Numerical Hydrodynamics
III

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Fluids: PH4031

18 February 2021

Complex Calculation: Required Components & considerations

Re-cap

- To solve any system numerically, we require

A method to divide the region (e.g. grids)
A method to describe the evolution of the region
(i.e. the set of fluid dynamics equations)
A method to describe the edge of the region (i.e. boundary conditions)
The initial properties of the system (i.e. initial conditions)

- Other considerations

Artificial terms
Timestepping
Resolution
Conservation laws to ensure accuracy

Resolution: Warning!

Re-cap

- Recall: decreasing *dx* by a factor 2
  - doubles the number of calculations per step
  - doubles the number of steps

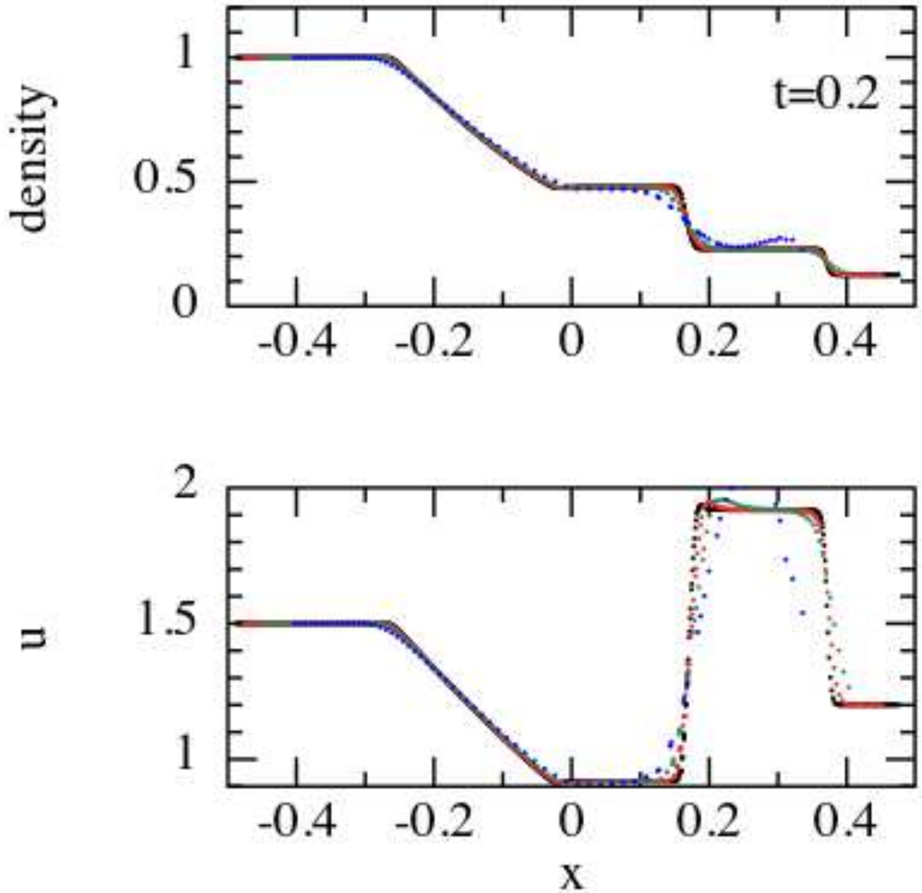
$$dt = C\frac{dx_i}{v_i} \quad \text{where} \quad C \leq 1$$

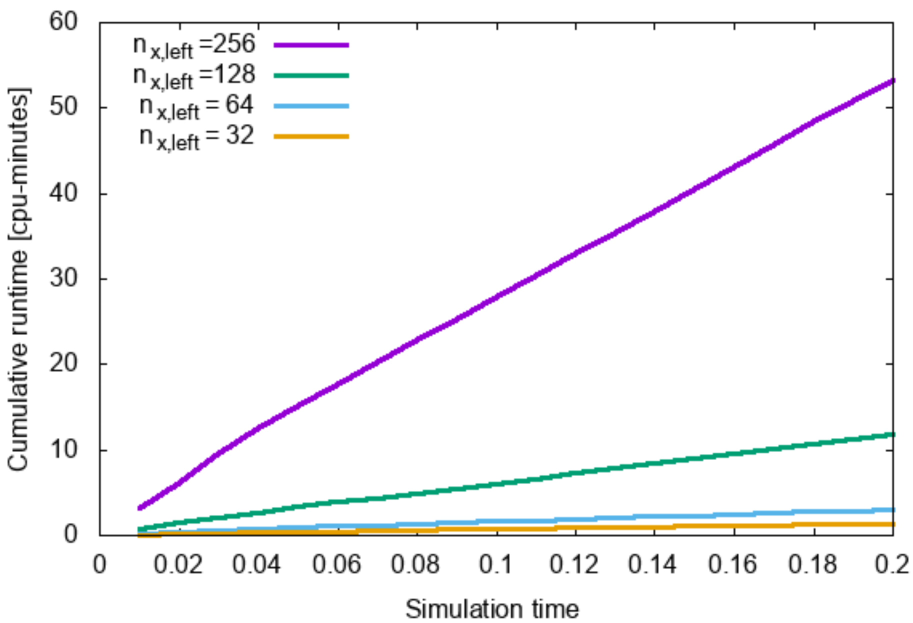
In numerical studies, the user must always balance resolution with runtime!

Resolution: Sod Shock

Re-cap

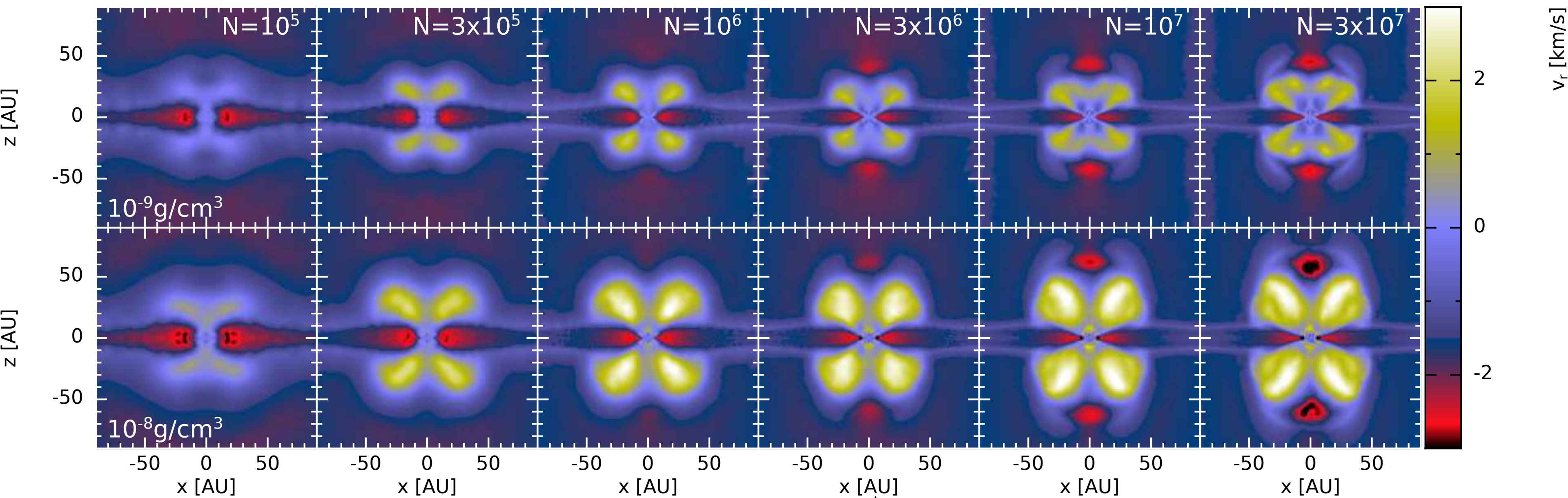
- Testing four resolutions: $n_{x,\mathrm{left}} = 32, 64, 128$ & 256
- Runtime is considerably longer for higher resolutions





Resolution: Star formation

- For realistic problems, we may not know the correct answer, so what resolution do we choose?
- This is the radial velocity (outflow) from a star formation simulation at two different times at various resolutions:

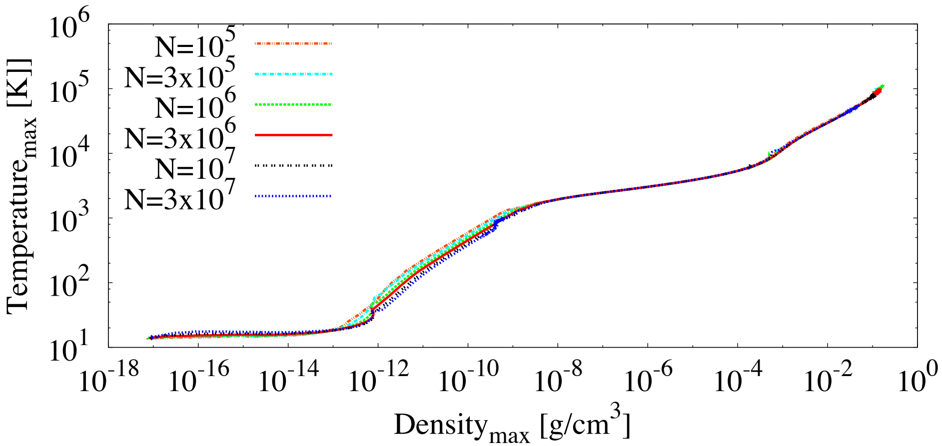


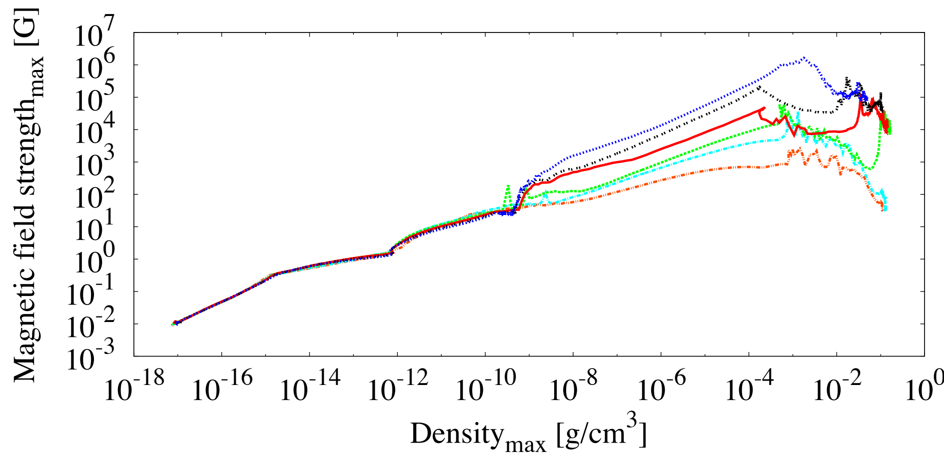
- Is my default resolution reasonable?

