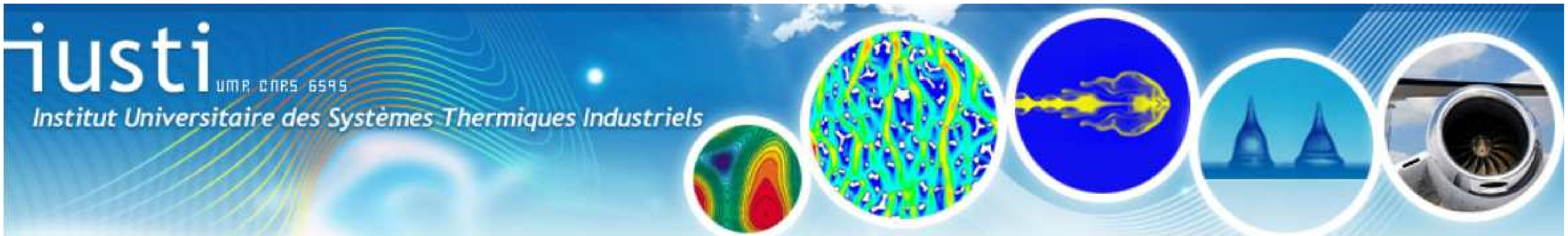
Aix*Marseille université

POLYTECH MARSEILLE

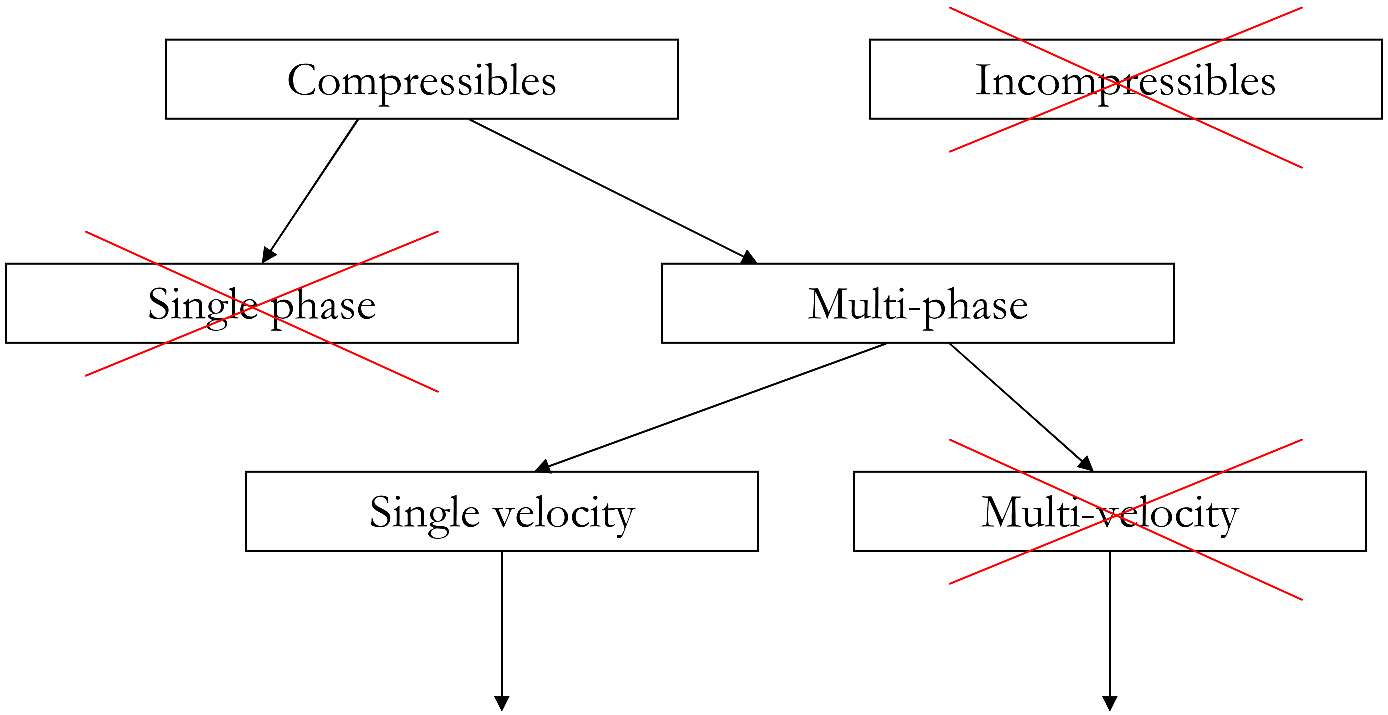
INRIA SOPHIA-ANTIPOLIS
Projet SMASH

Numerical simulation of compressible two-phase flows

F. Petitpas
SMASH Team - MARSEILLE



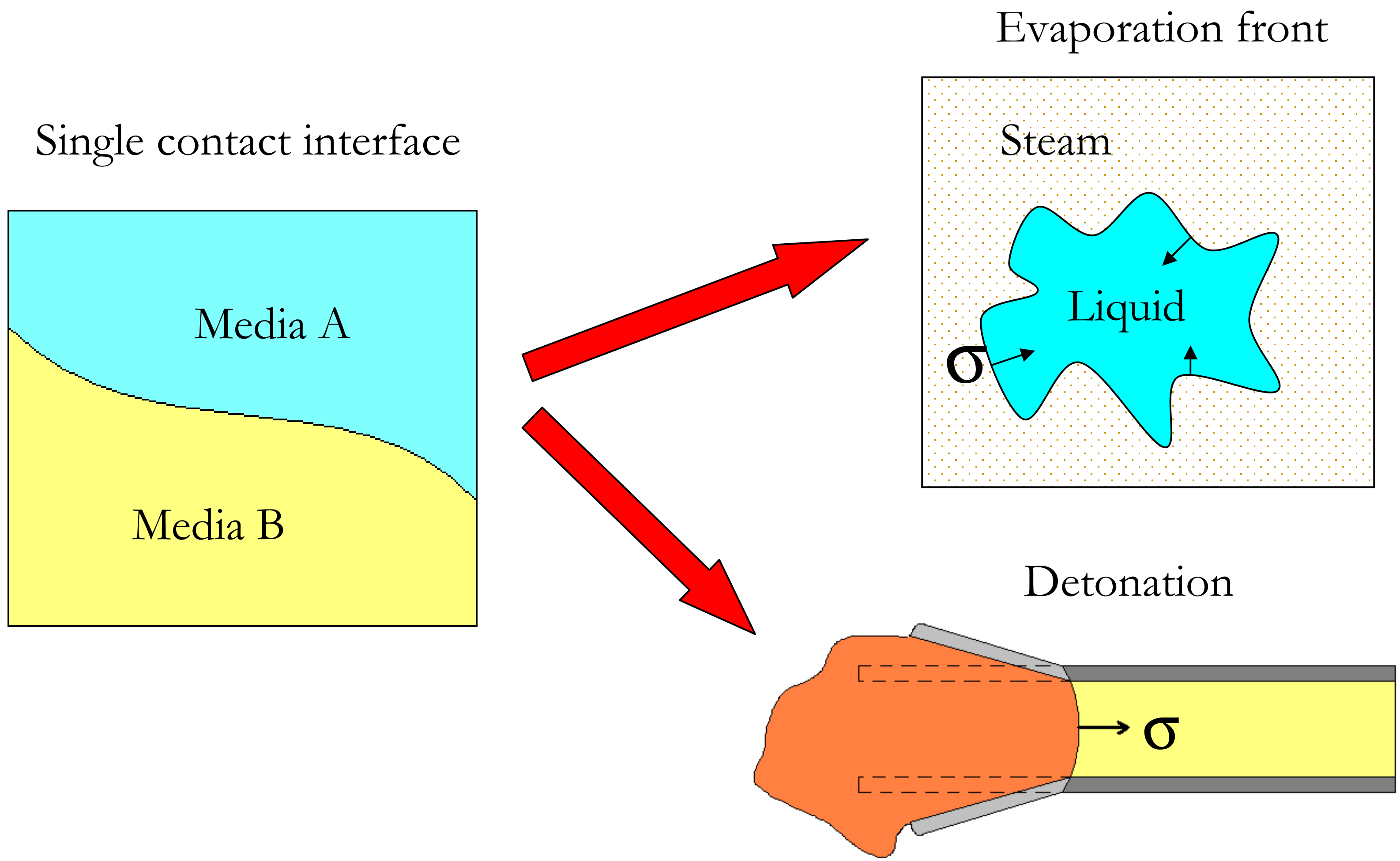
Flows zoology – Position of the topic



- Interface problems resolution
- Two-phase mixtures in mechanical equilibrium

- Non equilibrium two-phase mixtures
- General models

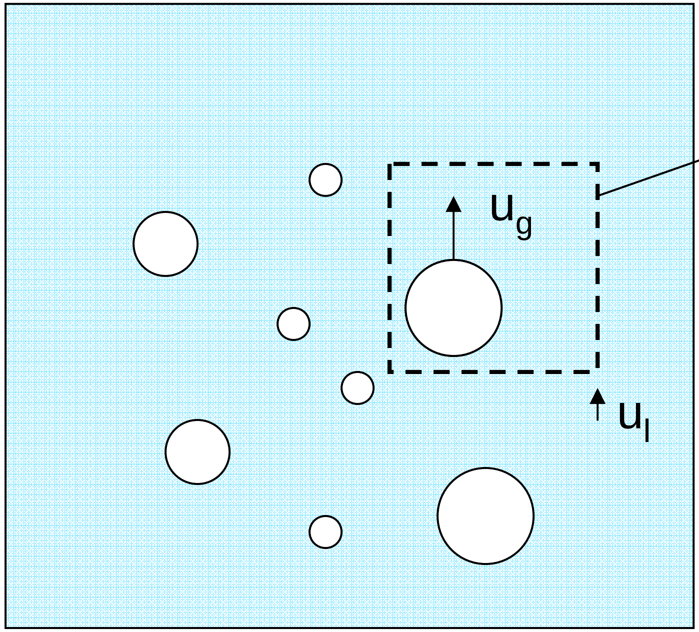
Single velocity flows / Interface problems

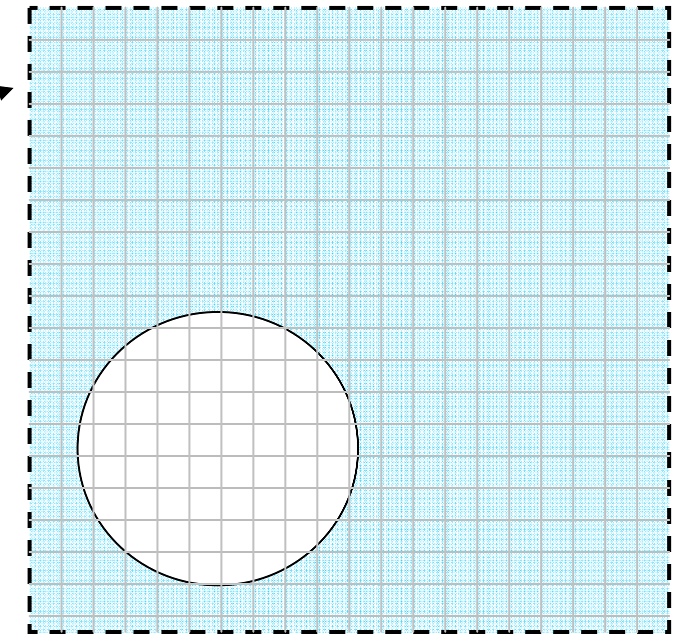


Some words about discretisation scales

"Macro" scale : Multi-velocity flow

« Micro » scale : Single velocity flow

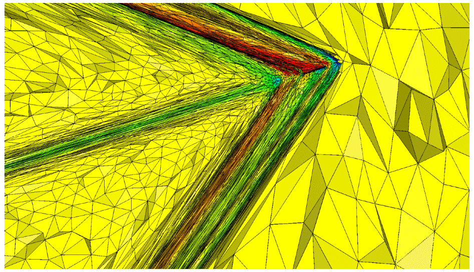




➡ An averaged model with two velocities is needed

➡ A reduced model for interface problems is enough

- Sharp interface methods
  - Lagrangian methods with moving meshes, ALE (Arbitrary Lagrangian Eulerian)



