

A MUSCL finite volume scheme for axisymmetric compressible Euler equations

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Main motivation

- Numerical simulation of inductive plasma torches (ICP: *Inductively Coupled Plasma Torch*)
- This study is part of a TRP (Technology Research Program) with ESA (European Space Agency)

Principle:

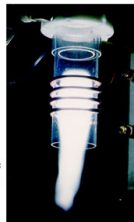
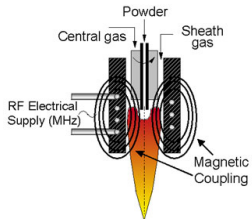
- A plasma torch is a quantitative chemical analysis technique (e.g. for detection of trace metals in environmental samples).
- It consists in ionizing a sample by injecting it in a plasma (generally in Argon): Atoms are ionized by a hot flame (6 000 to 8 000 K).
- The sample experiences **fusion** (solid), **vaporization**, and then **ionization**.
- High temperature is maintained by magnetic induction (thanks to a HF generator).
- Ions are detected either by **mass** or **emission spectrometry**.

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Summary

- A mathematical model for ICP
- Axisymmetric Euler equations
- A finite volume method
- MUSCL schemes
- Application to Euler equations
- Stationary radial solutions
- Numerical experiments

A mathematical model for ICP

Mathematical modelling of ICP takes into account various phenomena;

- **Electromagnetic Induction**: We use a quasi-static eddy current model (we neglect displacement currents). The major difficulty lies in the fact that an unknown part of the gas is transformed into plasma and becomes electrically conducting.
- **Gas Dynamics**: We are dealing with a compressible flow that we assume stationary and laminar.
- We use an **axisymmetric** description thanks to the device geometry.

1. Electromagnetism

Eddy current equations read in quasi-static regime (time harmonic):

$$\begin{cases} \mathbf{curl} \mathbf{H} = \mathbf{J} \\ i\omega\mu_0\mathbf{H} + \mathbf{curl} \mathbf{E} = 0 \\ \mathbf{J} = \sigma \mathbf{E} + \mathbf{J}_0 \end{cases}$$

\mathbf{J} : Current density

\mathbf{J}_0 : Source current

\mathbf{E} : Electric field

\mathbf{H} : Magnetic field

ω : Angular frequency

σ : Electric conductivity

μ_0 : Magnetic permeability of the free space

We neglect here current transport by the fluid flow (In fact, we have $\mathbf{J} = \sigma(\mathbf{E} + \mathbf{u} \times \mathbf{B}) + \mathbf{J}_0$).

In this model, we choose a formulation in terms of the electric field.

We have

$$\begin{cases} \operatorname{curl} \operatorname{curl} \mathbf{E} + i\omega\mu_0\sigma\mathbf{E} = -i\omega\mu_0\mathbf{J}_0 & \text{in } \mathbb{R}^3 \\ |\mathbf{E}(\mathbf{x})| = \mathcal{O}(|\mathbf{x}|^{-1}) & |\mathbf{x}| \rightarrow \infty \end{cases}$$

where $\sigma = \sigma(e)$ with

$$\sigma(e) = \begin{cases} 0 & \text{if } e \leq e_0, \\ > 0 & \text{otherwise} \end{cases}$$

where e is the internal energy and e_0 is the energy required for ionization.

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2. Flow of gas-plasma

We use compressible Euler equations (we neglect viscosity and thermal diffusion) with the following features:

- The gas motion is driven by the Lorentz force that we average on a time period.
- The energy source is given by Joule heating (also time averaged).

$$\nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \rho \mathbf{g} + \frac{\mu_0}{2} \operatorname{Re}(\mathbf{J} \times \overline{\mathbf{H}})$$

$$\nabla \cdot (\rho \mathbf{u}) = 0$$

$$\nabla \cdot ((E + p) \mathbf{u}) = \frac{1}{2} \operatorname{Re}(\mathbf{J} \cdot \overline{\mathbf{E}}) - R$$

$$p = p(\rho, e)$$

where \mathbf{u} is the velocity, p is the pressure, ρ is the density, \mathbf{g} is the gravity vector, e is the internal specific energy and E is the total energy defined by $E = \rho(e + \frac{1}{2} |\mathbf{u}|^2)$, R is a radiation source.

