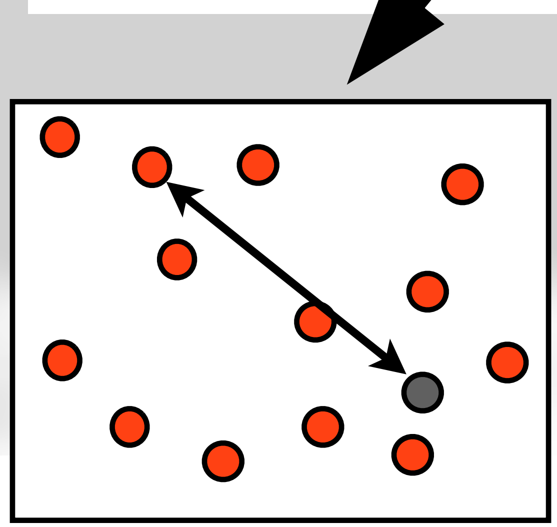
$$\frac{d}{dt}\mathbf{r}_j = \mathbf{p}_j / \sqrt{m^2 + p_j^2}$$

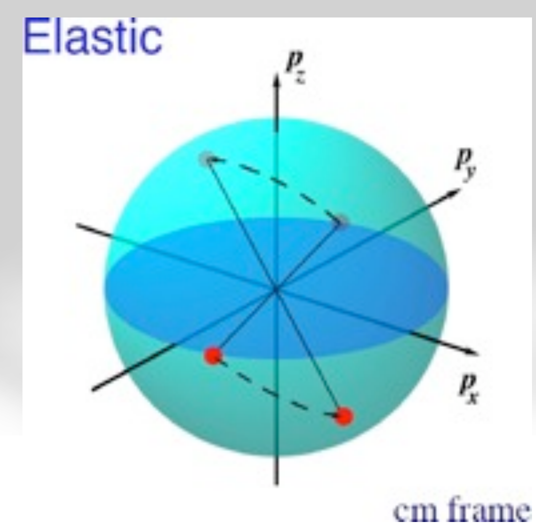
Strother & Bauer, Int. Journal Mod. Phys. D (2009),
Strother & Bauer, Journal of Phys. 230 (2010)

Grid for test-particle scattering

- Collisions by Direct Simulation Monte Carlo
- Random choice of scattering partners in a cell
- Collision is performed in the center-of-mass frame
- Random choice for orientation of outgoing velocity vector



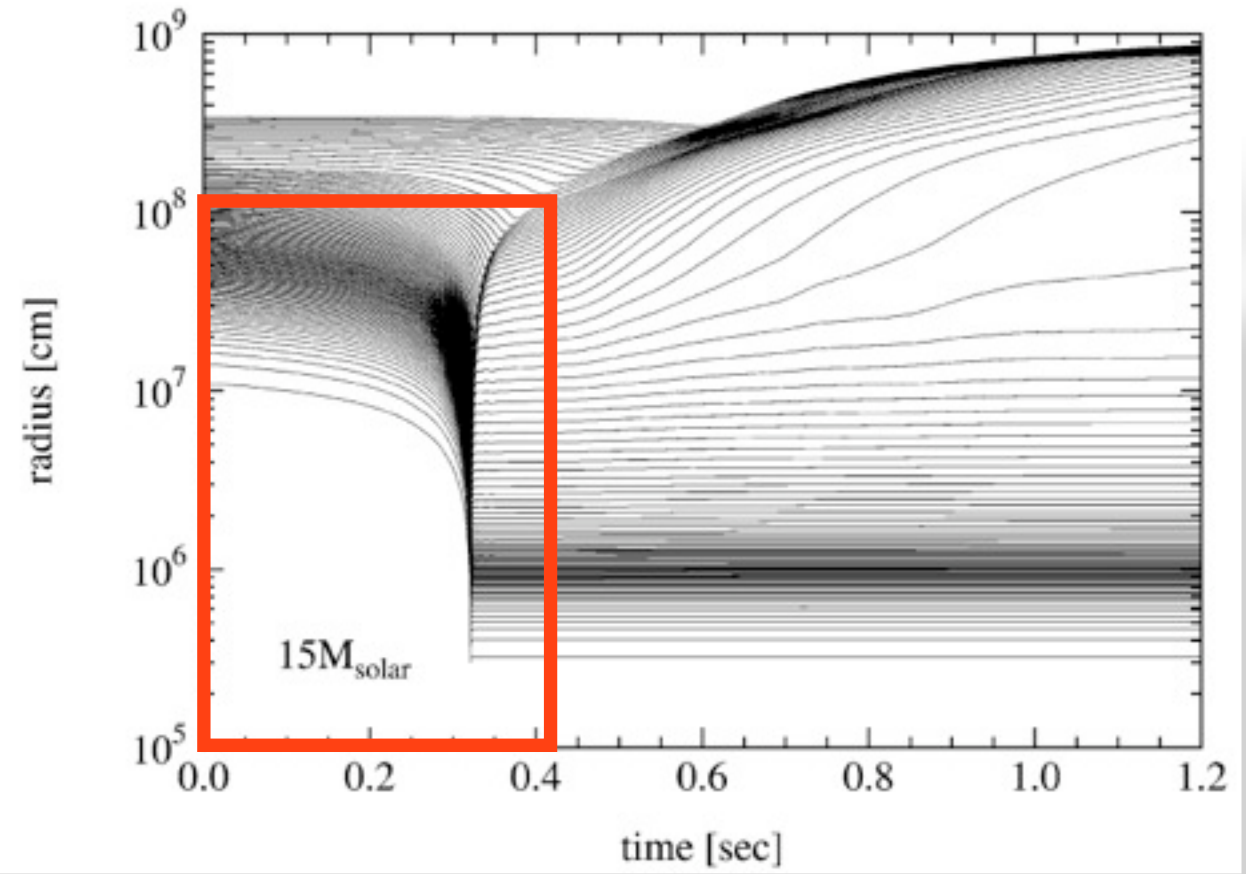


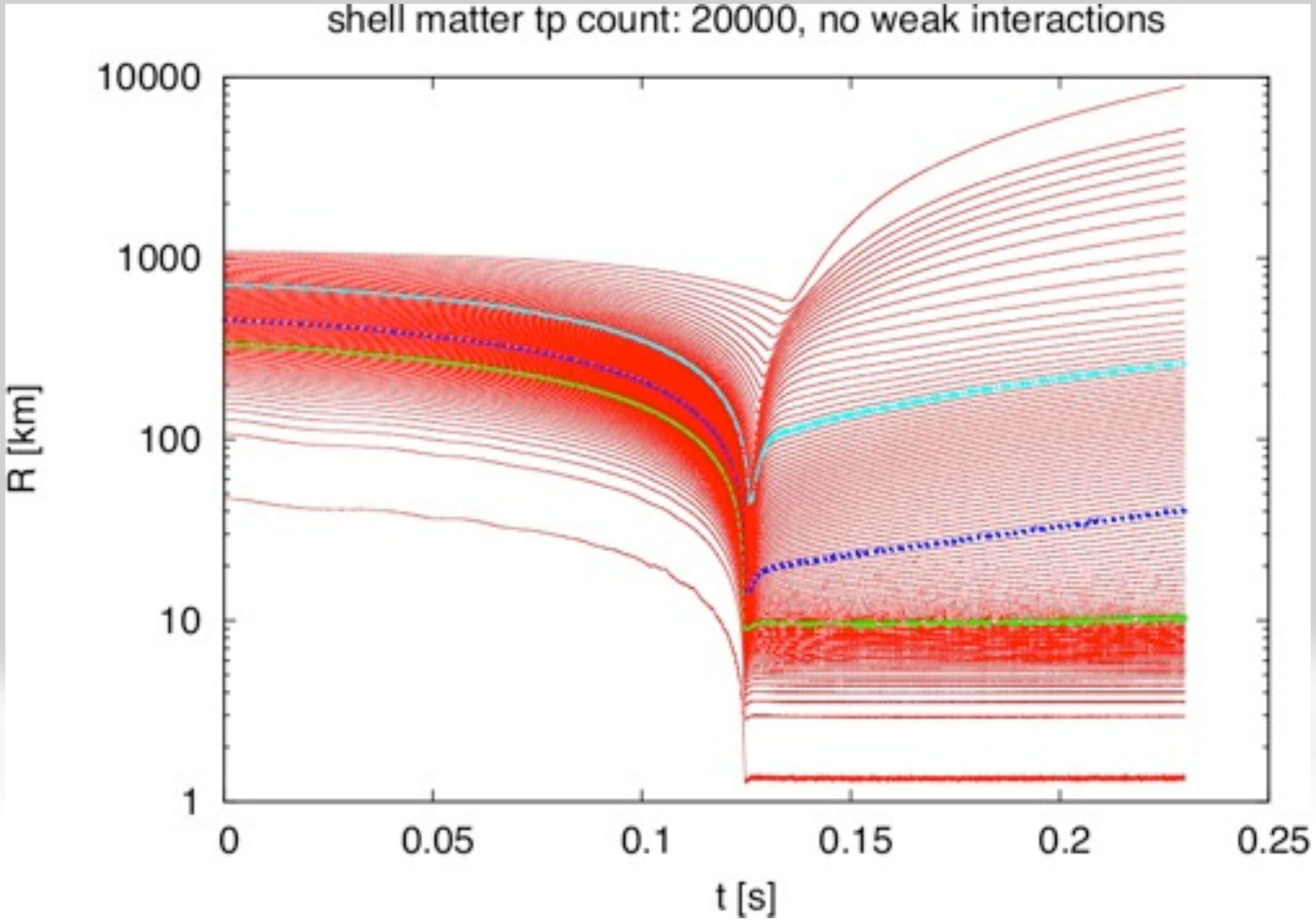


Strother & Bauer, Int. Journal Mod. Phys. D (2009),
Strother & Bauer, Journal of Phys. 230 (2010)

Previous studies

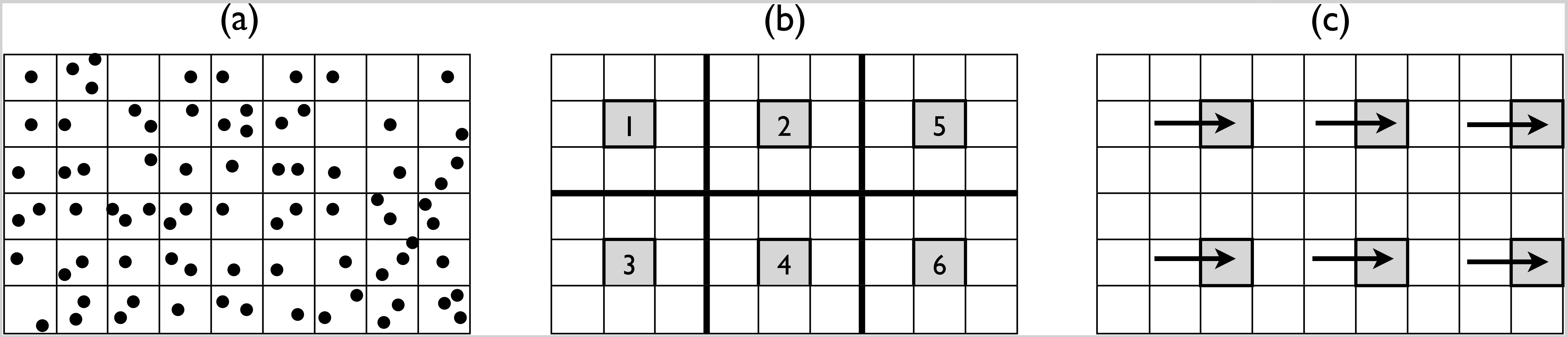
- 10^6 baryon test-particles
- Simple skyrme - type potential
- No iso-spin contribution
- Simulation via DSMC
- Collapse of the iron core of a $15M_{sun}$ star
- Comparison to 1D GR hydrodynamic simulation with Relativistic mean-field EoS
- Similarities in collapse phase and shock formation
- No neutrino transport
- Simulation ran on 1 CPU for one week (3D particle collision and propagation, 1D spherical gravity - Newtonian monopole approximation)





Top figure: Sumiyoshi et al. NPA 730 (2004)

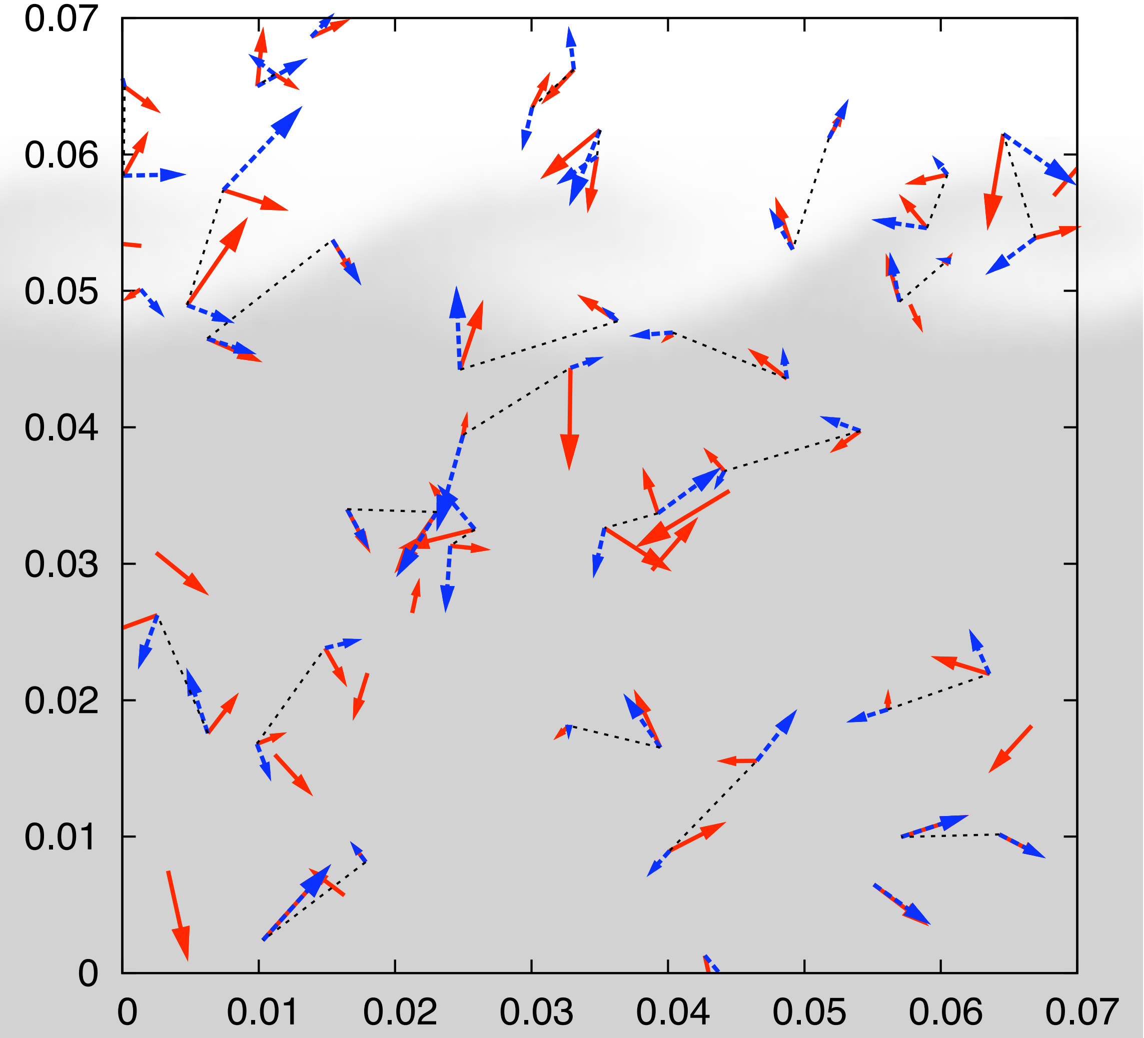
Large Scale DSMC Code



- Aim: Transport code that can handle N $\gg 10^6$ test particles in a computationally efficient way
- Divide simulation space into grid and allocate particles to its bins via linked list
- Parallel scattering partner search over *active* bins and their neighboring cells
- Particle interaction range must be smaller than bin size Δx
- Adaptive time step size: $\Delta t = \Delta x / v_{max}$
- Use one grid for calculations (c-bins) and one grid for output (o-bins)

Figs: I.S., D.Colbry, T.Strother, R.Pickett, W. Bauer JCP 266 (2014)

Collision detection via Point-of-Closest Approach



- Relative position change:

$$\chi = (\vec{r}_{\rm rel}(t) \cdot \vec{v}_{\rm rel}(t))(\vec{r}_{\rm rel}(t+\Delta t) \cdot \vec{v}_{\rm rel}(t+\Delta t))$$

$$\vec{r}_{\rm rel}(t) = \vec{r}_A(t) - \vec{r}_B(t), \quad \vec{r}_{rel}(t+\Delta t) = \vec{r}_A(t+\Delta t) - \vec{r}_B(t+\Delta t)$$