Good for solid weak deformation

Not adapted for fluids computation with extreme deformations

  - Front tracking, VOF, Level Set

Very impressive results

Generally non conservative regarding mass and energy

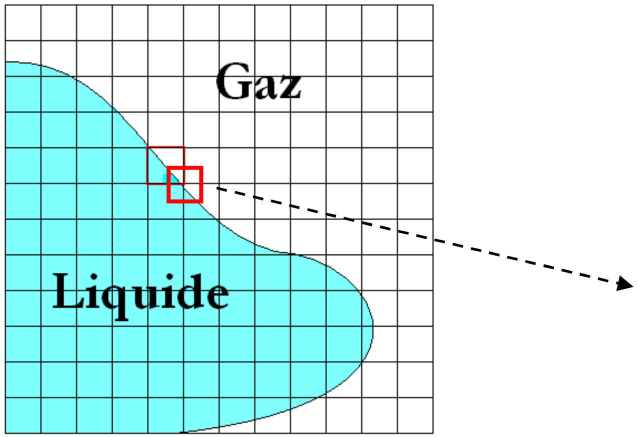
Heavy numerical treatment

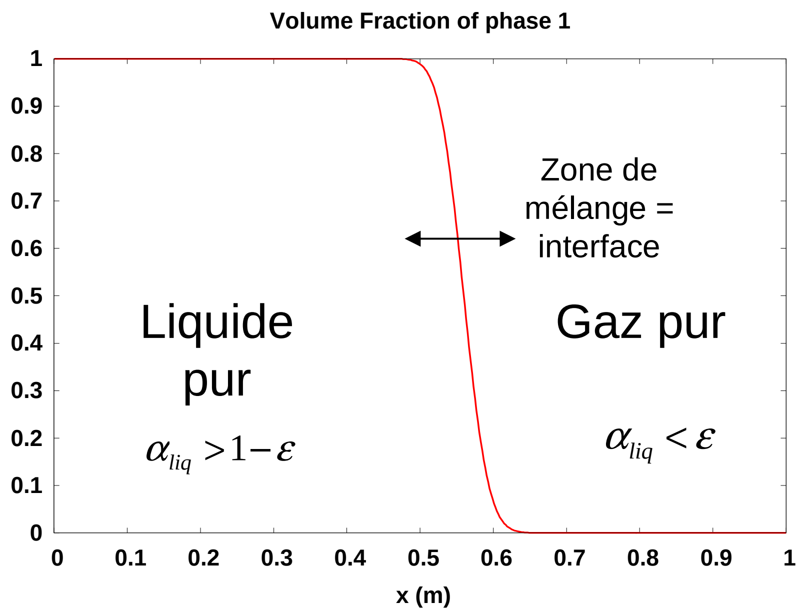
On the choice of the method

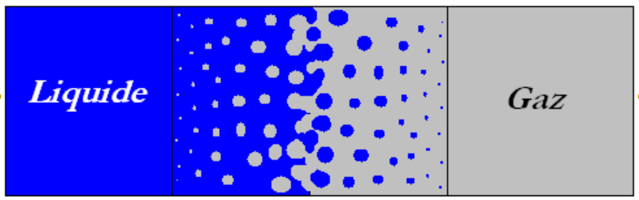
- Diffuse interface methods

These methods authorize numerical diffusion of interfaces. This presents several advantages:

- Interfaces are not tracked or reconstructed, they are captured by the numerical scheme as artificial diffusion zone.
- By the way disappearance or apparition of interfaces are naturally obtained
- Conservative







On the choice of the model

- Euler equations with liquid-vapor Equation of state for evaporation problems
  Single phase model with equilibrium EOS (T,p,g,u)
  - Able to compute liquid-vapor mixtures at Thermodynamical equilibrium
  - But metastable states are omitted
  - Unable to treat liquid-gas interfaces
- Multi-phase models
  - 4-equation : Euler + mass equation
    Thermal and mechanical equilibrium (T,p,u)
    - Largely use for gas mixtures where thermal equilibrium condition is not so restrictive
    - But unable to treat simple contact interface (interface condition of equal pressure and velocity are violated)
  - 5-equation : 4 equations + volume fraction equation (Kapila et al., 2001)
    Mechanical equilibrium (p,u)
    - Able to treat interfaces between non miscible fluids (liquid-gas)
    - Able to treat mixture evolving in mechanical equilibrium

  - 6-equation model
    Velocity equilibrium (u)
  - 7-equation (Baer & Nunziato, 1986)
    Total disequilibrium
    - Able to solve a large scale of problems
    - Difficult to solve numerically

Outline : The 5-equation model

- Topic 1 : Origins and properties of the 5-equation model
- Topic 2 : Numerical resolution
  - The Euler equations
  - The 5-equation model
- Topic 3 : Phase transition with the 5-equation model
- Topic 4 : Other extensions
  - Capillary effects
  - Compaction effects
  - Low Mach computing
  - Etc.

Topic 1 : Origins and properties of the 5-equation model

Starting point : origin of the 5-equation model (The 7-equation model)

Each phase obeys its own thermodynamics (pressure, density, internal energy) and has its own set of equations :

$$\frac{\partial \alpha_k}{\partial t} + \vec{\sigma}.\vec{\nabla}\alpha_k = \mu(P_k - P_{k'})$$

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \vec{\nabla}.(\alpha_k \rho_k \vec{u}_k) = 0$$

$$\frac{\partial \alpha_k \rho_k \vec{u}_k}{\partial t} + \vec{\nabla}.(\alpha_k (\rho_k \vec{u}_k \otimes \vec{u}_k + P_k \bar{I})) = P_I \vec{\nabla}\alpha_k + \lambda(\vec{u}_{k'} - \vec{u}_k)$$

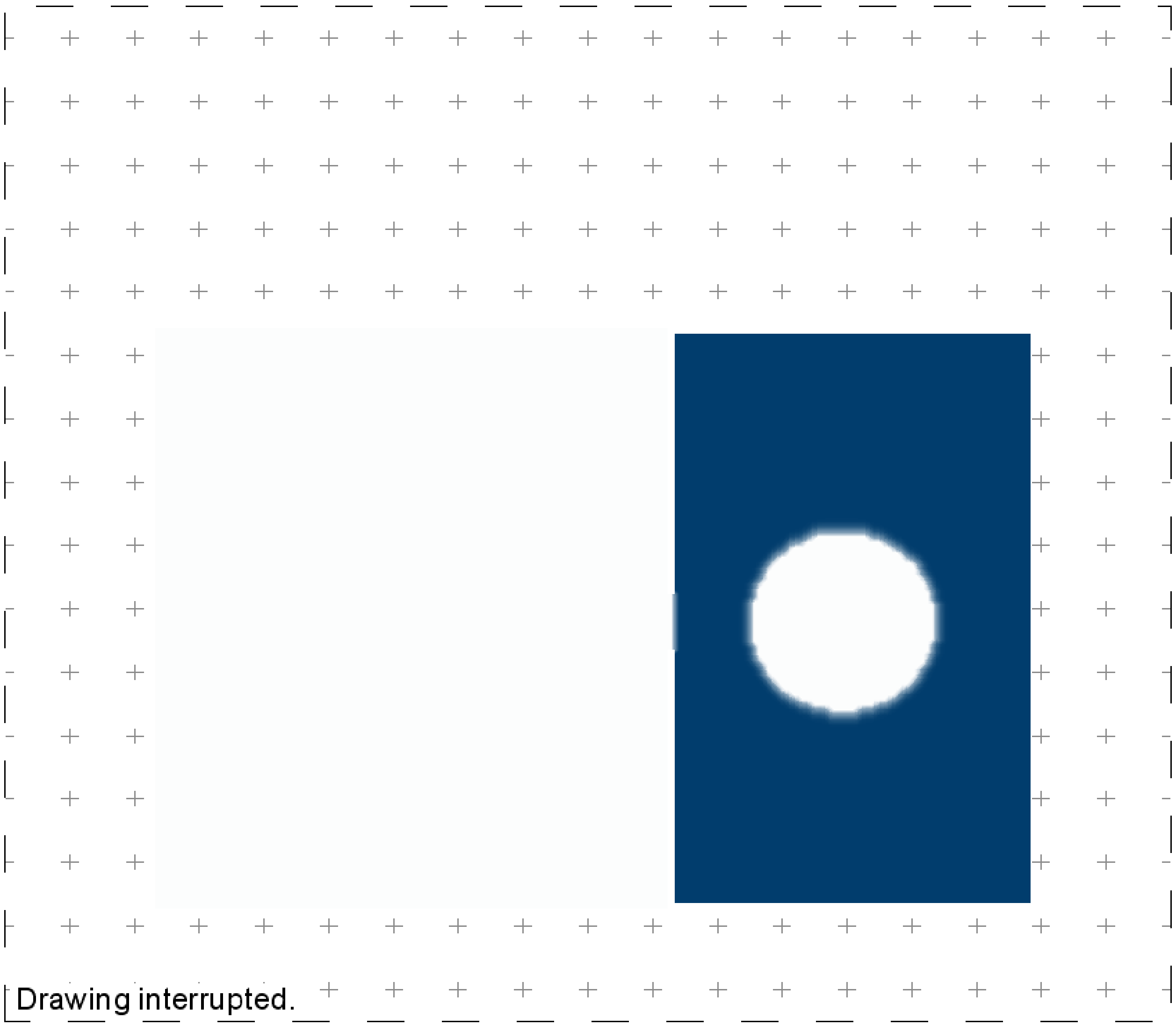
$$\frac{\partial \alpha_k \rho_k E_k}{\partial t} + \vec{\nabla}.(\alpha_k (\rho_k E_k + P_k)\vec{u}_k) = P_I \vec{\sigma}.\vec{\nabla}\alpha_k - \mu P_I (P_k - P_{k'}) + \lambda \vec{\sigma}.(\vec{u}_{k'} - \vec{u}_k)$$

$\vec{\sigma} = \vec{u}_2$ and $P_I = P_1$ — Baer & Nunziato (1986)

$$\vec{\sigma} = \frac{Z_1 \vec{u}_1 + Z_2 \vec{u}_2}{Z_1 + Z_2} \quad \text{and} \quad P_I = \frac{Z_1 P_2 + Z_2 P_1}{Z_1 + Z_2}$$

— Saurel & al. (2003); Chinnayya & al (2004)

Example of interface problem evolving to a two-velocity mixture



Simulation : Jacques Massoni, SMASH team

Asymptotic reduction of the 7-equation model

- Why it is interesting to use the 5-equation model instead of the 7-equation one ?
  - It is difficult to solve and implies heavy costs regarding CPU and memory.
  - It contains extra unuseful physics to treat interface problems (two velocities and two pressures)
  - Extra physical effects are difficult to introduce (as for example phase transition, capillary effects, etc.)