In the following, we restrict the model to an ideal gas

$$p = (\gamma - 1) \rho e \quad \gamma : \text{ratio of specific heats}$$

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Axisymmetric Euler equations

- We consider compressible time dependent Euler equations.
- The geometry of the domain suggests using an axisymmetric model.
- We don't take into account, in the sequel, sources (Joule and Lorentz)

Let (r, θ, z) stand for cylindrical coordinates and let (u_r, u_θ, u_z) stand for the components of a vector in this system, we obtain the system of equations (taking into account θ -invariance):

$$\begin{aligned}\frac{\partial}{\partial t}(r\rho) + \frac{\partial}{\partial r}(r\rho u_r) + \frac{\partial}{\partial z}(r\rho u_z) &= 0 \\ \frac{\partial}{\partial t}(r\rho u_r) + \frac{\partial}{\partial r}(r\rho u_r^2 + rp) + \frac{\partial}{\partial z}(r\rho u_r u_z) &= \rho u_\theta^2 + p \\ \frac{\partial}{\partial t}(r\rho u_z) + \frac{\partial}{\partial r}(r\rho u_r u_z) + \frac{\partial}{\partial z}(r\rho u_z^2 + rp) &= 0 \\ \frac{\partial}{\partial t}(r\rho u_\theta) + \frac{\partial}{\partial r}(r\rho u_\theta u_r) + \frac{\partial}{\partial z}(r\rho u_\theta u_z) &= -\rho u_\theta u_r \\ \frac{\partial}{\partial t}(rE) + \frac{\partial}{\partial r}(ru_r(E + p)) + \frac{\partial}{\partial z}(ru_z(E + p)) &= 0 \\ p &= (\gamma - 1)\rho e\end{aligned}$$

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We can write this system under the conservative formulation:

$$\frac{\partial}{\partial t}(rU) + \frac{\partial}{\partial r}(rF_r(U)) + \frac{\partial}{\partial z}(rF_z(U)) = G(U)$$

where

$$U = \begin{pmatrix} \rho \\ \rho u_r \\ \rho u_z \\ \rho u_\theta \\ E \end{pmatrix}, \quad F_r(U) = \begin{pmatrix} \rho u_r \\ \rho u_r^2 + p \\ \rho u_z u_r \\ \rho u_\theta u_r \\ u_r(E + p) \end{pmatrix}, \quad F_z(U) = \begin{pmatrix} \rho u_z \\ \rho u_r u_z \\ \rho u_z^2 + p \\ \rho u_\theta u_z \\ u_z(E + p) \end{pmatrix}, \quad G(U) = \begin{pmatrix} 0 \\ \rho u_\theta^2 + p \\ 0 \\ -\rho u_\theta u_r \\ 0 \end{pmatrix}$$

This formulation involves a divergence form that can be discretized by finite volumes, source terms being treated separately.

A finite volume method

Consider a triangulation of the domain Ω of parameters (r, z) . Let:

- T_i : Triangle, $1 \leq i \leq n_T$
- e_{ij} : Common edge to triangles T_i and T_j
- $\mathbf{n}_{ij} = (n_{ij,r}, n_{ij,z})$: Unit normal to the triangle T_i oriented toward T_j
- $\nu(i)$: Index set of the (3) neighbour triangles of T_i

Let us integrate the system of equations over a triangle T_i and use the divergence theorem. We get

$$\frac{d}{dt} \int_{T_i} U(r, z, t) r \, dr \, dz + \int_{\partial T_i} (F_r(U) n_{ij,r} + F_z(U) n_{ij,z}) r \, d\sigma = \int_{T_i} G(U) \, dr \, dz$$

Let $(t^n = n \delta t)_{n \in \mathbb{N}}$ denote a uniform subdivision of the interval $[0, \infty)$. We have

$$\begin{aligned} \int_{T_i} U(r, z, t^{n+1}) r \, dr \, dz &= \int_{T_i} U(r, z, t^n) r \, dr \, dz \\ &\quad - \int_{t^n}^{t^{n+1}} \int_{\partial T_i} (F_r(U) n_{ij,r} + F_z(U) n_{ij,z}) r \, d\sigma \, dt \\ &\quad + \int_{t^n}^{t^{n+1}} \int_{T_i} G(U) \, dr \, dz \, dt \end{aligned}$$