- Real overlap times:

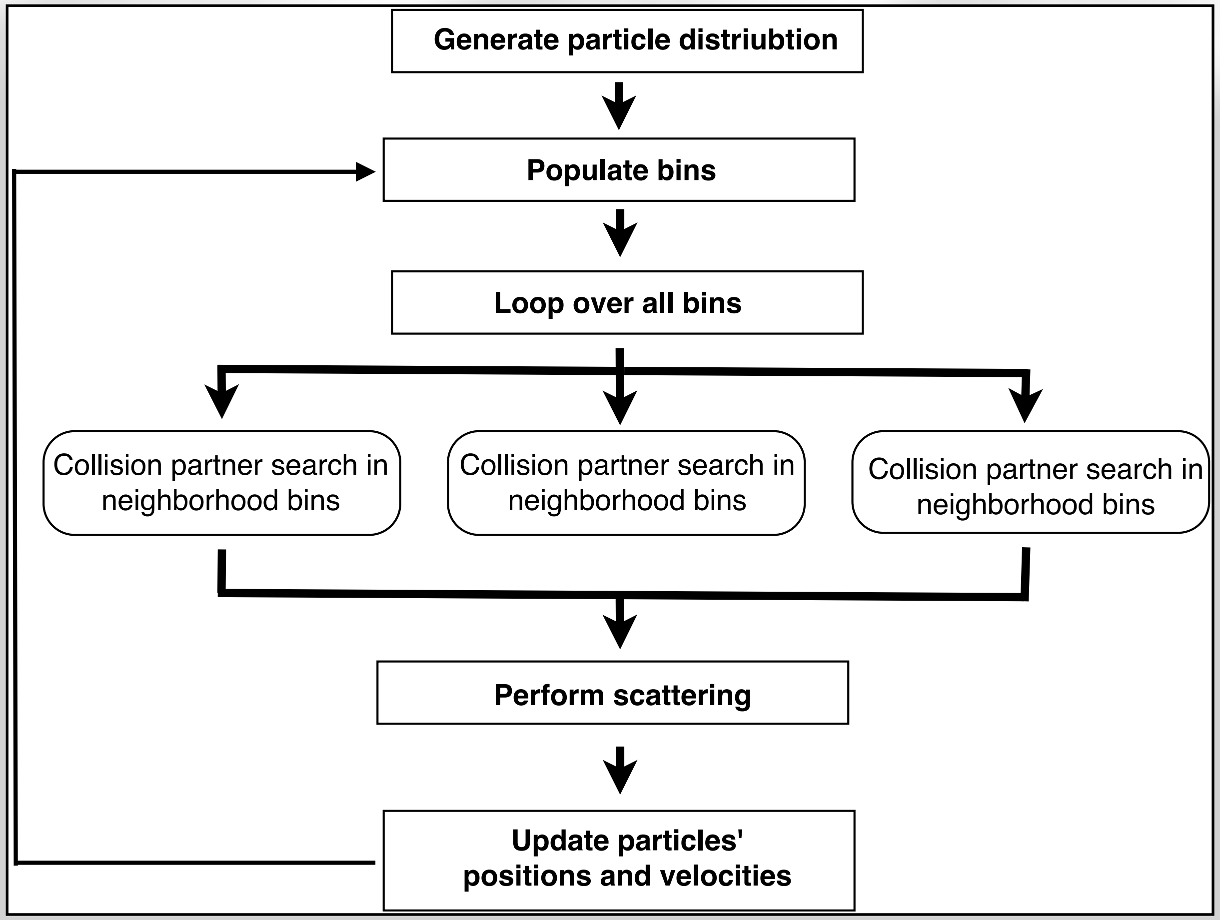
$$t_{o\,1,2} = \frac{1}{|\vec{v}_{\rm rel}|^2}\left[-(\vec{v}_{\rm rel} \cdot \vec{r}_{\rm rel})^2 \pm \sqrt{(\vec{v}_{\rm rel} \cdot \vec{r}_{\rm rel})^2 - |\vec{v}_{\rm rel}|^2\left(|\vec{r}_{\rm rel}|^2 - (r_{{\rm eff},A} + r_{{\rm eff},B})^2\right)}\right]$$

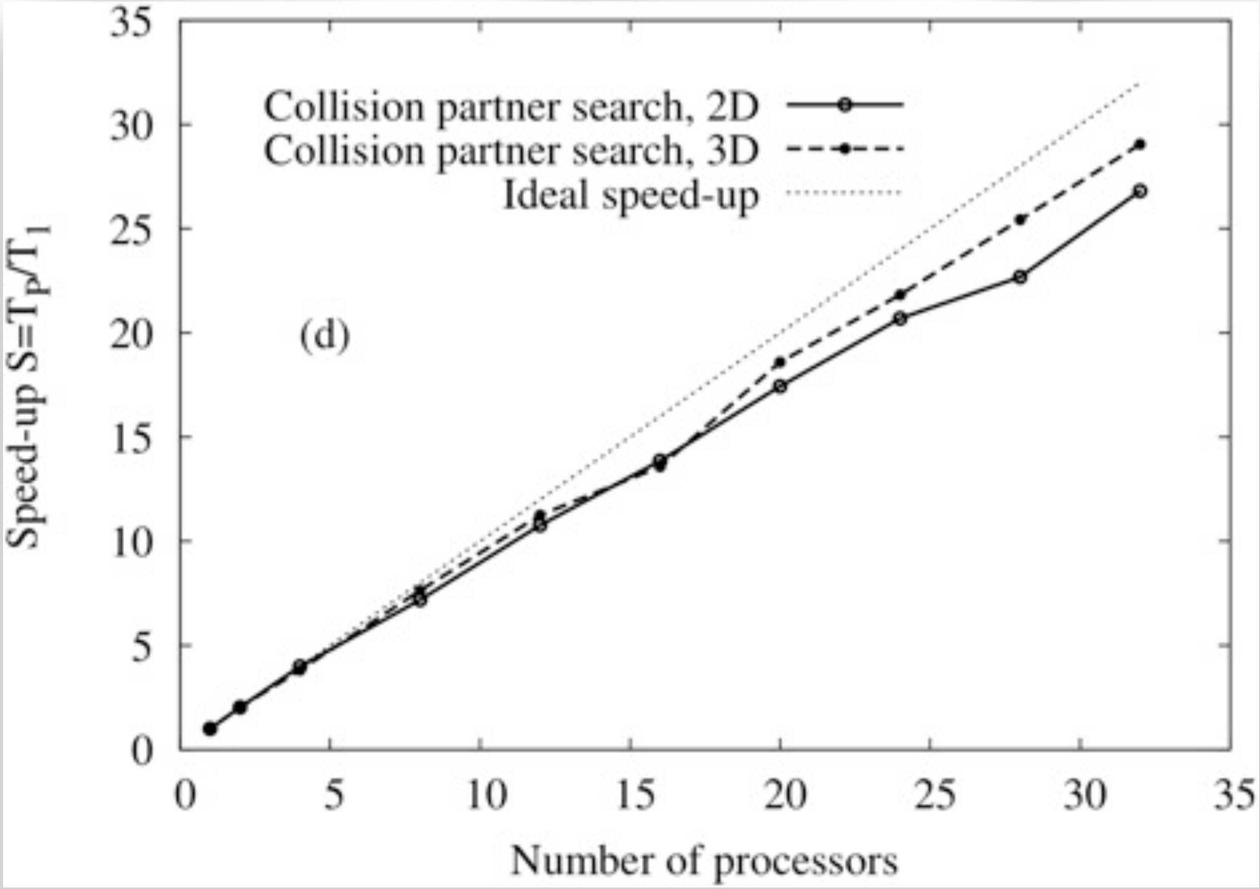
$$\lambda = (4\pi\, r_{\rm eff}^2\, n)^{-1}$$

- Final collision partner: Shortest collision time or smallest distance

Figs: Sagert., Bauer, Colbry, Howell, Pickett, Staber, Strother JCP 266 (2014)

Simulation overview





- Simulation space with 10^7 - 10^8 test-particles
- Parallel scattering partner search (currently OpenMP, MPI under development)
- Scattering partner by Point-closest-Approach
- Interactions: 2-body collisions
- Boundary conditions: reflective, periodic, free, random reflective, ...

Figs: Sagert., Bauer, Colbry, Howell, Pickett, Staber, Strother JCP 266 (2014)

Shock wave studies

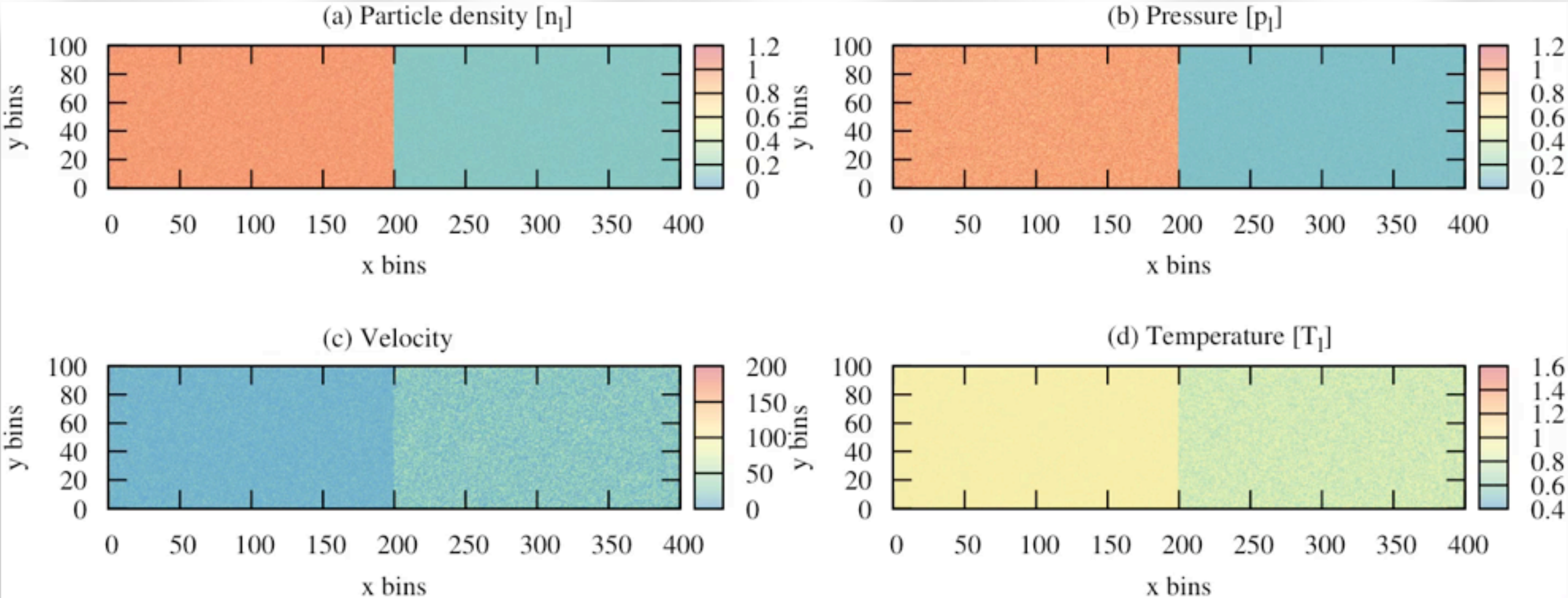
- Benchmark tests for hydrodynamic codes
- Many shock wave problems have analytic solution
- Allow evaluation of the performance of a code and comparison to other codes
- First tests: Sod tube test, Noh implosion test, Sedov blast wave test
- Output for analysis: density n, pressure p, velocity v (radial or bulk), temperature T

$$\boxed{\mathbf{P}_{\alpha\beta} = -\left(\sum_i m\,(v_{i,\alpha} - v_{b,\alpha})\,(v_{i,\beta} - v_{b,\beta}) + \frac{1}{2}\frac{1}{\Delta t}\sum_i \sum_{i\neq j} r_{ij,\alpha}\,\Delta p_{i,\beta}\right)}$$

$$\boxed{p_{2D} = -\frac{1}{V}\frac{\mathbf{P}_{xx} + \mathbf{P}_{yy}}{2}, \quad p_{3D} = -\frac{1}{V}\frac{\mathbf{P}_{xx} + \mathbf{P}_{yy} + \mathbf{P}_{zz}}{3}}$$

$$\boxed{v_{\mathrm{rms}} = \frac{1}{N}\left(\sum_{i=1}^{N}\left[(v_{i,x} - v_{b,x})^2 + (v_{i,y} - v_{b,y})^2 + (v_{i,z} - v_{b,z})^2\right]\right)^{1/2}} \qquad \boxed{T = v_{\mathrm{rms}}^2 m/f}$$

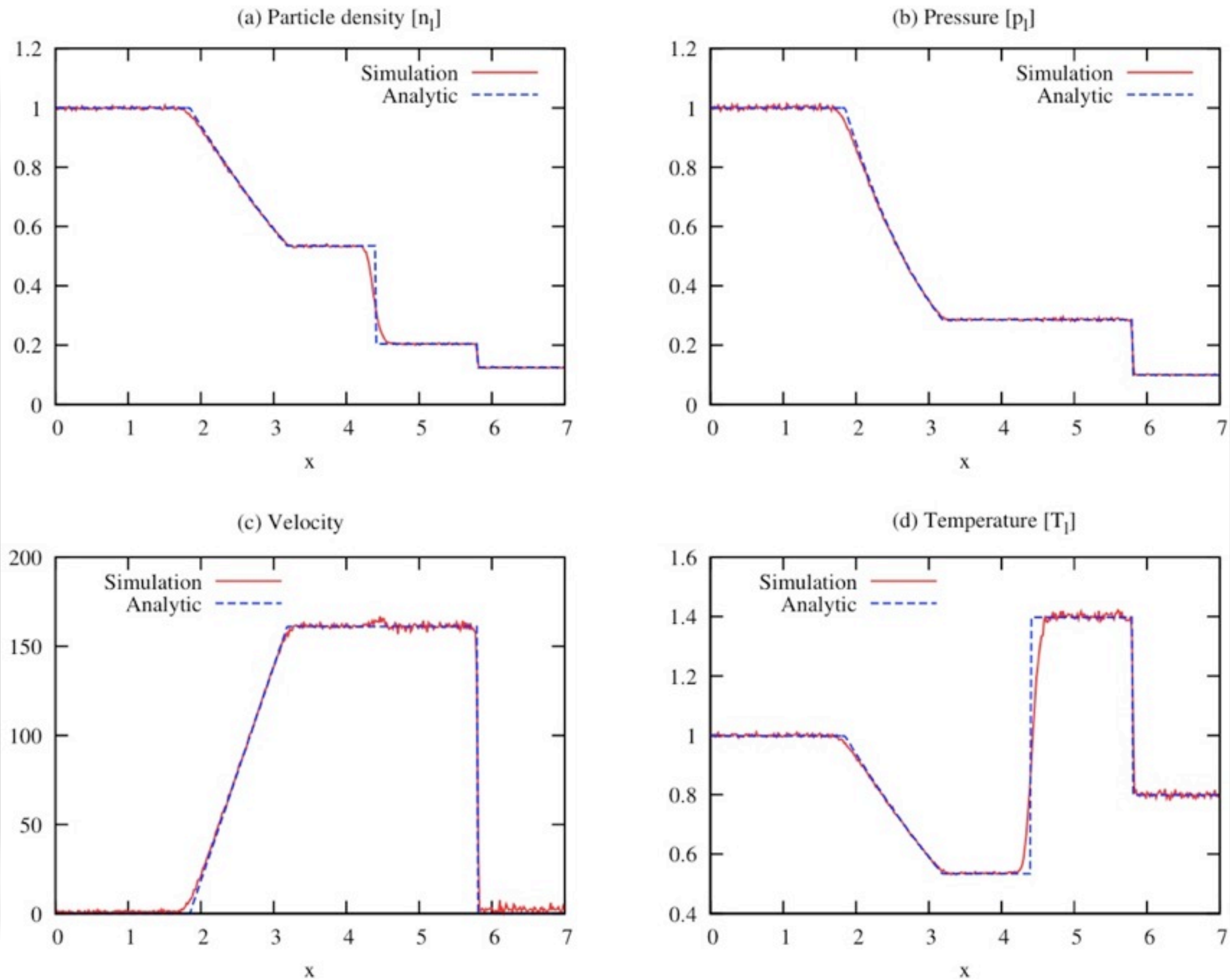
2D Sod Tests



Riemann problem with analytic solution

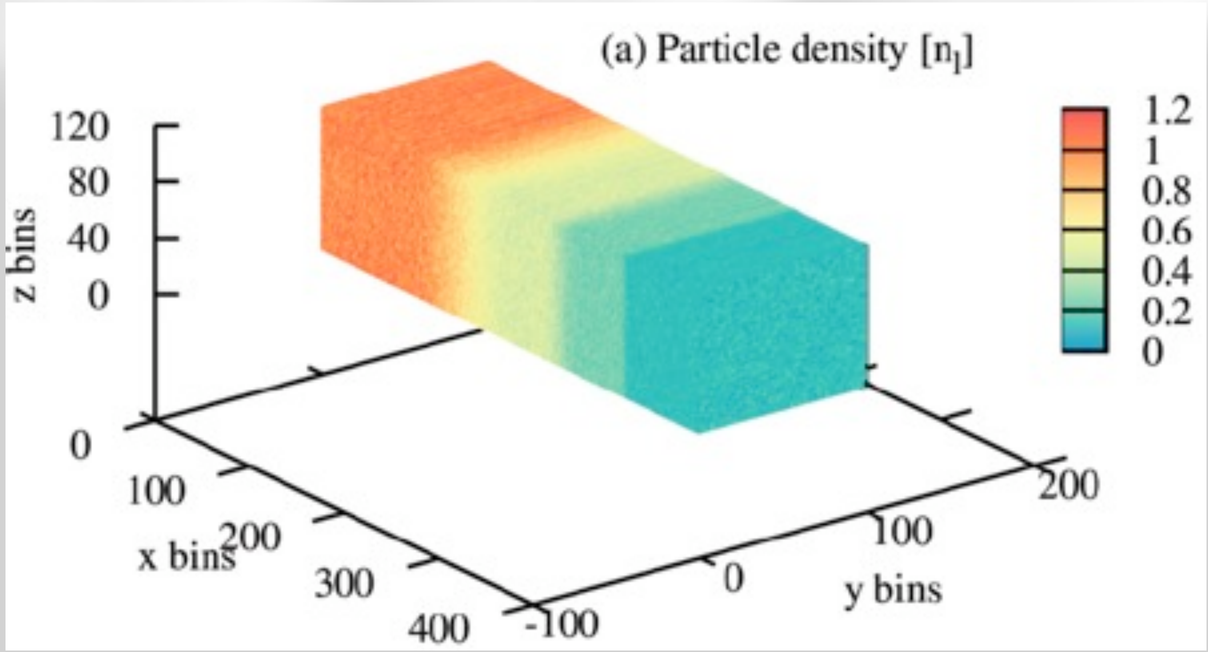
- Initial conditions: $n_1 = 1$, $n_2 = 0.125$, $p_1 = 1$, $p_2 = 0.1$, $v_1 = v_2 = 0$
- Analytic solution constraints: Shock front, contact discontinuity, and rarefaction wave
- Simulations: 2D, $N = 20{,}000{,}000$, $\lambda = 0.001\Delta x$, 2000×500 c-bins, 400×100 o-bins