Asymptotic reduction by the Chapman-Enskog method :

$\lambda, \mu = 1/\varepsilon \rightarrow \infty$ Relaxation parameters tend to infinity

$f = f^{o} + \varepsilon f^{1}$ Each flow variable is supporting small variation around an equilibrium state

The diffuse interface model (5-equation model)

4 conservative equations

$$\begin{cases} \dfrac{d\alpha_1}{dt} = \alpha_1\alpha_2\left(\dfrac{\rho_2 c_2^2 - \rho_1 c_1^2}{\alpha_2\rho_1 c_1^2 + \alpha_1\rho_2 c_2^2}\right)\dfrac{\partial u}{\partial x} \\ \dfrac{\partial \alpha_1\rho_1}{\partial t} + \dfrac{\partial \alpha_1\rho_1 u}{\partial x} = 0 \\ \dfrac{\partial \alpha_2\rho_2}{\partial t} + \dfrac{\partial \alpha_2\rho_2 u}{\partial x} = 0 \\ \dfrac{\partial \rho u}{\partial t} + \dfrac{\partial (\rho u^2 + p)}{\partial x} = 0 \\ \dfrac{\partial \rho E}{\partial t} + \dfrac{\partial (\rho E + p)u}{\partial x} = 0 \end{cases}$$

Equilibre mécanique

$$u_1 = u_2 = u$$

$$p_1 = p_2 = p$$

Variables de mélange :

$$\rho = \alpha_1\rho_1 + \alpha_2\rho_2$$

$$\rho E = \alpha_1\rho_1 E_1 + \alpha_2\rho_2 E_2$$

+ Équation d'état de mélange : $p = p(\rho, e, \alpha_k) = \dfrac{\rho e - \left(\dfrac{\alpha_1\gamma_1 p_{\infty,1}}{\gamma_1 - 1} + \dfrac{\alpha_2\gamma_2 p_{\infty,2}}{\gamma_2 - 1}\right)}{\dfrac{\alpha_1}{\gamma_1 - 1} + \dfrac{\alpha_2}{\gamma_2 - 1}}$

We will come back on thermodynamic closure in the following …

This is a mechanical equilibrium but each phase remains in thermal disequilibrium

Physical meaning of the volume fraction equation

$\rho_k c_k^2$ is the Bulk modulus of media k

It traduces the compressibility of a media

-Big when it is weakly compressible

-Small when it is strongly compressible

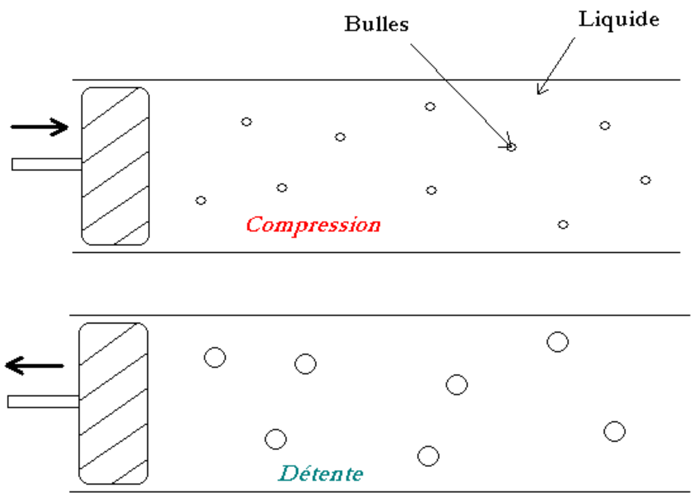
$$\begin{cases} \frac{d\alpha_1}{dt} = \alpha_1\alpha_2\left(\frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\alpha_2\rho_1 c_1^2 + \alpha_1\rho_2 c_2^2}\right)\frac{\partial u}{\partial x} \\ \frac{\partial \alpha_1\rho_1}{\partial t} + \frac{\partial \alpha_1\rho_1 u}{\partial x} = 0 \\ \frac{\partial \alpha_2\rho_2}{\partial t} + \frac{\partial \alpha_2\rho_2 u}{\partial x} = 0 \\ \frac{\partial \rho u}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} = 0 \\ \frac{\partial \rho E}{\partial t} + \frac{\partial(\rho E + p)u}{\partial x} = 0 \end{cases}$$

$$\frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} = K\frac{\partial u}{\partial x}$$

Exemple $K < 0$

Liquide : phase 1

Bulles gaz : phase 2

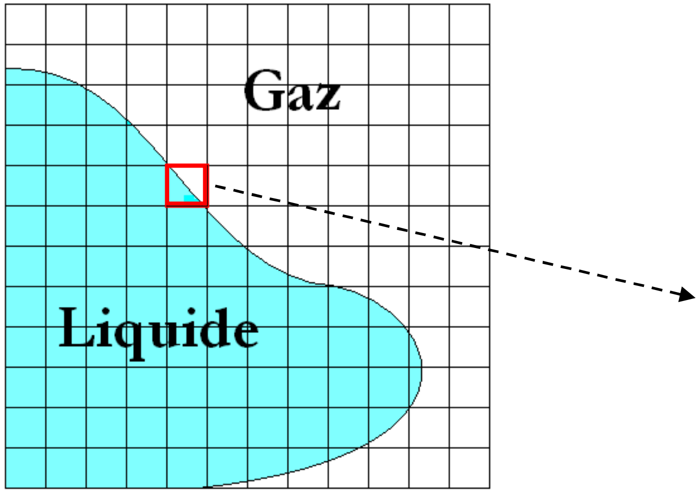


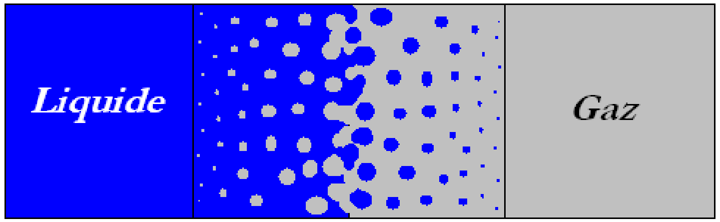
$\frac{\partial u}{\partial x} < 0 \Rightarrow \alpha_1$ increases

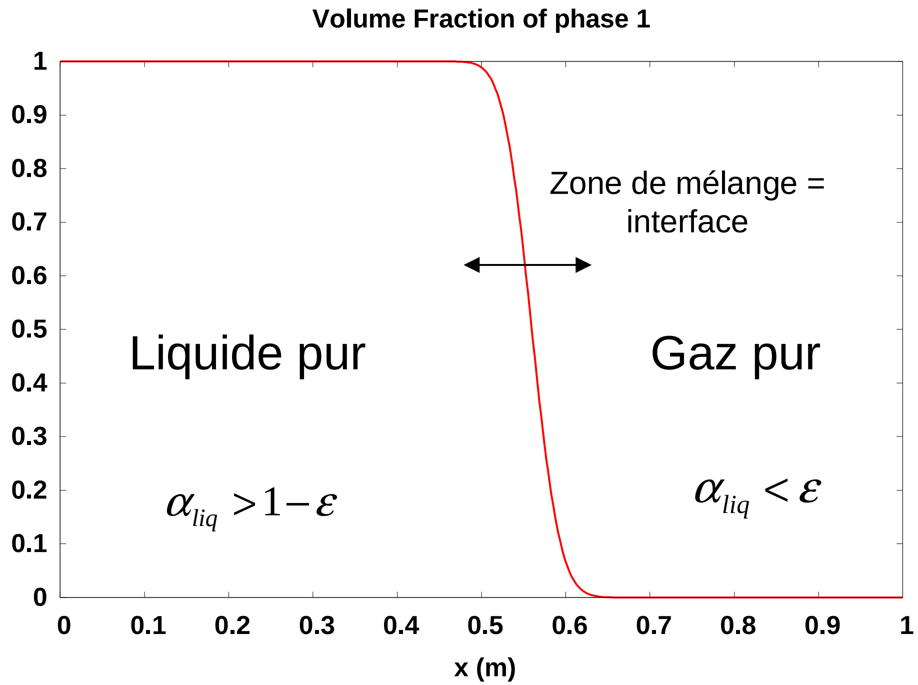
$\frac{\partial u}{\partial x} > 0 \Rightarrow \alpha_1$ decreases

Back to diffuse interface aptitude …

- Diffusion is due to numerical treatment : Artificial diffusion
- By the way, an interface looks like a mixture zone : $\varepsilon < \alpha_k < 1 - \varepsilon$
- The interface conditions of pressures and velocities equalities are automatically obtained !





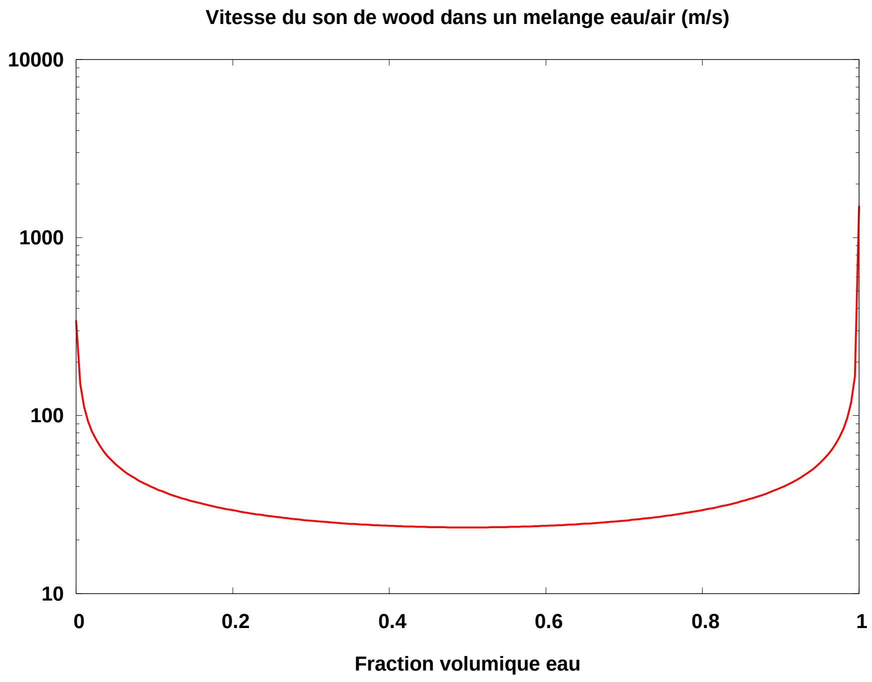


5-equation model properties

- Hyperbolic systems : 3 waves speeds.

$$u - c_w, u, u + c_w$$

- The speed of sound is those of Wood (1930)



$$\begin{cases} \dfrac{d\alpha_1}{dt} = K\,\mathrm{div}(\vec{u}) \\ \dfrac{\partial \alpha_1 \rho_1}{\partial t} + \mathrm{div}(\alpha_1 \rho_1 \vec{u}) = 0 \\ \dfrac{\partial \alpha_2 \rho_2}{\partial t} + \mathrm{div}(\alpha_2 \rho_2 \vec{u}) = 0 \\ \dfrac{\partial \rho u}{\partial t} + \mathrm{div}(\rho \vec{u} \otimes \vec{u}) + \vec{\nabla} p = 0 \\ \dfrac{\partial \rho E}{\partial t} + \mathrm{div}[(\rho E + p)\vec{u}] = 0 \end{cases}$$

$$\frac{1}{\rho c_w^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2}$$

Topic 2 : Numerical resolution considerations

- Basics for Euler conservative equations
- 5-equation model numerical resolution

Basics of numerical resolution for the Euler equations

- Euler equations:
  - Mass balance $$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \vec{u}) = 0$$
  - Momentum balance $$\frac{\partial \rho \vec{u}}{\partial t} + \mathrm{div}(\rho \vec{u} \otimes \vec{u}) + \mathrm{grad}(P) = 0$$
  - Total energy balance $$\frac{\partial \rho E}{\partial t} + \mathrm{div}((\rho E + P)\vec{u}) = 0$$

- 1D simplification:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + P}{\partial x} = 0$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial u(\rho E + P)}{\partial x} = 0$$

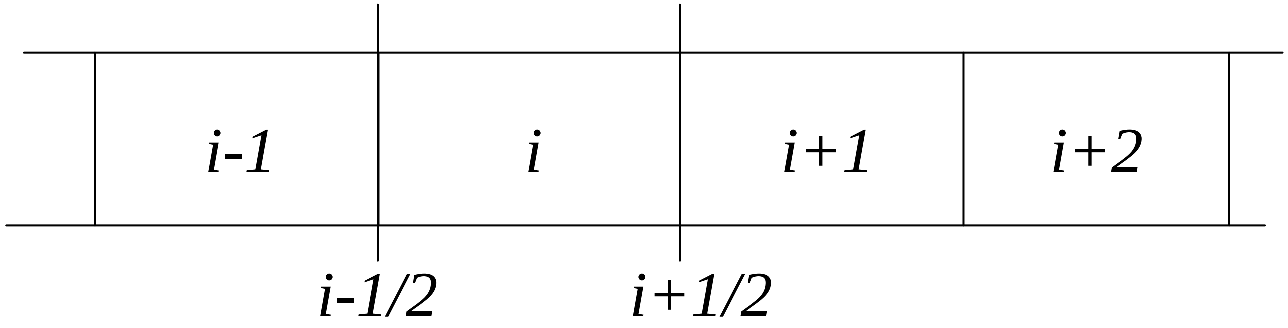
⇒

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0$$

$$U = (\rho, \rho u, \rho E)^T$$

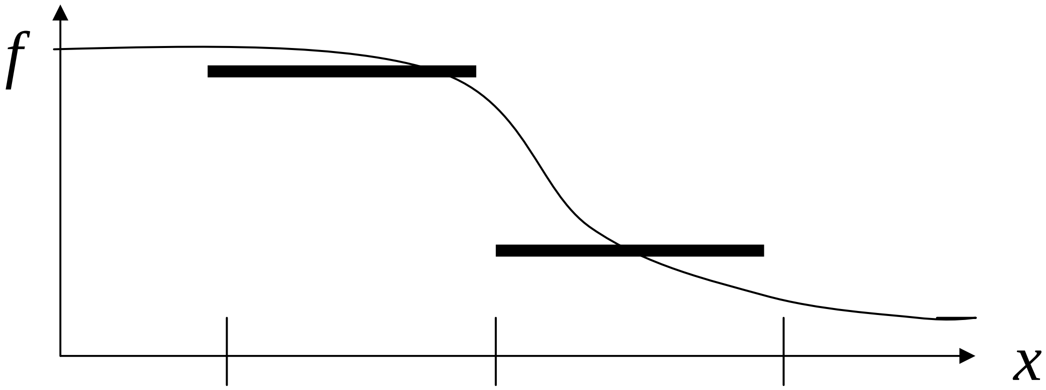
$$F = (\rho u, \rho u^2 + P, u(\rho E + P))^T$$

