A 3D Finite Volume Lagrangian Scheme

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Introduction

- Lagrangian fluid dynamics is critical for ICF:
  - **Strong** compressions,
  - Multi-material: avoid mixing.

  see P.H. MAIRE tomorrow
  R. ABGRALL, J. BREIL, P.H. MAIRE, and J. OVADIA. *A Lagrangian scheme for multidimensional compressible flow problems*. JCP, 2004. proposed alternatively to split p_r on each half-edge of each cell.
- Ongoing research about a new family of 3D Finite Volume schemes.
- In 2D this is based on B. DESPRÉS and C. MAZERAN. *Lagrangian Gas Dynamics in 2D and Lagrangian Schemes*, Arma 2005. . PhD thesis to be defended soon.
- Finite Volume collocated schemes have a great potential for **ALE** developments and **remeshing** techniques since

$$\rho, \mathbf{u} \text{ and } e = \varepsilon + \tfrac{1}{2}|u|^2$$

  are discretized at the same place.

Euler equations in Lagrangian coordinates

Euler equations in Eulerian coordinates

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot ((\rho \mathbf{u}) \mathbf{u}) + \nabla p = 0, \\ \partial_t (\rho e) + \nabla \cdot (e \mathbf{u}) + \nabla \cdot (p \mathbf{u}) = 0. \end{cases}$$

Here we choose $p = (\gamma - 1) \frac{\varepsilon}{\rho}$

Euler equations in Lagrangian coordinates

$$\begin{cases} \rho d_t \tau - \nabla \cdot \mathbf{u} = 0, \\ \rho d_t \mathbf{u} + \nabla p = 0, \\ \rho d_t e + \nabla \cdot (p \mathbf{u}) = 0, \end{cases}$$

where $\tau = \frac{1}{\rho}$.

Construction of the scheme in 3D

Introducing $\mathbf{C}_{jr}$

We construct a 3D scheme such that the density ρ_j^n, the velocity $\mathbf{u}_j^n$ and the **total energy** e_j^n are the unknowns given in cell j.

One can construct the vectors $\mathbf{C}_{jr} \in \mathbb{R}^3$

$$\mathbf{C}_{jr} = |\mathbf{C}_{jr}|\,\mathbf{n}_{jr}, \quad |\mathbf{C}_{jr}| \approx area, \quad |\mathbf{n}_{jr}| = 1.$$

such that the volume of cell j is

$$V_j = \frac{1}{3}\sum_r (\mathbf{C}_{jr}, \mathbf{x}_r)$$

and the derivative of the volume is

$$V_j'(t) = \sum_r (\mathbf{C}_{jr}, \mathbf{u}_r), \quad \mathbf{u}_r(t) = \mathbf{x}_r'(t).$$

For tetrahedra $\mathbf{C}_{jr}$ are *uniquely* defined.
For other cell types $\mathbf{C}_{jr}$ are ***not*** *uniquely* defined.

Discretization of the divergence

Define the mass of the lagrangian cell

$$M_j = \rho_j(t) V_j(t).$$

One has

$$M_j \frac{d}{dt}\left(\frac{1}{\rho_j(t)}\right) = V_j'(t) = \sum_r (\mathbf{C}_{jr}, \mathbf{u}_r)\,.$$

Therefore

$$\sum_r (\mathbf{C}_{jr}, \mathbf{u}_r) \approx \int_{\partial j} (\mathbf{u}, \mathbf{n}) d\sigma \qquad \left(= \int_j \nabla \cdot \mathbf{u}\; dx\right)$$

is our Finite Volume discretization of the divergence operator.

$\Longrightarrow$ The $\mathbf{C}_{jr}$'s give the discretization of the divergence operator.

Discretization of the gradient

We use the idea of a **compatible discretization** of all discrete operators. One has the formula

$$\sum_r \mathbf{C}_{jr} p_r \approx \int_{\partial j} \mathbf{n} p \, d\sigma \qquad \left(= \int_j \nabla p \, dx \right).$$

We have also

$$\sum_r (\mathbf{C}_{jr}, \mathbf{u}_r) p_r \approx \int_{\partial j} (\mathbf{u}, \mathbf{n}) p \, d\sigma = \int_{\partial j} (\mathbf{u}, p\mathbf{n}) \, d\sigma \left(= \int_j \nabla \cdot (p\mathbf{u}) \, dx \right).$$

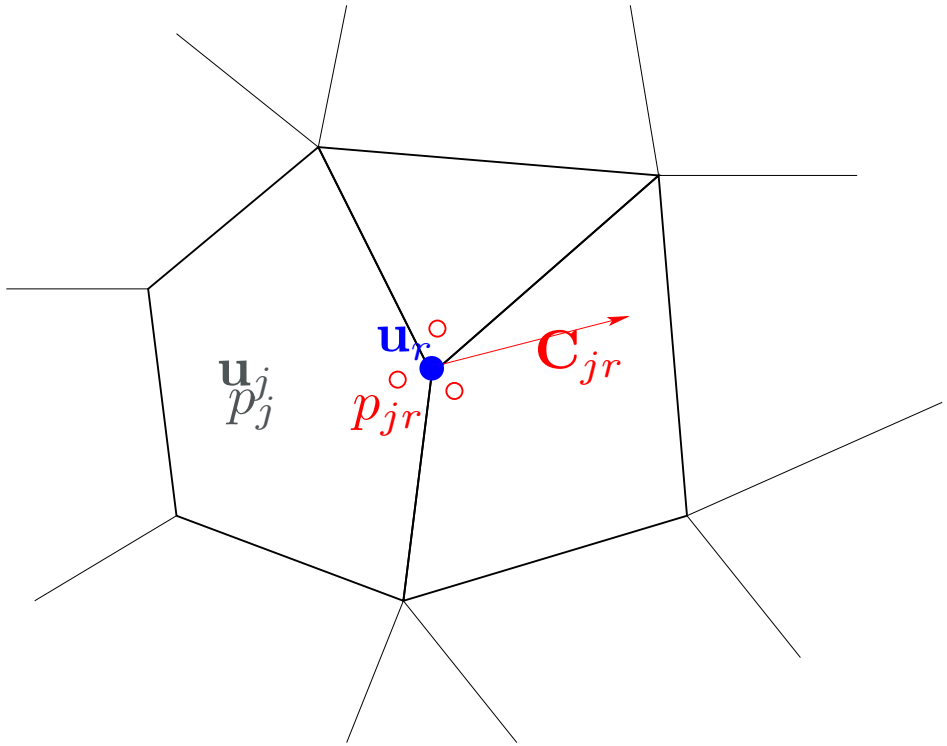
This gives the structure of the Finite Volume Lagrangian scheme