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$$|T_i| = \int_{T_i} dr dz, \quad |T_i|_r = \int_{T_i} r dr dz, \quad |e_{ij}| = \int_{e_{ij}} d\sigma, \quad |e_{ij}|_r = \int_{e_{ij}} r d\sigma,$$

and define the approximation

$$U_i^n \approx \frac{1}{|T_i|_r} \int_{T_i} U(r, z, t^n) r dr dz.$$

We consider the approximate flux:

$$F_{ij}^n \approx \frac{1}{\delta t |e_{ij}|_r} \int_{t^n}^{t^{n+1}} \int_{e_{ij}} (F_r(U) n_{ij,r} + F_z(U) n_{ij,z}) r d\sigma dt$$

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$$G_i^n \approx \frac{1}{\delta t |T_i|} \int_{t^n}^{t^{n+1}} \int_{T_i} G(U) dr dz dt.$$

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$$|T_i|_r U_i^{n+1} = |T_i|_r U_i^n - \delta t \sum_{j \in \nu(i)} |e_{ij}|_r F_{ij}^n + \delta t |T_i| G(U_i^n) \quad 1 \leq i \leq n_T.$$

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The finite volume scheme is entirely determined by the choice of F_{ij}^n and G_i^n .
For instance, the **Rusanov** scheme consists in defining the flux:

$$F_{ij}^n = \frac{1}{2}(F_r(U_i) + F_r(U_j))n_{ij,r} + \frac{1}{2}(F_z(U_i) + F_z(U_j))n_{ij,z} - \lambda_{ij}(U_j - U_i)$$

where λ_{ij} is large enough to ensure stability.

Other alternative schemes:

- **Godunov**: It consists in solving exactly the obtained Riemann problems.
- **HLL** (Harten, Lax, Van Leer): Approximate solution of Riemann problems.
- **HLLC** (+ Contact): Adaptation of HLL to contact discontinuities.

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A second-order scheme (MUSCL)

- The first MUSCL scheme (*Monotonic Upwind Scheme for Conservation Laws*) is due to Van Leer ('79) for the 1-D case.
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- T. Buffard, S. Clain and V. Clauzon have proposed a new extension based on the calculation of directional derivatives.

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Consider the conservation law:

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0 \quad x \in \mathbb{R}, t > 0$$

The basic finite volume scheme uses a piecewise constant approximation. For instance, the first-order upwind scheme reads:

$$\frac{du_i}{dt} + \frac{f(u_i) - f(u_{i-1})}{\delta x} = 0$$

This scheme is known to be very diffusive *i.e.* it smooths Shocks and discontinuities.

To obtain less numerical diffusion, we can consider a piecewise linear approximation like:

$$\frac{du_i}{dt} + \frac{f(u_{i+\frac{1}{2}}) - f(u_{i-\frac{1}{2}})}{\delta x} = 0$$

where

$$u_{i+\frac{1}{2}} := \frac{1}{2}(u_i + u_{i+1}), \quad u_{i-\frac{1}{2}} := \frac{1}{2}(u_{i-1} + u_i).$$

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The total variation is defined by:

$$TV(u) = \sum_i |u_{i+1} - u_i|.$$

A scheme is said to be **TVD** (Total Variation Diminishing) if

$$\frac{d}{dt} TV(u) \leq 0$$

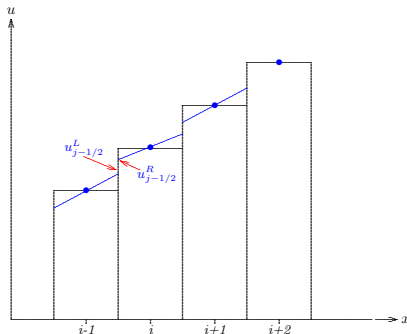
or, after time discretization:

$$TV(u^{n+1}) \leq TV(u^n).$$

We can then use a MUSCL scheme:

$$\frac{du_i}{dt} + \frac{f_{i+\frac{1}{2}}^* - f_{i-\frac{1}{2}}^*}{\delta x} = 0$$

Numerical fluxes $f_{i\pm\frac{1}{2}}^*$ correspond to a nonlinear combination of first and second order approximations of $f(u)$.



