Modelling of Inductively Coupled Plasma Torches

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- Numerical simulation of inductively coupled plasma torches (ICP)
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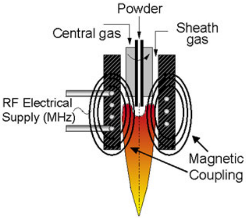
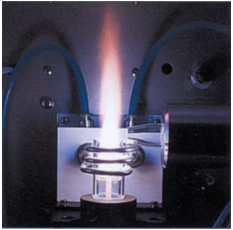
PRINCIPLE:

- The use of plasma torches is a chemical analytical technique to detect trace metals in environmental samples.
- It consists in ionizing a sample by injecting it in a plasma (in general Argon): Atoms are ionized by a hot flame (6 000 – 8 000 K).
- The sample experiences melting (solid), vaporization, then ionization.
- Temperature is maintained by magnetic induction (using a HF generator).
- Ions are detected either by mass spectrometry or by emission spectrométry.


Powder
Central gas
Sheath gas
RF Electrical Supply (MHz)
Magnetic Coupling



Outline

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

A mathematical model for ICP

Mathematical modelling of the ICP process takes into account the following phenomena:

- Electromagnetic induction: We use a quasi-static eddy current model (Displacement currents are neglected). The main difficulty comes from the fact that only a part (unknown) of the gas transforms into plasma and is then electrically conducting.

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- Radiative Transfer: We consider, for this study, a rather simple modelling.
- Due to the particular geometry of the setup, we use an axisymmetric description.

1. Electromagnetics

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

$$\begin{cases} \textbf{curl}\, \boldsymbol{H} = \boldsymbol{J} \\ i\omega\mu_0 \boldsymbol{H} + \textbf{curl}\, \boldsymbol{E} = 0 \\ \boldsymbol{J} = \sigma\, \boldsymbol{E} \end{cases}$$

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Here we have neglected current transport by the fluid
(In fact $\boldsymbol{J} = \sigma\,(\boldsymbol{E} + \mu_0 \boldsymbol{u} \times \boldsymbol{H})$).

We choose to formulate the problem in terms of the electric field. We have

$$\begin{cases} \mathbf{curl}\,\mathbf{curl}\,\boldsymbol{E} + i\omega\mu_0\sigma\boldsymbol{E} = 0 & \text{in } \mathbb{R}^3 \\ |\boldsymbol{E}(\boldsymbol{x})| = \mathcal{O}(|\boldsymbol{x}|^{-1}) & |\boldsymbol{x}| \to \infty \end{cases}$$

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

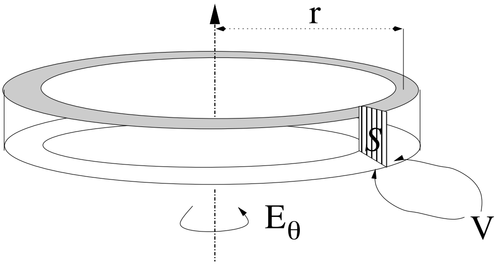
$$\sigma(e) = \begin{cases} 0 & \text{if } e \leq e_0, \\ > 0 & \text{otherwise} \end{cases}$$

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

The current source is maintained by voltages V_k supplied in each inductor Ω_k, such that we have the energy identity

$$\int_{\mathbb{R}^3} |\,\mathbf{curl}\,\boldsymbol{E}|^2 + i\omega\mu_0 \int_\Omega \sigma|\boldsymbol{E}|^2 = i\omega\mu_0 \sum_k V_k \int_{S_k} \sigma \boldsymbol{E}\cdot\boldsymbol{n}$$

where $\Omega = \cup_k \Omega_k$ is the union of conductors and S_k is a "cut" in the inductor Ω_k, *i.e.* such that $\Omega_k \setminus S_k$ is simply connected.