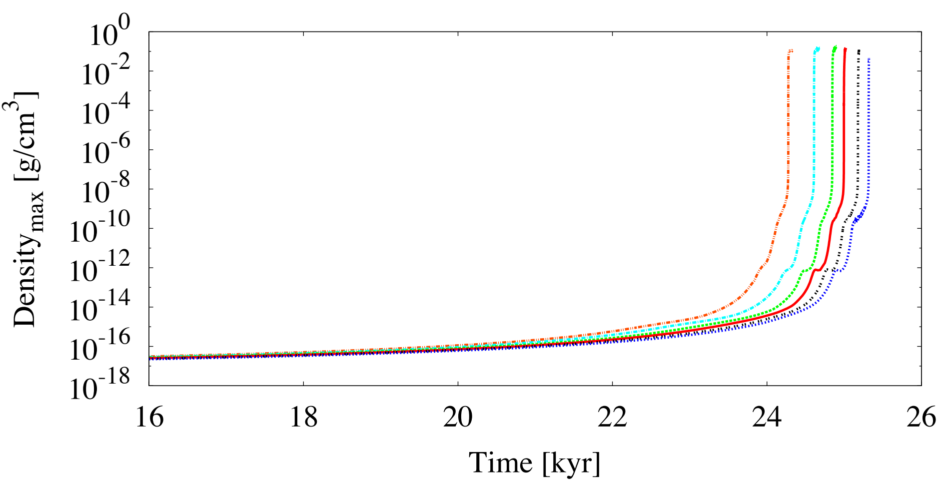
default

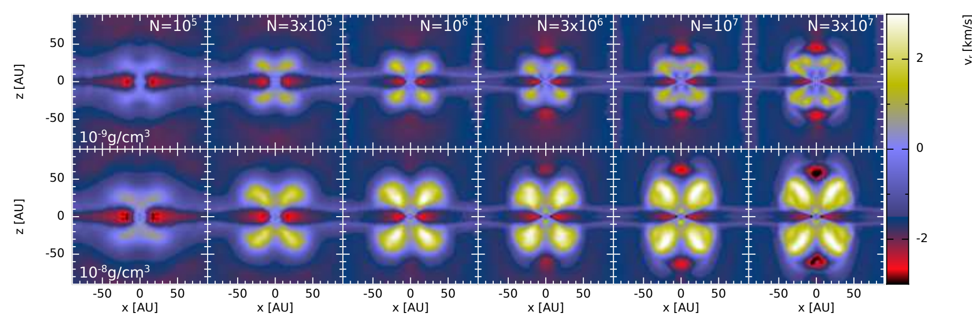
Resolution: Star formation

- For realistic problems, we may not know the correct answer, so what resolution do we choose?
- Consider convergence



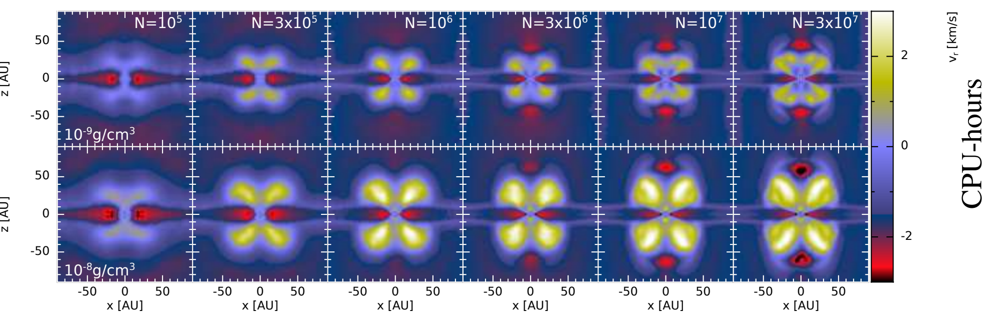


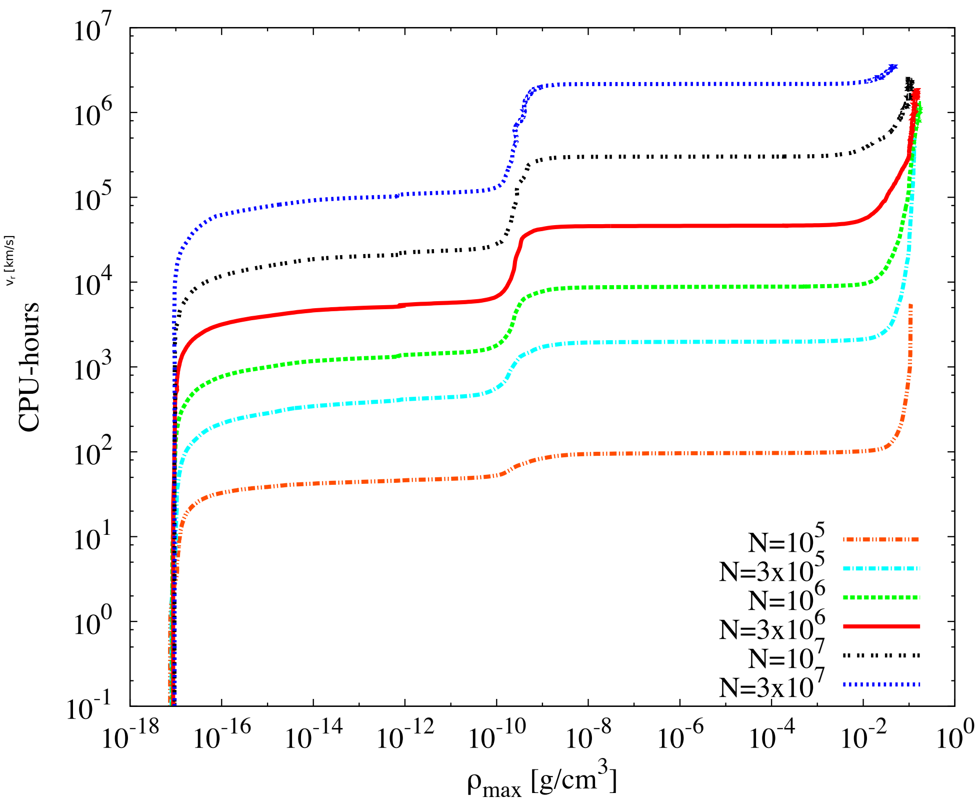




Resolution: Star formation

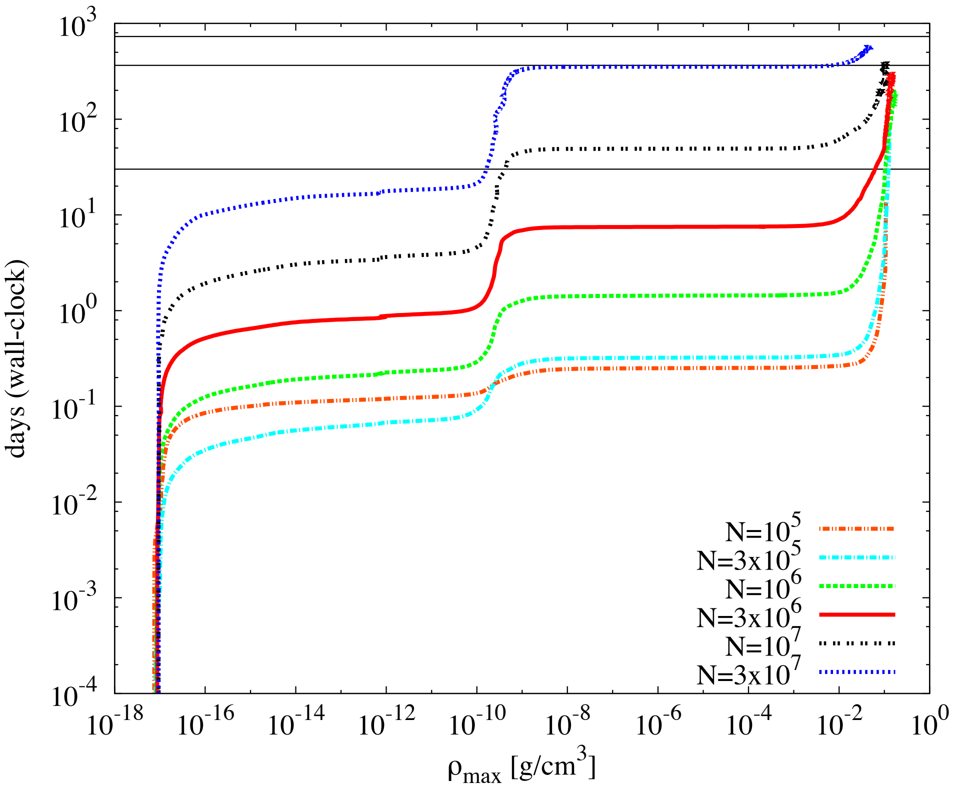
- For realistic problems, we may not know the correct answer, so what resolution do we choose?
- Consider the runtime

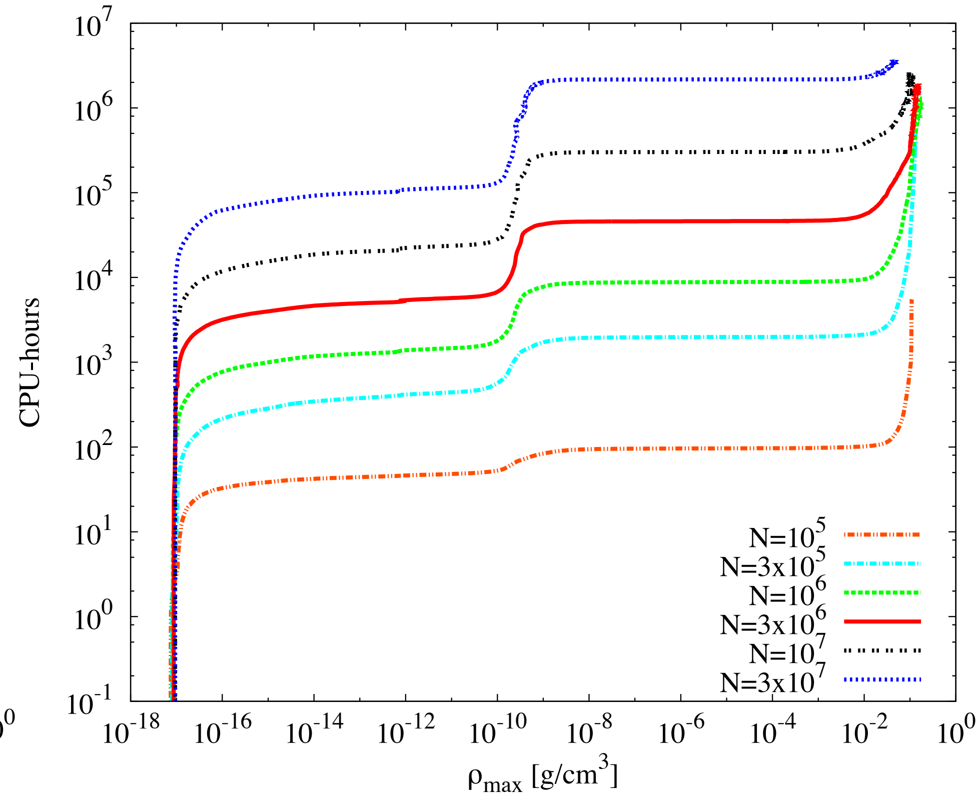




Resolution: Star formation

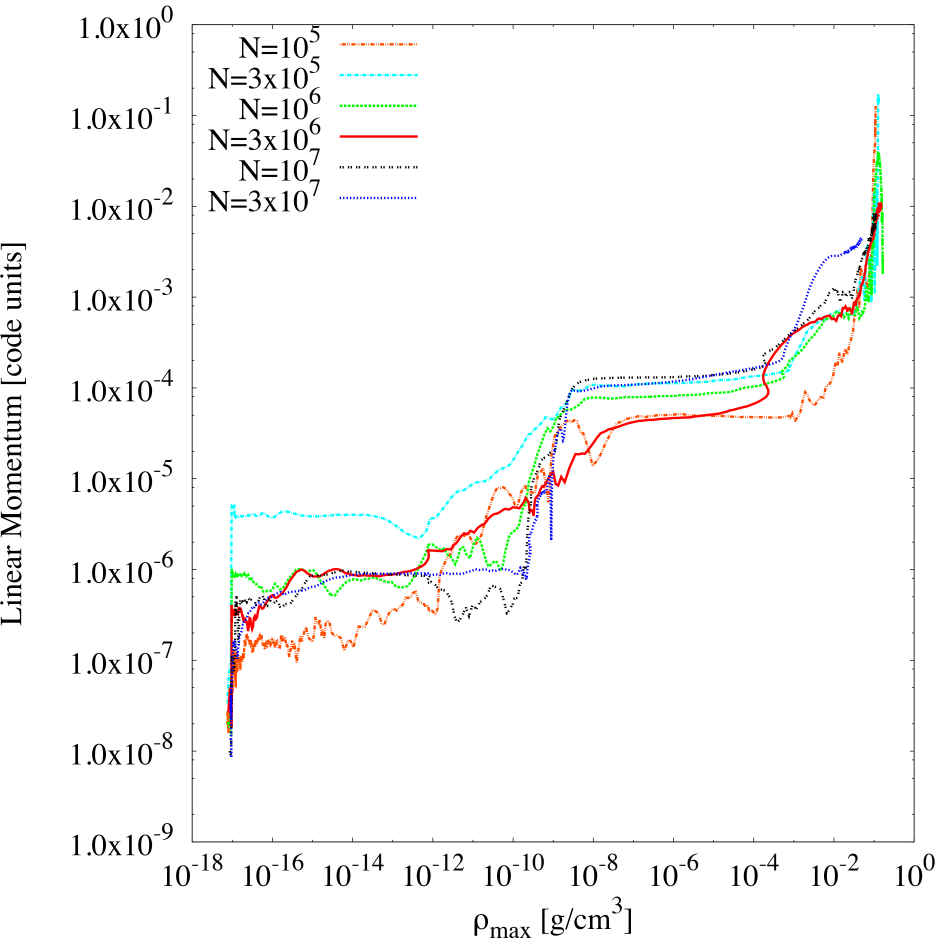
- CPU-hours represents the number of computer-hours required, which should scale with the number of processors
- Wall-hours represent the actual passage of time as perceived by us (left: grey lines at 30d, 1yr & 2yrs)