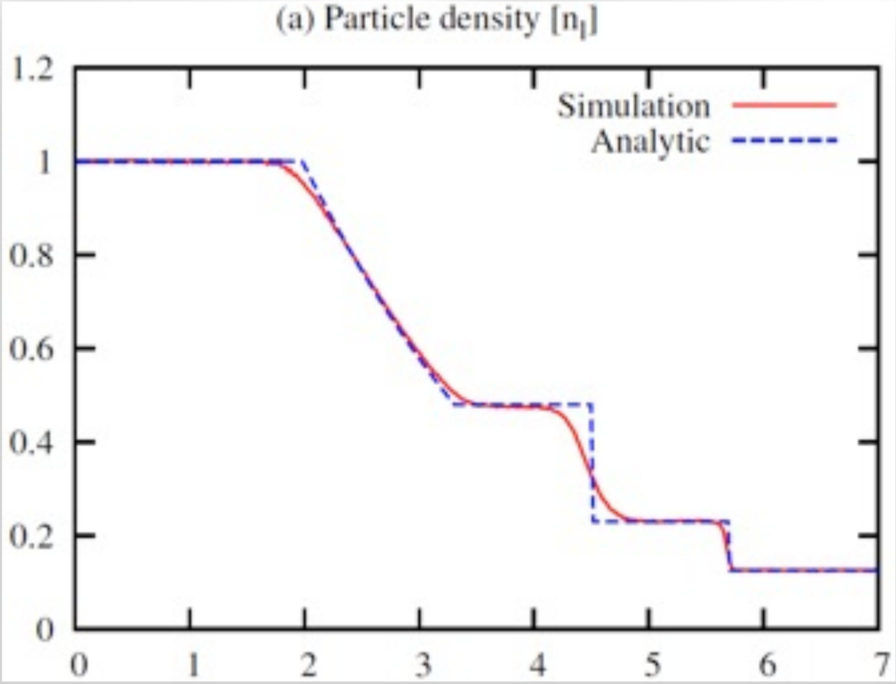
Figs: Sagert., Bauer, Colbry, Howell, Pickett, Staber, Strother JCP 266 (2014)

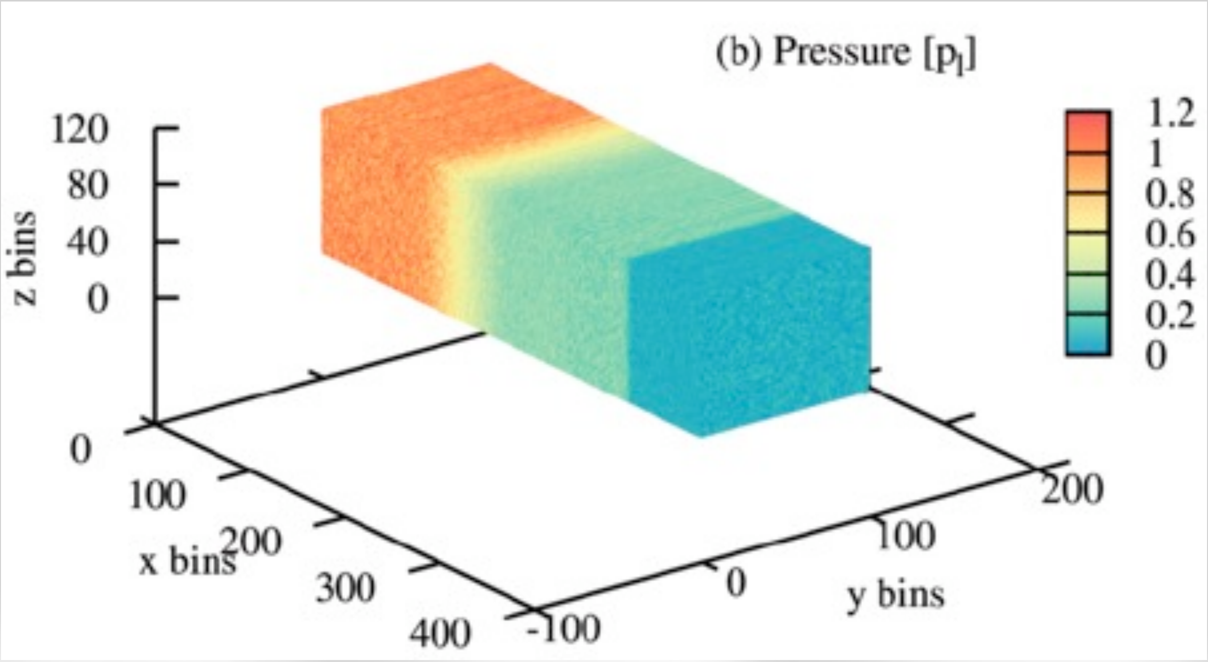


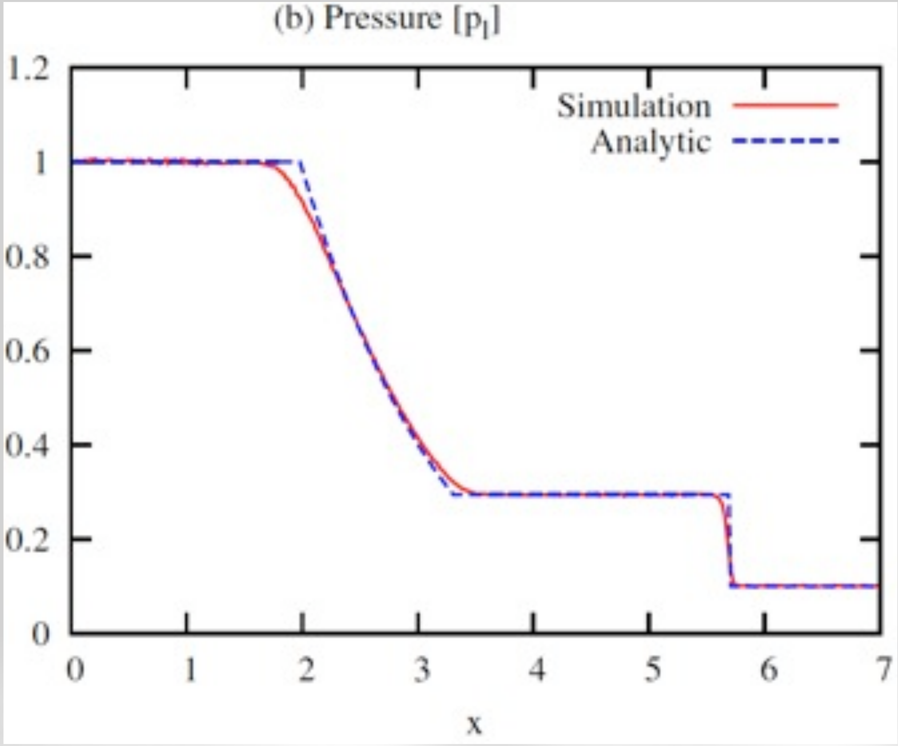
Figs: Sagert., Bauer, Colbry, Howell, Pickett, Staber, Strother JCP 266 (2014)

3D Sod Tests







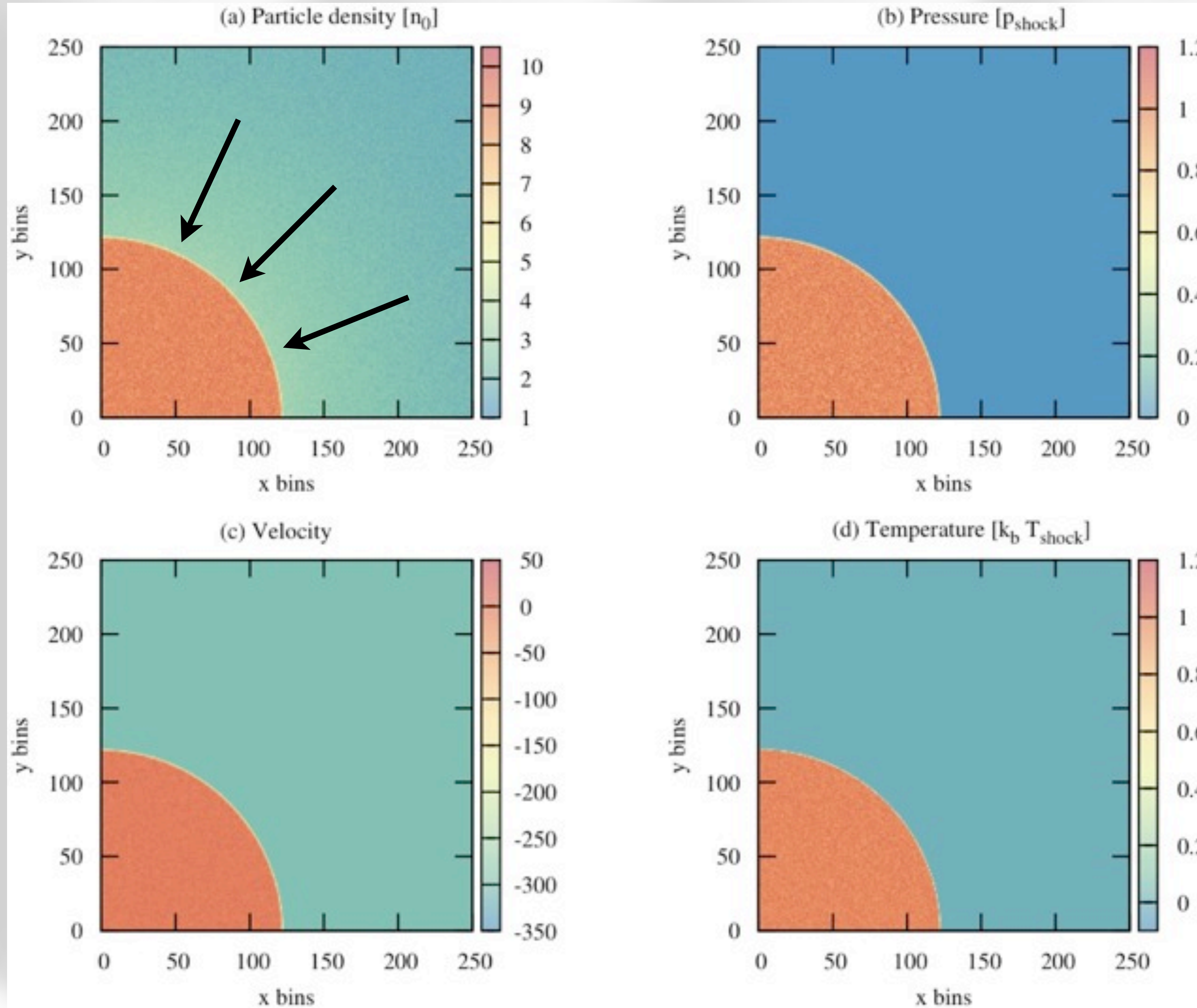


- Simulations: 3D, N = 80,000,000, $\lambda = 0.001\Delta x$, 400×100×100 c-bins and o-bins

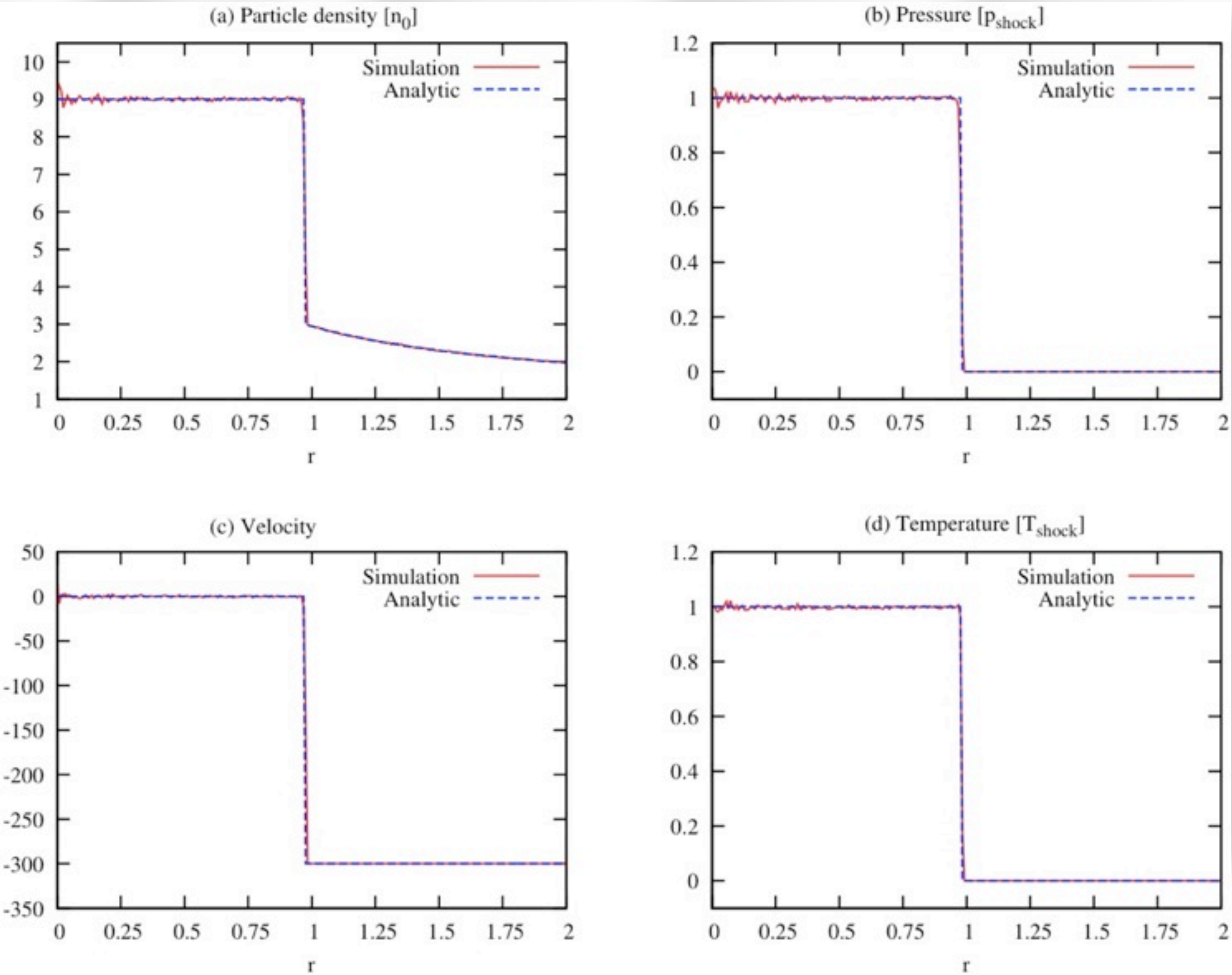
2D Noh Test

Collapsing gas: Cold, ideal gas with uniform, radially inward speed

- Matter piles up at the origin and is trapped by incoming particles
- Shock front forms at the origin and moves outwards
- Hydrodynamic codes often experience anomalous wall-heating due to artificial viscosity
- 2D Simulations: N = 20,000,000; $\lambda = 0.001\Delta x$, 2000×2000 c-bins, 500×500 o-bins