We use cylindrical coordinates and assume rotational symmetry.
For all k, Λ_k is the domain of parameters:

$$\Lambda_k := \{(r,z);\ (r\sin\theta, r\cos\theta, z) \in \Omega_k\ \forall\ \theta \in (0,2\pi]\}.$$

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We obtain for $E := E_\theta$ the problem:

$$\begin{cases} -\dfrac{\partial}{\partial r}\Big(\dfrac{1}{r}\dfrac{\partial}{\partial r}(rE)\Big) - \dfrac{\partial^2 E}{\partial z^2} + i\omega\mu_0\sigma E = \dfrac{i\omega\mu_0\sigma}{2\pi r}\displaystyle\sum_k V_k \mathbf{1}_{\Lambda_k} & \text{in } \mathbb{R}^3 \\ |E(r,z)| = \mathcal{O}((r^2+z^2)^{-\frac{1}{2}}) & (r^2+z^2) \to \infty \end{cases}$$

2. Gas–Plasma Flow

We use compressible Euler equations (*i.e.* we neglect viscosity and thermal conductivity effects) with the following features:

- Gas flow is generated by the Lorentz force (averaged on one time period).
- Energy source is given by Joule power density (also averaged).

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

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

$$\nabla \cdot ((\mathcal{E} + p)\, \boldsymbol{u}) = \frac{1}{2} \mathrm{Re}\,(\boldsymbol{J} \cdot \overline{\boldsymbol{E}}) - R$$

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

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

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In the following, we restrict the presentation to an ideal gas:

$$p=(\gamma-1)\,\rho e \qquad \gamma\text{: Ratio of specific heats}$$

Axisymmetric Euler Equations

We consider time dependent compressible Euler equations.
Denoting by (r, θ, z) the cylindrical coordinates and by (u_r, u_θ, u_z) the components of a vector in this system, we obtain the system (taking into account θ–invariance):

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

where f_r and f_z are r and z components of the Lorentz force.

This system can be written in the conservative form:

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

where

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

This formulation involves a divergence form that can be handled by a finite volume method. The right-hand side can be treated as a source term.

A finite volume method

Let us consider a triangulation of the domain Ω of parameters (r, z). We define:

- T_i : Triangle, $1 \leq i \leq n_T$
- e_{ij} : Common edge to triangles T_i and T_j
- $\boldsymbol{n}_{ij} = (n_{ij,r}, n_{ij,z})$: Unit normal to triangle T_i pointing to T_j
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Integrating the system of equations on a triangle T_i and using the divergence theorem, we obtain

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

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

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

We set

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

and define the approximation

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

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We define the approximate flux:

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

and the source term

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We then introduce the scheme

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

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

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

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Other possible schemes:

- Godunov: It consists in solving exactly the resulting Riemann problems.
- HLL (Harten, Lax, Van Leer): Uses an approximation of Riemann problems
- HLLC (+ Contact) : Adaptation of the HLL scheme to contact discontinuities

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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We have extended this extension for the axisymmetrical case.

Consider the conservation law:

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A basic finite volume scheme uses a piecewise constant approximation. Let us consider, for instance if $f' \geq 0$, the first-order upwind scheme:

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

This scheme is known to be diffusive, *i.e.* it smooths shocks and discontinuities.

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In order 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

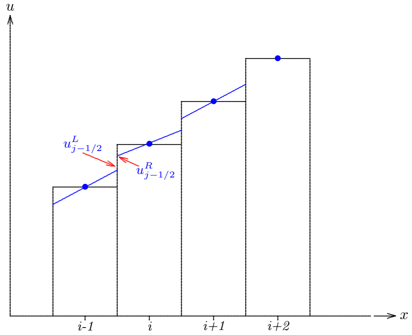
$$u_{i+\frac{1}{2}} := \frac{1}{2}(u_i + u_{i+1}), \quad u_{i-\frac{1}{2}} := \frac{1}{2}(u_{i-1} + u_i).$$

This scheme is more accurate but is oscillating (non TVD).

We can then resort to MUSCL type schemes:

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

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



We define:

$$u^*_{i\pm\frac{1}{2}} = u^*_{i\pm\frac{1}{2}}(u^L_{i\pm\frac{1}{2}}, u^R_{i\pm\frac{1}{2}})$$

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

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

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

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

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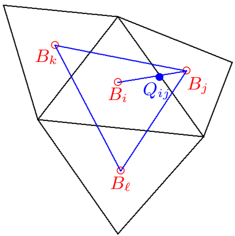
For instance, the limiter minmod is defined by

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

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



MUSCL schemes for Euler equations

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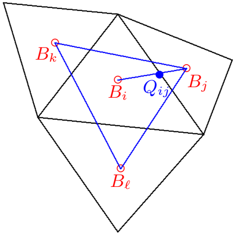

We introduce barycentric coordinates $(\rho_{ij})_{j\in\nu(i)}$ by

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

We assume that B_i is strictly in the interior of the triangle having barycenters of neighboring triangles as vertices. Thus $\rho_{ij} > 0$.