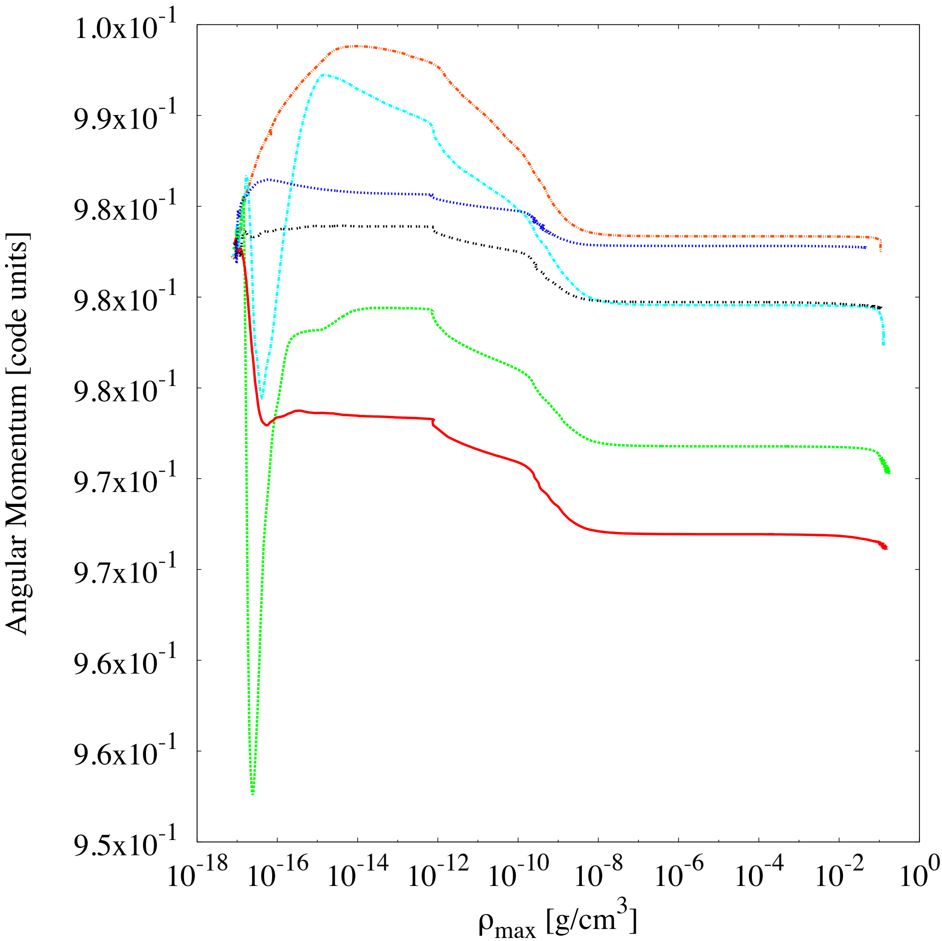




Resolution & Conservation: Star formation

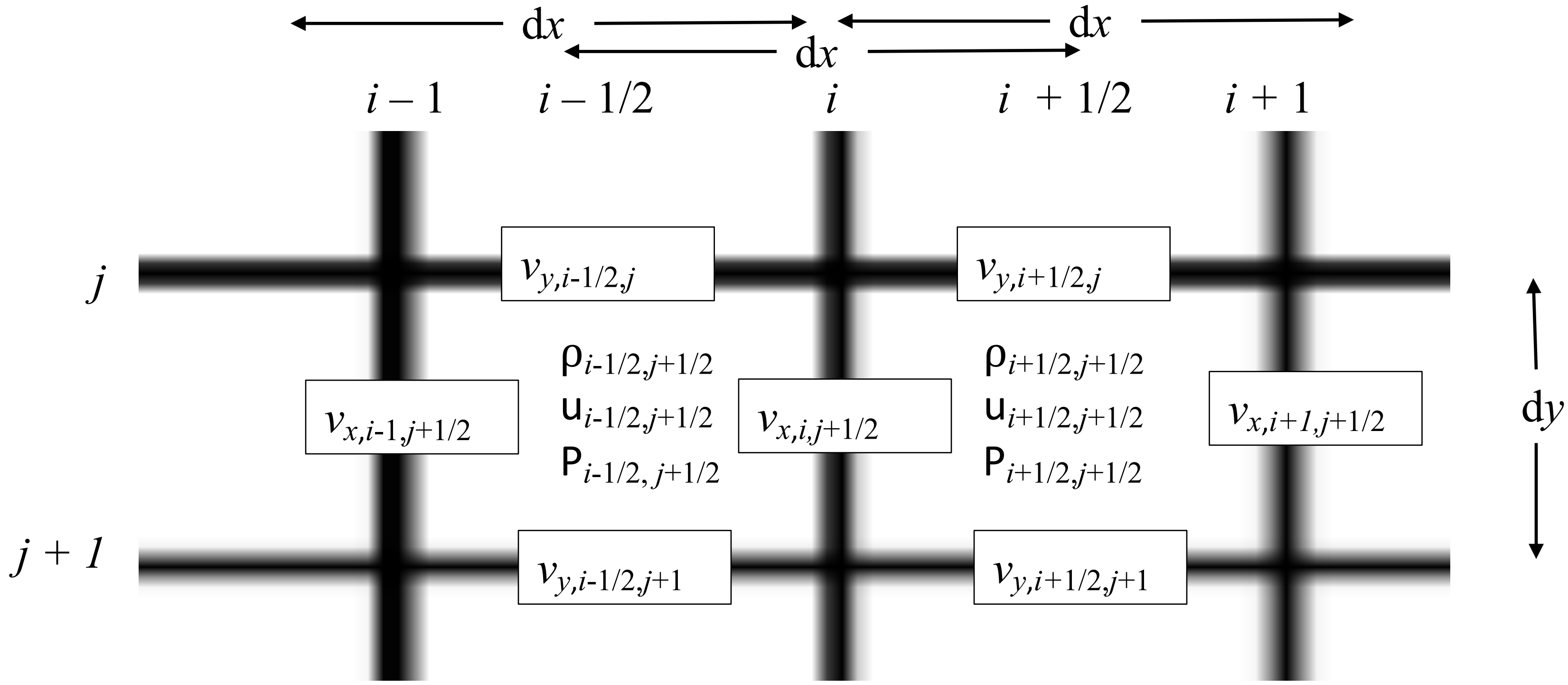
➢ Momentum is decently well conserved





Defining your problem: Defining quantities on a 2D grid

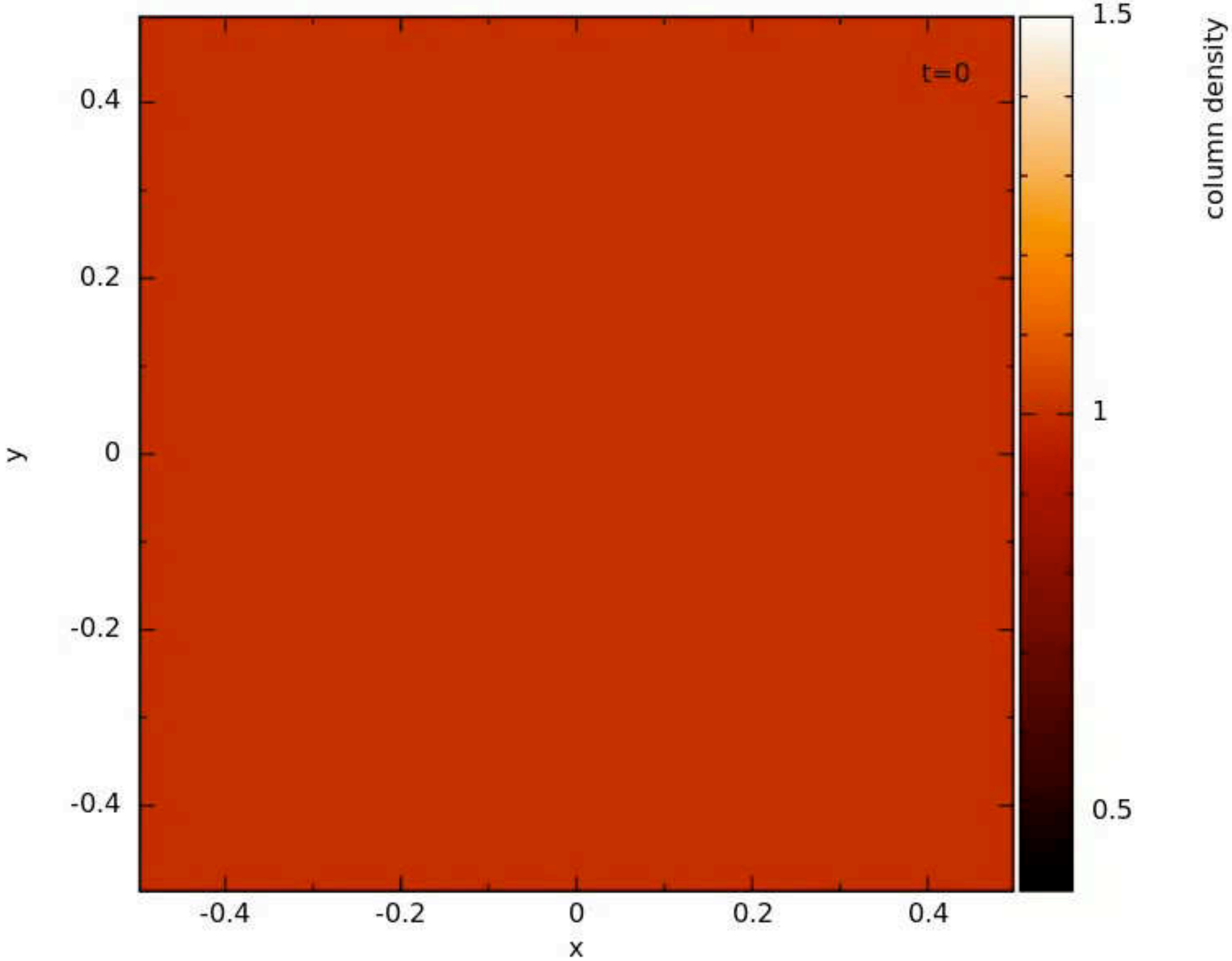
- Eulerian grid: grid of constant spacing