We define:

$$u_{i\pm\frac{1}{2}}^* = u_{i\pm\frac{1}{2}}^*(u_{i\pm\frac{1}{2}}^L, u_{i\pm\frac{1}{2}}^R)$$

$$u_{i+\frac{1}{2}}^L = u_i + \frac{1}{2}\phi(r_i)(u_{i+1} - u_i)$$

$$u_{i+\frac{1}{2}}^R = u_{i+1} - \frac{1}{2}\phi(r_{i+1})(u_{i+2} - u_{i+1})$$

$$r_i = \frac{u_i - u_{i-1}}{u_{i+1} - u_i}$$

The function ϕ is a slope limiter ensuring that the obtained solution is TVD, with

$$\phi(r) = 0 \quad \text{if } r \leq 0, \quad \phi(1) = 1.$$

The literature contains a large variety of slope limiters.

For instance the limiter **minmod** is defined by

$$\phi(r) = \max(0, \min(1, r)), \quad \lim_{r \rightarrow \infty} \phi(r) = 1.$$

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$$r_i = \frac{u_i - u_{i-1}}{u_{i+1} - u_i}$$

The function ϕ is a slope limiter ensuring that the obtained solution is TVD, with

$$\phi(r) = 0 \quad \text{if } r \leq 0, \quad \phi(1) = 1.$$

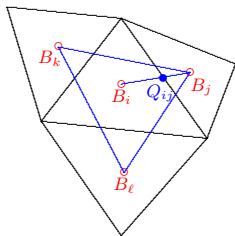
The literature contains a large variety of slope limiters.

For instance the limiter **minmod** is defined by

$$\phi(r) = \max(0, \min(1, r)), \quad \lim_{r \rightarrow \infty} \phi(r) = 1.$$

MUSCL schemes for Euler equations

For a triangle T_i , we denote by B_i its centroid and by Q_{ij} the intersection of the segment $[B_i, B_j]$ with the edge e_{ij} for all $j \in \nu(i)$.



We introduce the barycentric coordinates $(\rho_{ij})_{j \in \nu(i)}$ by

$$\sum_{j \in \nu(i)} \rho_{ij} B_j = B_i, \quad \sum_{j \in \nu(i)} \rho_{ij} = 1.$$

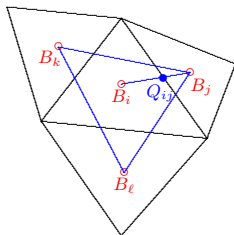
We assume that B_i is strictly in the interior of the triangle formed by the centroids of neighbour triangles. Thus $\rho_{ij} > 0$.

We define the direction

$$t_{ij} = \frac{B_i B_j}{|B_i B_j|}$$

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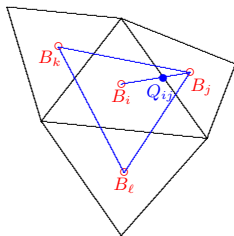
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We obtain the decomposition

$$t_{ij} = \sum_{\substack{j \in \nu(i) \\ k \neq i}} \beta_{ijk} t_{ik}, \quad \beta_{ijk} = -\frac{\rho_{ik}}{\rho_{ij}} \frac{|B_i B_k|}{|B_i B_j|}$$

We want now to reconstruct the values U_{ij} on the edge e_{ij} .

Let v denote any component of U (piecewise constant).

We define a first **downwind** slope by

$$p_{ij}^+ = \frac{v_j - v_i}{|B_i B_j|} \quad \forall j \in \nu(i), 1 \leq i \leq n_T.$$

Therefore p_{ij}^+ is an approximation of the derivative of v in the direction t_{ij} .

The **upwind** slope is defined by:

$$p_{ij}^- = - \sum_{\substack{k \in \nu(i) \\ k \neq j}} \beta_{ijk} p_{ik}^+ \quad \forall j \in \nu(i), 1 \leq i \leq n_T.$$

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$$p_{ij} := \text{minmod}(p_{ij}^+, p_{ij}^-)$$

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$$p_{ij} := \text{minmod}(p_{ij}^+, p_{ij}^-)$$

and the reconstruction of v on e_{ij} is given by

$$v_{ij} := v_i + p_{ij} |B_i Q_{ij}|$$

Remarks

- This reconstruction is exact for affine functions: $v(Q_{ij}) = v_{ij}$ if v is piecewise linear.
- The main advantage is that the reconstruction is typically 1-D. This enables using classical 1-D slope limiters.
- The property $p_{ij} > 0$ implies $\beta_{ijk} < 0$. Therefore, if v_i is a local extremum, we have $p_{ij}^+ p_{ij}^- \leq 0$. Hence $p_{ij} = 0$. This means that extrema do not increase.
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Stationary radial solutions