Computational mesh



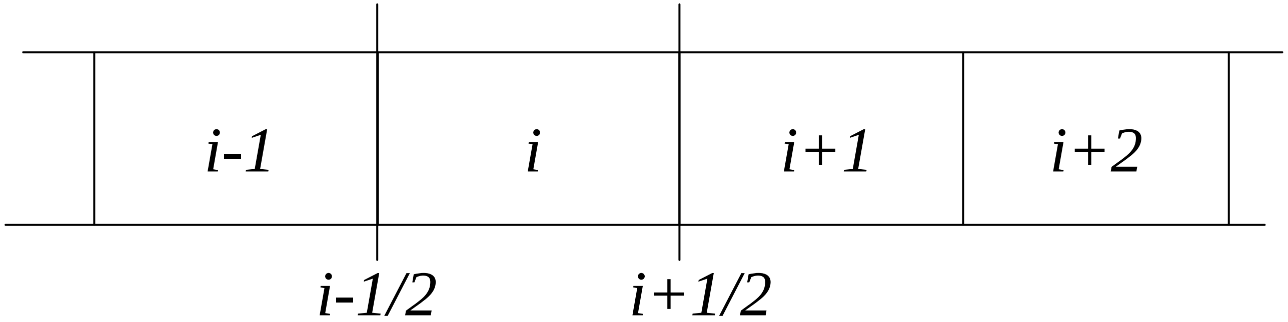
- The cell 'i' is bounded by inlet and outlet sections i-1/2 and i+1/2.
- The fluxes cross over these cell boundaries.
- The unknowns are computed at the cell center and are piecewise constant functions in the cell.

Example at a given time



How to obtain average cells variables form on time step to an other one

Numerical approximation



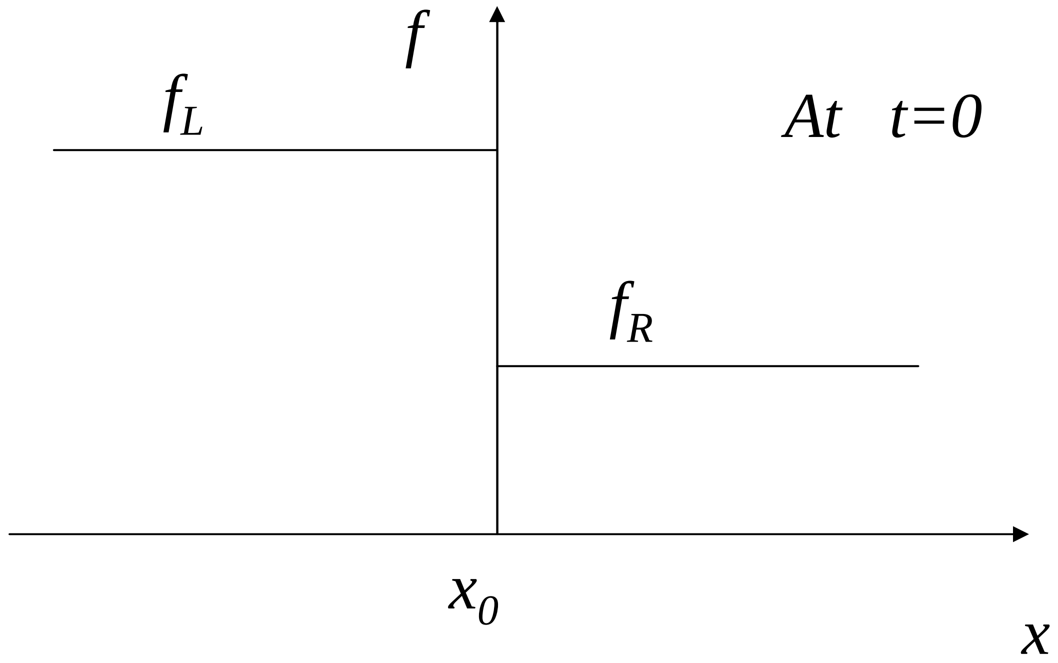
Integration on cell i over time :

$$\iint_{\Delta t\, V} \left[\frac{\partial U}{\partial t} + \mathrm{div}(F) \right] dV dt = 0 \quad \Rightarrow \quad U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}\left(F^*_{i+1/2} - F^*_{i-1/2} \right)$$

The '*' superscript is for : Solution of the Riemann problem at cell boundary

The Flux F at cell boundaries has been supposed to be constant during integration time step ⇒ CFL condition

The Riemann problem

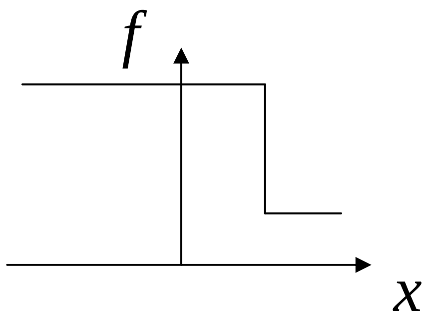


- The initial data are know at a given time and are constant on the right and left side.
- A discontinuity connects the two state.
- Question: How does the solution evolves at t>0 ?

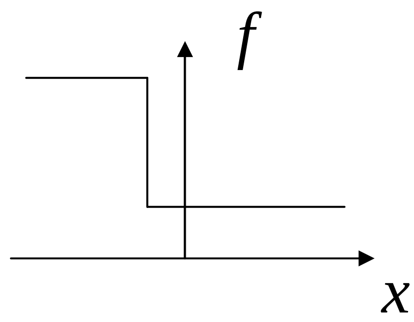
The Riemann problem solution (advection)

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = 0$$

The two possible solutions are:

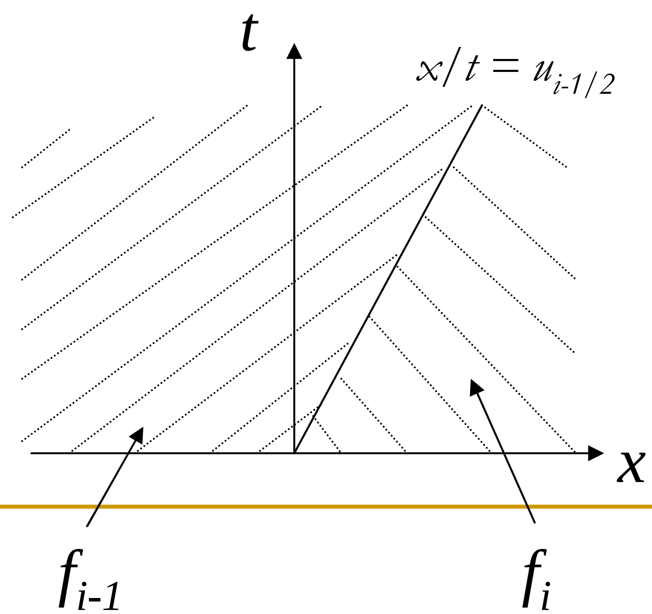


$u_{i-1/2} > 0$



$u_{i-1/2} < 0$

In the (x,t) diagram



The solution is:

$$f(x/t) = \begin{cases} f_{i-1} & \text{if } x/t < u_{i-1/2} \\ f_i & \text{if } x/t > u_{i-1/2} \end{cases}$$

For the linearized Euler equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + P}{\partial x} = 0$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial u(\rho E + P)}{\partial x} = 0$$

$$\Rightarrow \begin{cases} \dfrac{\partial W}{\partial t} + A(W)\dfrac{\partial W}{\partial x} = 0 \\ W = (\rho, u, P)^T \\ A(W) = \begin{pmatrix} u & \rho & 0 \\ 0 & u & 1/\rho \\ 0 & \rho c^2 & u \end{pmatrix} \end{cases}$$

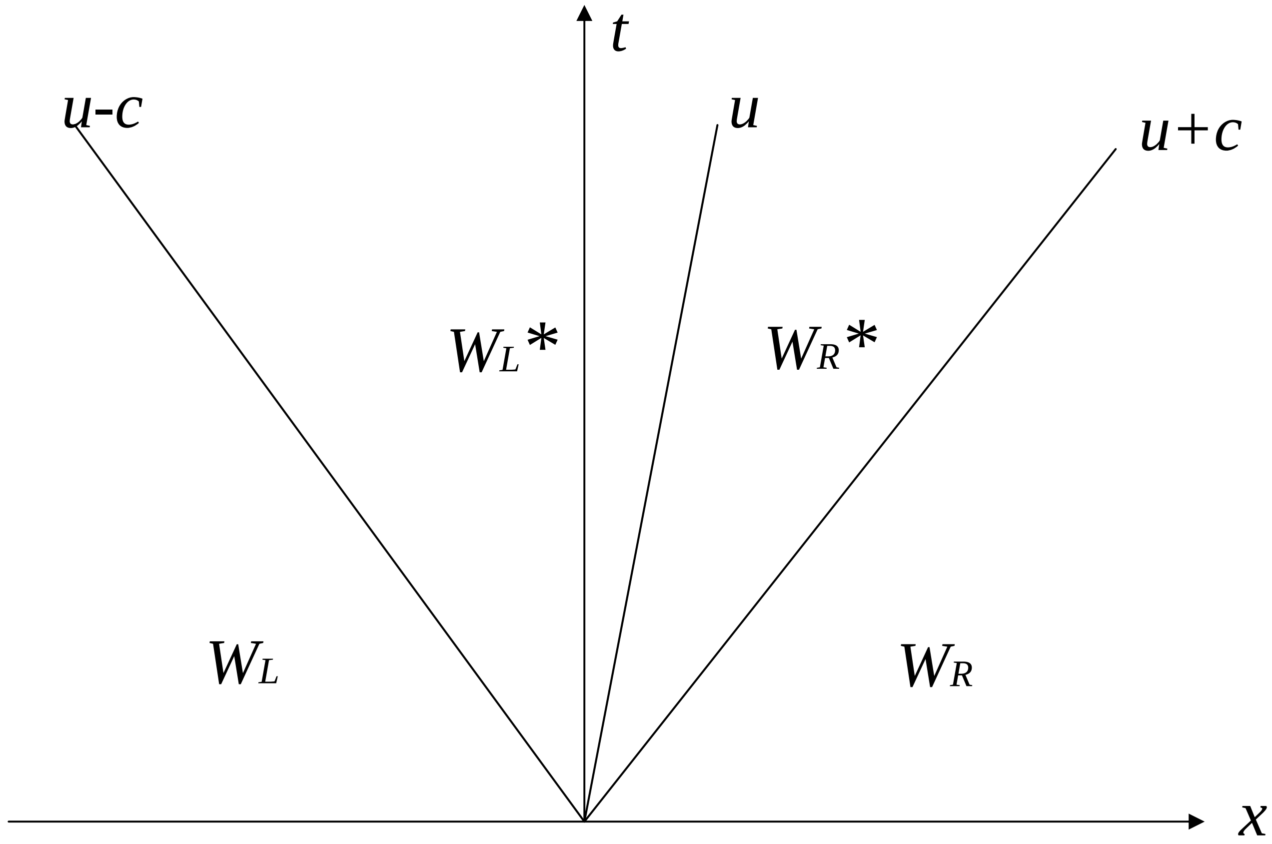
analogue of $\dfrac{\partial f}{\partial t} + u\dfrac{\partial f}{\partial x} = 0$