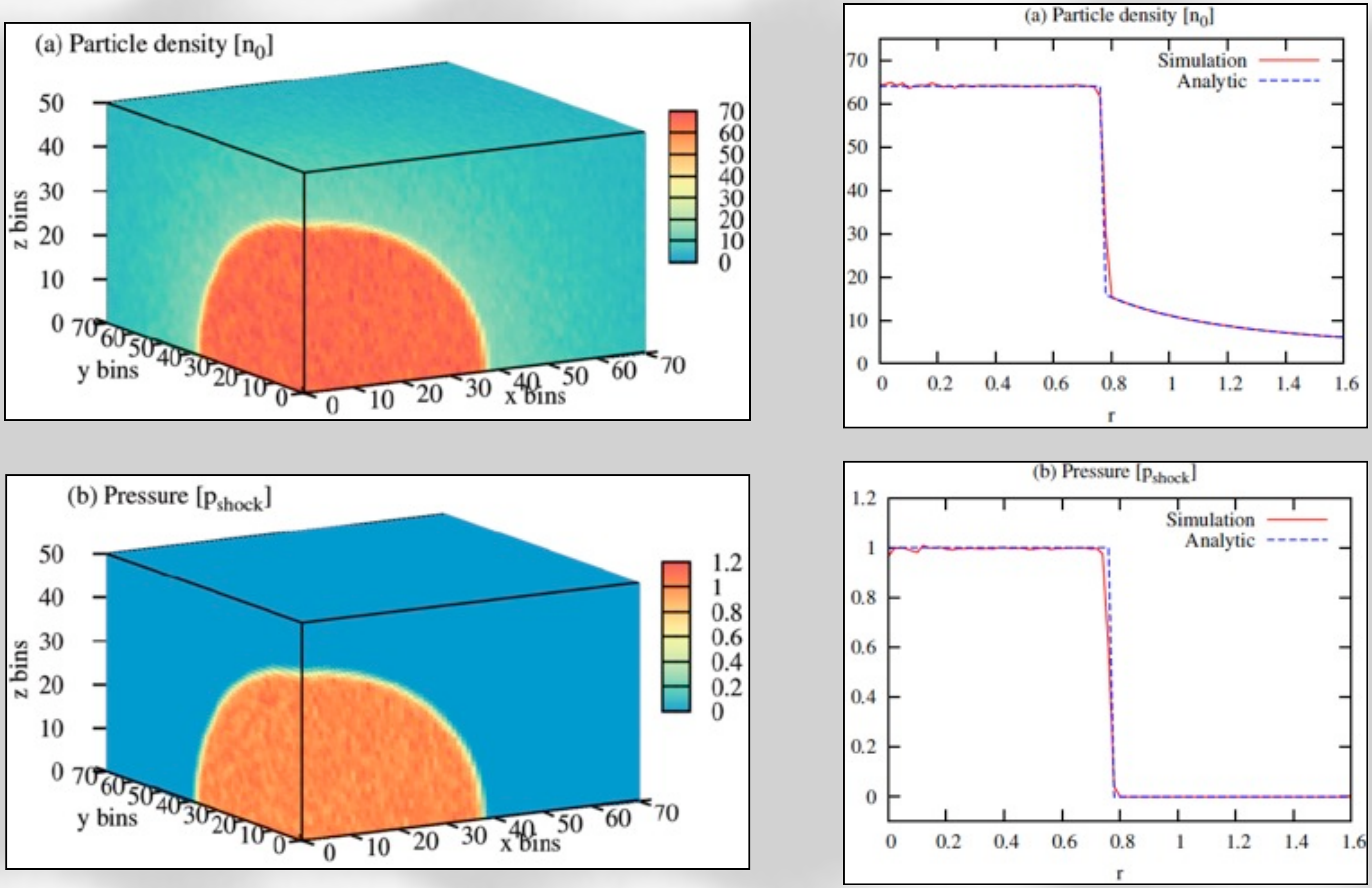


2D Noh Test



Figs: Sagert., Bauer, Colbry, Howell, Pickett, Staber, Strother JCP 266 (2014)

3D Noh Test



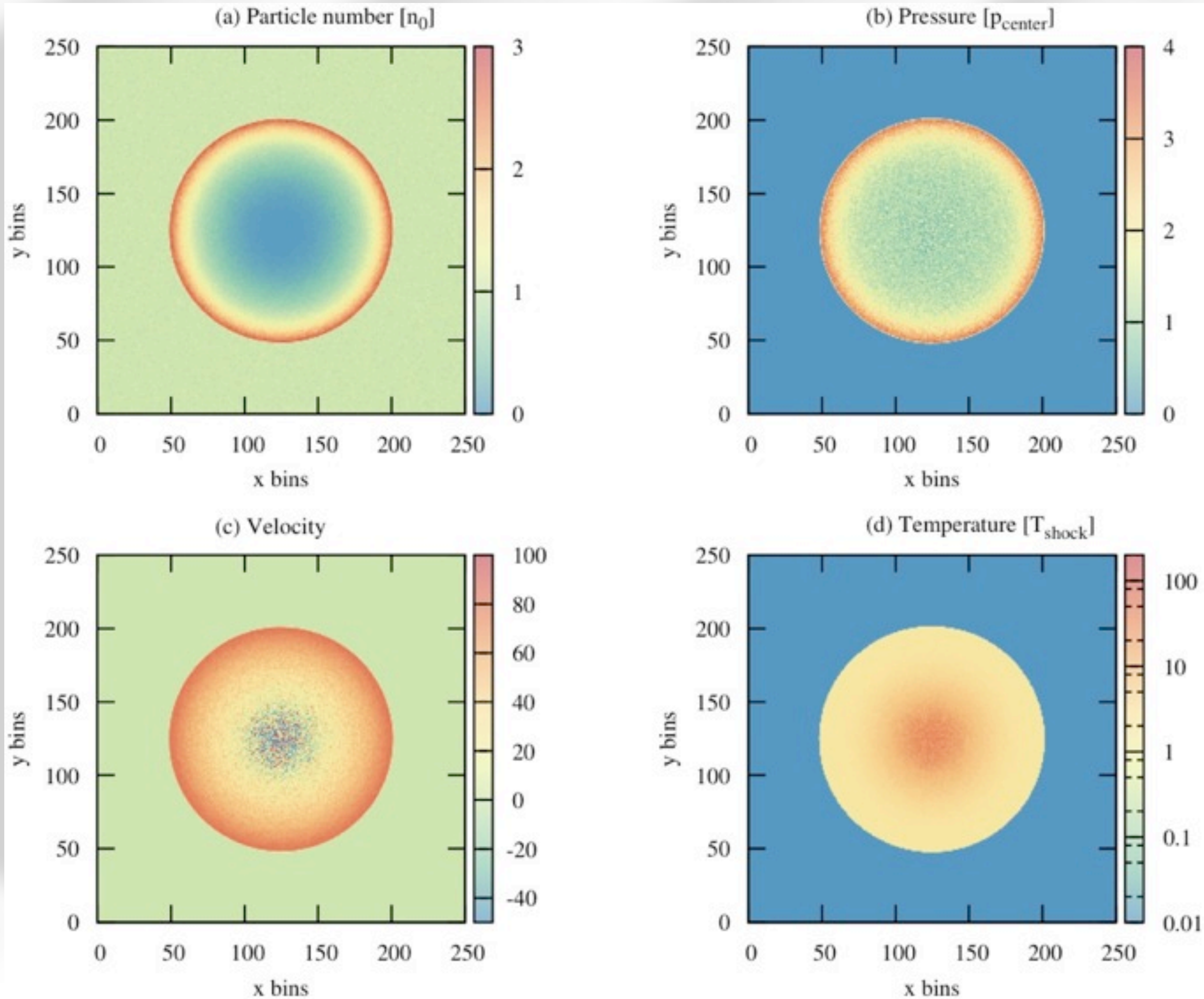
- 3D Simulations: N = 80,000,000; $\lambda = 0.001\Delta x$, 400×400×400 c-bins, 200×200×200 o-bins

Figs: Sagert., Bauer, Colbry, Howell, Pickett, Staber, Strother JCP 266 (2014)

2D Sedov Test

Spherical shock wave caused by energy deposition in the center of simulation space

- Similarities to core-collapse supernova shock wave
- General numerical difficulties: finite size energy injection region, vanishingly small densities at the origin
- 2D Simulations: N = 35,000,000, $\lambda = 0.001\Delta x$, 2000×2000 c-bins, 250×250 o-bins



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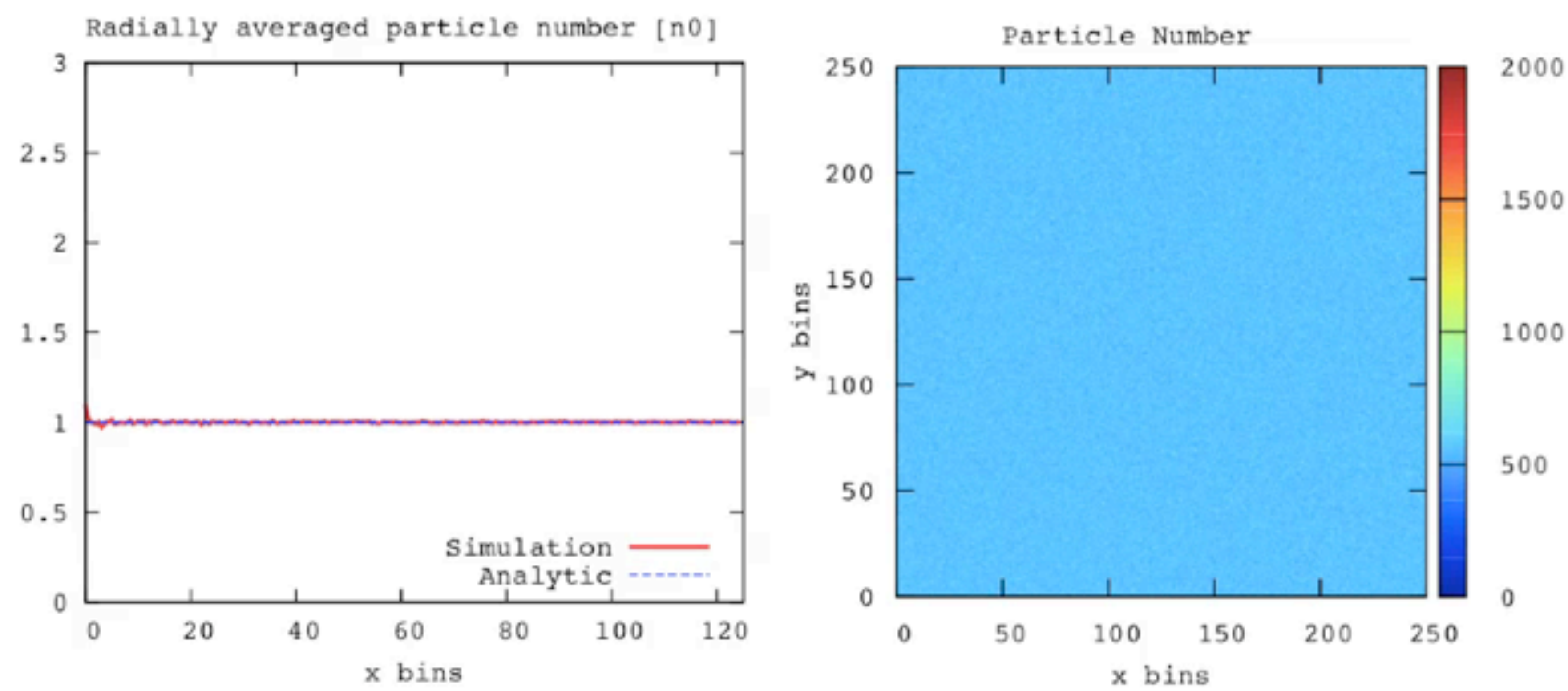
2D Sedov Test



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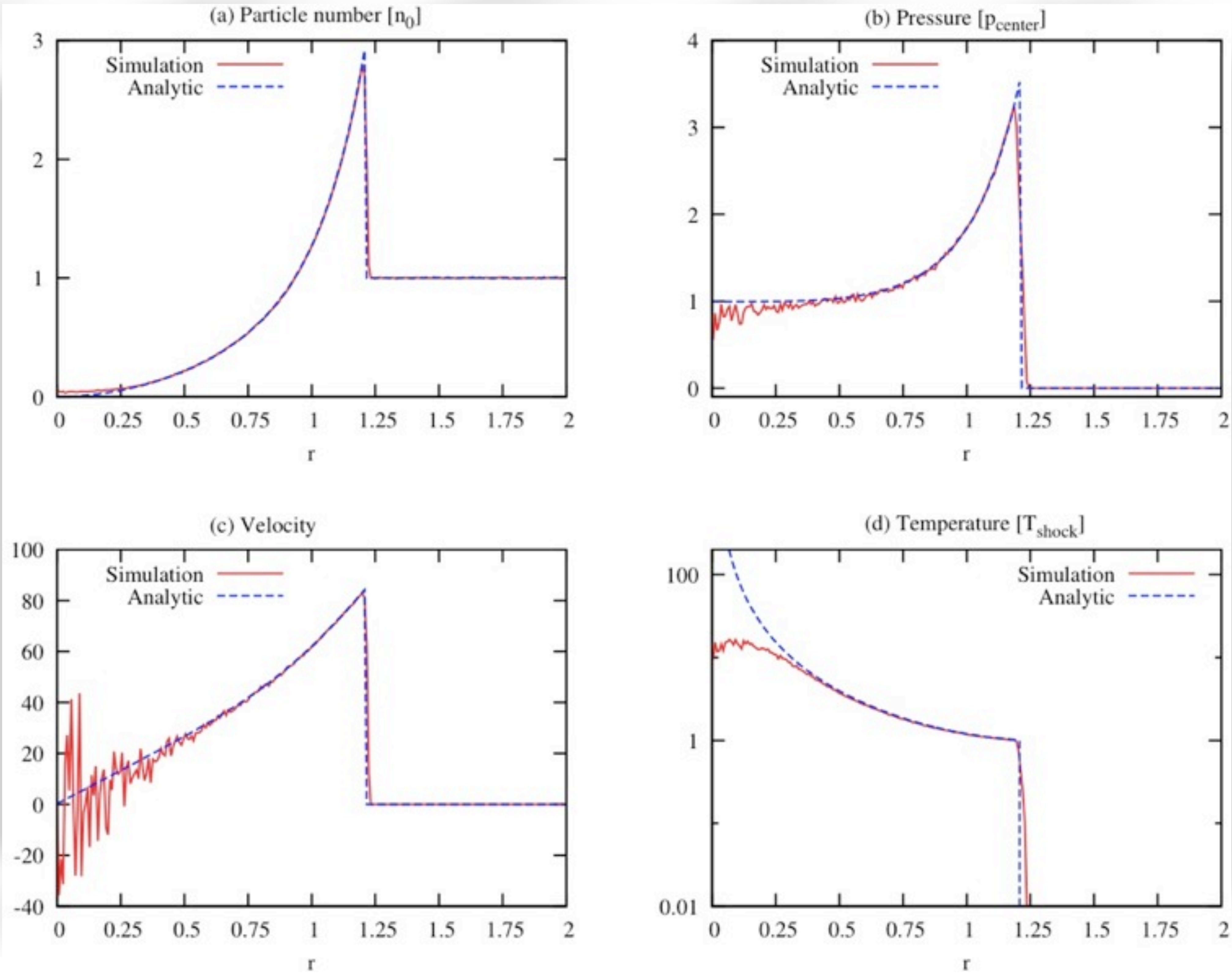
2D Sedov Test