$$\begin{cases} V_j'(t) = \sum_r (\mathbf{C}_{jr}, \mathbf{u}_r), \\ M_j \mathbf{u}_j'(t) = -\sum_r \mathbf{C}_{jr} p_r, \\ M_j e_j'(t) = -\sum_r (\mathbf{C}_{jr}, \mathbf{u}_r) p_r. \end{cases}$$

Construction of the fluxes

At this stage we know only the unknowns inside the cells, that is $\rho_j(t)$, $\mathbf{u}_j(t)$ and $e_j(t)$. So we need a formula to construct the $\mathbf{u}_r$'s and p_r's. We use mainly three ideas.

- The p_r are replaced by some p_{jr}'s.



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- The p_r are replaced by some p_{jr}'s.
- We assume the Riemann-invariant-like formula along $\mathbf{n}_{jr}$

$$p_{jr} - p_j + \rho_j c_j \left(\mathbf{u}_r - \mathbf{u}_j, \mathbf{n}_{jr}\right) = 0.$$

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$$p_{jr} - p_j + \rho_j c_j \left(\mathbf{u}_r - \mathbf{u}_j, \mathbf{n}_{jr}\right) = 0.$$

- We force the local conservativity of forces around node r

$$\sum_j \mathbf{C}_{jr} p_{jr} = \sum_j |\mathbf{C}_{jr}| \, \mathbf{n}_{jr} p_{jr} = 0.$$

There is a unique solution to these requirements.

Solution

After elimination of the p_{jr}'s, the equation for $\mathbf{u}_r$ is

$$\left(\sum_j \rho_j c_j \left| \mathbf{C}_{jr} \right| \mathbf{n}_{jr} \otimes \mathbf{n}_{jr} \right) \mathbf{u}_r$$

$$= \left(\sum_j \mathbf{C}_{jr} p_j \right) + \left(\sum_j \rho_j c_j \left| \mathbf{C}_{jr} \right| \mathbf{n}_{jr} \otimes \mathbf{n}_{jr} \mathbf{u}_j \right) .$$

Since the matrix is symetric and positive

$$A_r = \left(\sum_j \rho_j c_j \left| \mathbf{C}_{jr} \right| \mathbf{n}_{jr} \otimes \mathbf{n}_{jr} \right) = A_r^t > 0$$

there is is a unique solution $\mathbf{u}_r$. Then we compute the p_{jr}'s thanks to

$$p_{jr} - p_j + \rho_j c_j \left(\mathbf{u}_r - \mathbf{u}_j, \mathbf{n}_{jr} \right) = 0.$$

Scheme in 3D

- Cell quantities ($M_j, V_j, \mathbf{x}_j, \rho_j, e_j, \mathbf{u}_j$ and p_j) are given
- Compute $\mathbf{C}_{jr}$ on the current configuration
- We take $\Delta t \leq \min_j \left(\frac{\sum_r |\mathbf{C}_{jr}|}{3V_j} c_j \right)$.
- $A_r = \sum_j \rho_j c_j \, \mathbf{C}_{jr} \otimes \mathbf{n}_{jr}$.
- $\mathbf{u}_r = A_r^{-1} \sum_j (\mathbf{C}_{jr} p_j + \rho_j c_j \, \mathbf{C}_{jr} \otimes \mathbf{n}_{jr} \, \mathbf{u}_j)$.
- $p_{jr} = p_j + \rho_j c_j \, (\mathbf{u}_j - \mathbf{u}_r, \mathbf{n}_{jr})$
- $\mathbf{u}_j^{n+1} = \mathbf{u}_j^n - \frac{\Delta t}{M_j} \sum_r \mathbf{C}_{jr} p_r$
- $e_j^{n+1} = e_j^n - \frac{\Delta t}{M_j} \sum_r (\mathbf{C}_{jr}, \mathbf{u}_r) \, p_r$
- $\mathbf{x}_r^{n+1} = \mathbf{x}_r^n + \Delta t \, \mathbf{u}_r$
- Update V_j, ρ_j and p_j

Conservativity

- Mass conservation: the scheme imposes M_j to be constant.
- Momentum conservation:

$$\begin{aligned}\sum_j M_j \mathbf{u}_j^{n+1} &= \sum_j M_j \mathbf{u}_j^n - \sum_j \Delta t \sum_r \mathbf{C}_{jr} p_r \\ &= \sum_j M_j \mathbf{u}_j^n - \Delta t \sum_r \sum_j \mathbf{C}_{jr} p_r \\ &= \sum_j M_j \mathbf{u}_j^n\end{aligned}$$

- Total energy conservation:

$$\begin{aligned}\sum_j M_j e_j^{n+1} &= \sum_j M_j e_j^n - \sum_j \Delta t \sum_r \left(\mathbf{C}_{jr}, \mathbf{u}_r\right) p_r \\ &= \sum_j M_j e_j^n - \Delta t \sum_r \left(\sum_j \mathbf{C}_{jr} p_r, \mathbf{u}_r\right) \\ &= \sum_j M_j e_j^n\end{aligned}$$

$\Longrightarrow$ the scheme is **locally** conservative.

It is also stable and consistant.