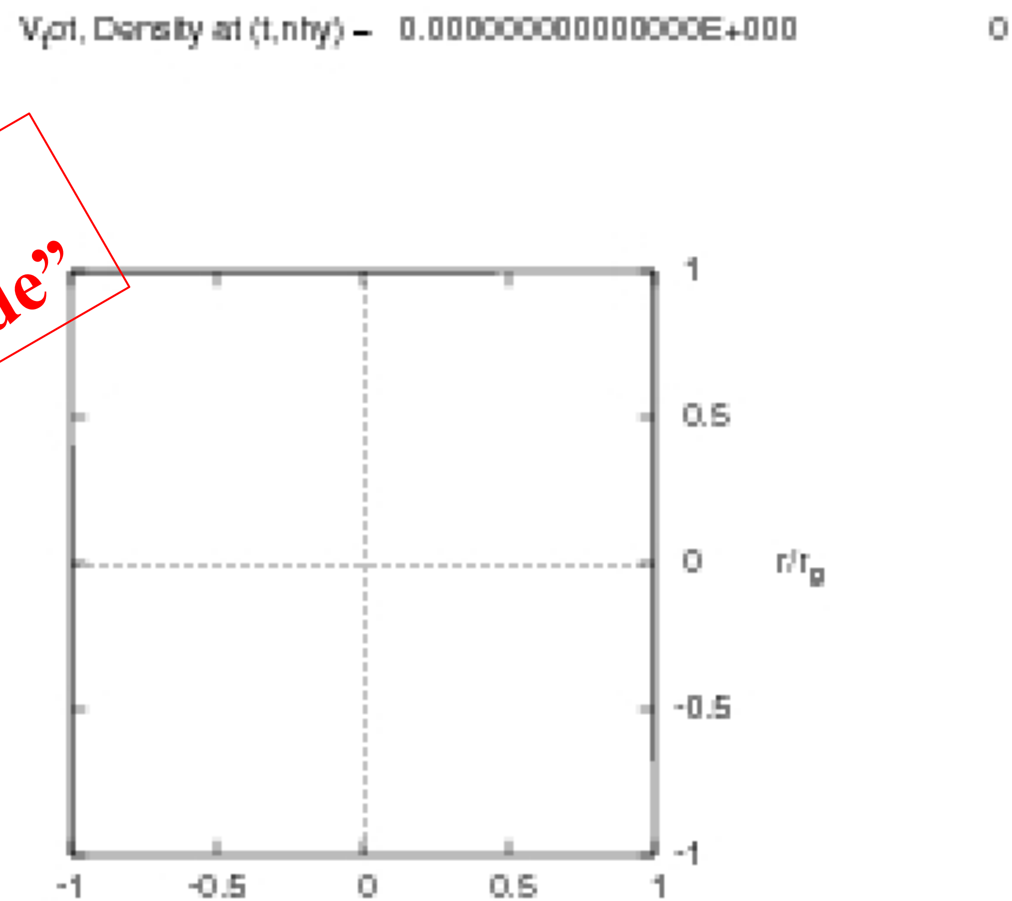
- Scalars are calculated at *cell-centre*
- Vectors are calculated at *cell-interface*

Sedov blast wave

- Energy injected into the centre and allowed to evolve

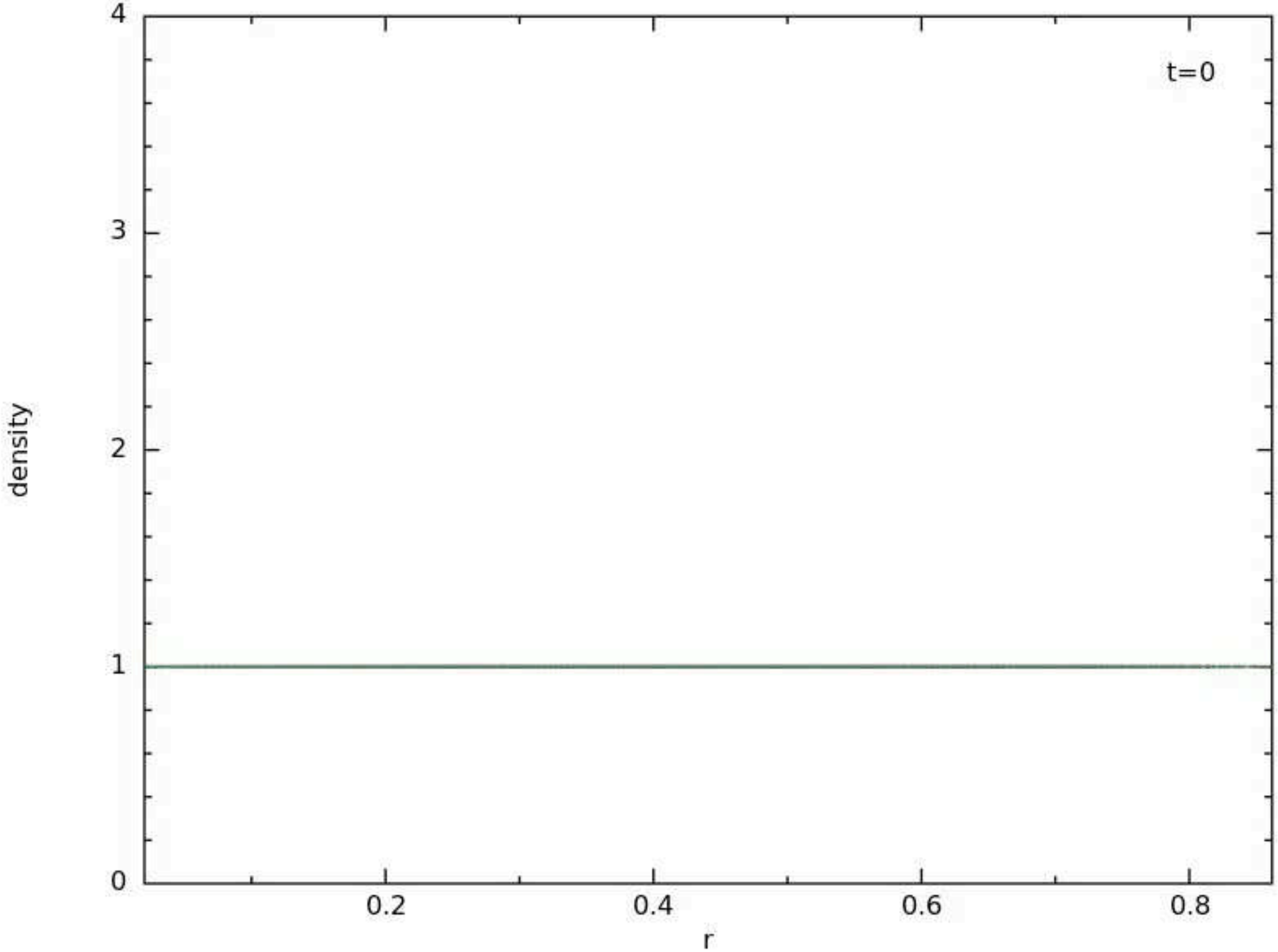


Sedov blast wave: When there's a bug!

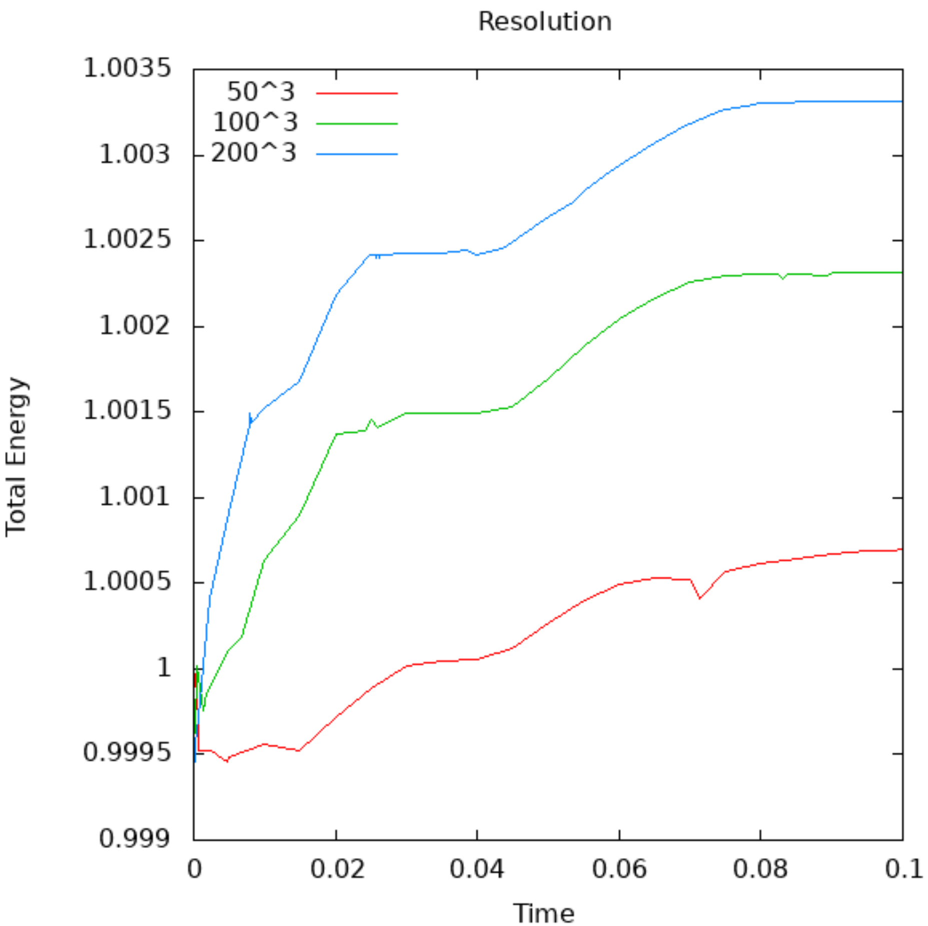


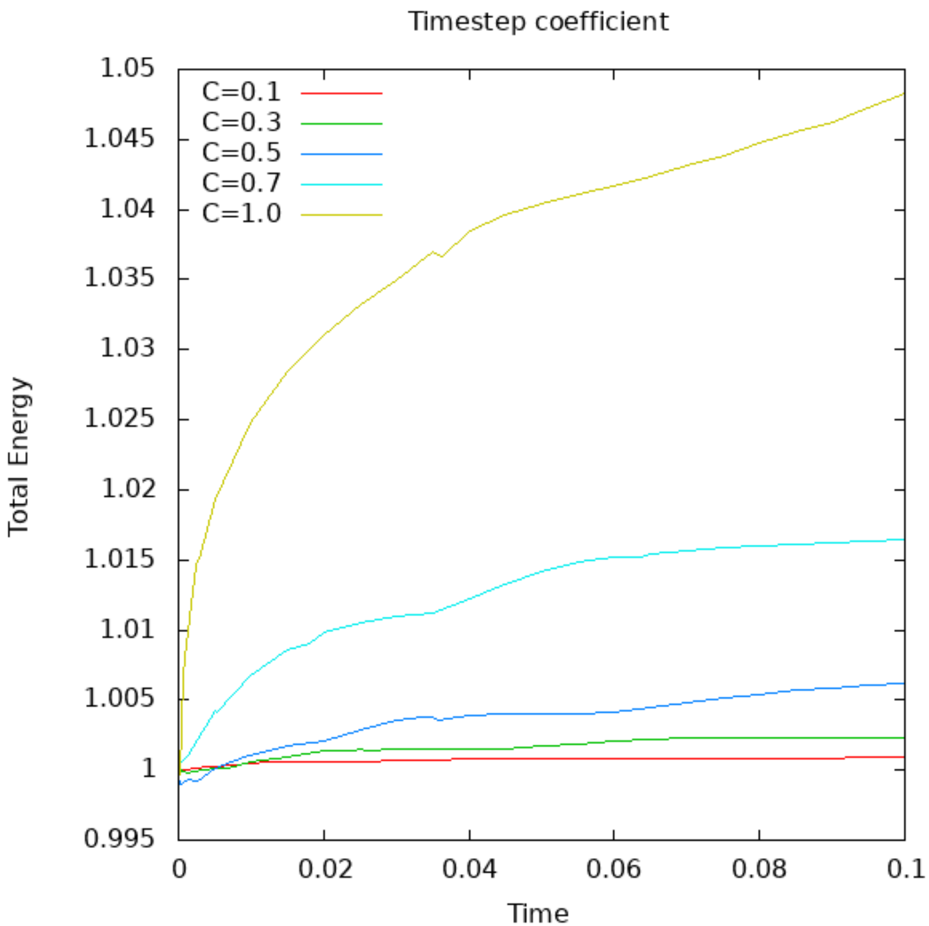
Evil clown says "Debug your Code"