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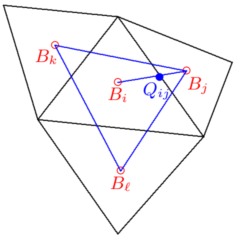

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We define the direction

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

We have then obtained a decomposition

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

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Let us define a reconstruction of the values U_{ij} on the edges e_{ij}.
Let v denote any component of U (piecewise constant).
We define a first set of downwind slopes by

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

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

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Let us define a reconstruction of the values U_{ij} on the edges e_{ij}.
Let v denote any component of U (piecewise constant).
We define a first set of downwind slopes by

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The slopes p_{ij} are then obtained by a limiter. For instance

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

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

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

Remarks

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- For positivity reasons, the reconstruction must be carried out on physical variables and not on conservative ones.

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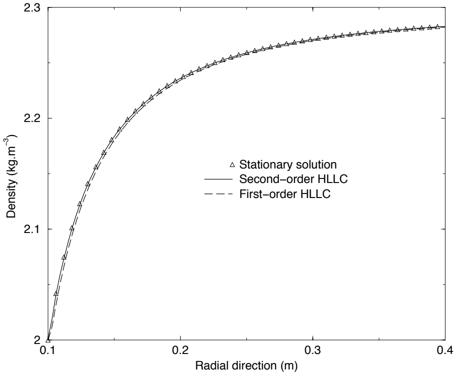
We deduce, for $\alpha, \beta \in \mathbb{R}$

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

Numerical tests

1. Stationary radial solutions
2. Shock tube (SOD): Some configurations
3. Supersonic flow in a channel

Stationary radial solutions



Shock Tube

Let us define the domain of parameters

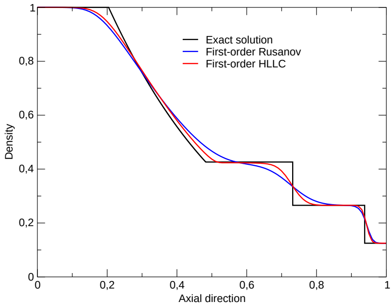
$$\Lambda = \{(r, z);\ r \in [0, 1),\ z \in (0, 1)\}.$$

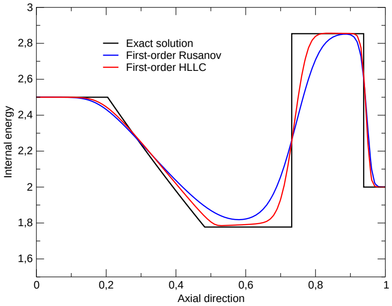
We define $\Lambda_L = (0, 1) \times (0, \frac{1}{2})$, $\Lambda_R = (0, 1) \times (\frac{1}{2}, 1)$ and the initial conditions:

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

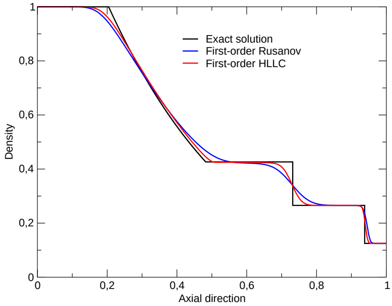
We test a configuration with a left rarefaction wave, a contact discontinuity and a right shock wave. We prescribe for this:

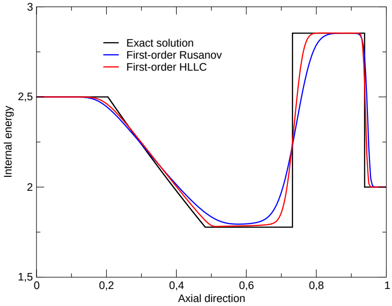
$$\rho_L = 1,\ \rho_R = 0.125, \quad u_L = u_R = 0, \quad p_L = 1,\ p_R = 0.1$$