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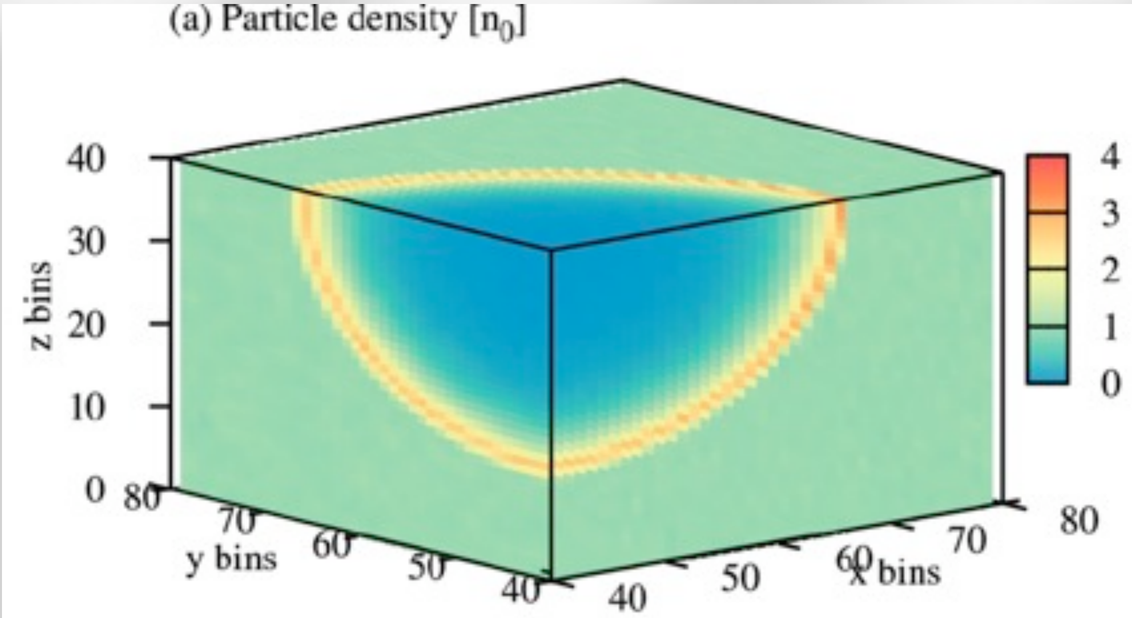
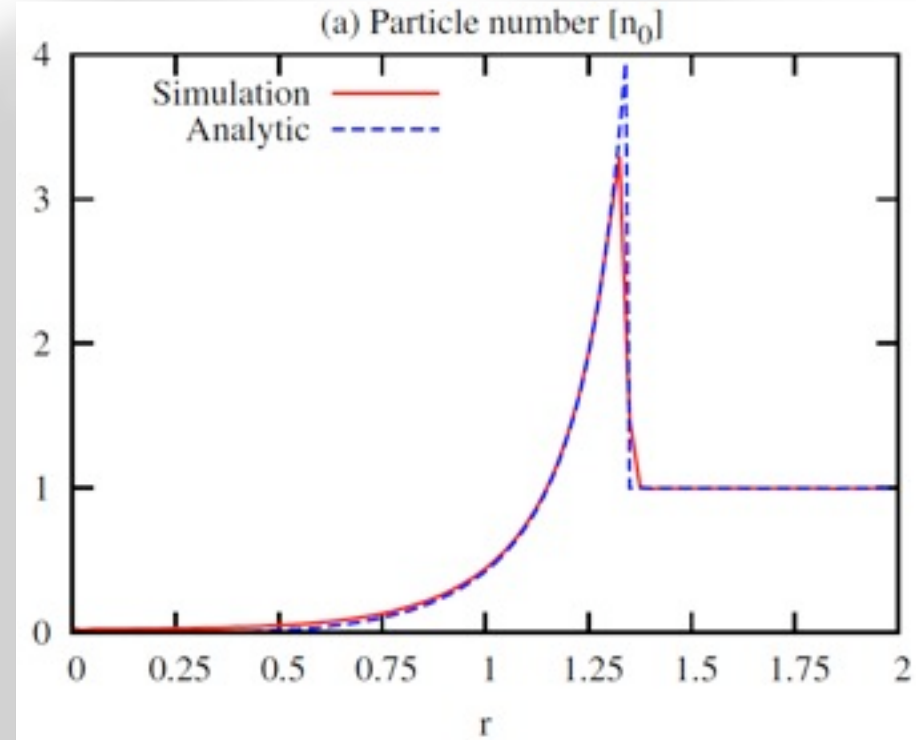
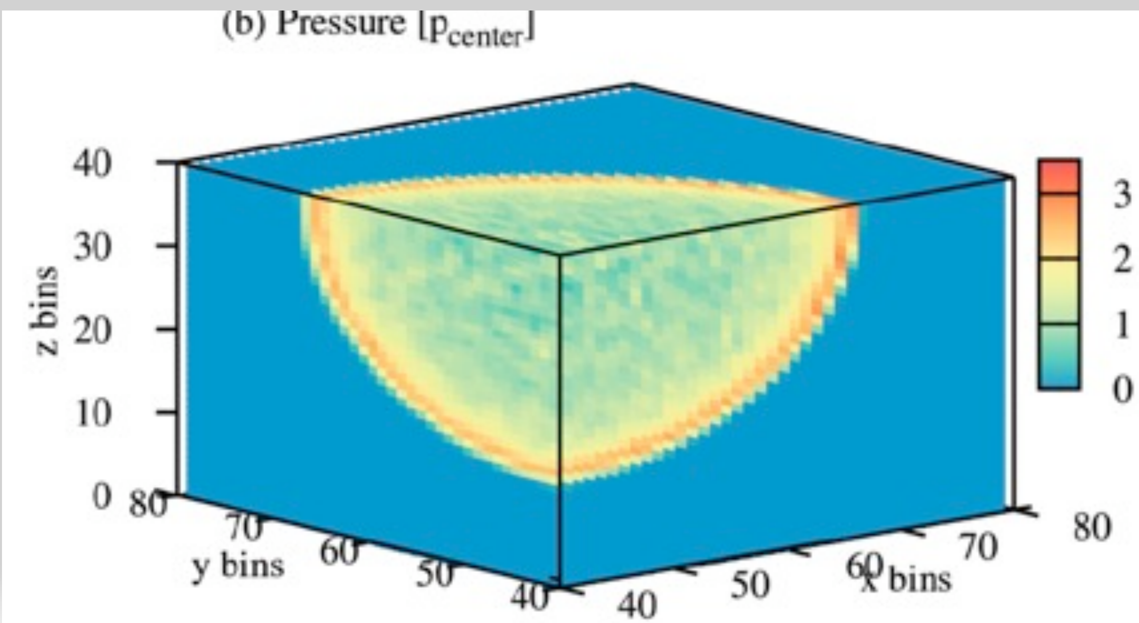
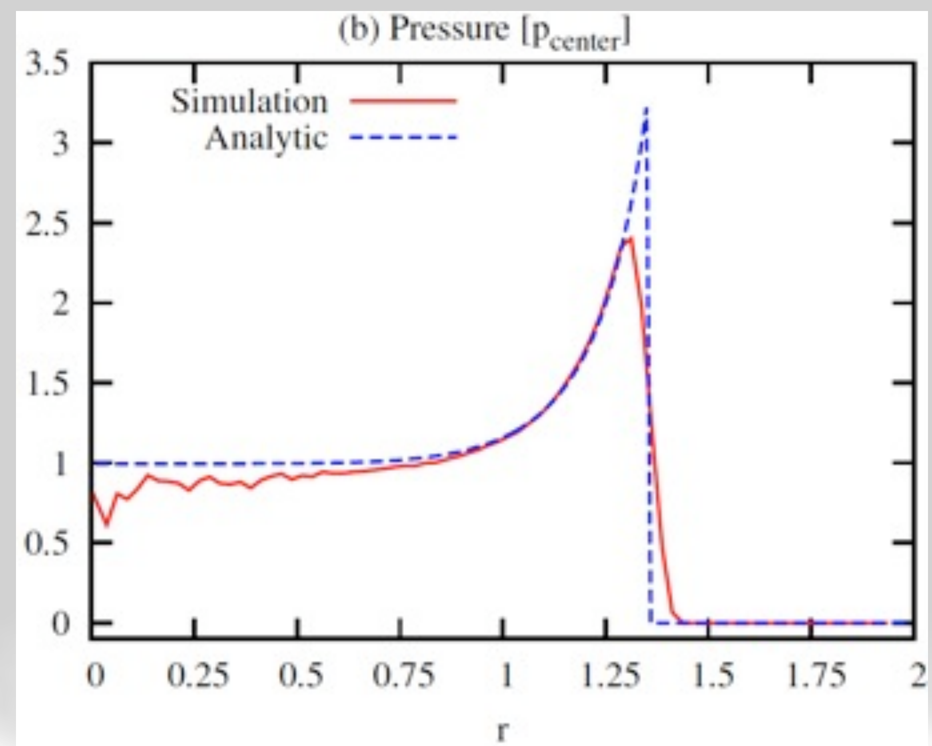
3D Sedov Test





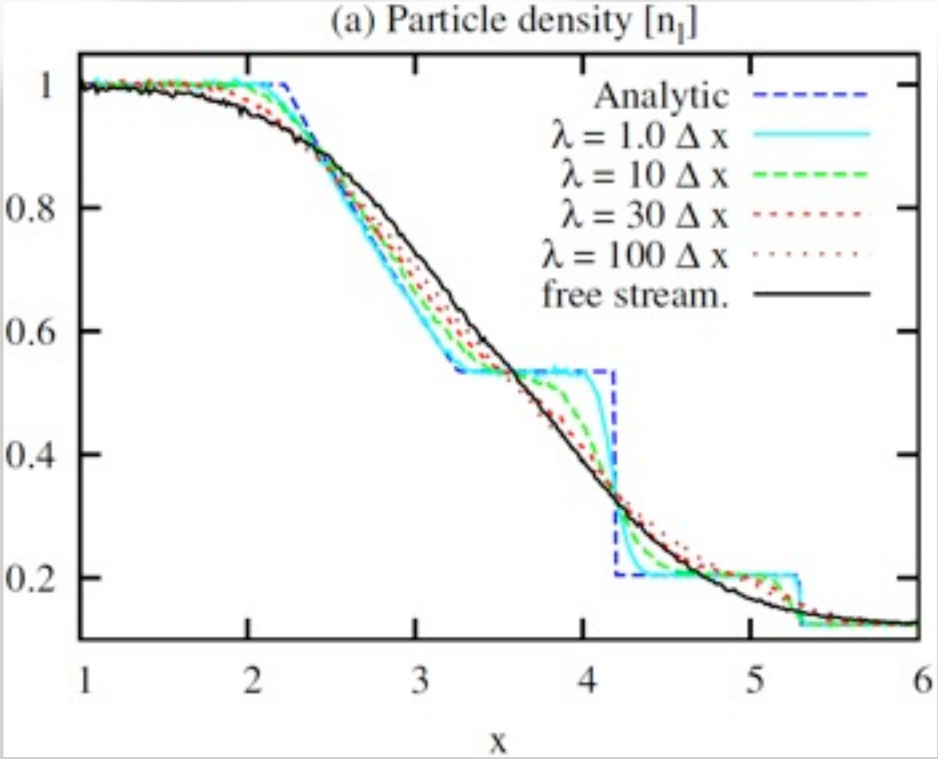


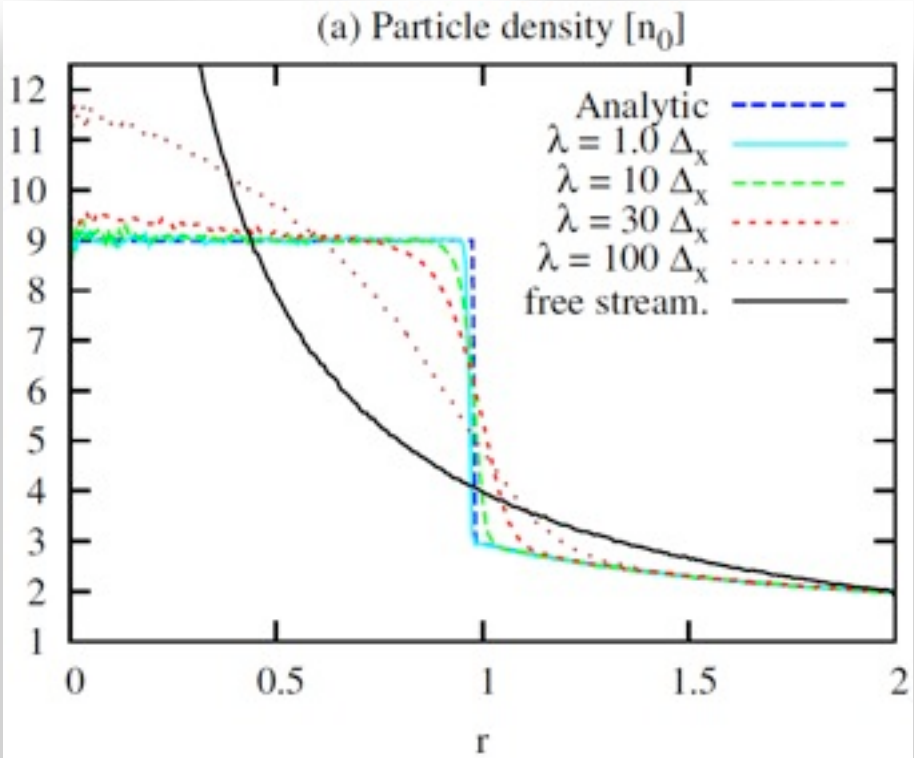


- 3D Simulations: N = 200,000,000, $\lambda = 0.001\Delta x$, 400×400×400 c-bins, 80×80×80 o-bins

Figs: Sagert., Bauer, Colbry, Howell, Pickett, Staber, Strother JCP 266 (2014)

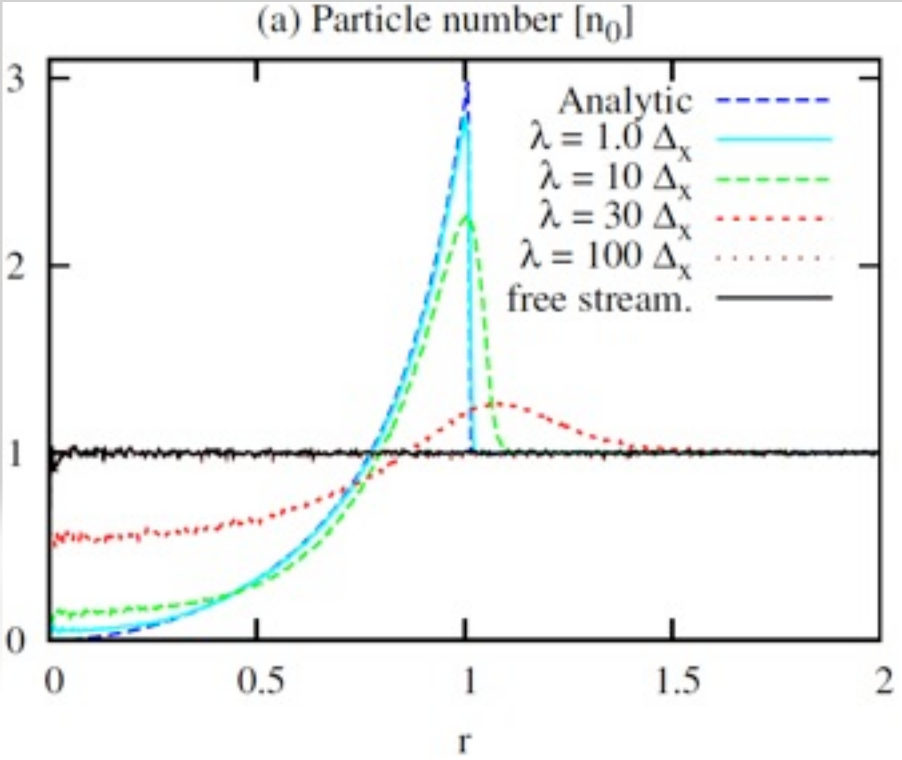
Mean-free path studies





Repeat 2D Sod, Noh, Sedov test with larger particle mean free paths

- Important test for e.g. ability of code to handle neutrinos in core-collapse supernova simulations
- Similar tests have only been performed for the Sod test, not for the Noh or Sedov test
- Initial conditions as in the 2D shock tests



Figs: Sagert., Bauer, Colbry, Howell, Pickett, Staber, Strother JCP 266 (2014)

Rayleigh-Taylor Instabilities

A layer of heavier fluid is placed on top of a layer of lighter fluid in the presence of gravitational acceleration