Sedov blast wave: Resolution



Sedov blast wave: Total Energy



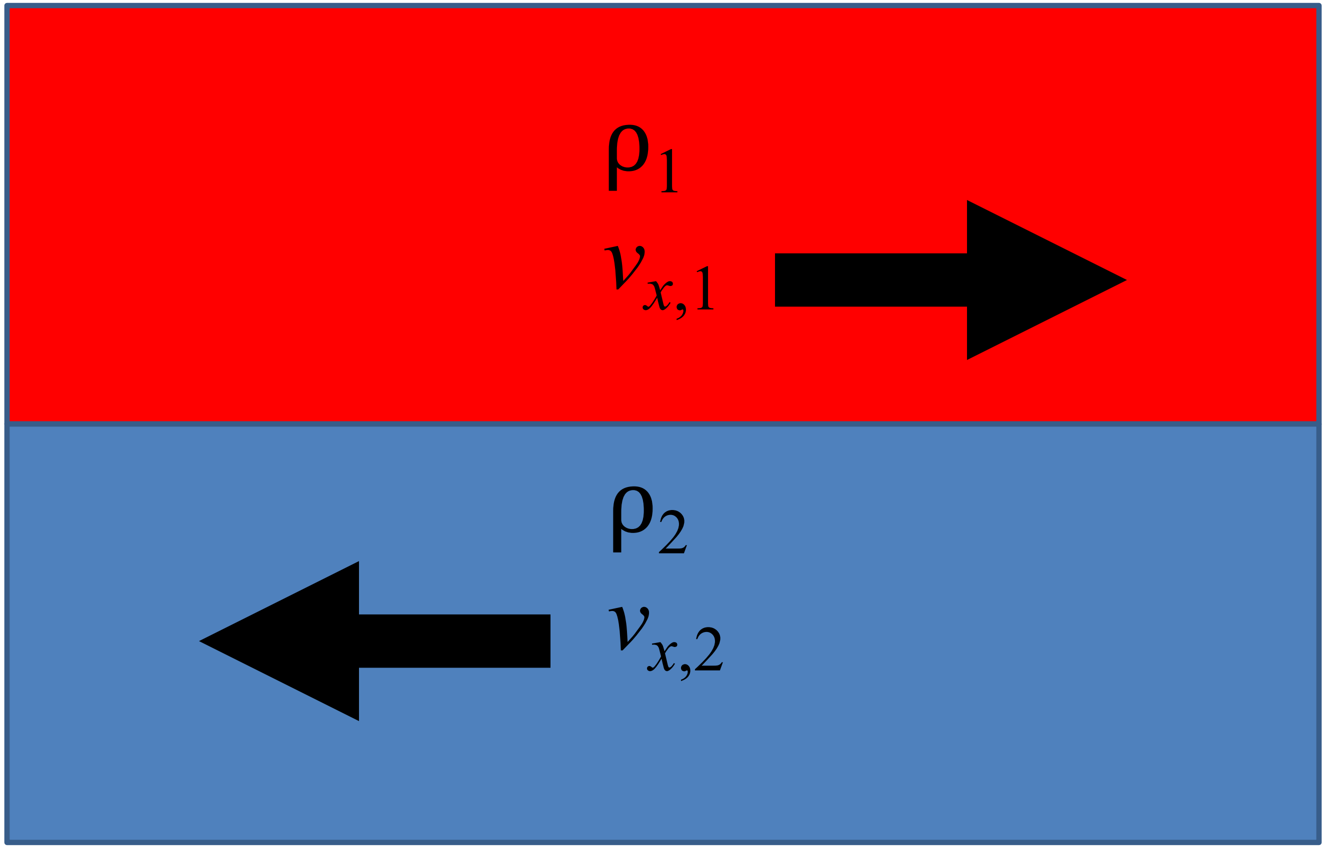


Complex Calculation: Kelvin-Helmholtz instability

- Recall the rolling clouds: This demonstrates the Kelvin-Helmholtz instability

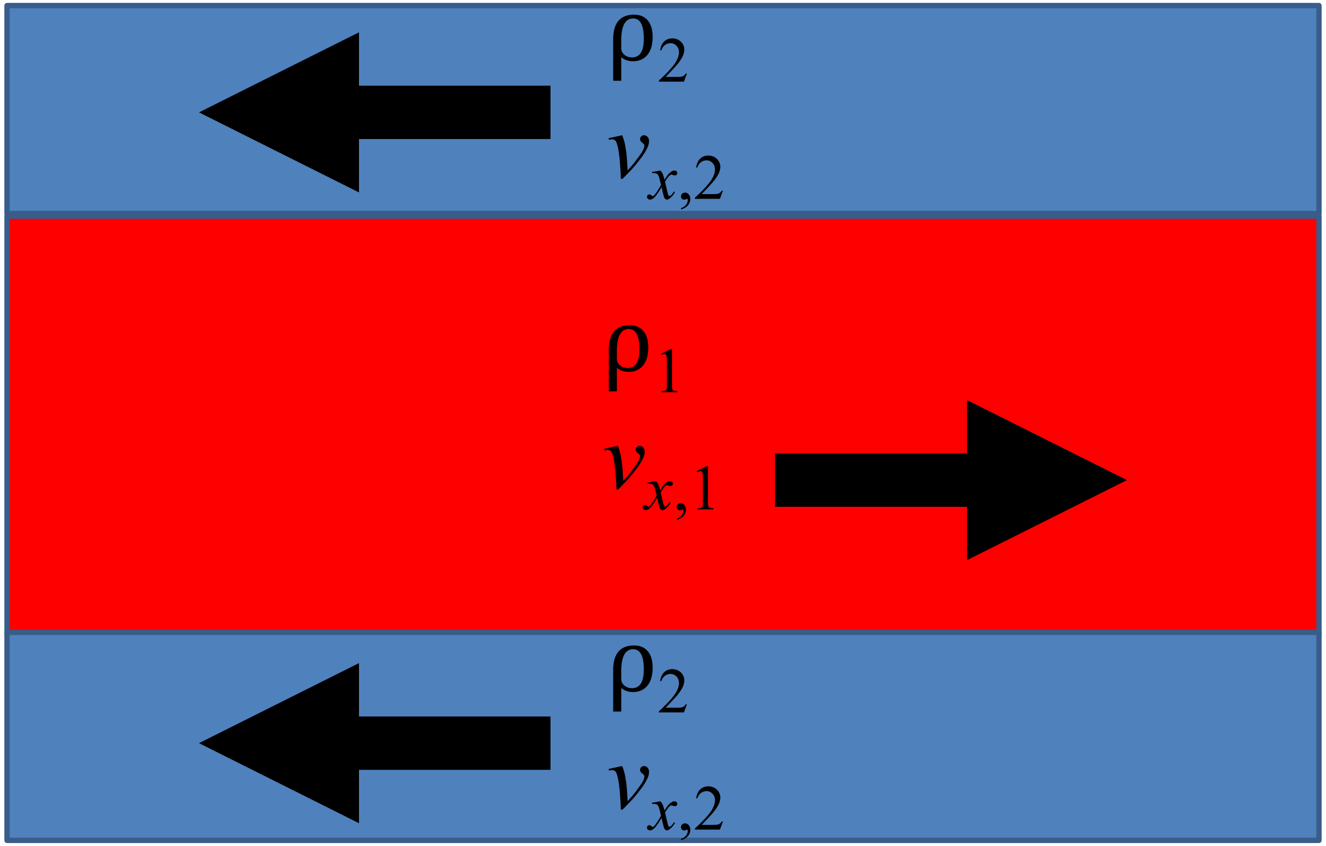
Complex Calculation: Kelvin-Helmholtz instability

- This models the shear layer between fluids of different densities:
  - Periodic boundaries in the *x*-direction; fixed in *y*-direction



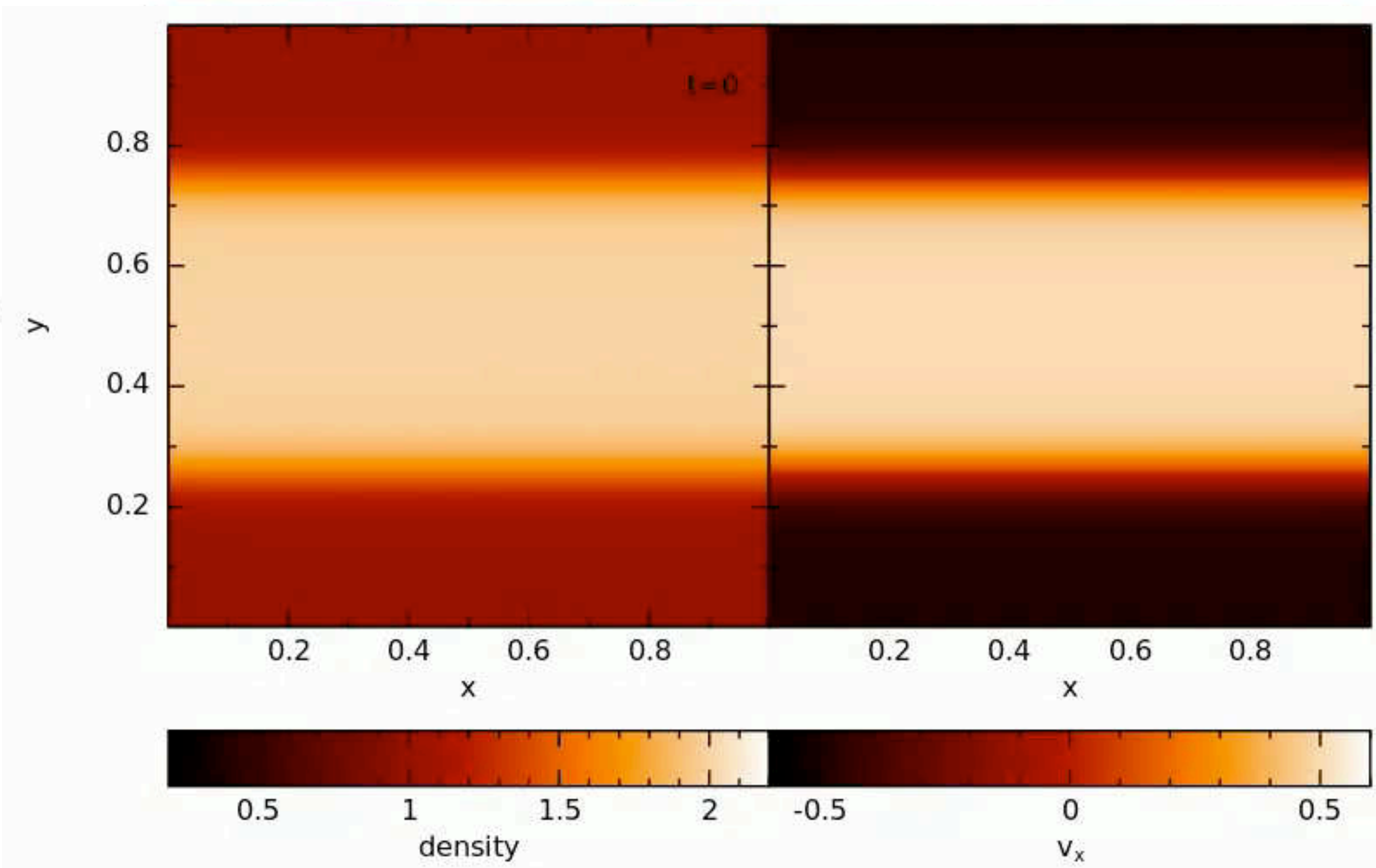
Complex Calculation: Kelvin-Helmholtz instability

- This models the shear layer between fluids of different densities:
  - Periodic boundaries in all directions



Complex Calculation: Kelvin-Helmholtz instability

- This models the shear layer between fluids of different densities:



Complex Calculation: Required Components

- To solve any system numerically, we require

  A method to divide the region (e.g. grids)
  A method to describe the evolution of the region
  (i.e. the set of fluid dynamics equations)
  A method to describe the edge of the region (i.e. boundary conditions)
  The initial properties of the system (i.e. initial conditions)
  Multi-dimensional scheme

- How complex can these calculations get?