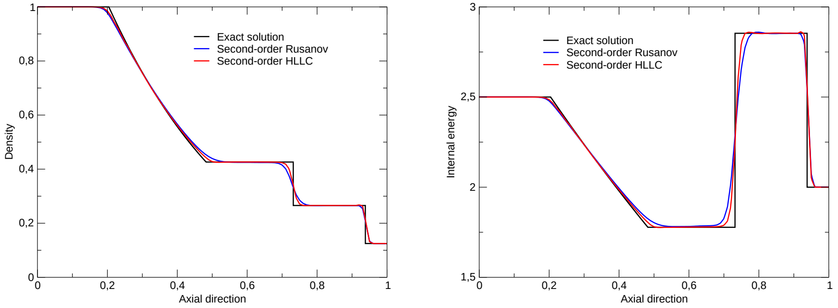
Order 1: Rusanov Schemes and HLLC schemes. Mesh 1/100





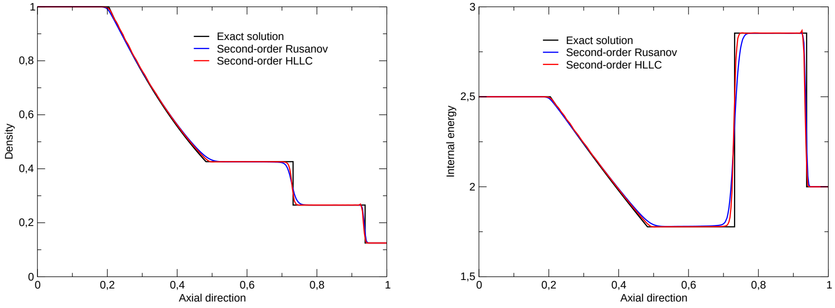
Order 1: Rusanov and HLLC schemes. Mesh 1/200

Shock Tube: Test 1



Order 2: Rusanov and HLLC schemes. Mesh 1/100

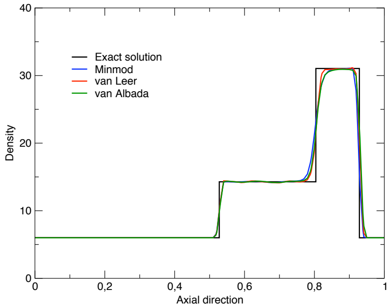
Shock Tube: Test 1

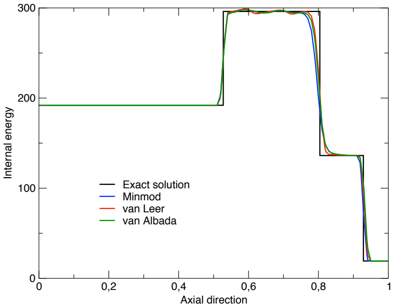


Order 2: Rusanov and HLLC schemes. Mesh 1/200

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

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

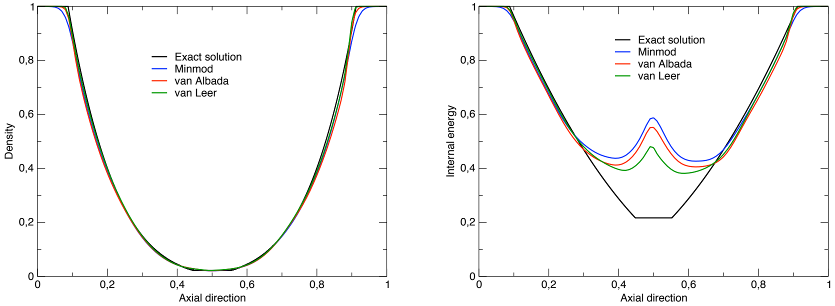




Order 2: Rusanov and HLLC schemes. Mesh 1/200

We test a configuration with 2 rarefactions and a contact discontinuity where the solution is close to vacuum state. This is obtained by the conditions:

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



Order 2: Rusanov and HLLC shemes. Mesh 1/200

Supersonic flow in a channel

We consider a channel flow 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: Iso-density curves

Animation

Cone: iso-Mach curves

Animation

ICP: A time integration scheme

We integrate in time until convergence to a stationary solution.