Second order extension

- Goal
  - Improve the accuracy of the scheme.
  - Diminish scheme dissipation
- Method. Muscl reconstruction + Van-Leer slope limiter:
  - $\bar{\mathbf{u}}_j(\mathbf{x}) = \mathbf{u}_j + \Phi^{\mathrm{vl}} \nabla \mathbf{u}_j (\mathbf{x} - \mathbf{x}_j)$
  - $\bar{p}_j(\mathbf{x}) = p_j + \Phi^{\mathrm{vl}} \nabla p_j \cdot (\mathbf{x} - \mathbf{x}_j)$

  $\Phi^{\mathrm{vl}} \in [0,1]$ is chosen so that $\bar{p}_j$ and $|\bar{\mathbf{u}}_j|$ respect some maximum principle.

Second order fluxes are

- $\mathbf{u}_r = A_r^{-1} \sum_j (\mathbf{C}_{jr} \bar{p}_j(\mathbf{x}_r) + \rho_j c_j \, \mathbf{C}_{jr} \otimes \mathbf{n}_{jr} \; \bar{\mathbf{u}}_j(\mathbf{x}_r))$.
- $p_{jr} = \bar{p}_j(\mathbf{x}_r) + \rho_j c_j \, (\bar{\mathbf{u}}_j(\mathbf{x}_r) - \mathbf{u}_r, \mathbf{n}_{jr})$

The scheme is order 1 in time, so we need smaller time steps to avoid the anti-dissipative term of the equivalent equation

Second order extension

- Second Method. Muscl reconstruction + LW procedure + Van-Leer slope limiter:
  - $\bar{\mathbf{u}}_j(\mathbf{x}) = \mathbf{u}_j + \Phi^{\mathrm{vl}}(1-\nu)\nabla\mathbf{u}_j(\mathbf{x}-\mathbf{x}_j)$
  - $\bar{p}_j(\mathbf{x}) = p_j + \Phi^{\mathrm{vl}}(1-\nu)\nabla p_j \cdot (\mathbf{x}-\mathbf{x}_j)$

  $\Phi^{\mathrm{vl}} \in [0,1]$ is chosen so that $\bar{p}_j$ and $|\bar{\mathbf{u}}_j|$ respect some maximum principle.

Second order fluxes are still

- $\mathbf{u}_r = A_r^{-1} \sum_j (\mathbf{C}_{jr}\bar{p}_j(\mathbf{x}_r) + \rho_j c_j\, \mathbf{C}_{jr} \otimes \mathbf{n}_{jr}\ \bar{\mathbf{u}}_j(\mathbf{x}_r))$.
- $p_{jr} = \bar{p}_j(\mathbf{x}_r) + \rho_j c_j\, (\bar{\mathbf{u}}_j(\mathbf{x}_r) - \mathbf{u}_r, \mathbf{n}_{jr})$

The scheme is formally order 2 in time and space for simple 1D problems

Numerical results

Numerical results

We compute the results of some basic shock tube problems in various geometries

Sod shock tube

$$\gamma = 1.4, u = 0 \qquad \begin{cases} p(x) = 1 & \rho(x) = 1 & \text{if } x < 0.5, \\ p(x) = 0.1 & \rho(x) = 0.125 & \text{else.} \end{cases}$$

Shestakov shock tube

$$\gamma = \tfrac{5}{3} \quad u = 0 \quad p = \tfrac{2}{3} \times 10^{14} \quad x_{min}(0) = 0 \quad x_{max}(0) = 0.75$$

$$u(x_{max}(t)) = 2.5 \times 10^7$$

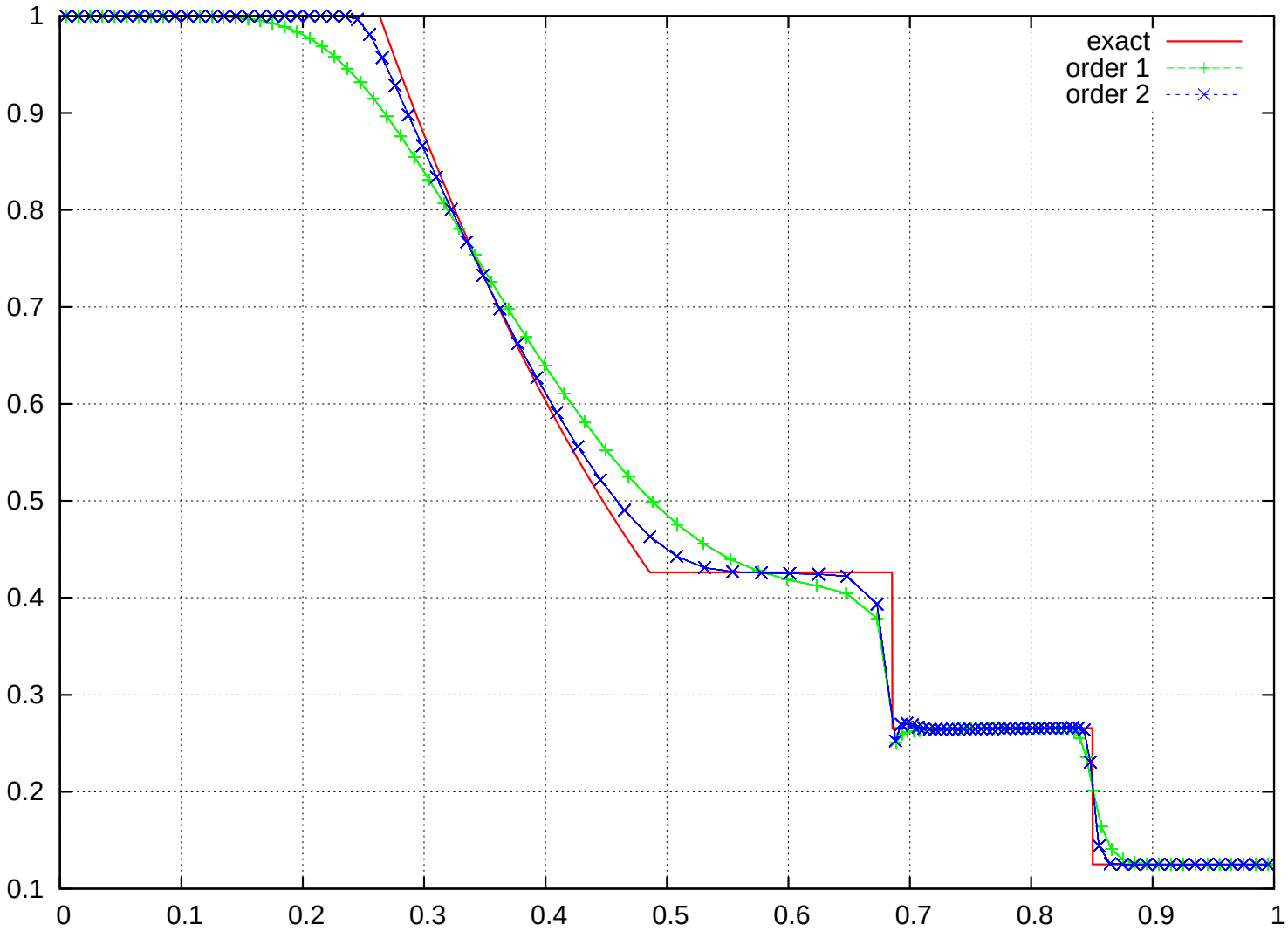
$$u(x_{min}(t)) = \begin{cases} 10^8 \left((1 - 10^8 t)^{-0.25} - 1 \right), & \text{if } 0 \leq t < 0.9 \times 10^{-8}, \\ 10^8 (10^{0.25} - 1) \approx 7.8 \times 10^7 & \text{if } 0.9 \times 10^{-8} \leq t < 10^{-8}, \\ 0 & \text{else.} \end{cases}$$