Adding complexity: Other 'fluid' components

- Continuum Equations:

$$\text{Continuity equation:} \quad \frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\nabla\cdot\boldsymbol{v}$$

$$\text{Equation of motion:} \quad \frac{\mathrm{D}\boldsymbol{v}}{\mathrm{D}\mathrm{t}} = -\frac{1}{\rho}\nabla P$$

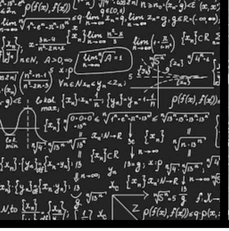
$$\text{Energy equation:} \quad \frac{\mathrm{D}u}{\mathrm{D}t} = -\frac{P}{\rho}\nabla\cdot\boldsymbol{v}$$

$$\text{Equation of state:} \quad P = (\gamma - 1)\,\rho u$$

- Where

$$\frac{\mathrm{D}}{\mathrm{Dt}} \equiv \frac{\partial}{\partial t} + \boldsymbol{v}\cdot\boldsymbol{\nabla}$$

is the Lagrangian (or co-moving) derivative

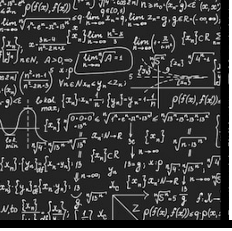


Adding complexity: Other ‘fluid’ components

- Many astrophysical phenomena include magnetic fields. The fluid equations become

$$
\begin{aligned}
\frac{\mathrm{D}\rho}{\mathrm{D}t} &= -\rho\nabla\cdot\boldsymbol{v} \\
\frac{\mathrm{D}\boldsymbol{v}}{\mathrm{Dt}} &= -\frac{1}{\rho}\nabla\left[\left(P+\frac{B^2}{2\mu_0}\right)\mathbb{I}-\frac{1}{\mu_0}\boldsymbol{B}\boldsymbol{B}\right] \\
\frac{\mathrm{D}\boldsymbol{B}}{\mathrm{D}t} &= \boldsymbol{\nabla}\times(\boldsymbol{v}\times\boldsymbol{B}) \\
\frac{\mathrm{D}u}{\mathrm{D}t} &= -\frac{P}{\rho}\nabla\cdot\boldsymbol{v}
\end{aligned}
$$

- Magnetic fields are vectors, thus numerically treated like velocity fields
- Requires artificial resistivity, similar in to artificial viscosity and artificial conductivity



Adding complexity: Other 'fluid' components

- Many astrophysical phenomena include magnetic fields.
- The fluid equations intrinsically contain magnetic monopoles:

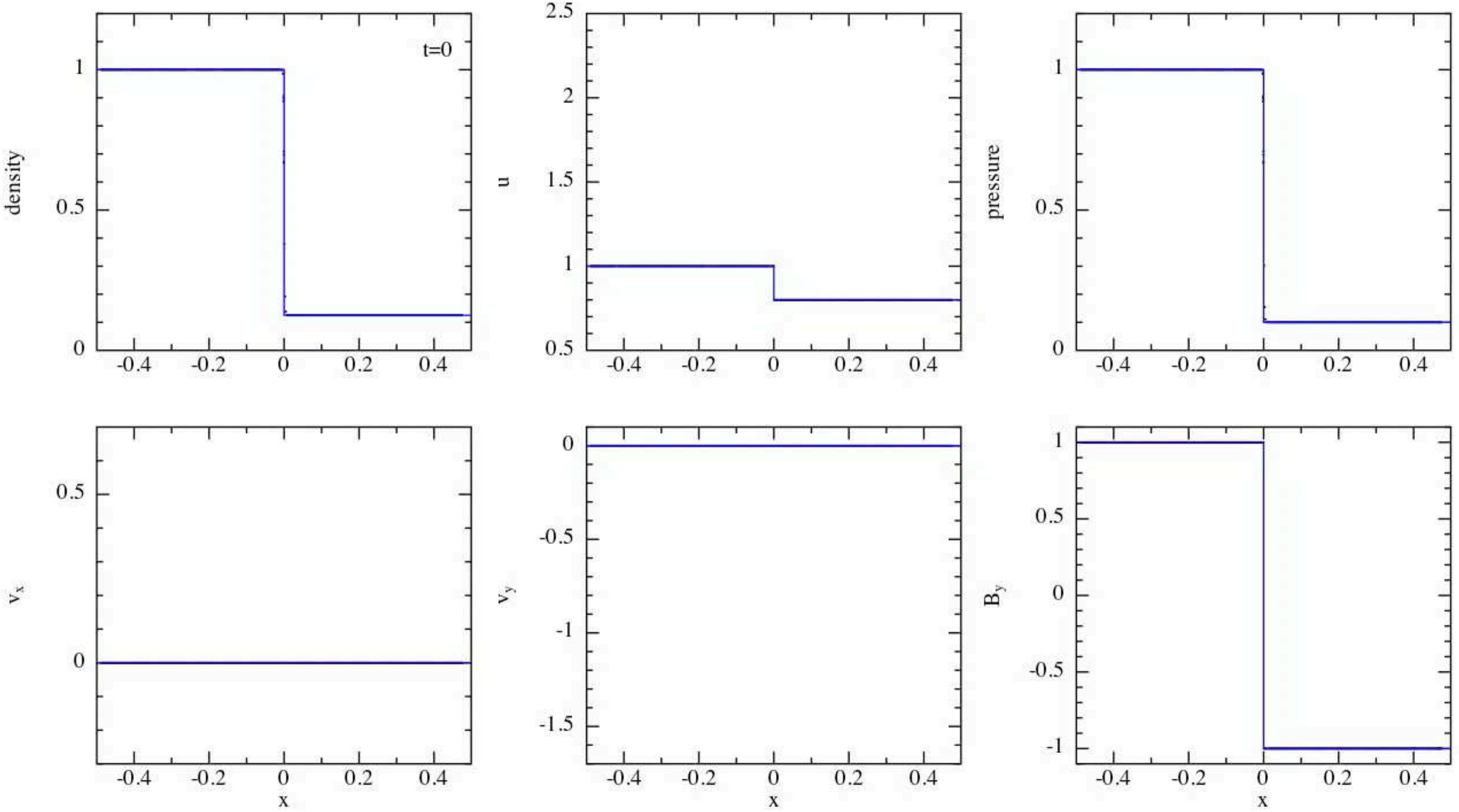
$$
\begin{aligned}
\frac{\mathrm{D}\boldsymbol{v}}{\mathrm{Dt}} &= -\frac{1}{\rho}\nabla\left[\left(P+\frac{B^2}{2\mu_0}\right)\mathbb{I}-\frac{1}{\mu_0}\boldsymbol{B}\boldsymbol{B}\right] \\
&= -\frac{\nabla P}{\rho}-\frac{1}{\mu_0\rho}\left[\frac{1}{2}\nabla B^2-\nabla\cdot(\boldsymbol{B}\boldsymbol{B})\right] \\
&= -\frac{\nabla P}{\rho}-\frac{1}{\mu_0\rho}\left[\frac{1}{2}\nabla B^2-\left\{\frac{1}{2}\nabla B^2-\boldsymbol{B}\times(\nabla\times\boldsymbol{B})+\boldsymbol{B}\,(\nabla\cdot\boldsymbol{B})\right\}\right] \\
&= -\frac{\nabla P}{\rho}+\frac{(\nabla\times\boldsymbol{B})\times\boldsymbol{B}}{\mu_0\rho}+\boxed{\frac{\boldsymbol{B}\,(\nabla\cdot\boldsymbol{B})}{\mu_0\rho}}
\end{aligned}
$$

Analytically zero
Numerically non-zero (possibly)

- Requires 'cleaning' method to remove numerical magnetic monopoles

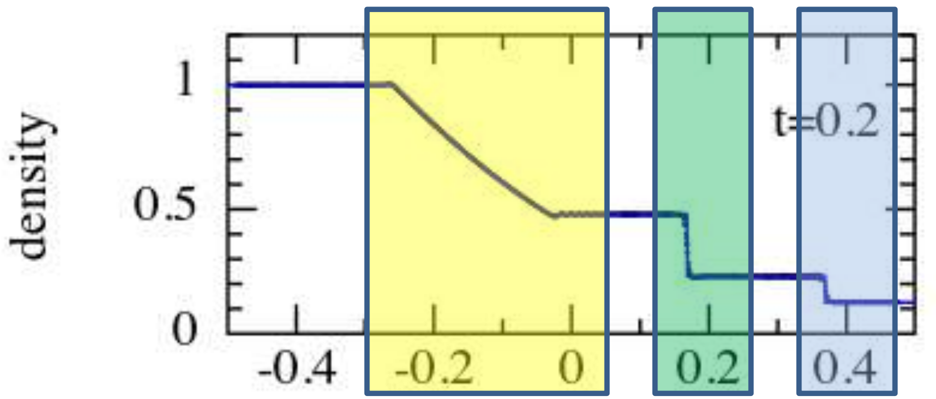
Adding complexity: Other 'fluid' components

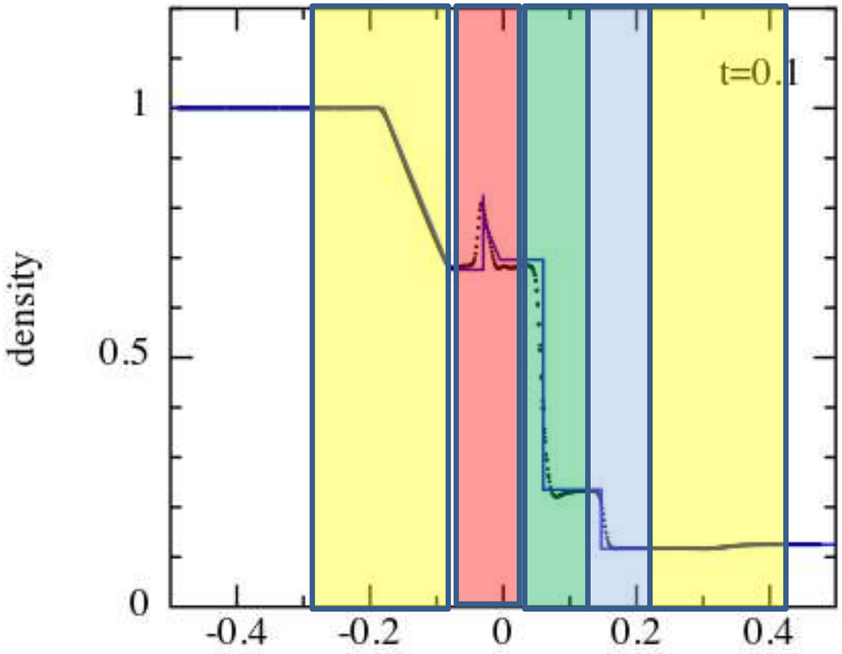
- Many astrophysical phenomena include magnetic fields.