In order to test the numerical scheme, we construct a radial steady state solution of the equations: We look for a solution $(u_r, u_\theta, u_z, p, e)$ that depends on r only and such that $u_z = u_\theta = 0$. We obtain the system:

$$\frac{d}{dr}(r\rho u_r) = 0$$

$$\frac{d}{dr}(r(\rho u_r^2 + p)) = p$$

$$\frac{d}{dr}(r u_r (e + p)) = 0$$

$$p = (\gamma - 1)\rho e$$

We deduce for $\alpha, \beta \in \mathbb{R}$

$$\frac{d\rho}{dr} = \frac{\rho}{\left(\alpha\rho^2 r^2 - \frac{\gamma+1}{2(\gamma-1)}\right)(\gamma-1)r}, \quad u_r = \frac{\beta}{\rho r}$$

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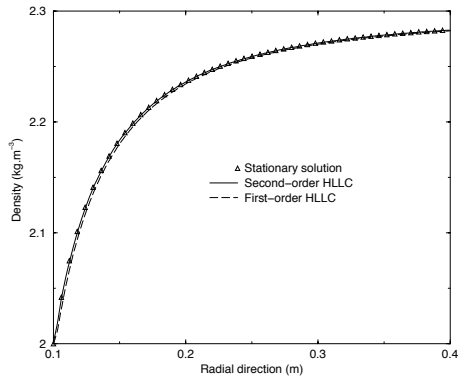
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Numerical tests

- 1 A stationary radial solution
- 2 Shock tube (SOD)
- 3 A supersonic flow in a channel

A stationary radial solution



Shock tube

Let Ω denote the domain of parameters

$$\Omega = \{(r, z); \ r \in [0, 1), \ z \in (0, 1)\}.$$

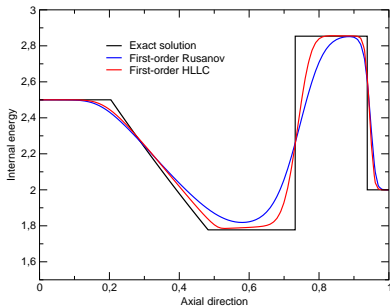
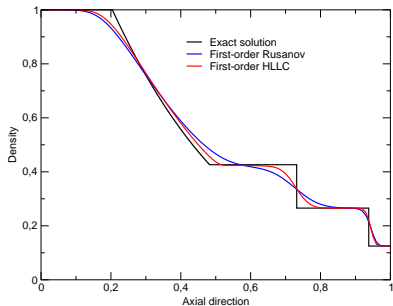
We define $\Omega_L = (0, 1) \times (0, \frac{1}{2})$, $\Omega_R = (0, 1) \times (\frac{1}{2}, 1)$ and the initial conditions:

$$U(t=0) = \begin{cases} U_L & \text{in } \Omega_L \\ U_R & \text{in } \Omega_R \end{cases}$$

Shock tube: Test 1

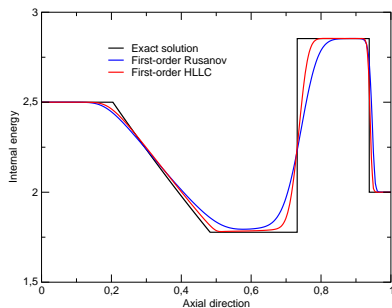
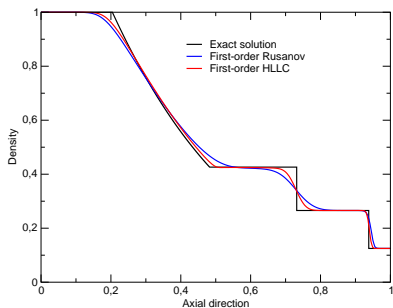
We test a configuration with a left rarefaction wave, a contact discontinuity and a right shock wave. For this we prescribe:

$$\rho_L = 1, \rho_R = 0.125, \quad u_L = u_R = 0, \quad p_L = 1, p_R = 0.1$$



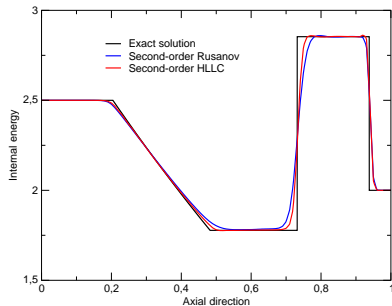
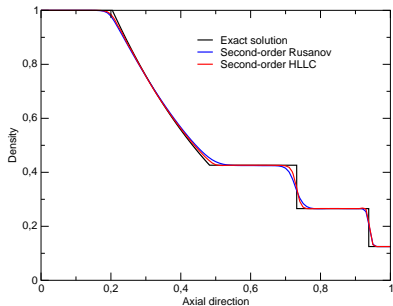
First Order: Rusanov and HLLC schemes: Mesh size 1/100