Sod shock tube in 2D and 3D

$$\gamma = 1.4, u = 0 \qquad \begin{cases} p(r) = 1 & \rho(r) = 1 & \text{if } x > 0.5, \\ p(r) = 0.1 & \rho(r) = 0.125 & \text{else.} \end{cases}$$

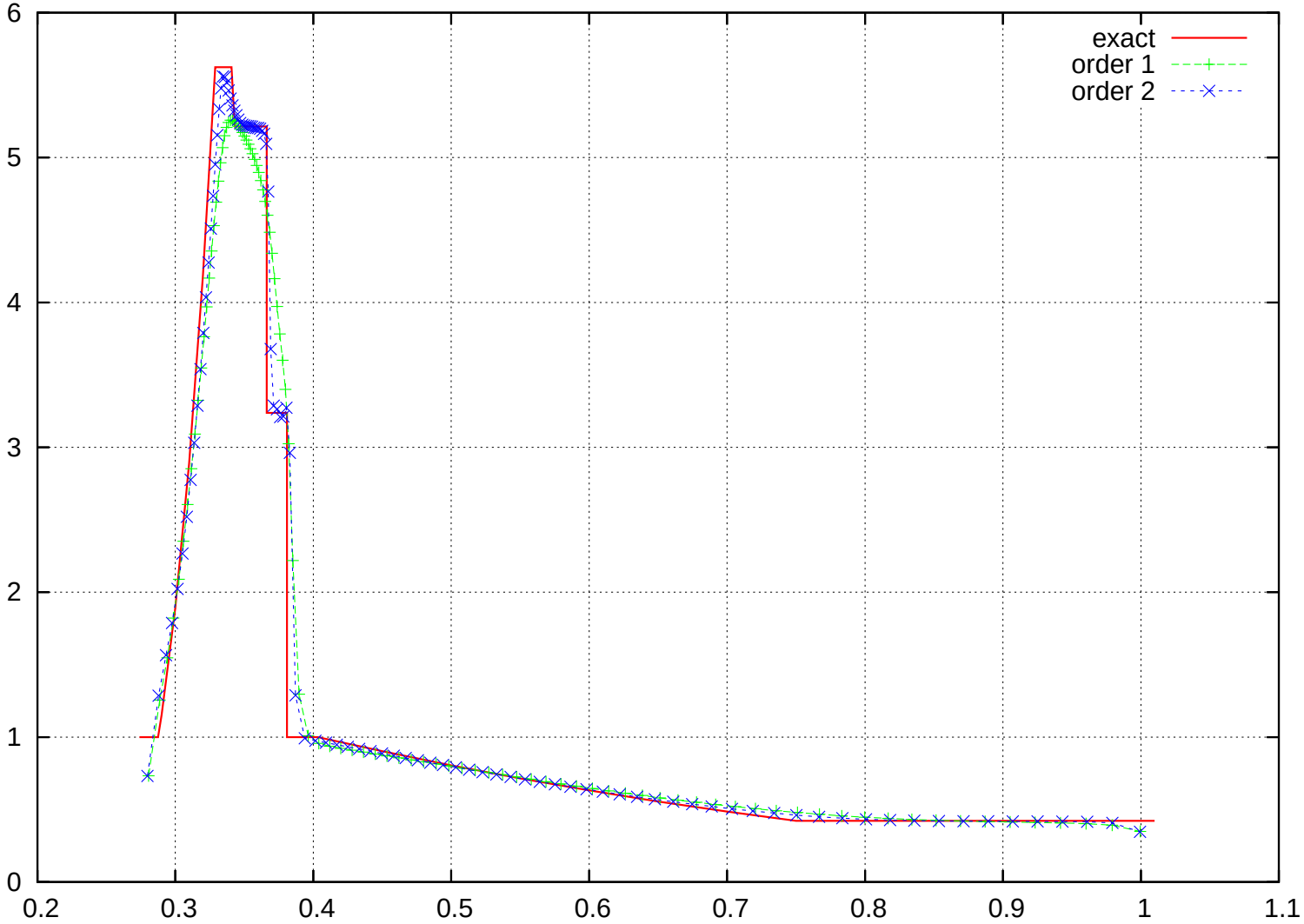
Sod shock tube - 1D