Adding complexity:
Other 'fluid' components: Shocks

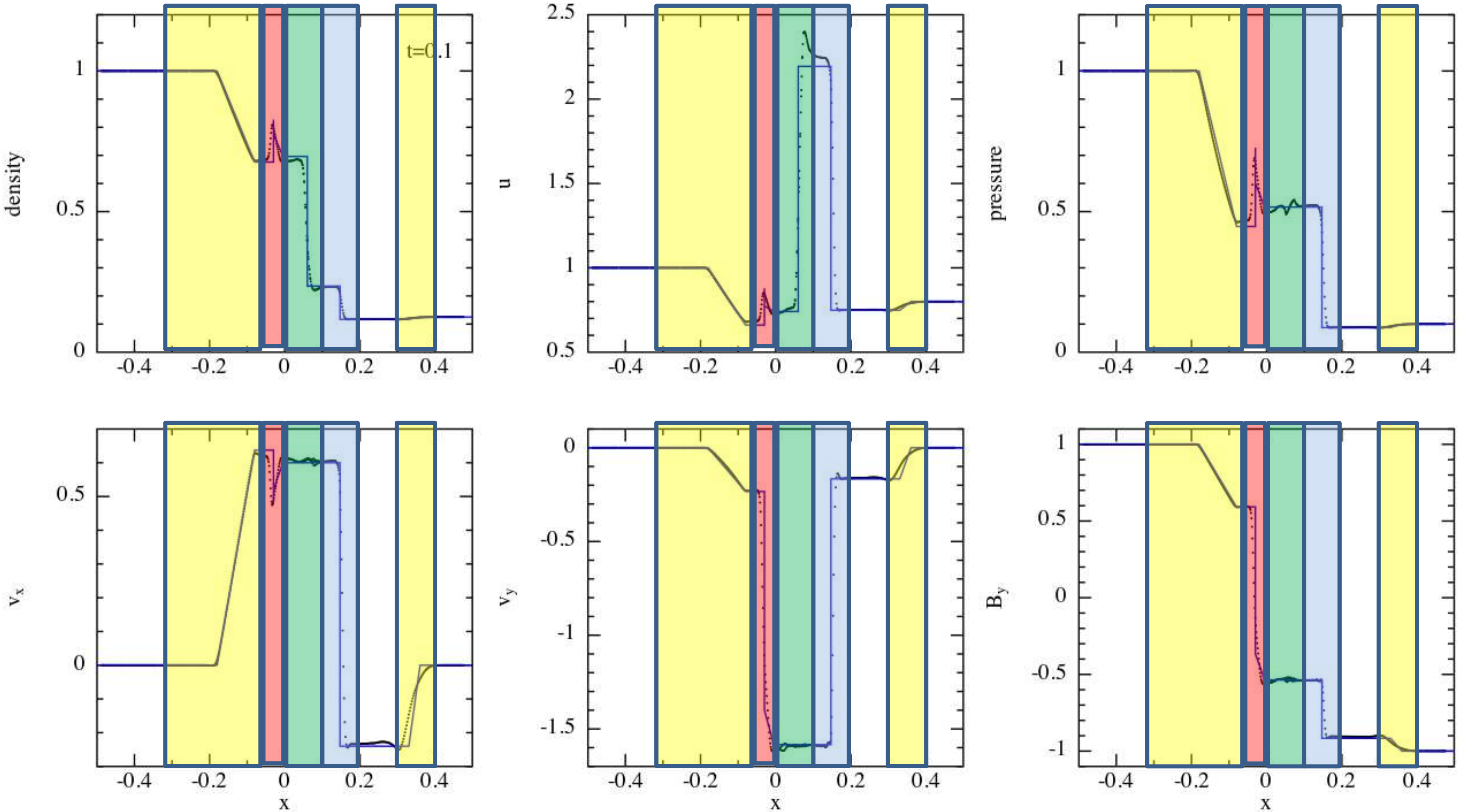
- Sod shock tube (hydro) vs Brio Wu shock tube (MHD)
  - Rarefaction wave
  - Compound wave
  - Contact discontinuity
  - Shock wave





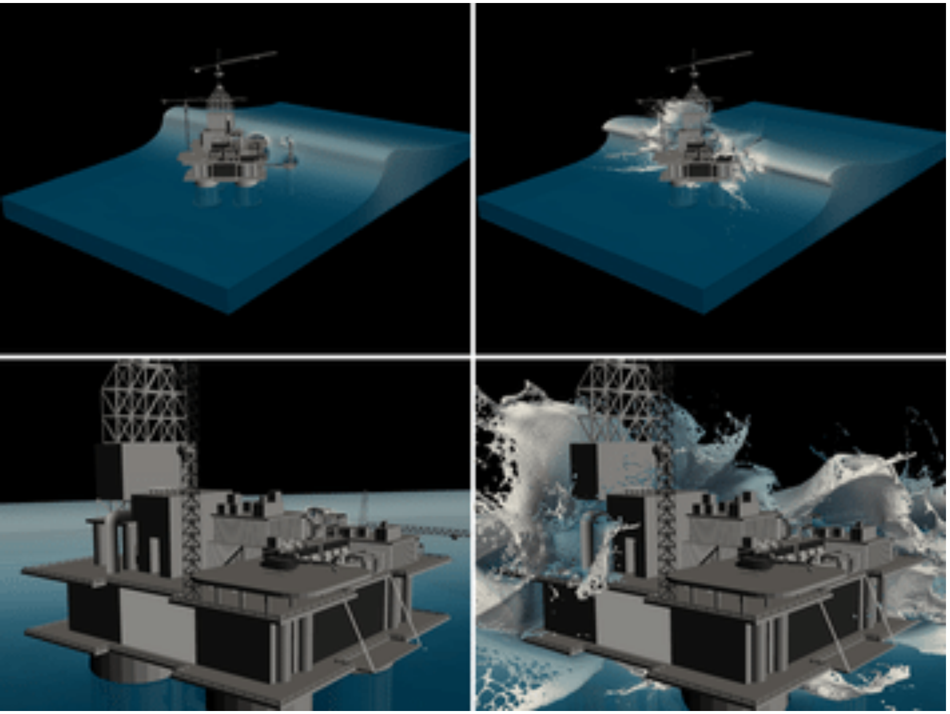
Adding complexity: Other 'fluid' components

- Many astrophysical phenomena include magnetic fields.



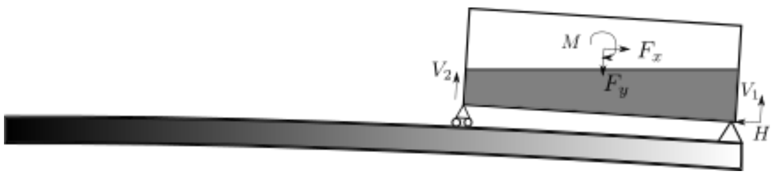
Interaction with non-fluids

- Many engineering simulations require
  - complex boundary conditions (left)
  - the fluid to interact with solid, but moveable, objects (right)

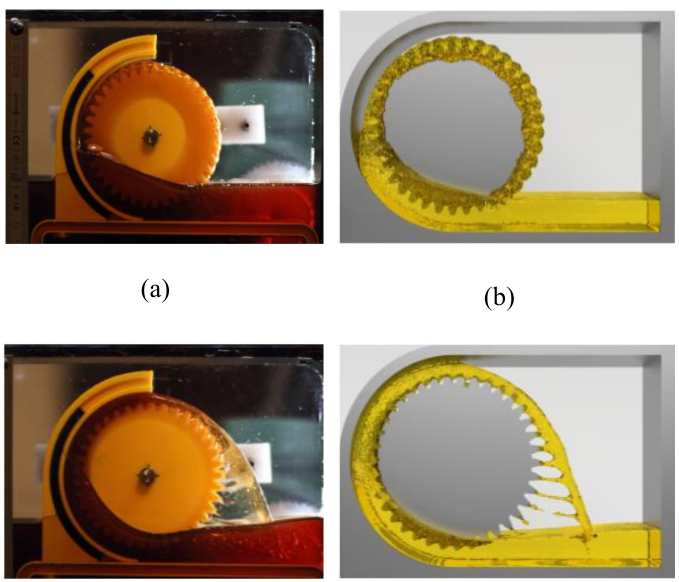


Interaction with non-fluids: Non-uniform Boundaries

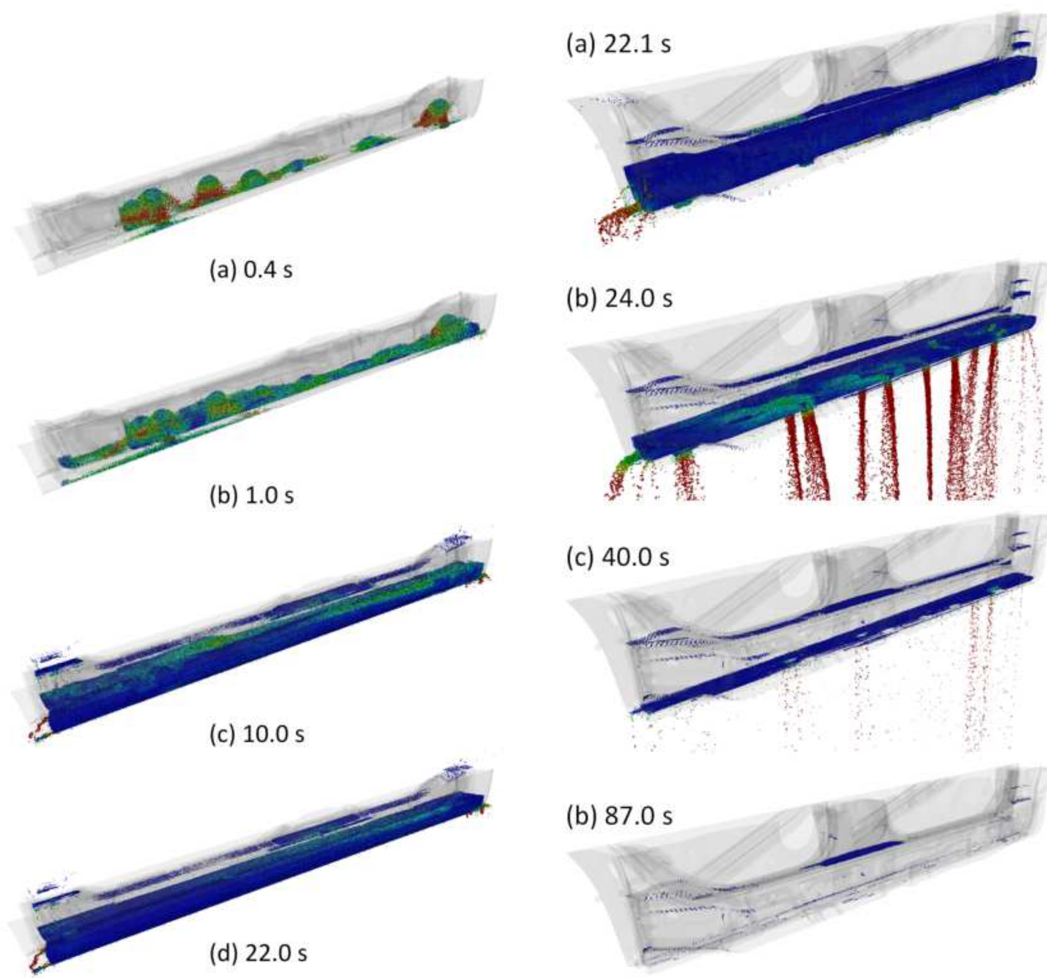
- To minimise sloshing in aircraft wings (Calderon-Sanchez + 2019)



- Lubricating a gearbox (Bannier+ 2019)



- Coating car cavities with wax (Chitneedi, Peng & Verma 2019)



Interaction with non-fluids

- Many astrophysical phenomena include non-fluid components
  - Dust
  - Stars
  - Dark matter
- These non-fluid components typically interact via gravity or drag
- If only gas:

$$
\begin{aligned}
\frac{\mathrm{D}\rho}{\mathrm{D}t} &= -\rho\nabla\cdot\boldsymbol{v} \\
\frac{\mathrm{D}\boldsymbol{v}}{\mathrm{Dt}} &= -\frac{1}{\rho}\nabla P - \nabla\Phi \\
\frac{\mathrm{D}u}{\mathrm{D}t} &= -\frac{P}{\rho}\nabla\cdot\boldsymbol{v} \\
\nabla^2\Phi &= 4\pi G\rho
\end{aligned}
$$

Interaction with non-fluids

- Many astrophysical phenomena include non-fluid components
  - Dust
  - Stars
  - Dark matter
- These non-fluid components are pressureless and typically interact via gravity or drag
- If gas, stars and dark matter:

$$
\begin{aligned}
\frac{\mathrm{D}\rho_{\mathrm{g}}}{\mathrm{D}t} &= -\rho_{\mathrm{g}} \nabla \cdot \boldsymbol{v}_{\mathrm{g}} \\
\frac{\mathrm{D}\boldsymbol{v}_{\mathrm{g}}}{\mathrm{Dt}} &= -\frac{1}{\rho_{\mathrm{g}}} \nabla P_{\mathrm{g}} - \nabla \Phi \\
\frac{\mathrm{D}\boldsymbol{v}_{\mathrm{s}}}{\mathrm{Dt}} &= -\nabla \Phi \\
\frac{\mathrm{D}\boldsymbol{v}_{\mathrm{dm}}}{\mathrm{Dt}} &= -\nabla \Phi \\
\frac{\mathrm{D}u_{\mathrm{g}}}{\mathrm{D}t} &= -\frac{P_{\mathrm{g}}}{\rho_{\mathrm{g}}} \nabla \cdot \boldsymbol{v}_{\mathrm{g}} \\
\nabla^2 \Phi &= 4\pi G \rho
\end{aligned}
$$