Plays the role of a propagation velocity

The eigenvalues of A are the waves speeds:

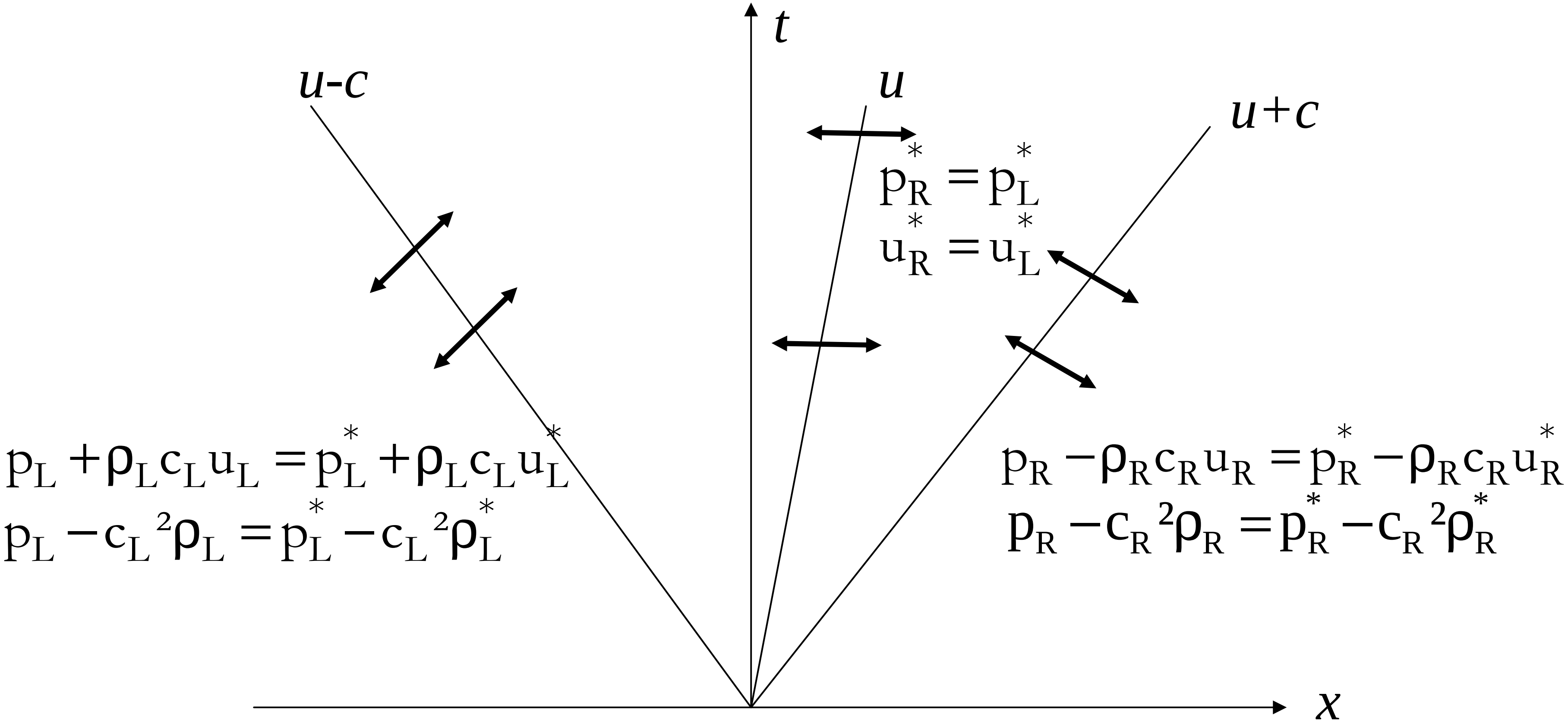
$$\lambda^+ = u + c \;,\; \lambda^- = u - c \;,\; \lambda^0 = u$$

The Riemann problem for linearized Euler equations



Solving the Riemann problem consist in determining the perturbed states W_L* and W_R* after waves propagation from the known states W_L and W_R.

The Riemann problem solution for linearized Euler equations



From this algebraic set of 6 equations the two intermediate states

W_L* and W_R* are readily obtained.

Riemann problem solution

$$u^* = \frac{p_L - p_R + Z_R u_R + Z_L u_L}{Z_R + Z_L}$$

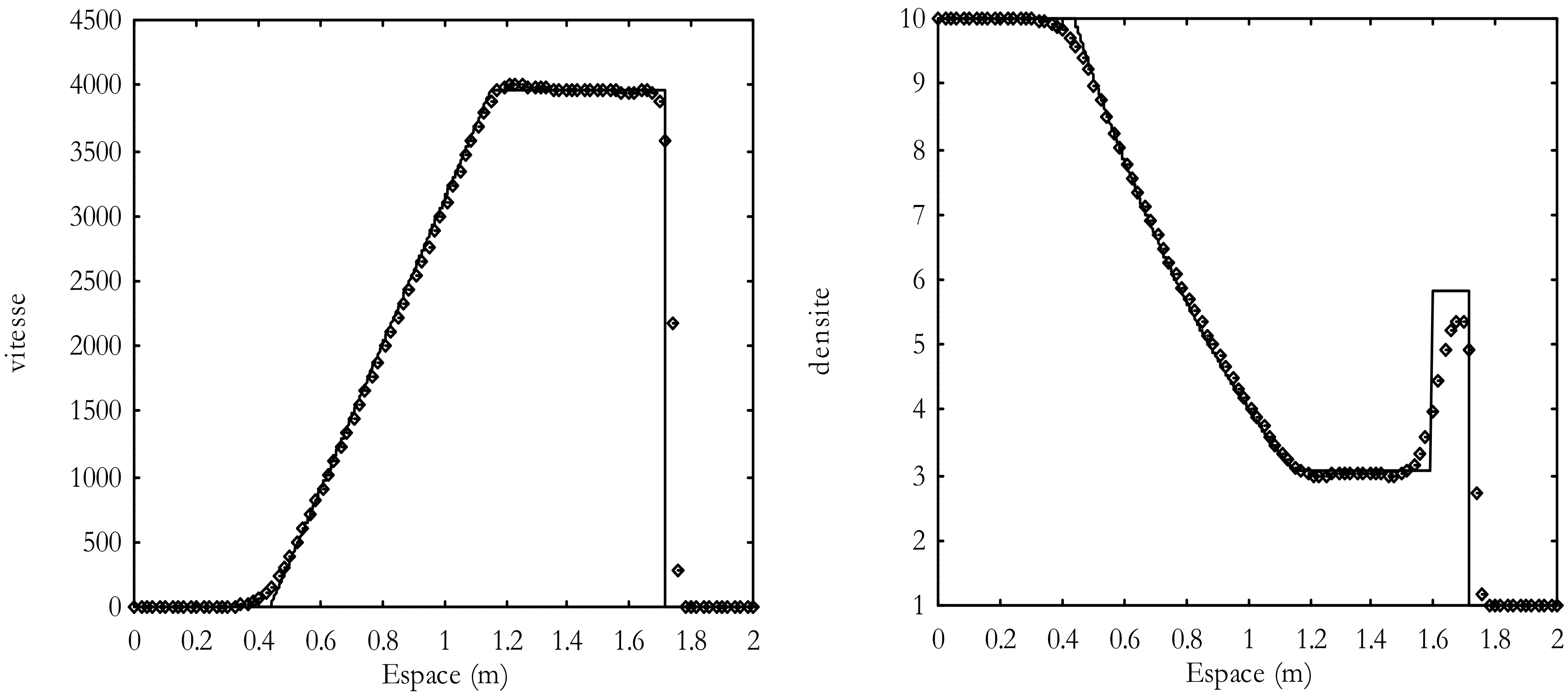
$$p^* = \frac{Z_R p_L + Z_L p_R + Z_R Z_L (u_L - u_R)}{Z_R + Z_L}$$

$$\rho_R^* = \rho_R + \frac{p^* - p_R}{c_R{}^2}$$

$$\rho_L^* = \rho_L + \frac{p^* - p_L}{c_L{}^2}$$

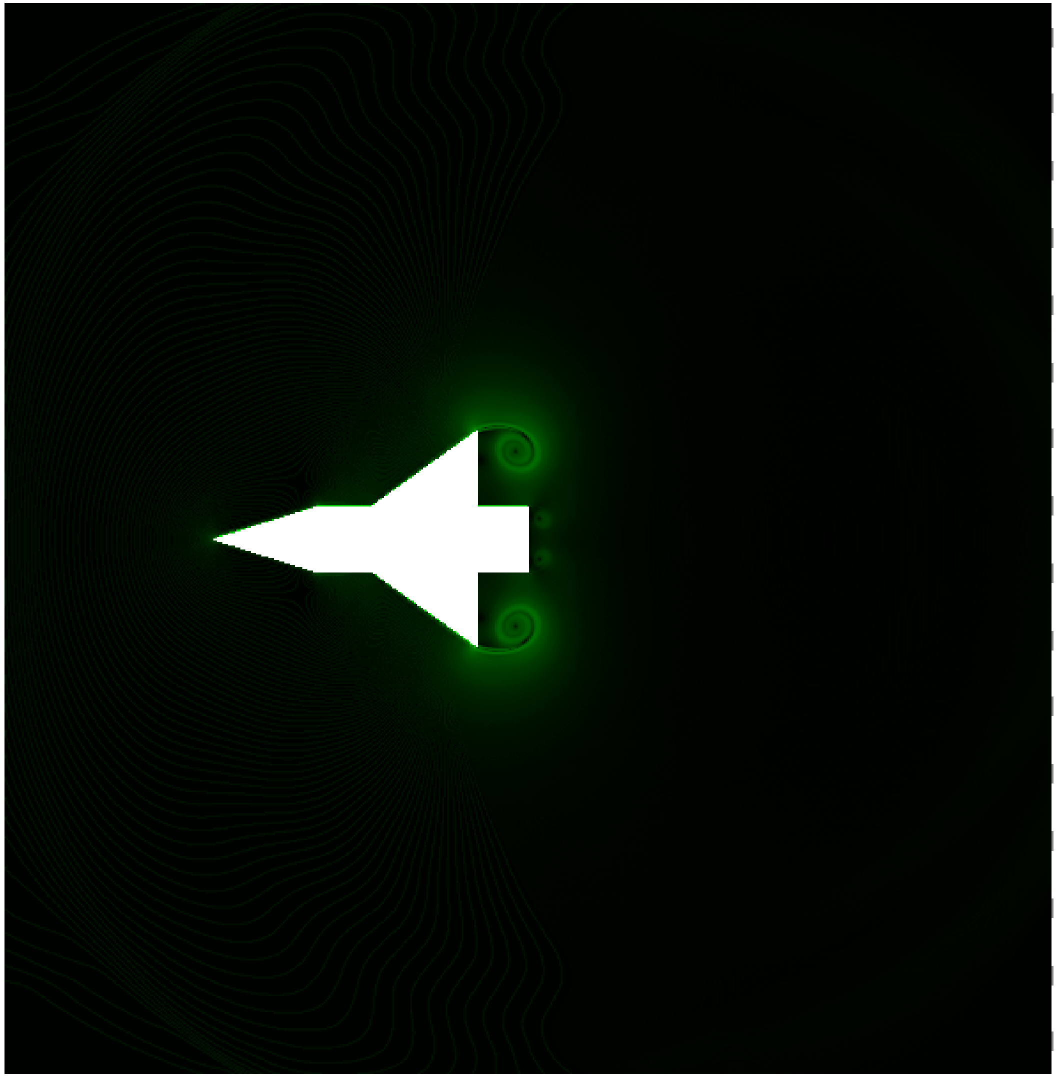
Example: shock tube

P=10 000 bars	P=1 bar
u=0 m/s	u=0 m/s
ϱ=10 kg /m3	ϱ=1 kg /m3



Exact solution (lines) / Computed results with Godunov (symbols)