Density 100 cells, $t = 0.2s$



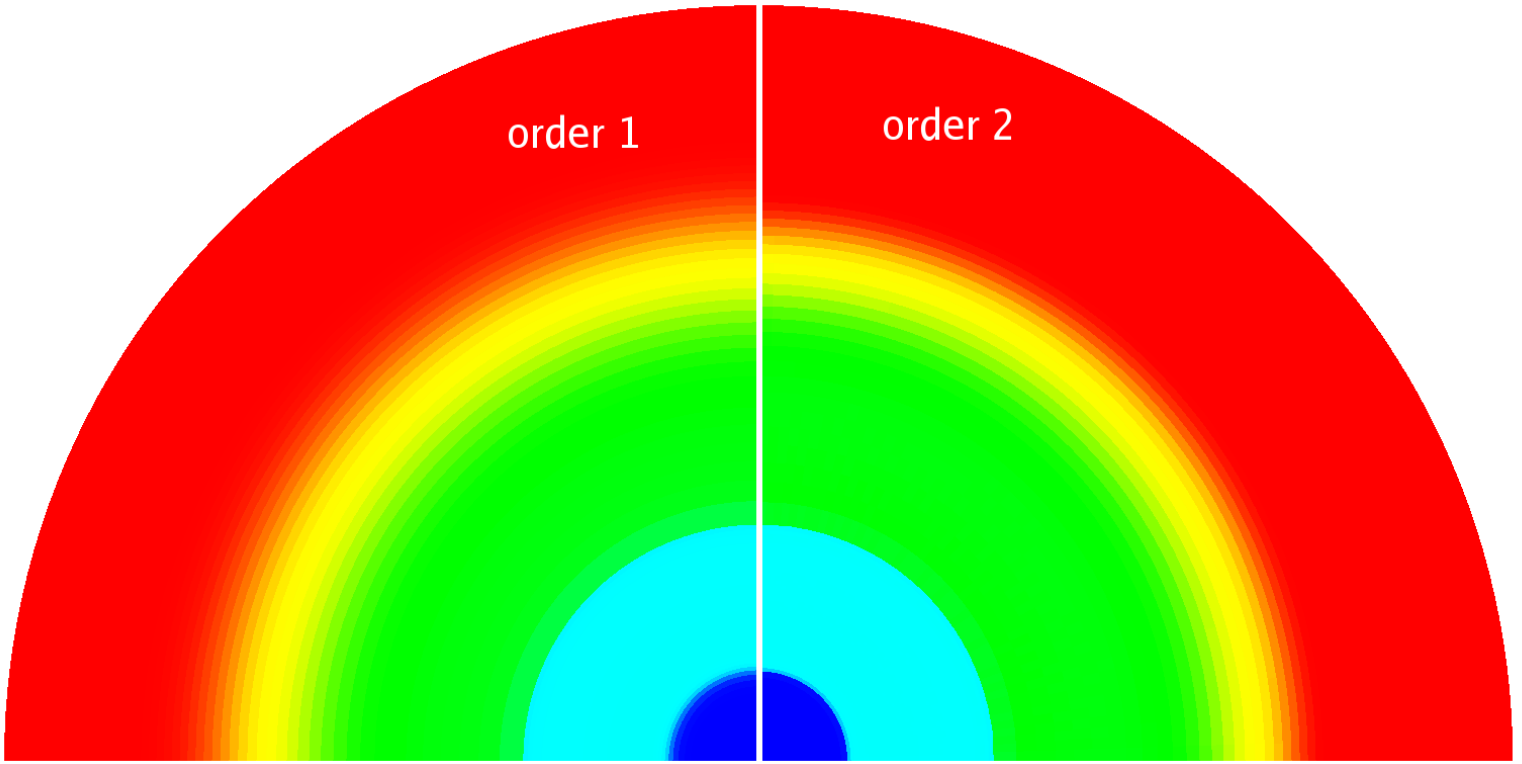
Shestakov shock tube - 1D

Density 100 cells, $t = 10.4 \times 10^{-9} s$



Sod shock tube - 2D

Density 100×50 cells, $t = 0.2s$



Sod shock tube - 2D