Interaction with non-fluids

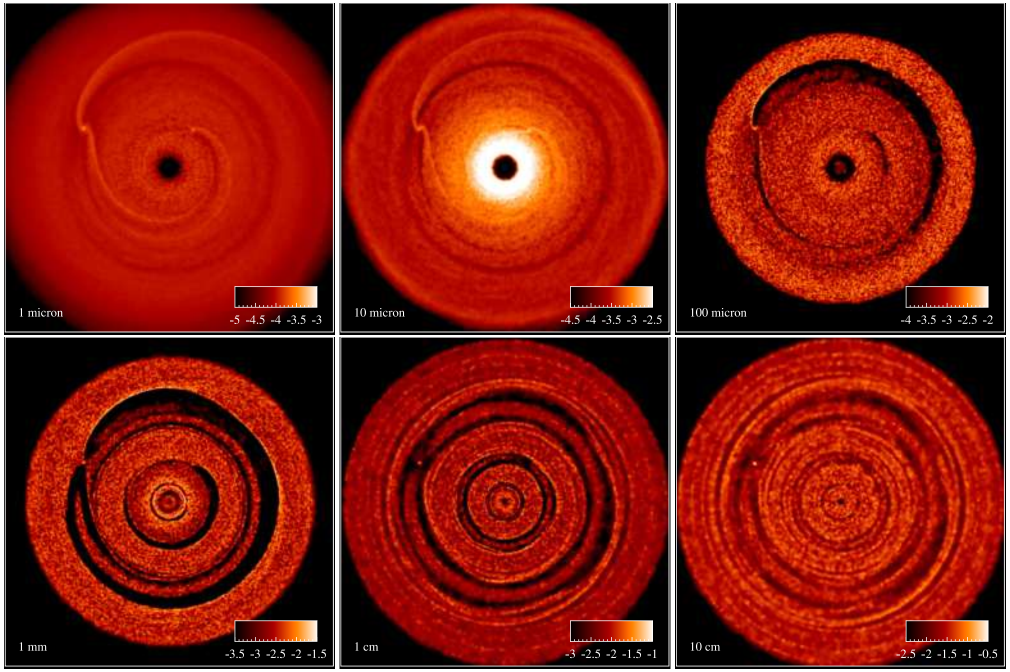
- Many astrophysical phenomena include non-fluid components
  - Dust
  - Stars
  - Dark matter
- These non-fluid components are pressureless and typically interact via gravity or drag
- If gas & dust:

$$\frac{\partial \rho_{\mathrm{g}}}{\partial t} + \nabla \cdot \left(\rho_{\mathrm{g}} \boldsymbol{v}_{\mathrm{g}}\right) = 0,$$

$$\frac{\partial \rho_{\mathrm{d}}}{\partial t} + \nabla \cdot \left(\rho_{\mathrm{d}} \boldsymbol{v}_{\mathrm{d}}\right) = 0,$$

$$\rho_{\mathrm{g}} \left(\frac{\partial \boldsymbol{v}_{\mathrm{g}}}{\partial t} + \boldsymbol{v}_{\mathrm{g}} \cdot \nabla \boldsymbol{v}_{\mathrm{g}} \right) = \rho_{\mathrm{g}} \boldsymbol{f} + K(\boldsymbol{v}_{\mathrm{d}} - \boldsymbol{v}_{\mathrm{g}}) - \nabla P_{\mathrm{g}},$$

$$\rho_{\mathrm{d}} \left(\frac{\partial \boldsymbol{v}_{\mathrm{d}}}{\partial t} + \boldsymbol{v}_{\mathrm{d}} \cdot \nabla \boldsymbol{v}_{\mathrm{d}} \right) = \rho_{\mathrm{d}} \boldsymbol{f} - K(\boldsymbol{v}_{\mathrm{d}} - \boldsymbol{v}_{\mathrm{g}}),$$

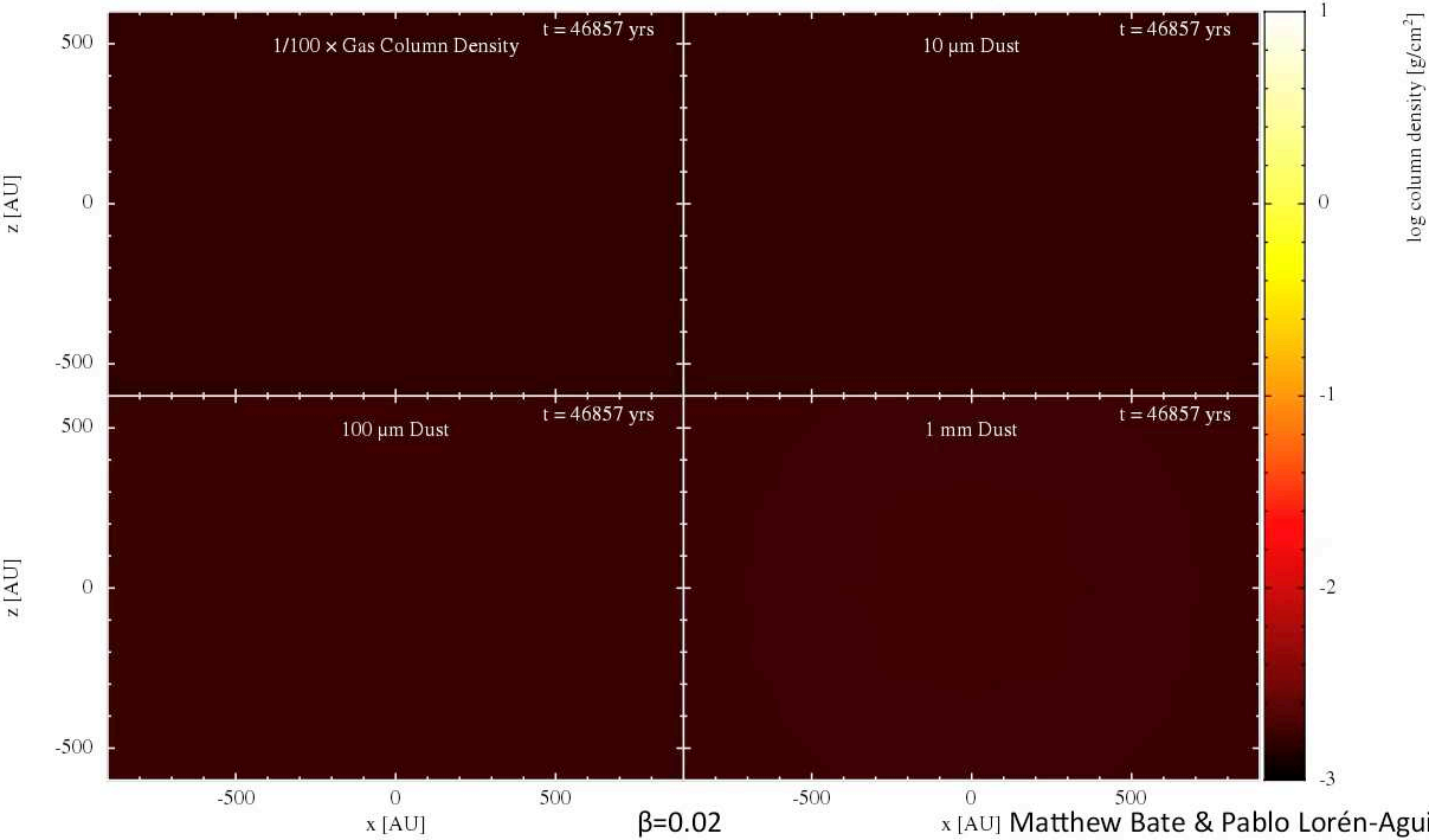


Laibe & Price (2014); Lagrangian formalism so $\frac{\mathrm{D}}{\mathrm{Dt}} \equiv \frac{\partial}{\partial t}$

Dipierro+ (2015)

Interaction with non-fluids

- Gas + Dust simulations

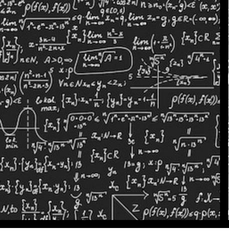


β=0.02

Matthew Bate & Pablo Lorén-Aguilar

Sub-grid physics

- Resolution is chosen based upon the size of the object you want to study and the computational resources
- What about physical processes that are below the resolution?
  - Implement 'sub-grid' models:
    - Use the macroscopic (resolved) properties to predict how something smaller than a resolved element would behave
    - Use the results from the sub-grid model to predict how this would influence the macroscopic properties; modify as required
  - Often resolution dependent
  - Require careful calibration and often 'fine-tuning'
  - Example: feedback from supernovae when modelling galaxy evolution



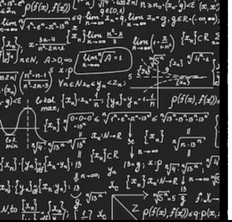
Sub-grid physics:
Example: AGN feedback sub-grid models

- Each row represents one component of the sub-grid model
  - Analytical accretion rate; analytical feedback rate; numerical accretion method; artificial black hole advection method; particle accretion condition
- Each column represents one possible option; shaded options represent free parameters

$\dot{M}_{\rm B} = \frac{4\pi\alpha G^2 M_{\rm BH}^2 \rho}{(c_{\rm s}^2 + v_{\rm rel}^2)^{3/2}}$	$\dot{M}_{\rm drag} = \epsilon_{\rm drag} \frac{L_{\rm RSF}}{c^2} \left(1 - {\rm e}^{-\tau_{\rm RSF}}\right)$	$\dot{M}_{\rm visc} = 3\pi\delta\Sigma \frac{c_{\rm s}^2}{\Omega}$
$\dot{E}_{\rm feed} = \epsilon_{\rm f}\epsilon_{\rm r}\dot{M}_{\rm BH}c^2$	$\dot{E}_{\rm feed} = \epsilon_{\rm r} L_{\rm jet}$	$\dot{p} = \tau \frac{L}{c}$
Stochastic-Unconditional	Stochastic-Conditional	Continual-Conditional

Couple to gas particle	Tracer mass	Δl along stellar gradients	Δl towards centre of mass
$d < h_{\rm BH}$ $v_{\rm rel} < f\, c_{\rm s}$	$d < h_{\rm BH}$ $v_{\rm rel} < v_{\rm circ}$	$d < \varepsilon_{\rm S2}$ gravitationally bound	$d < h_{\rm BH}$

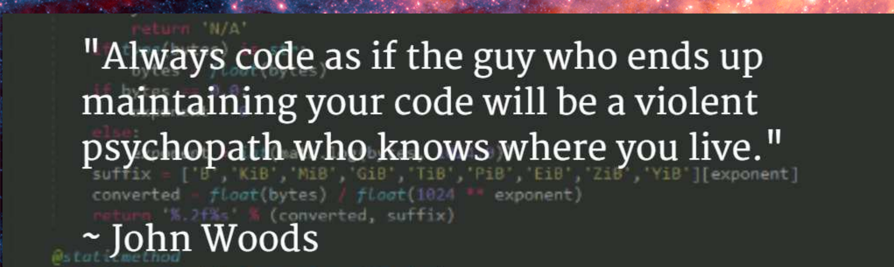
Wurster & Thacker (2013a,b)



Complex calculation: Put it all together!

Illustris Simulation: Vogelsberger+(2014): https://www.youtube.com/watch?v=QSivydIyeG4

Coding Words of Wisdom



For any questions on numerical hydrodynamics or computational astrophysics, please feel free to contact me: jhw5@st-andrews.ac.uk