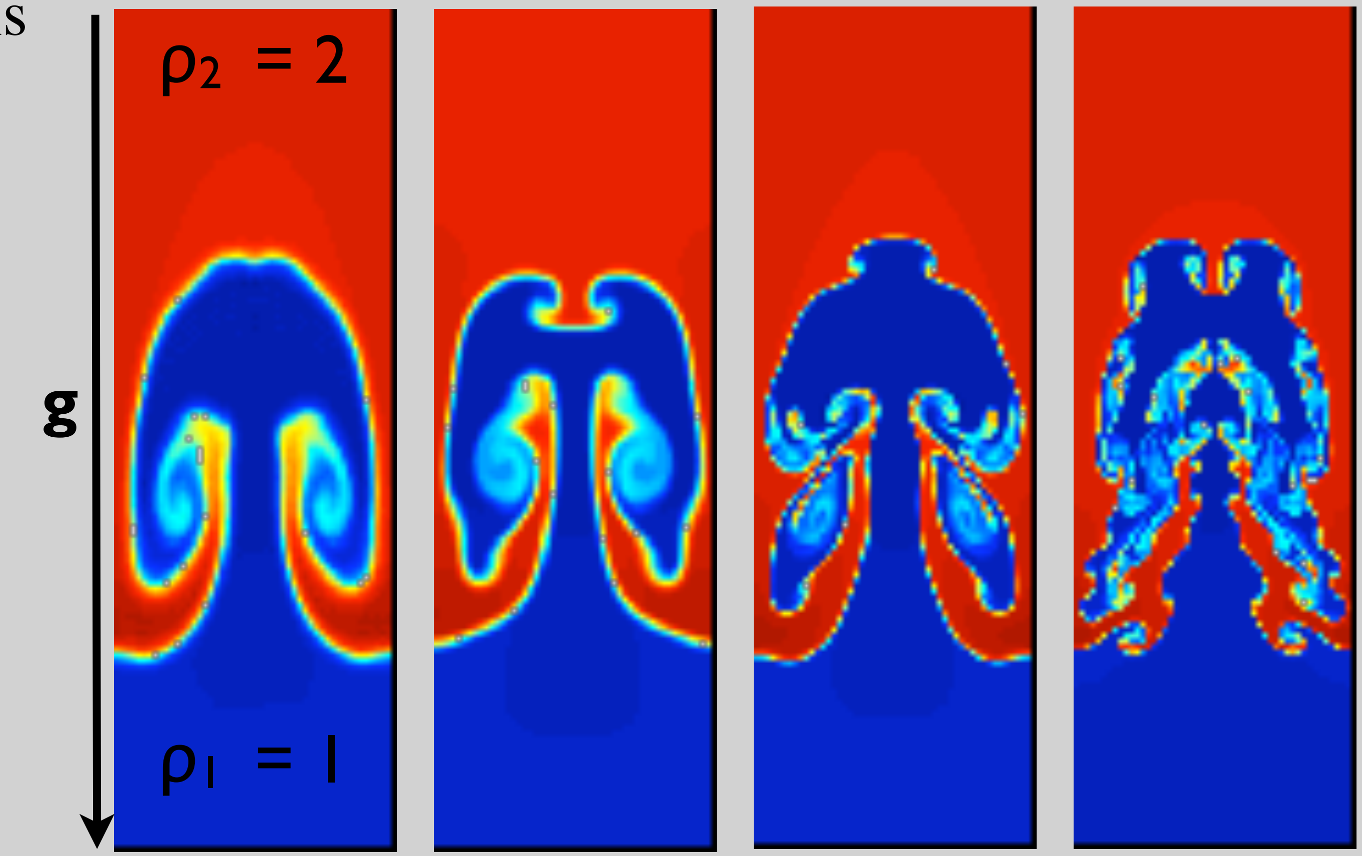
The interface between the light and heavy fluid is unstable

At early times, the growth rate can be predicted from linear theory

$$\eta(x,t) = \frac{1}{2}\left(e^{\gamma t} + e^{-\gamma t}\right)\eta(x, t=0),$$

$$\gamma = \sqrt{Ag\alpha} \qquad \alpha = 2\pi/\lambda,$$

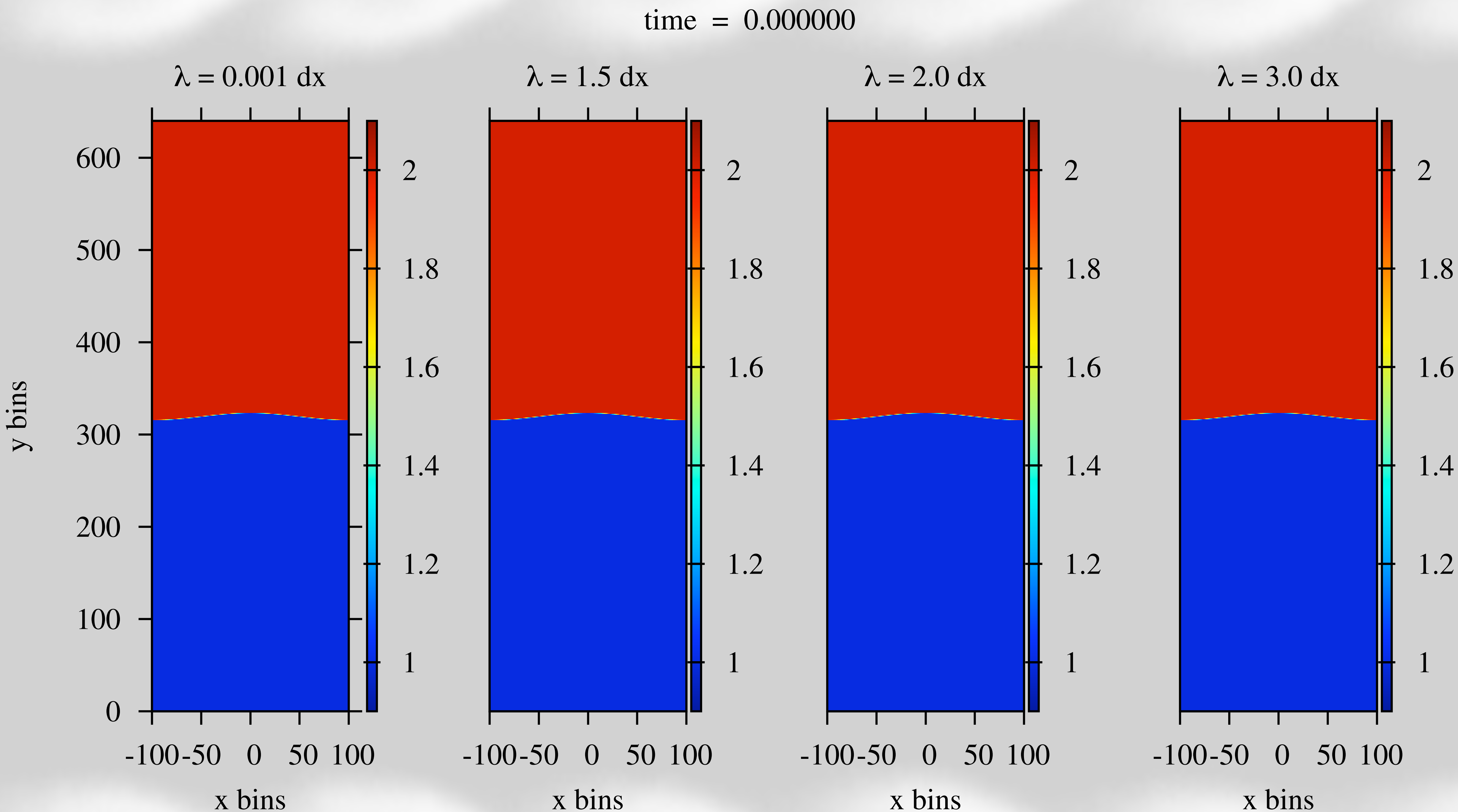
$$A = \frac{\rho_2 - \rho_1}{\rho_2 + \rho_1}$$



http://www-troja.fjfi.cvut.cz/~liska/CompareEuler/compare8/

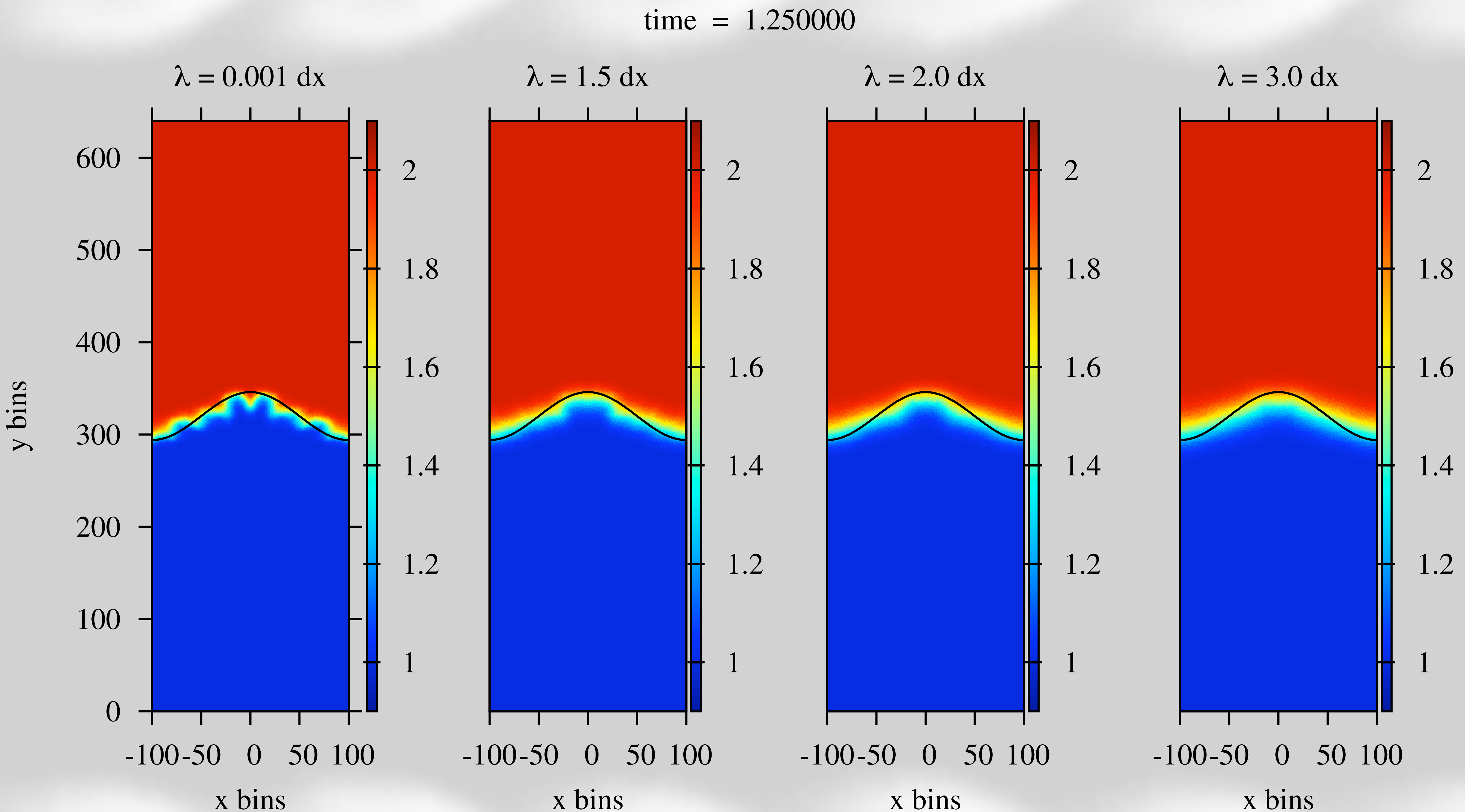
Structures which appear in the non-linear regime are sensitive to the initial perturbations.

Rayleigh-Taylor Instabilities



- 2D Simulations: $N = 40{,}000{,}000$, $\lambda = 0.001\Delta x$, 800×5120 c-bins, 100×640 o-bins
- ca. 100,000 timesteps for $t = 3.0$

Rayleigh-Taylor Instabilities



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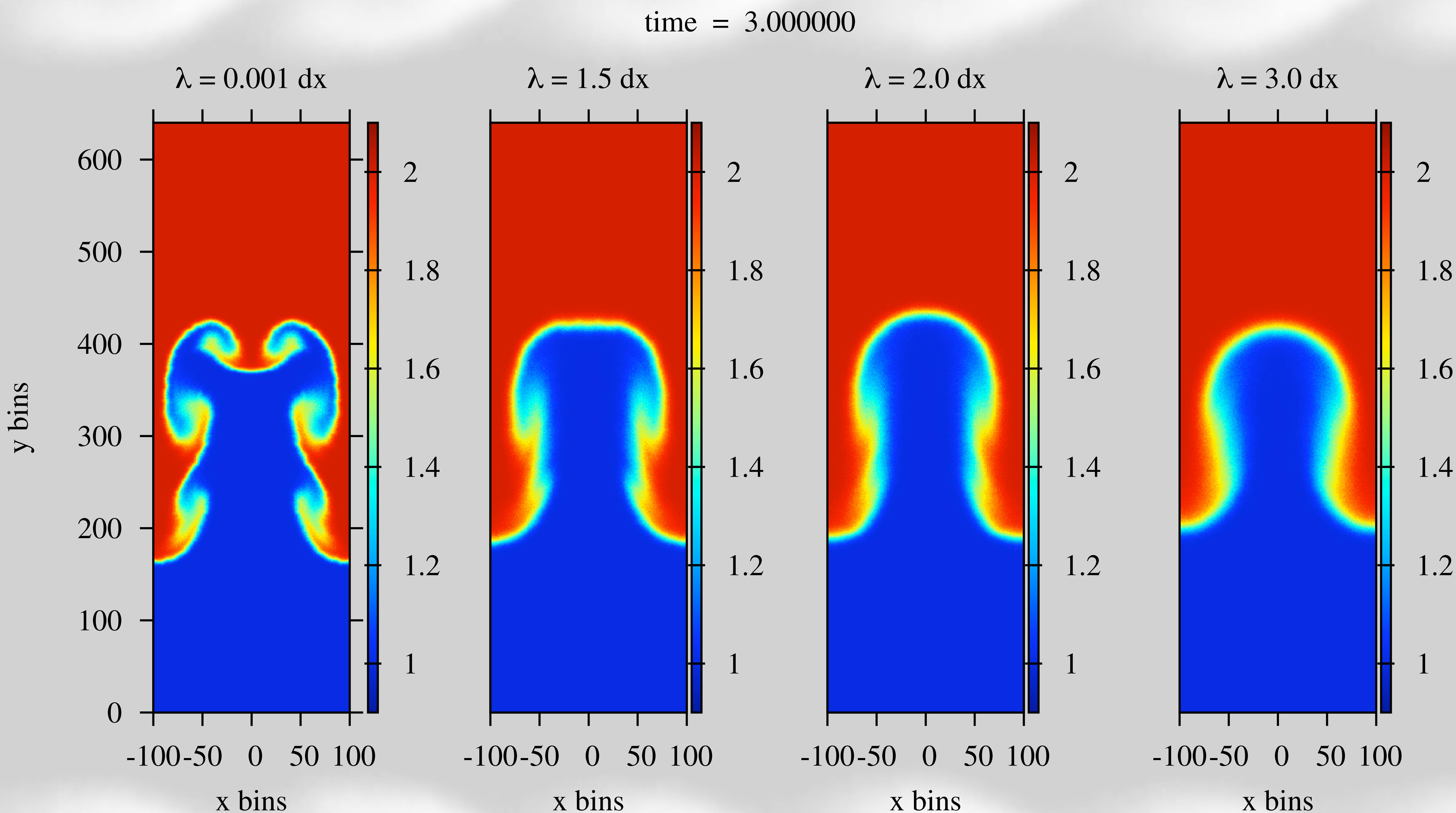
Rayleigh-Taylor Instabilities