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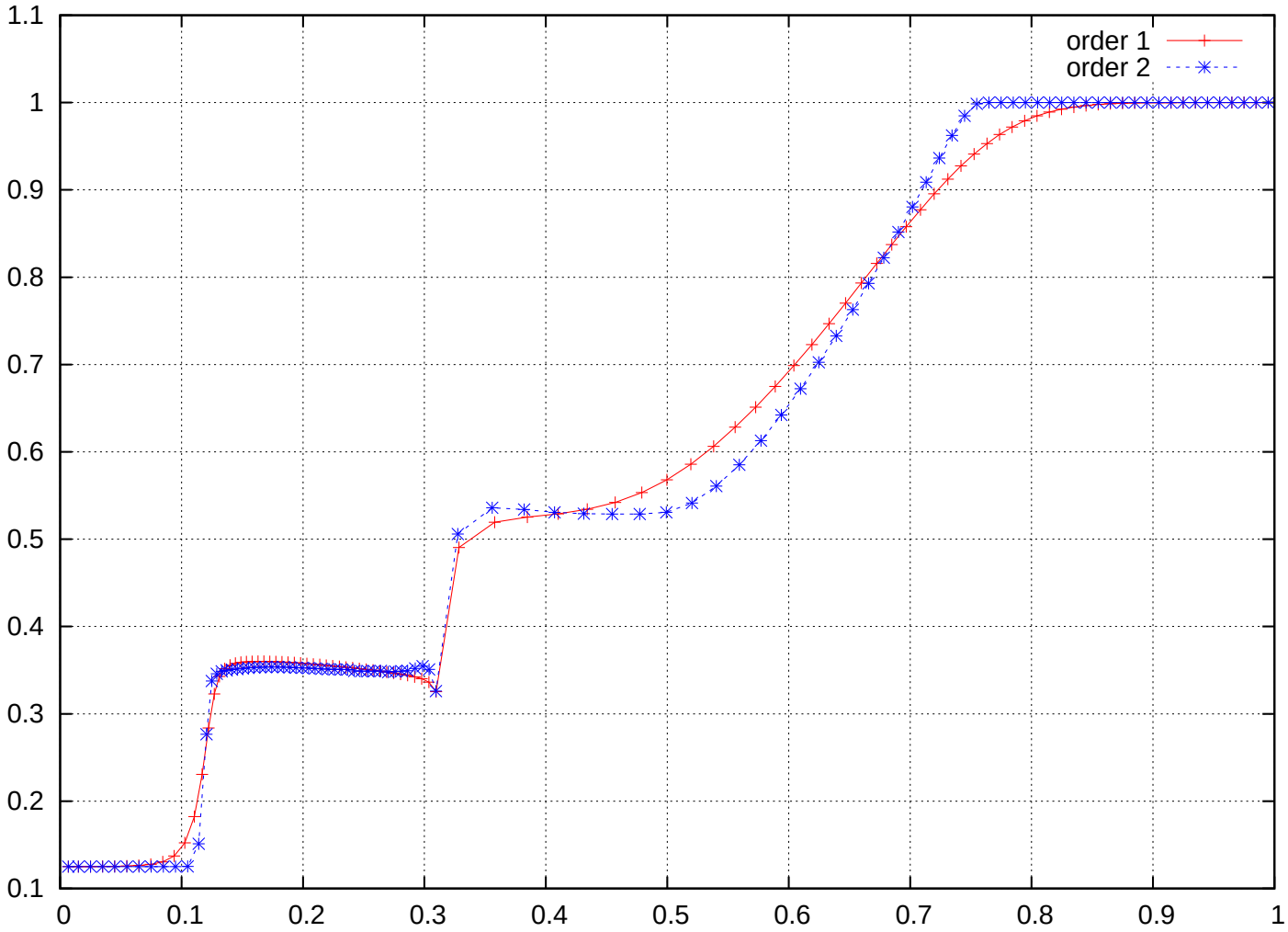
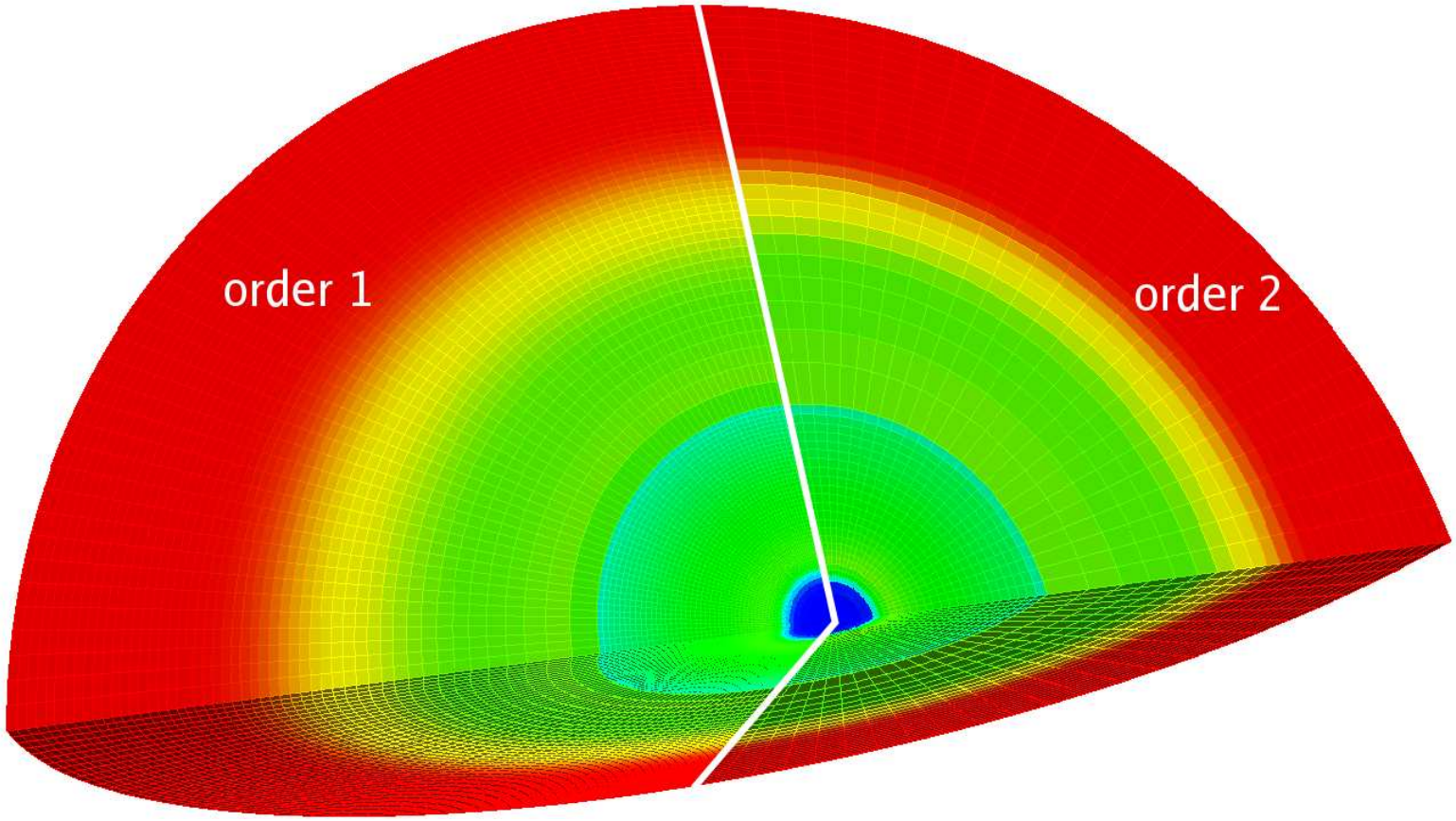


Sod shock tube - 3D

Density $187\,500$ and $21\,600$ cells, $t = 0.2s$ (Parallel computation)