- Given $\boldsymbol{E}^n$, $\boldsymbol{U}^n$, we compute $\boldsymbol{B}^n = \frac{i}{\omega}\,\textbf{curl}\,\boldsymbol{E}^n$.
- We set $\sigma^n := \sigma(e^n)$ and solve the electromagnetic problem, which yields $\boldsymbol{E}^{n+1}$.
- We deduce

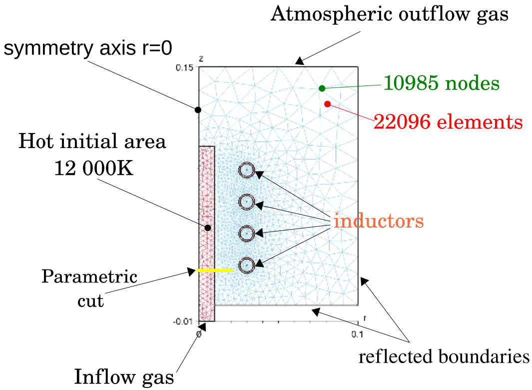
$$\boldsymbol{J}^{n+1} = \sigma^n \boldsymbol{E}^{n+1},\ \ \boldsymbol{B}^{n+1} = \frac{i}{\omega}\,\textbf{curl}\,\boldsymbol{E}^{n+1}$$

  and the sources

$$\boldsymbol{f}_L^{n+1} = \boldsymbol{J}^{n+1} \times \boldsymbol{B}^{n+1},\ \ f_J^{n+1} = \boldsymbol{J}^{n+1} \cdot \boldsymbol{E}^{n+1},\ \ R^{n+1} = R(e^n).$$

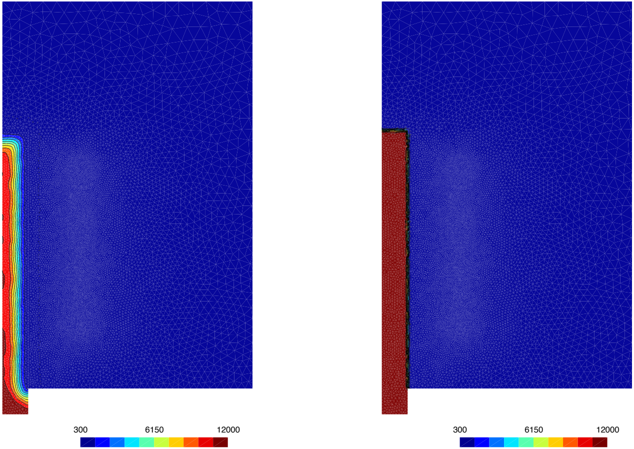
- We perform a time step of the Euler system without source terms: $\boldsymbol{U}^{n+\frac{1}{2}}$.
- We update by adding the source term using implicit approximation:

$$\rho^{n+1} = \rho^{n+\frac{1}{2}},$$
$$\rho^{n+1}\boldsymbol{u}^{n+1} = \rho^n \boldsymbol{u}^n + \Delta t\, \boldsymbol{f}_L^n,$$
$$\mathcal{E}^{n+1} = \mathcal{E}^{n+\frac{1}{2}} + \Delta t\,(f_J^{n+\frac{1}{2}} - R^{n+\frac{1}{2}}).$$


Atmospheric outflow gas
symmetry axis r=0
z
0.15
10985 nodes
22096 elements
Hot initial area
12 000K
inductors
Parametric
cut
-0.01
0
r
0.1
reflected boundaries
Inflow gas

Test with 0 V

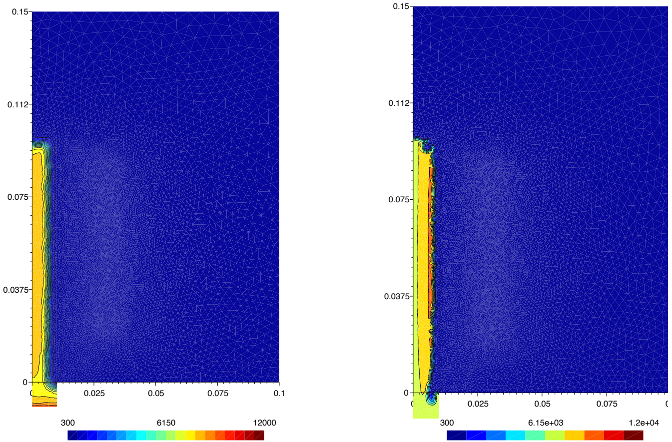
We take $V_k = 0$ for all k. In this case, we have a Riemann problem with a contact discontinuity.



The contact discontinuity is preserved with the HLLC flux (*right*). The Rusanov flux (*left*) is more dissipative.

Test with 1500 V

We choose $V_k = 1500$ volts for all k and add the radiation term



After $100\,\mu s$, we obtain by the HLLC flux HLLC a stationary solution. Using the Rusanov flux, the temperature decreases until extinction.