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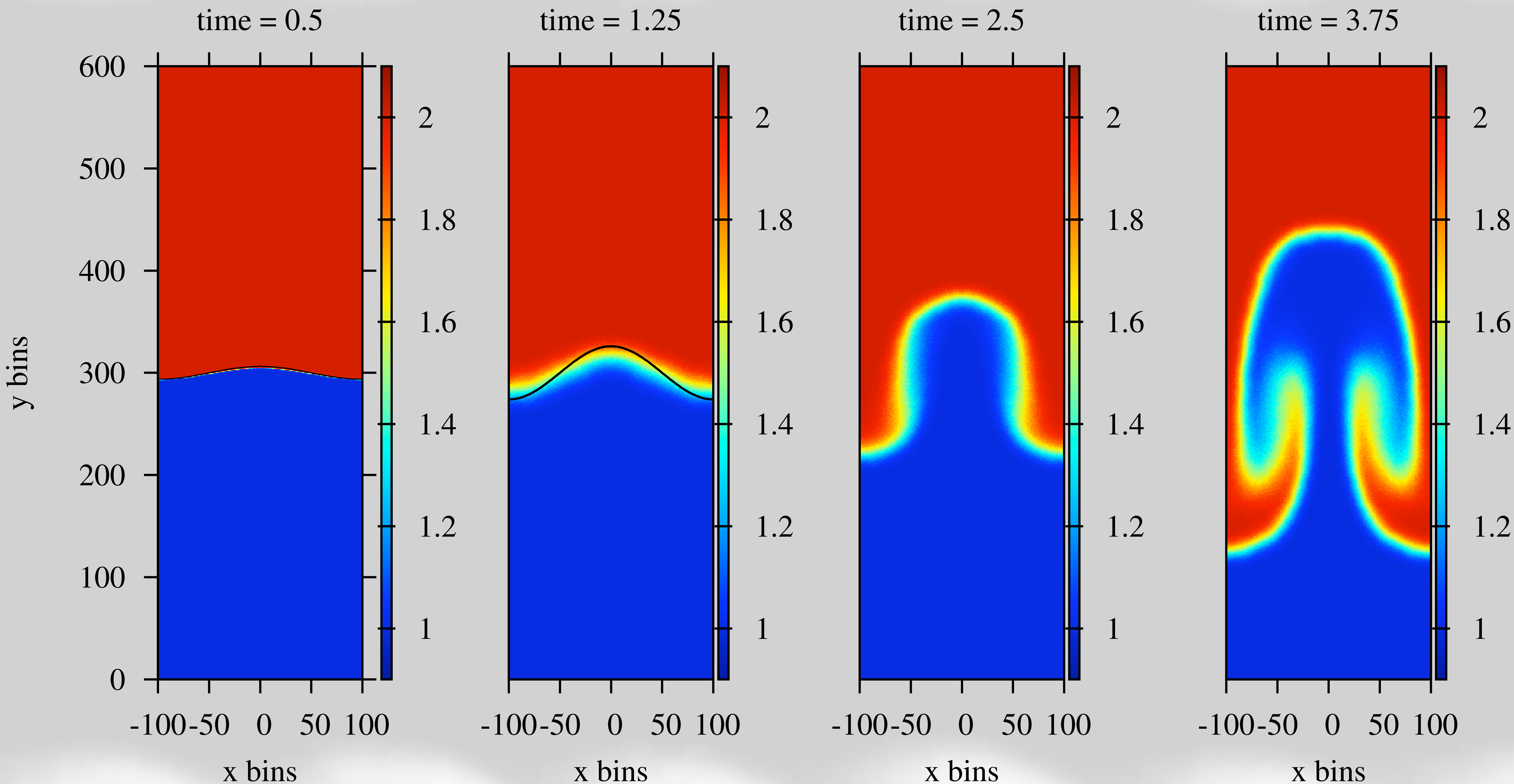
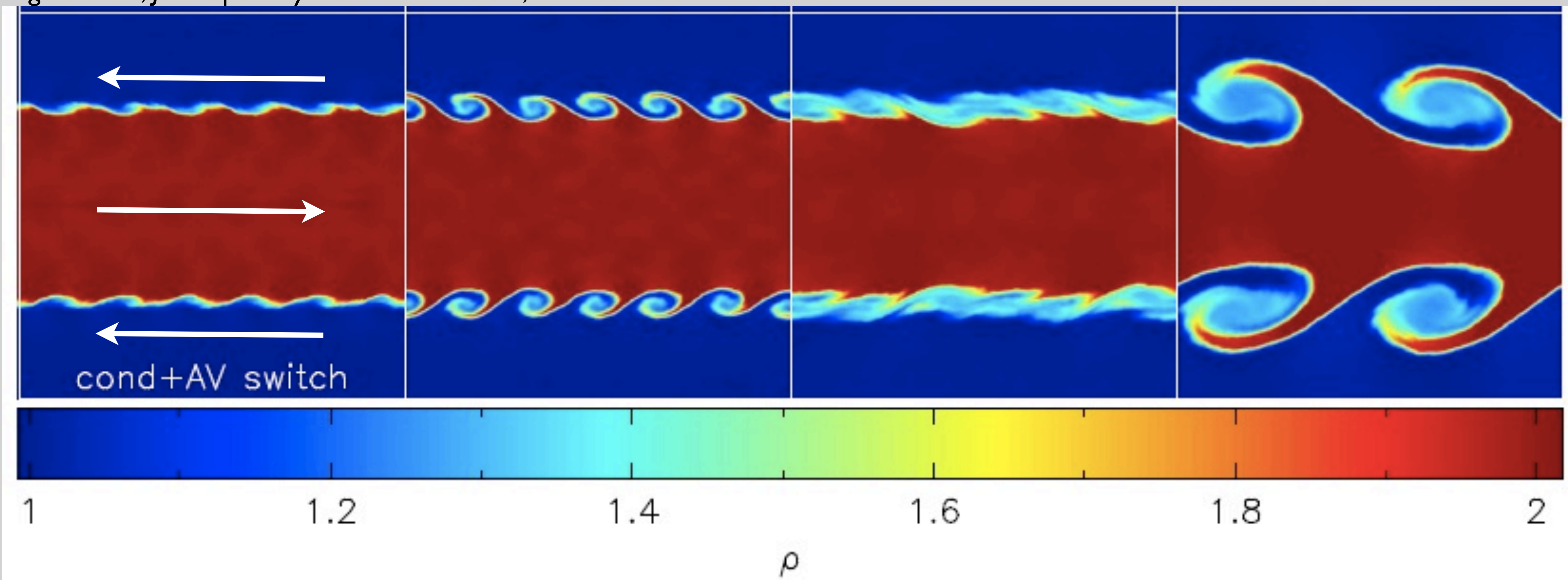
Rayleigh-Taylor Instabilities



- 2D Simulations: $N = 40{,}000{,}000$, $\lambda = 0.001\Delta x$, 800×5120 c-bins, 100×640 o-bins
- Diffusion suppression for $t < 0.5$

Kelvin Helmholtz Instability

Fig. D. Price, J.Comput.Phys.227:10040-10057,2008

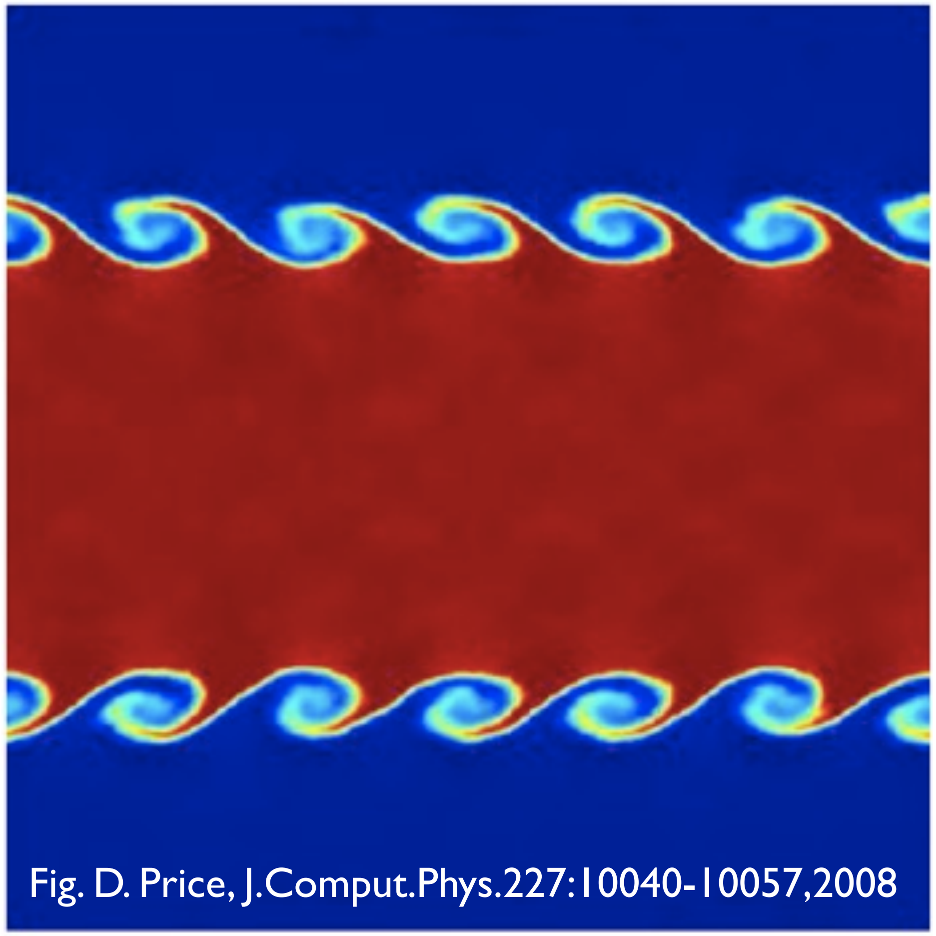


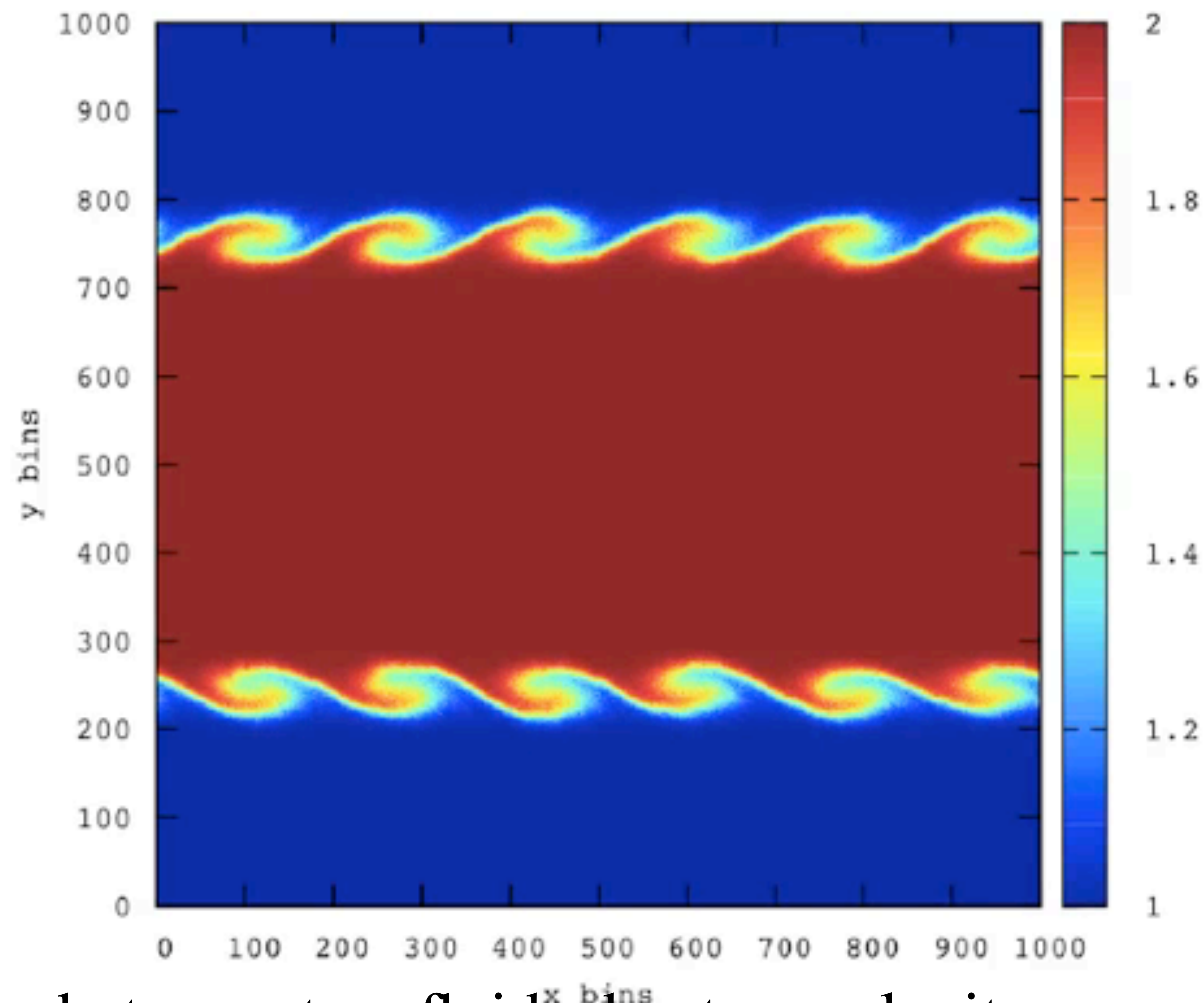
Instability which develops at the interface between two fluids due to a velocity difference

- Initial conditions: $n_1 = 2n_2$, p=2.5 everywhere, v_1 = -0.5, v_2 = 0.5
- Seed: Perturbation of y-velocity

$$v_y = \begin{cases} A\sin\left[-2\pi(x+0.5)/\lambda\right] & |y-0.25| < 0.025, \\ A\sin\left[2\pi(x+0.5)/\lambda\right] & |y+0.25| < 0.025. \end{cases}$$

Kelvin-Helmholtz Instability



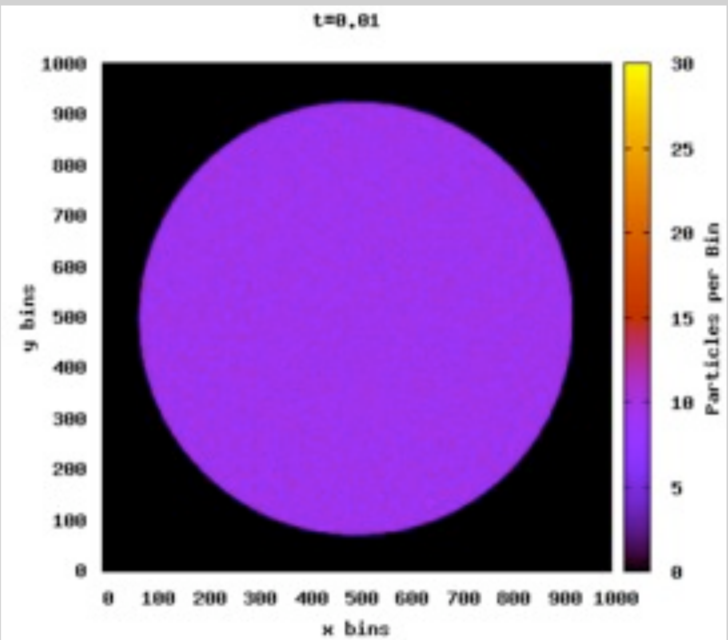


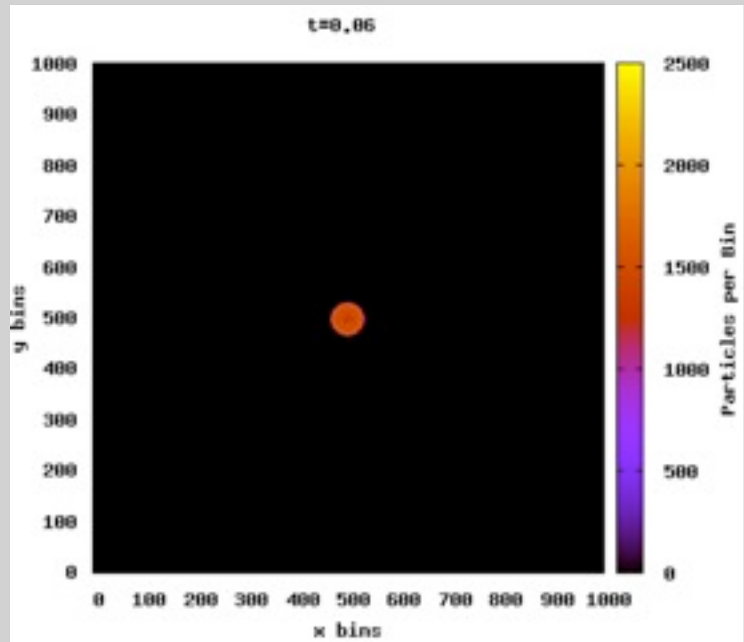
Instability which develops at the interface between two fluids due to a velocity difference

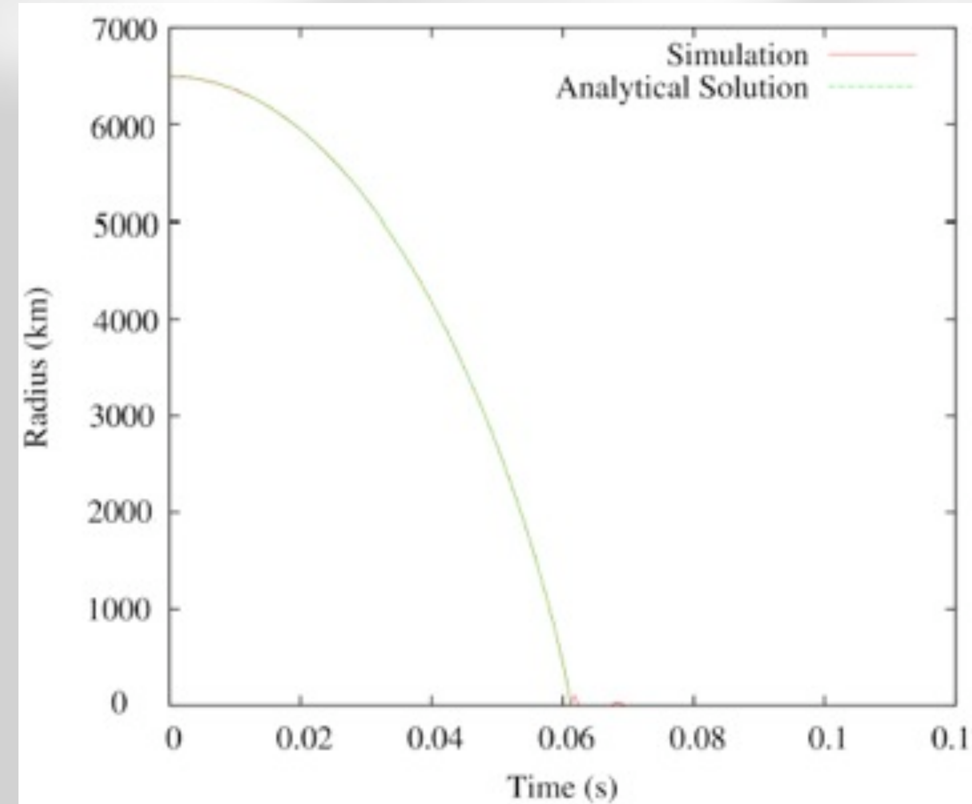
- Initial conditions: $n_1 = 2n_2$, p=2.5 everywhere, $v_1 = 0.5$, $v_2 = -0.5$
- Seed: Perturbation of y-velocity

$$v_y = \begin{cases} A\sin\left[-2\pi(x+0.5)/\lambda\right] & |y-0.25| < 0.025, \\ A\sin\left[2\pi(x+0.5)/\lambda\right] & |y+0.25| < 0.025. \end{cases}$$