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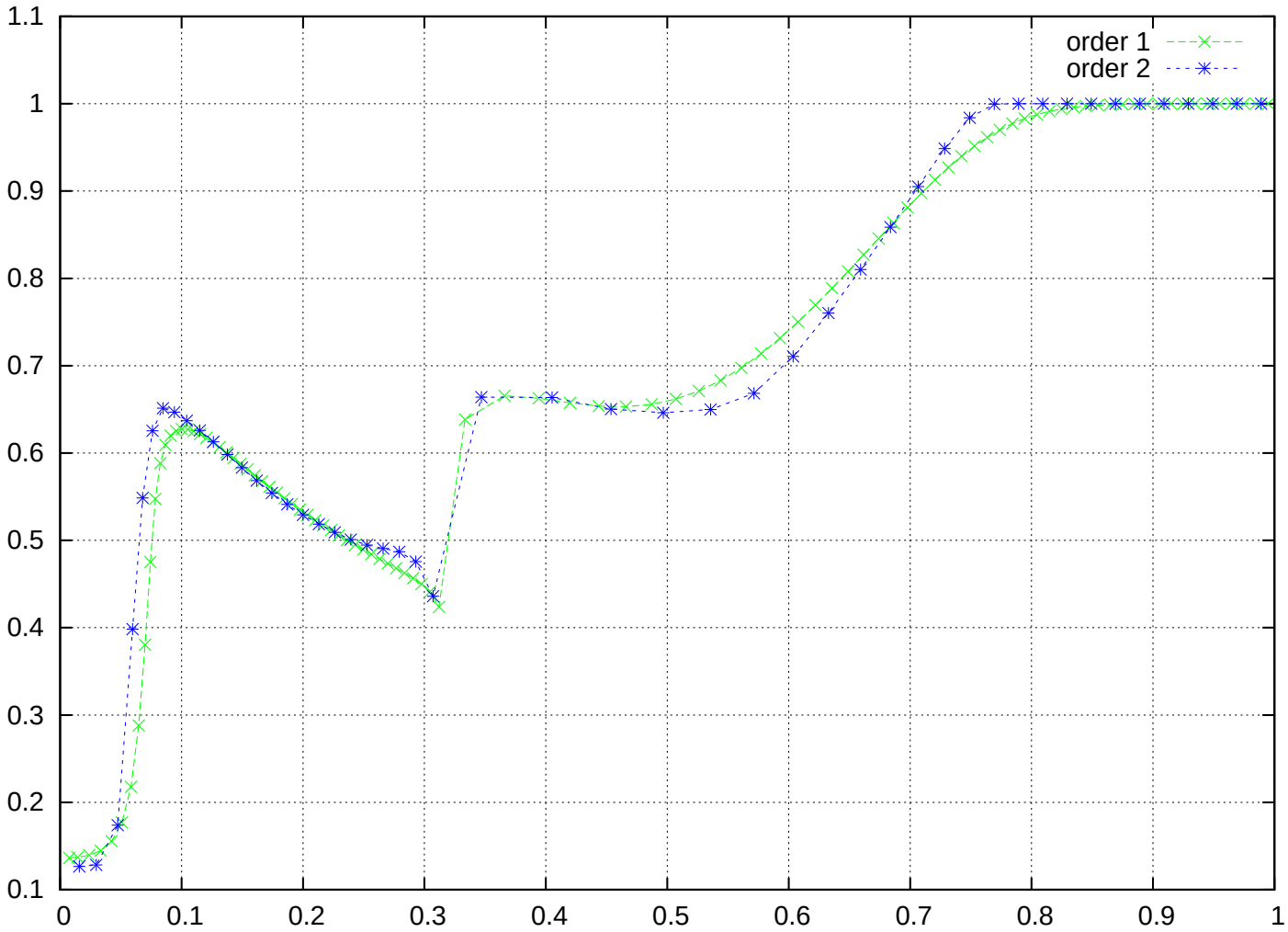
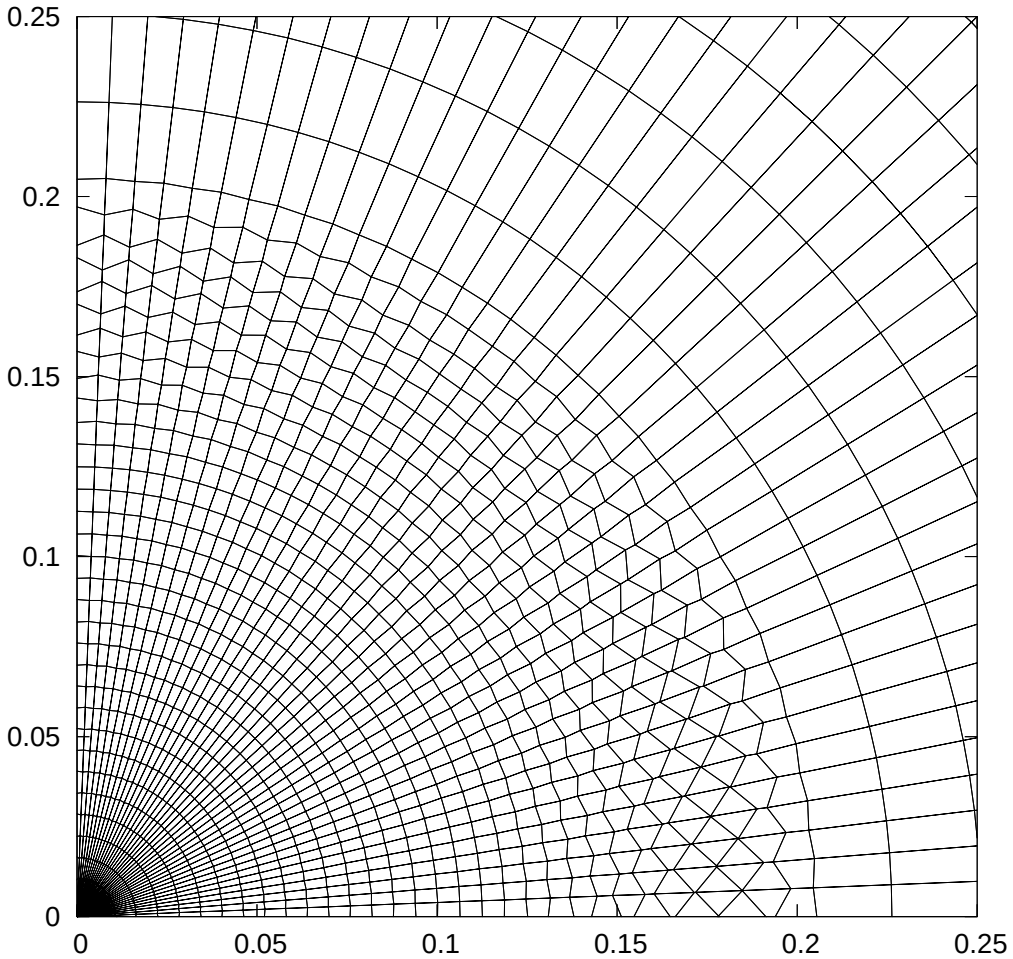