Shock tube: Test 1



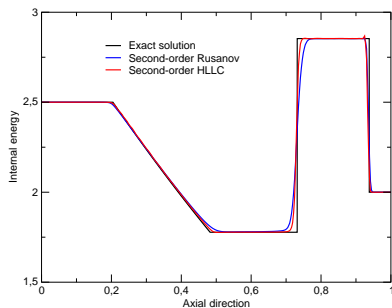
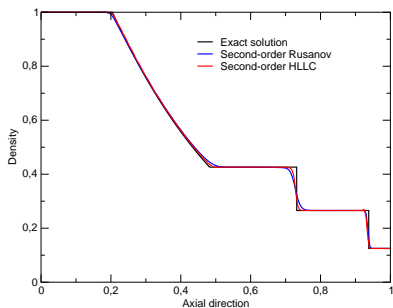
First Order: Rusanov and HLLC schemes: Mesh size 1/200

Shock tube: Test 1



Second Order: Rusanov and HLLC schemes: Mesh size 1/100

Tube à choc : Test 1

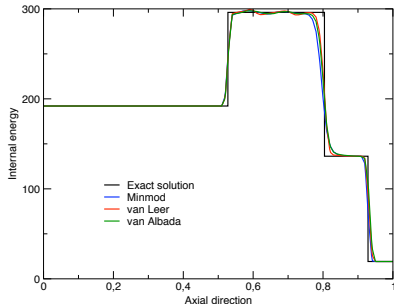
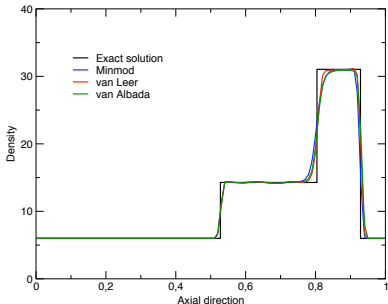


Second order: Rusanov and HLLC schemes: Mesh size 1/200

Shock tube: Test 2

We consider a configuration with a double shock and a contact discontinuity. This is obtained from the conditions:

$$\rho_L = \rho_R = 6, \quad u_L = 19.6, \quad u_R = -6.2, \quad p_L = 460, \quad p_R = 46$$

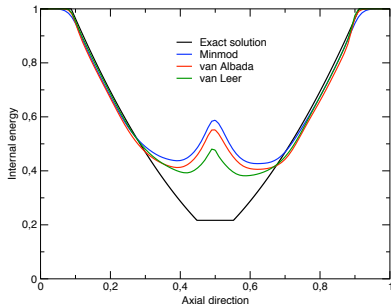
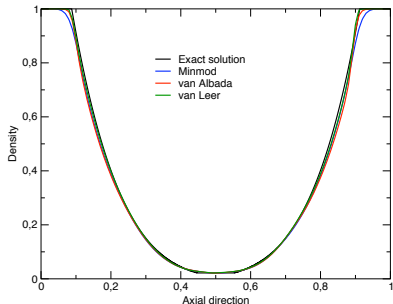


Second order: Rusanov and HLLC schemes: Mesh size 1/200

Shock tube: Test 3

We now test a configuration with 2 rarefactions and a contact discontinuity and where the solution presents a vacuum like situation. This is obtained with the conditions:

$$\rho_L = \rho_R = 1, \quad u_L = -2, \quad u_R = 2, \quad p_L = 1, \quad p_R = 0.4$$



Second Order: Rusanov and HLLC: Mesh size 1/200

Supersonic flow in a channel

We consider a compressible Euler flow in a channel with an oblique obstacle (10 degrees) forming a cone.

Problem data:

$$P_{\infty} = 10^5 Pa, \rho_{\infty} = 1.16 Kg/m^3, M_{\infty} = 2$$

Mesh: 5176 triangles.

Cone: Density contours

Animation

Cone: Mach contours

Animation