Gravitational Collapse of a Gas Cloud







Alec Staber, "Implosion and Collapses within a Kinetic Monte Carlo Approach" (MSU, senior thesis)

Spherical cloud of noninteracting gas collapses under own gravitational pressure

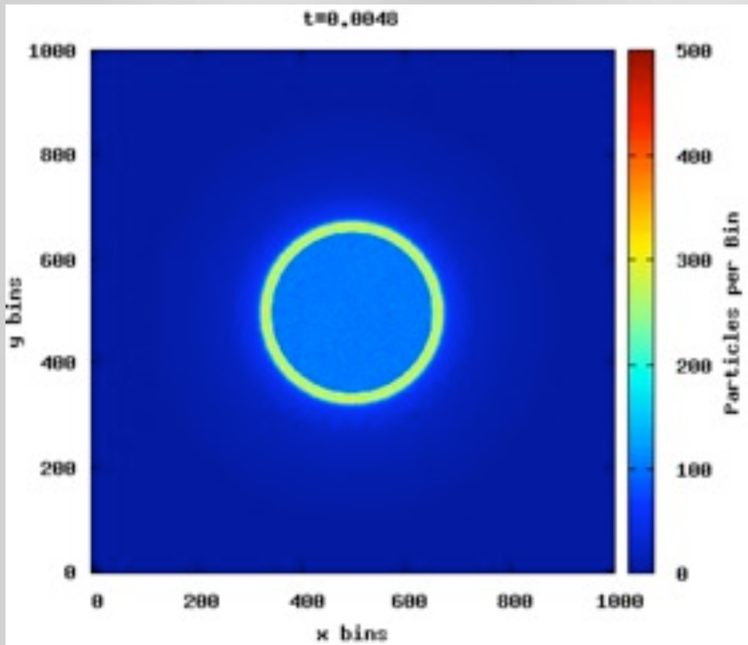
Collapse timescales for 2D given by:

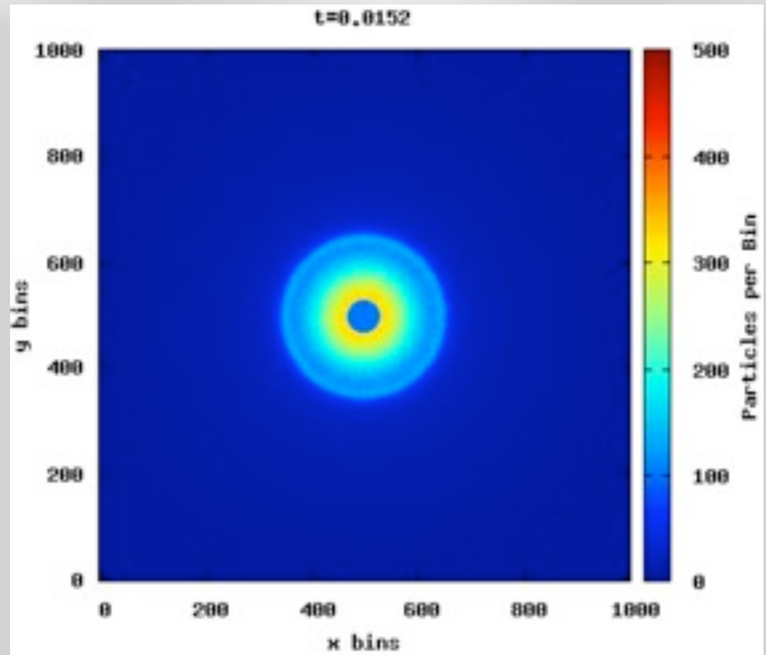
$$t = \frac{1}{\sqrt{4Gm}} \int_{r_0}^{r} \frac{dr}{\sqrt{ln(r_0/r)}} = \sqrt{\frac{\pi}{Gm}} \frac{r_0}{2} \mathrm{Erf}[\sqrt{\ln(r_0/r)}]$$

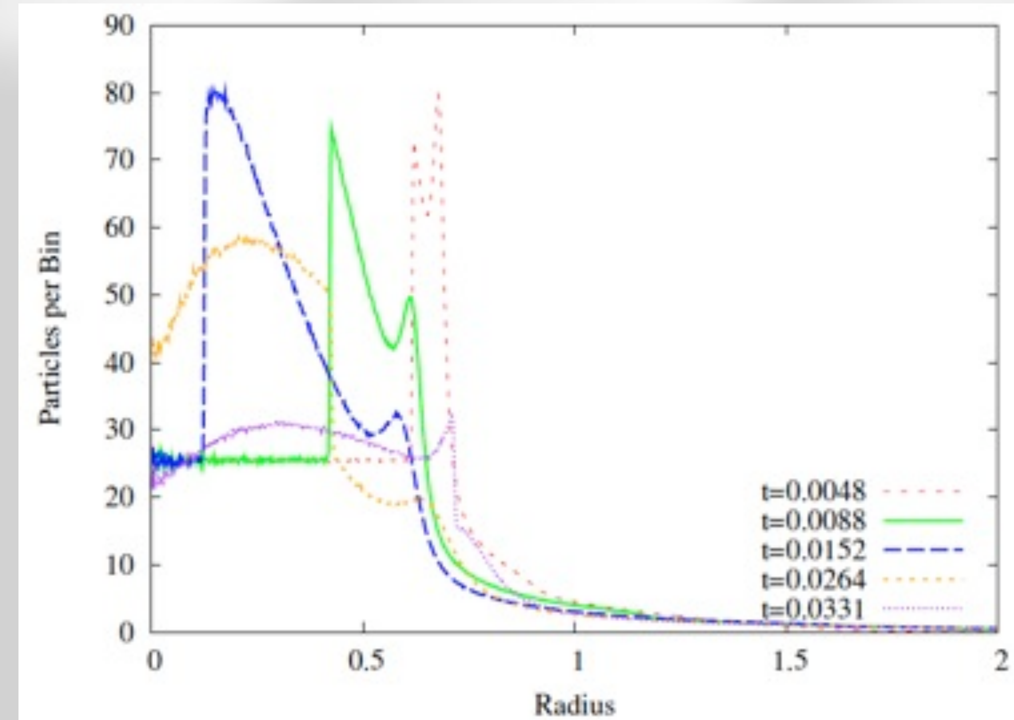
- Total mass: 1.326×10^{26} kg, radius $R = 6.5 \times 10^{6}$ km, Simulations in 2D and 3D
- Gravity implementation

$$\mathbf{F}_{Grav(j)} = -G \frac{m_{tp}^2 \left\{ i \in \{1, ..., N_{tp}\} : |\mathbf{r}_i| < |\mathbf{r}_j| \right\} \mathbf{r_j}}{\mathbf{r}_j^3}$$

Implosion of a sphere

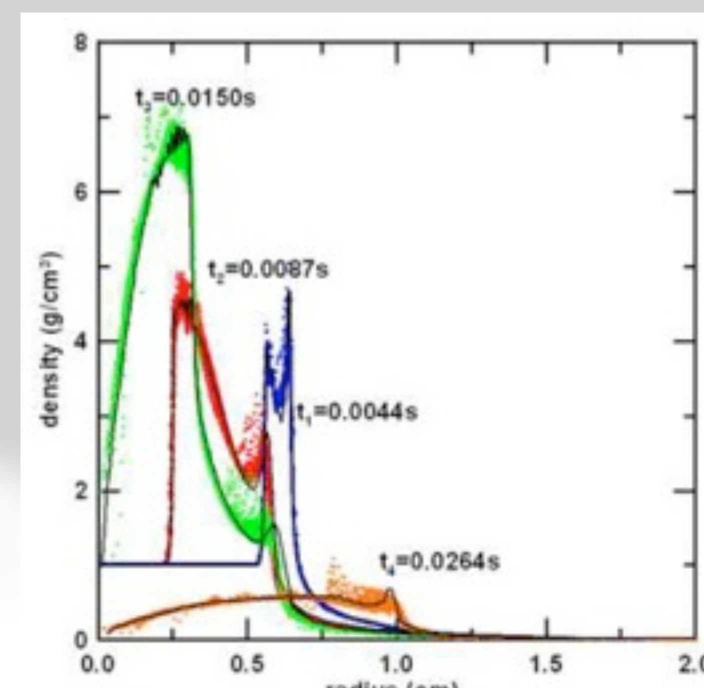






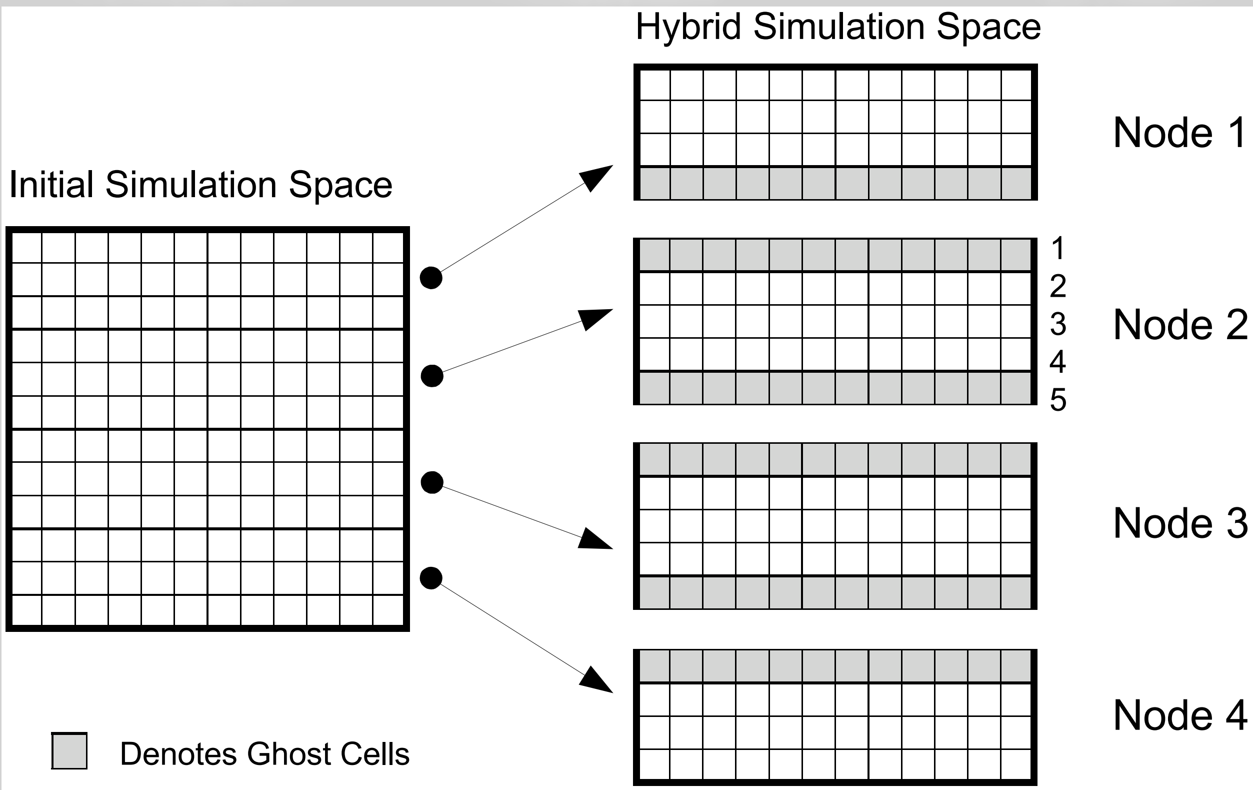
Alec Staber, "Implosion and Collapses within a Kinetic Monte Carlo Approach" (MSU, senior thesis)

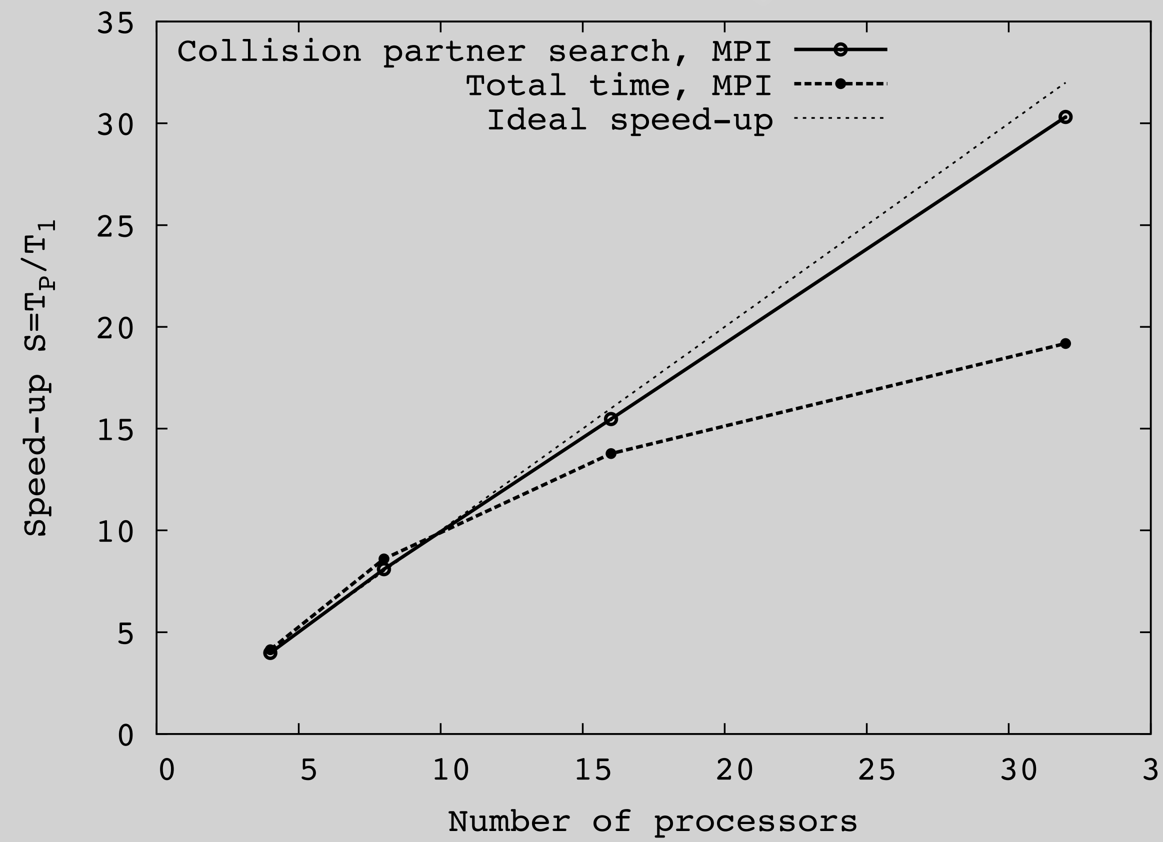
Ablation of homogeneous sphere by deposition of kinetic energy in its outer layers (Garcia-Senz et al. , MNRAS 392 (2009). Linear internal energy deposition profile with E(r=R) = 10^4 E(r=0.8R)



- Shock wave forms in the outer layer and travels inward, bounces of itself at the center and travels radially outward
- Simulations were done in 2D and 3D

MPI parallelization





Jim Howell, (MSU senior) (*Parallelization of Kinetic Theory Simulations, PNP 2014, Howell et al*.)

Shared memory parallelization (e.g OpenMP) is limited by the number of CPUs per core (≤ 64 at HPCC). Distributed memory parallelization (MPI) is in principle limitless but has some overhead due to node communication

- First implementation and tests of MPI version of KineticSN (gravitational collapse, RTI instabilities)
- Speed up of collision partner search looks promising

Summary

- Transport models can describe matter in and out of equilibrium, shock wave phenomena, fluid instabilities ...
- ➔ Large scale hydrodynamic simulation via Kinetic Theory
- Comparisons to hydrodynamic codes look promising
- Current development: Transport code that can handle $\gg 10^6$ test particles in a computationally efficient way
- First hydrodynamic tests to reproduce shock wave phenomena
- Current work: MPI parallelization, extension of test suite (fluid instabilities)
- Future work: Nuclear and gravitational forces, neutrino test-particles and interactions, relativistic effects, ...