Example – Supersonic flow around plane profil



Summary for Euler equations

- The Riemann problem solution is a local solution of the Euler equations between two discontinuous initial states.
- It is the cornerstone of all numerical schemes used in gas dynamics, shallow water and modern multiphase codes

- Recommended literature:

  E.F. Toro (1997) Riemann solvers and numerical methods for fluid dynamics. Springer Verlag

The diffuse interface model (5-equation model)

4 conservative equations

$$\begin{cases} \dfrac{d\alpha_1}{dt} = \alpha_1\alpha_2\left(\dfrac{\rho_2 c_2^2 - \rho_1 c_1^2}{\alpha_2\rho_1 c_1^2 + \alpha_1\rho_2 c_2^2}\right)\dfrac{\partial u}{\partial x} \\ \dfrac{\partial \alpha_1\rho_1}{\partial t} + \dfrac{\partial \alpha_1\rho_1 u}{\partial x} = 0 \\ \dfrac{\partial \alpha_2\rho_2}{\partial t} + \dfrac{\partial \alpha_2\rho_2 u}{\partial x} = 0 \\ \dfrac{\partial \rho u}{\partial t} + \dfrac{\partial(\rho u^2 + p)}{\partial x} = 0 \\ \dfrac{\partial \rho E}{\partial t} + \dfrac{\partial(\rho E + p)u}{\partial x} = 0 \end{cases}$$

Equilibre mécanique

$$u_1 = u_2 = u$$

$$p_1 = p_2 = p$$

Variables de mélange :

$$\rho = \alpha_1\rho_1 + \alpha_2\rho_2$$

$$\rho E = \alpha_1\rho_1 E_1 + \alpha_2\rho_2 E_2$$

+ Équation d'état de mélange : $$p = p(\rho, e, \alpha_k) = \frac{\rho e - \left(\dfrac{\alpha_1\gamma_1 p_{\infty,1}}{\gamma_1 - 1} + \dfrac{\alpha_2\gamma_2 p_{\infty,2}}{\gamma_2 - 1}\right)}{\dfrac{\alpha_1}{\gamma_1 - 1} + \dfrac{\alpha_2}{\gamma_2 - 1}}$$

We will come back on thermodynamic closure in the following …

⚠ This is a mechanical equilibrium but each phase remains in thermal disequilibrium

Numerical resolutions: issues

1) Volume fraction positivity: How to treat the non-conservative term in the volume fraction equation when shocks or strong rarefaction waves are present ?

$$\frac{\partial \alpha_1}{\partial t} + \vec{u}.\vec{\nabla}\alpha_1 = \frac{(\rho_2 c_2^2 - \rho_1 c_1^2)}{\dfrac{\rho_1 c_1^2}{\alpha_1} + \dfrac{\rho_2 c_2^2}{\alpha_2}} \vec{\nabla}.\vec{u}$$

Difficulty to guarantee that $0 < \alpha_1 < 1$

2) The volume fraction varies across acoustic waves: Riemann solver difficult to construct.

6+1-equation model

- Previous difficulties are circumvented using a pressure non-equilibrium model

$$\frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} = \mu(p_1 - p_2)$$

$$\frac{\partial \alpha_1\rho_1}{\partial t} + \frac{\partial \alpha_1\rho_1 u}{\partial x} = 0$$

$$\frac{\partial \alpha_2\rho_2}{\partial t} + \frac{\partial \alpha_2\rho_2 u}{\partial x} = 0$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + (\alpha_1 p_1 + \alpha_2 p_2)}{\partial x} = 0$$

$$\frac{\partial \alpha_1\rho_1 e_1}{\partial t} + \frac{\partial \alpha_1\rho_1 e_1 u}{\partial t} + \alpha_1 p_1 \frac{\partial u}{\partial x} = -p_I \mu(p_1 - p_2)$$

$$\frac{\partial \alpha_2\rho_2 e_2}{\partial t} + \frac{\partial \alpha_2\rho_2 e_2 u}{\partial t} + \alpha_2 p_2 \frac{\partial u}{\partial x} = p_I \mu(p_1 - p_2)$$

$$\rho = \alpha_1\rho_1 + \alpha_2\rho_2$$

$$\rho E = \alpha_1\rho_1 E_1 + \alpha_2\rho_2 E_2$$

- The pressure equilibrium 5-equation model is obtained from this 6-equation model in the asymptotic limit of stiff pressure relaxation coefficient,
- The speed of sound is monotonic,

$$c_f^2 = Y_1 c_1^2 + Y_2 c_2^2$$

- The volume fraction is constant through right- and left-facing waves when relaxation effects are absent $(\mu=0)$.

6 equations + 1 redundant equation (coming from the summation of energies):

$$\frac{\partial \rho(Y_1 e_1 + Y_2 e_2 + \frac{1}{2}u^2)}{\partial t} + \frac{\partial u\left(\rho(Y_1 e_1 + Y_2 e_2 + \frac{1}{2}u^2) + (\alpha_1 p_1 + \alpha_2 p_2)\right)}{\partial x} = 0$$

3-step methods

a) The (6+1)-equation model is solved without relaxation effects: Godunov-type scheme,
b) Stiff pressure relaxation procedure,
c) Energies reset (in order to ensure energy conservation)

⇒ The 5-equation model is solved

1st step: Godunov-type scheme

- Without relaxation terms, the 6+1 equation model becomes:

$$\frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} = 0$$

$$\frac{\partial \alpha_1\rho_1}{\partial t} + \frac{\partial \alpha_1\rho_1 u}{\partial x} = 0$$

$$\frac{\partial \alpha_2\rho_2}{\partial t} + \frac{\partial \alpha_2\rho_2 u}{\partial x} = 0$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + (\alpha_1 p_1 + \alpha_2 p_2)}{\partial x} = 0$$

$$\frac{\partial \alpha_1\rho_1 e_1}{\partial t} + \frac{\partial \alpha_1\rho_1 e_1 u}{\partial t} + \alpha_1 p_1 \frac{\partial u}{\partial x} = 0$$

$$\frac{\partial \alpha_2\rho_2 e_2}{\partial t} + \frac{\partial \alpha_2\rho_2 e_2 u}{\partial t} + \alpha_2 p_2 \frac{\partial u}{\partial x} = 0$$

An advection equation

$$\frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} = 0$$

+ A conservative part

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0$$

with

$$U = \left((\alpha\rho)_1,\ \ (\alpha\rho)_2,\ \ \rho u,\ \ \rho E\right)^T$$

$$F = \left((\alpha\rho)_1 u,\ \ (\alpha\rho)_1 u,\ \ \rho u^2 + p,\ \ (\rho E + p)u\right)^T$$

+ A non conservative one

$$\frac{\partial \alpha_1\rho_1 e_1}{\partial t} + \frac{\partial \alpha_1\rho_1 e_1 u}{\partial t} + \alpha_1 p_1 \frac{\partial u}{\partial x} = 0$$

$$\frac{\partial \alpha_2\rho_2 e_2}{\partial t} + \frac{\partial \alpha_2\rho_2 e_2 u}{\partial t} + \alpha_2 p_2 \frac{\partial u}{\partial x} = 0$$

1^{st} step: Godunov-type scheme

Godunov scheme for advection equation

$$\frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} = 0 \quad \Longrightarrow \quad \alpha_{1_i}^{n+1} = \alpha_{1_i}^{n} - \frac{\Delta t}{\Delta x}\left((u\alpha_1)^*_{i+1/2} - (u\alpha_1)^*_{i-1/2} - \alpha_{1_i}^{n}(u^*_{i+1/2} - u^*_{i-1/2})\right)$$

+ Godunov scheme for conservative equations

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0 \quad \Longrightarrow \quad U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}\left(F^*(U_i^n, U_{i+1}^n) - F^*(U_{i-1}^n, U_i^n)\right)$$

with

$$U = \left((\alpha\rho)_1,\ (\alpha\rho)_2,\ \rho u,\ \rho E\right)^T$$

$$F = \left((\alpha\rho)_1 u,\ (\alpha\rho)_1 u,\ \rho u^2 + p,\ (\rho E + p)u\right)^T$$

+ A non conventional scheme for non conservative internal energies equations

$$\frac{\partial \alpha_1\rho_1 e_1}{\partial t} + \frac{\partial \alpha_1\rho_1 e_1 u}{\partial t} + \alpha_1 p_1 \frac{\partial u}{\partial x} = 0$$

$$\frac{\partial \alpha_2\rho_2 e_2}{\partial t} + \frac{\partial \alpha_2\rho_2 e_2 u}{\partial t} + \alpha_2 p_2 \frac{\partial u}{\partial x} = 0$$

$$\Longrightarrow \quad (\alpha\rho e)_{ki}^{n+1} = (\alpha\rho e)_{ki}^{n} - \frac{\Delta t}{\Delta x}\left((\alpha\rho e u)^*_{ki+1/2} - (\alpha\rho e u)^*_{ki-1/2} + (\alpha p)_{ki}^{n}\left(u^*_{i+1/2} - u^*_{i-1/2}\right)\right)$$

Riemann solver

$$\frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} = 0$$

$$\frac{\partial \alpha_1\rho_1}{\partial t} + \frac{\partial \alpha_1\rho_1 u}{\partial x} = 0$$

$$\frac{\partial \alpha_2\rho_2}{\partial t} + \frac{\partial \alpha_2\rho_2 u}{\partial x} = 0$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + (\alpha_1 p_1 + \alpha_2 p_2)}{\partial x} = 0$$

$$\frac{\partial \alpha_1\rho_1 e_1}{\partial t} + \frac{\partial \alpha_1\rho_1 e_1 u}{\partial t} + \alpha_1 p_1 \frac{\partial u}{\partial x} = 0$$

$$\frac{\partial \alpha_2\rho_2 e_2}{\partial t} + \frac{\partial \alpha_2\rho_2 e_2 u}{\partial t} + \alpha_2 p_2 \frac{\partial u}{\partial x} = 0$$

$$\frac{\partial W}{\partial t} + A(W)\frac{\partial W}{\partial x} = 0$$

$$W = (\alpha_1, s_1, s_2, u, p_1, p_2)^T$$

$$A(W) = \begin{pmatrix} u & 0 & 0 & 0 & 0 & 0 \\ 0 & u & 0 & 0 & 0 & 0 \\ 0 & 0 & u & 0 & 0 & 0 \\ \frac{p_1 - p_2}{\rho} & 0 & 0 & u & \frac{\alpha_1}{\rho} & \frac{\alpha_2}{\rho} \\ 0 & 0 & 0 & \rho_1 c_1^2 & u & 0 \\ 0 & 0 & 0 & \rho_2 c_2^2 & 0 & u \end{pmatrix}$$

3 waves speeds $\lambda^+ = u + c_f \;,\; \lambda^- = u - c_f \;,\; \lambda^0 = u$

with $c_f{}^2 = Y_1 c_1^2 + Y_2 c_2^2$

Riemann problem solution

$$u^* = \frac{p_L - p_R + Z_R u_R + Z_L u_L}{Z_R + Z_L}$$

$$p^* = \frac{Z_R p_L + Z_L p_R + Z_R Z_L (u_L - u_R)}{Z_R + Z_L}$$

$$\alpha_{kL}^* = \alpha_{kL}$$

$$\alpha_{kR}^* = \alpha_{kR}$$

$$s_{kR}^* = s_{kR}$$

$$s_{kL}^* = s_{kL}$$

with

$$p = \alpha_1 p_1 + \alpha_2 p_2$$

$$\rho = \alpha_1 \rho_1 + \alpha_2 \rho_2$$

$$Z = \rho c$$

$$c_f^2 = Y_1 c_1^2 + Y_2 c_2^2$$

→ Similar to Euler Riemann solver

2^{nd} step: Pressure relaxation

Already solved by the 1^{st} step

$\frac{\partial \alpha_1}{\partial t} + u\frac{\partial \alpha_1}{\partial x} =$	$\mu(p_1 - p_2)$
$\frac{\partial \alpha_1\rho_1}{\partial t} + \frac{\partial \alpha_1\rho_1 u}{\partial x} = 0$	
$\frac{\partial \alpha_2\rho_2}{\partial t} + \frac{\partial \alpha_2\rho_2 u}{\partial x} = 0$	
$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + (\alpha_1 p_1 + \alpha_2 p_2)}{\partial x} = 0$	
$\frac{\partial \alpha_1\rho_1 e_1}{\partial t} + \frac{\partial \alpha_1\rho_1 e_1 u}{\partial t} + \alpha_1 p_1 \frac{\partial u}{\partial x} =$	$-p_I\mu(p_1 - p_2)$
$\frac{\partial \alpha_2\rho_2 e_2}{\partial t} + \frac{\partial \alpha_2\rho_2 e_2 u}{\partial t} + \alpha_2 p_2 \frac{\partial u}{\partial x} =$	$p_I\mu(p_1 - p_2)$

$$\frac{\partial \alpha_1}{\partial t} = \mu(p_1 - p_2)$$
$$\frac{\partial \alpha_1\rho_1 e_1}{\partial t} = -p_I\mu(p_1 - p_2)$$
$$\frac{\partial \alpha_2\rho_2 e_2}{\partial t} = p_I\mu(p_1 - p_2)$$
$$\frac{\partial \alpha_1\rho_1}{\partial t} = 0$$
$$\frac{\partial \alpha_2\rho_2}{\partial t} = 0$$
$$\frac{\partial \rho u}{\partial t} = 0$$
$$\frac{\partial \rho E}{\partial t} = 0$$