Fix-up and optimizations

Hourglass with Noh

This has already been identified in 2D.

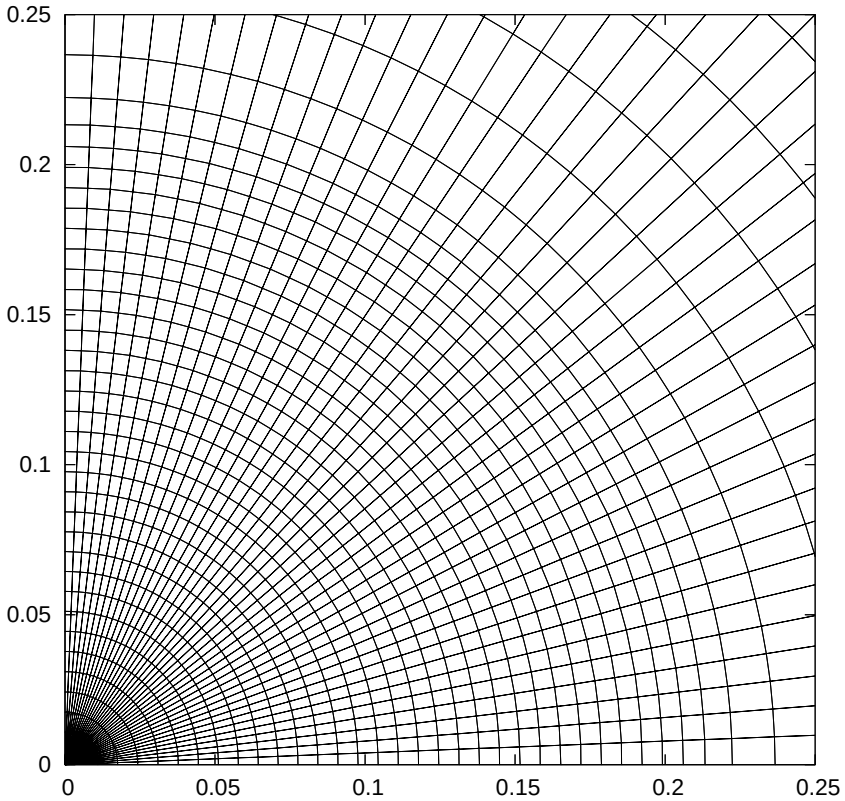
Noh problem in 2D: $\gamma = \frac{5}{3}$, $\rho = 1$, $p = 0 (\approx 10^{-6})$, $\mathbf{u} = -\mathbf{e}_r$.
Using a polar mesh, one obtains



A fix-up

- $c_j \ll 1 \implies A_r$ nearly singular.
- Noh: $c_j \approx 10^{-3} \implies A_r = \sum_j \rho_j c_j \, \mathbf{C}_{jr} \otimes \mathbf{n}_{jr} \approx 0$.

  $\mathbf{u}_r = A_r^{-1} \sum_j (\mathbf{C}_{jr} \bar{p}_j(\mathbf{x}_r) + \rho_j c_j \, \mathbf{C}_{jr} \otimes \mathbf{n}_{jr} \, \bar{\mathbf{u}}_j(\mathbf{x}_r))$.
- Idea: increase c when it is too small for the fluxes calculus (more dissipative scheme).



Time step optimization

In order to increase the time step, we can replace

$$p_{jr} - p_j + \rho_j c_j \left(\mathbf{u}_r - \mathbf{u}_j, \mathbf{n}_{jr}\right) = 0$$

by

$$p_{jr} - p_j + \lambda_j \rho_j c_j \left(\mathbf{u}_r - \mathbf{u}_j, \mathbf{n}_{jr}\right) = 0.$$

It can be shown that the optimal λ_j is

$$\lambda_j = \sum_r \frac{|\mathbf{C}_{jr}|}{\Lambda} \in [1, \sqrt{3}],$$

where Λ is the maximum eigenvalue of

$$\sum_r \frac{\mathbf{C}_{jr} \otimes \mathbf{C}_{jr}}{|\mathbf{C}_{jr}|}.$$

Finally $\Delta t \leq \min_j \left(\lambda_j \frac{\sum_r |\mathbf{C}_{jr}|}{3V_j} c_j \right)$

Conclusions et perspectives

- The whole scheme relies on the definition of

$$\mathbf{C}_{jr}.$$

  - This is straightforward only for tetrahedrons.
  - But there is no unique definition for other kind of meshes in 3D. So we need to compare all possible definition of theses quantities.
  - The situation is different in 2D (unicity of the definition for all meshes).
- We still work on boundary conditions and the second order Muscl reconstruction.
- We have begun the evaluation of the coupling with ALE and remeshing.
- We shall start coupling with other physics to test this scheme for ICF simulations.
- ...