Relaxation system

2nd step: Pressure relaxation

$$\frac{\partial \alpha_1}{\partial t} = \mu(p_1 - p_2)$$
$$\frac{\partial \alpha_1 \rho_1 e_1}{\partial t} = -p_I \mu(p_1 - p_2)$$
$$\frac{\partial \alpha_2 \rho_2 e_2}{\partial t} = p_I \mu(p_1 - p_2)$$

$$\frac{de_1}{dt} + p_I \frac{dv_1}{dt} = 0$$
$$\frac{de_2}{dt} + p_I \frac{dv_2}{dt} = 0$$

time integration

$$\boxed{e_k - e_k^0 + \hat{p}_{Ik}\left(v_k - v_k^0\right) = 0}$$

$$\hat{p}_{Ik} = \frac{1}{v_k - v_k^0} \int_0^{\Delta t} p_I \frac{dv_k}{dt} dt = 0$$

$$\sum_k \Rightarrow Y_1 e_1 - Y_1 e_1^0 + Y_2 e_2 - Y_2 e_2^0 + \hat{p}_{I1}\left(Y_1 v_1 - Y_1 v_1^0\right) + \hat{p}_{I2}\left(Y_2 v_2 - Y_2 v_2^0\right) = 0$$

$$e - e^0 + \left(\hat{p}_{I1} - \hat{p}_{I2}\right)\left(Y_1 v_1 - Y_1 v_1^0\right) = 0 \quad \Rightarrow \quad \hat{p}_{I1} = \hat{p}_{I2} = \hat{p}_I$$

Using mass equations

Possible choice $\hat{p}_I = p$

Entropy inequality is verified

2^{nd} step: Pressure relaxation

Using EOS :

$$e_1(p, v_1) - e_1^0(p_1^0, v_1^0) + p(v_1 - v_1^0) = 0$$

$$e_2(p, v_2) - e_2^0(p_2^0, v_2^0) + p(v_2 - v_2^0) = 0$$

$$v_1 = v_1(p)$$

$$v_2 = v_2(p)$$

Closure relation: $\alpha_1 + \alpha_2 = 1 \Leftrightarrow (\alpha\rho)_1^0 v_1(p) + (\alpha\rho)_2^0 v_2(p) = 1$

Zero function to solve $f(p) = (\alpha\rho)_1^0 v_1(p) + (\alpha\rho)_2^0 v_2(p) - 1$

Then, we determine: $p \rightarrow v_k(p) \rightarrow \alpha_k = (\alpha\rho)_k v_k$

3^{th} step: Internal energy reset

- We have in the 2^{nd} step determined: p, v_k, α_k
- We forget the relaxed pressure but keep volume fractions:

$$\cancel{p} \longrightarrow \alpha_k$$

- It is then possible to determine mixture pressure by the mixture EOS. By this way, energy conservation is ensured:

$$p_{new}(\rho, e, \alpha_1, \alpha_2) = \frac{\rho e - \left(\frac{\alpha_1 \gamma_1 p_{\infty 1}}{\gamma_1 - 1} + \frac{\alpha_2 \gamma_2 p_{\infty 2}}{\gamma_2 - 1} \right)}{\frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1}}$$

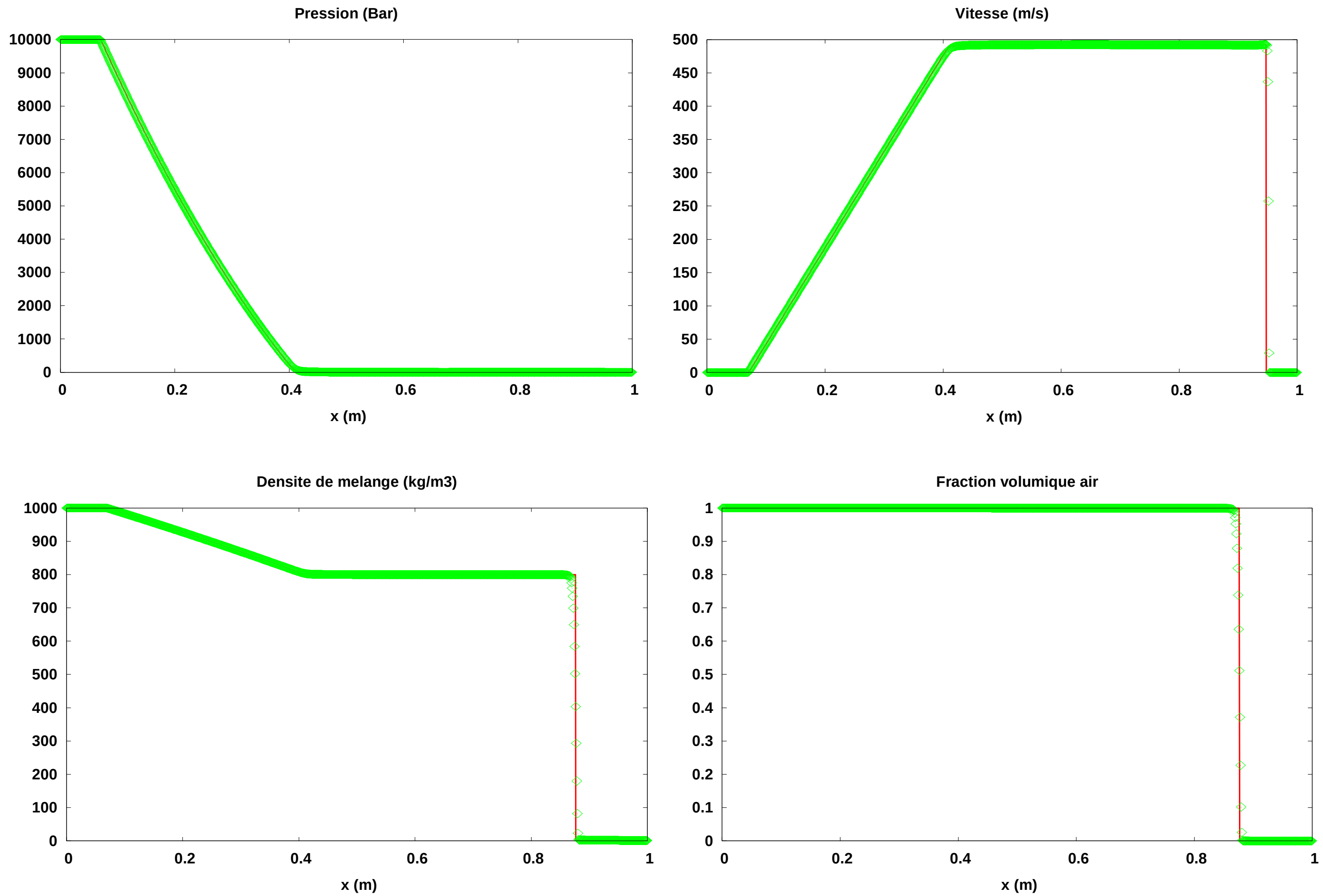
- Phasic EOS permits to reset internal energies:

$$e_k = e_k(p_{new}, \alpha_k \rho_k, \alpha_k)$$

Conservative and good treatment of wave dynamics from both sides of the interface

1D example:
Water-Air shock tube

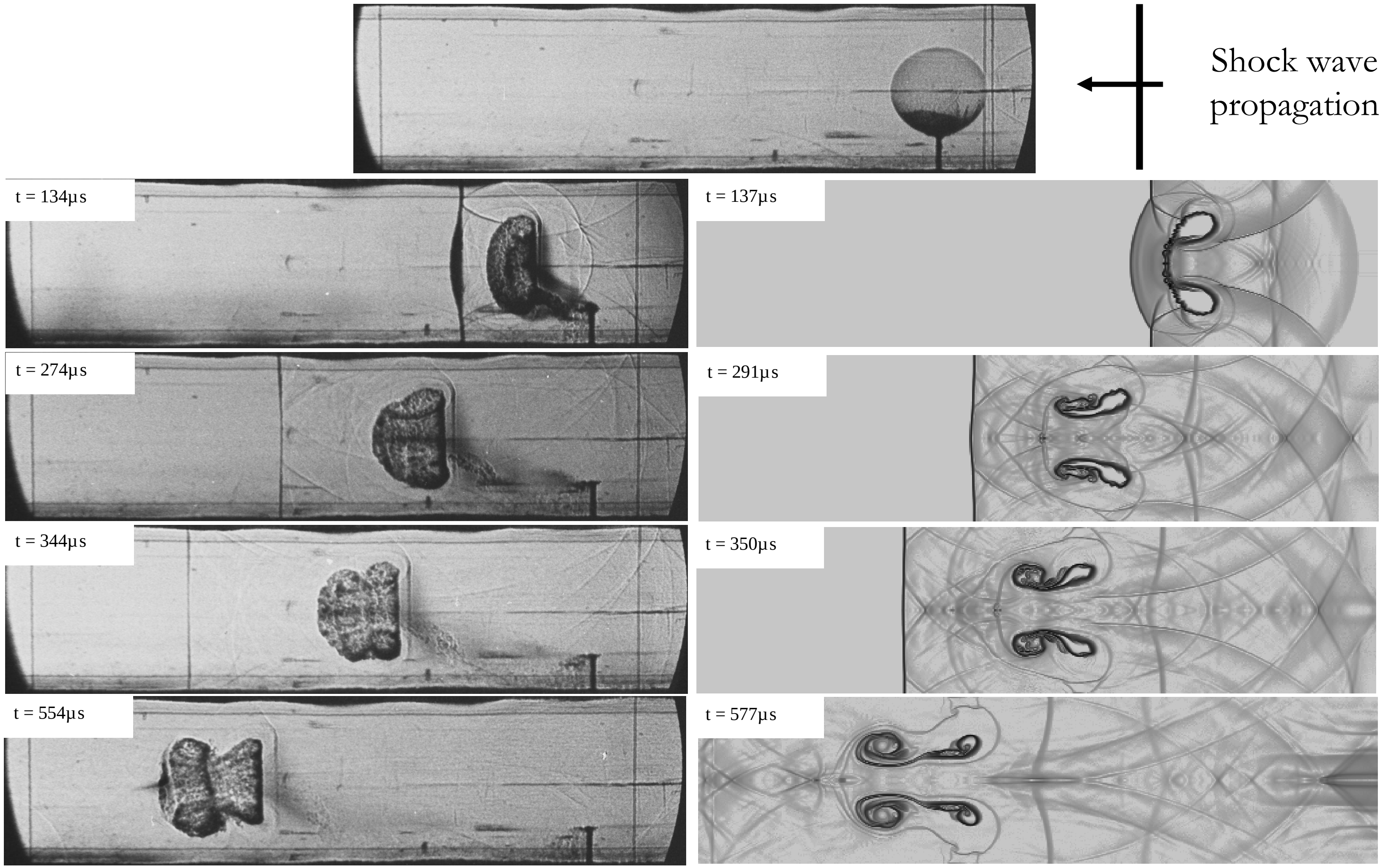
EAU	AIR
$P_{eau} = 10\,000$ bar $\varrho_{eau} = 1000\ kg/m^3$	$P_{eau} = 1$ bar $\varrho_{eau} = 1\ kg/m^3$



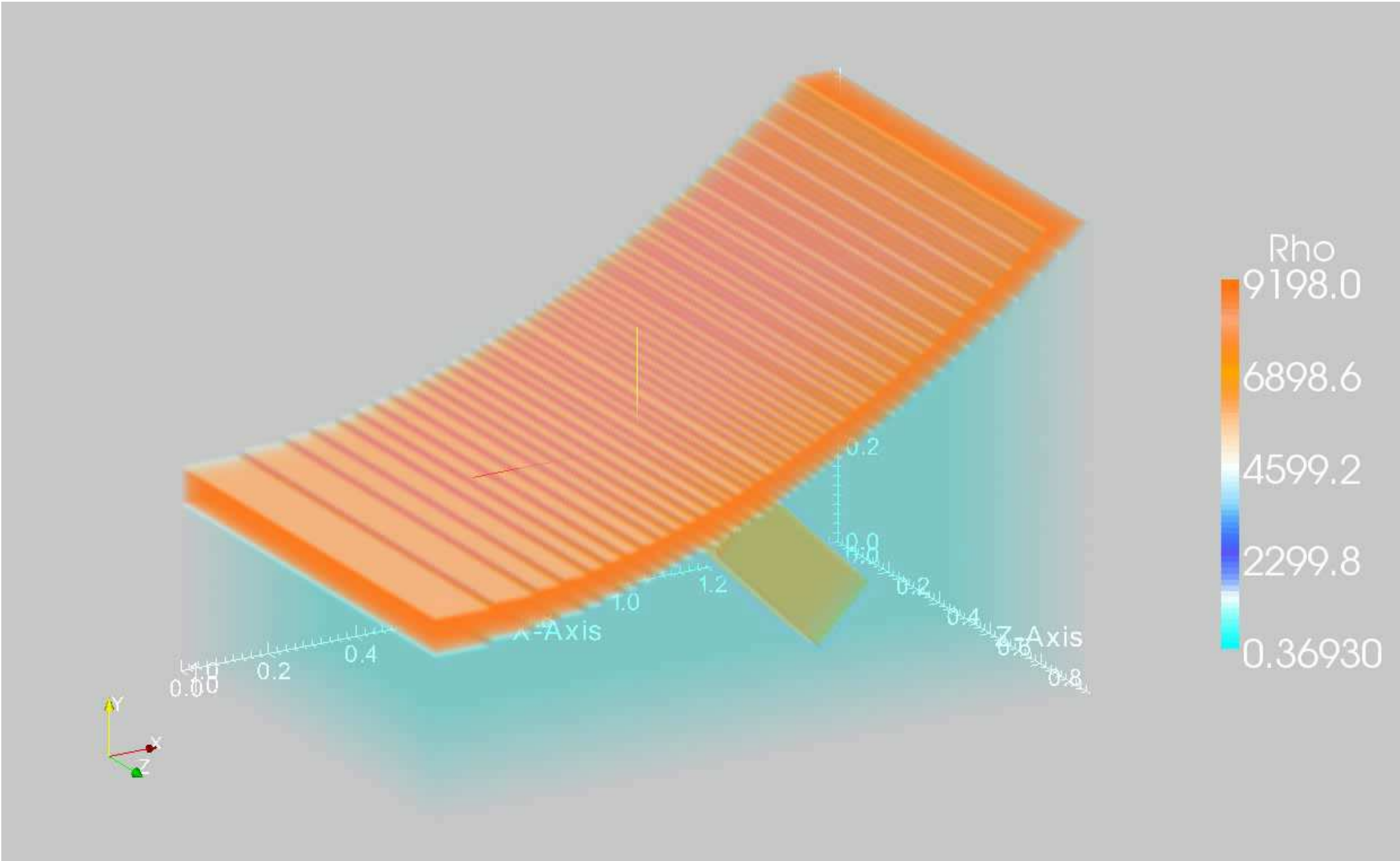
Solution exacte

Solution numérique

Résultats 2D - Expériences IUSTI (Layes, Jourdan, Houas)

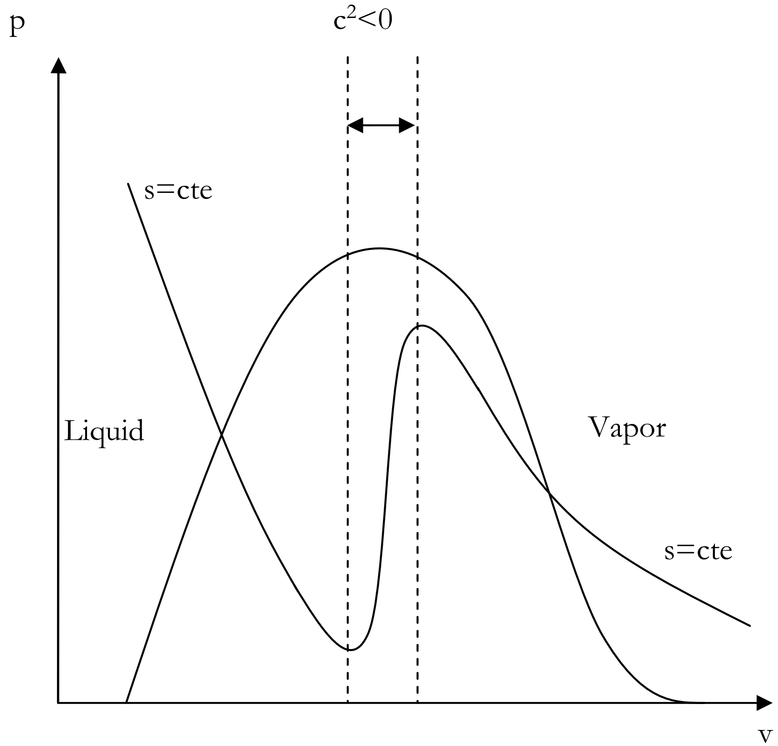


3D example : Missile impact on a metal plate



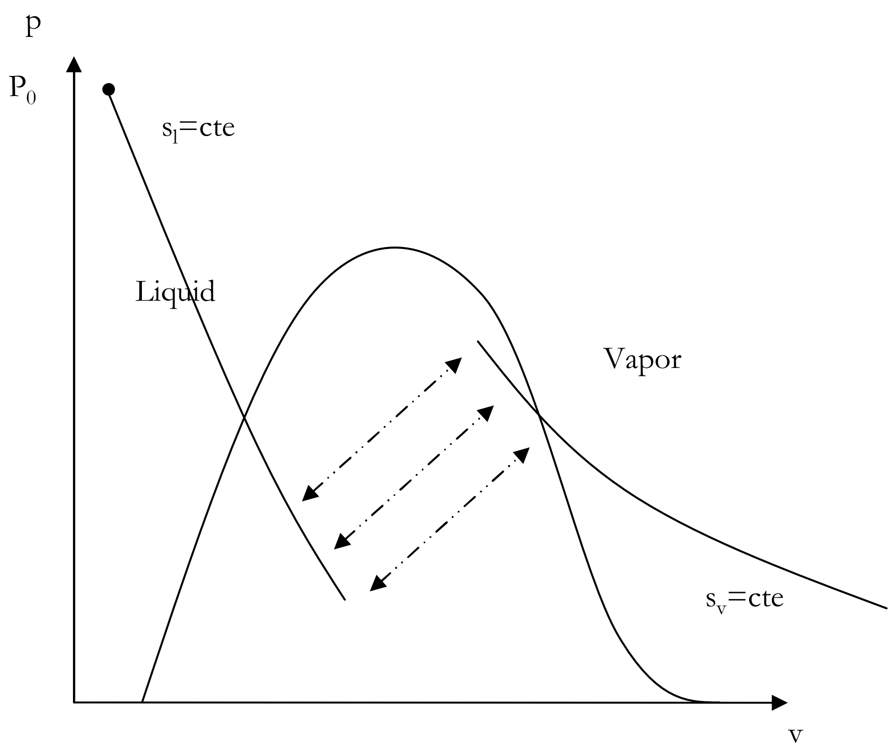
Topic 3 : Phase transition with the 5-equation model

Why is the 5-equation model a good candidate for phase transition ?



Thermodynamic path using the Van de Waals representation

$$c^2 = -v^2 \left.\frac{\partial p}{\partial v}\right)_{s=cte} < 0$$



Kinetic path with the 5-equation model and two separate EOS

Liquid and Vapor isentropes are linked by a kinetic process

Hyperbolicity is lost into the phase diagram

Hyperbolicity is preserved in the entire domain

Phase transition modeling

1) Mass transfer modifies mass equations:

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \mathrm{div}(\alpha_1 \rho_1 \vec{u}) = \dot{m}_1 = \rho \dot{Y}_1$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \mathrm{div}(\alpha_2 \rho_2 \vec{u}) = -\dot{m}_1 = -\rho \dot{Y}_1$$

Avec $\dot{Y}_1 = \frac{dY_1}{dt} = \frac{d}{dt}\left(\frac{\alpha_1 \rho_1}{\rho}\right)$

2) Volume fractions change during phase transition:

$$\frac{d\alpha_1}{dt} = K\mathrm{div}(\vec{u}) + AQ_1 + \frac{\dot{m}_1}{\rho_I}$$

This « interfacial » density has to be determined in order to close the model.

Two-phase model for interface problems with phase transition

$$\frac{\partial \alpha_1\rho_1}{\partial t} + \mathrm{div}(\alpha_1\rho_1\vec{u}) = \rho\nu(g_2 - g_1)$$

$$\frac{\partial \alpha_2\rho_2}{\partial t} + \mathrm{div}(\alpha_2\rho_2\vec{u}) = -\rho\nu(g_2 - g_1)$$

$$\frac{\partial \rho\vec{u}}{\partial t} + \mathrm{div}(\rho\vec{u}\otimes\vec{u}) + \vec{\nabla}(p) = 0$$

$$\frac{\partial \rho E}{\partial t} + \mathrm{div}((\rho E + p)\vec{u}) = 0$$

$$\frac{\partial \alpha_1}{\partial t} + \vec{u}.\vec{\nabla}(\alpha_1) = \frac{(\rho_2 c_2^2 - \rho_1 c_1^2)}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}}\mathrm{div}(\vec{u}) + \rho\nu(g_2 - g_1)\frac{\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2}}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}} + H(T_2 - T_1)\frac{\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2}}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}}$$

Entropy analysis for each phase and for the mixture

Mechanical relaxation — Mass transfer — Heat transfer

Lois d'état :

$$\begin{cases} e_1(\rho_1, p) = \dfrac{p + \gamma_1 p_{\infty,1}}{(\gamma_1 - 1)\rho_1} + e_{0,1} & \text{For the liquid} \\ e_2(\rho_2, p) = \dfrac{p}{(\gamma_2 - 1)\rho_2} + e_{0,2} & \text{For vapor} \end{cases}$$

$$\rho e = \alpha_1\rho_1 e_1 + \alpha_2\rho_2 e_2$$

$$p(\rho, e, \alpha_1, \alpha_2) = \frac{\rho e - \left(\frac{\alpha_1\gamma_1 p_{\infty 1}}{\gamma_1 - 1} + \frac{\alpha_2\gamma_2 p_{\infty 2}}{\gamma_2 - 1}\right)}{\frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1}}$$

$$\text{Kinetic parameters : } \nu, H = \begin{cases} +\infty & \text{at interfaces (thermodynamical equilibrium)} \\ 0 & \text{elsewhere (metastable state)} \end{cases}$$

Thermodynamic closure

Assumption : Each fluid is governed by the stiffened gas EOS:

$$p(\rho, e) = \underbrace{(\gamma - 1)\,\rho\,(e - q)}_{\text{Repulsive effects (gas, liquids and solids)}}\ \underbrace{-\,\gamma p_\infty}_{\text{Attractive effects (liquids and solids)}}$$

Repulsive effects (gas, liquids and solids)	Attractive effects (liquids and solids)

Other useful forms for the SG EOS :

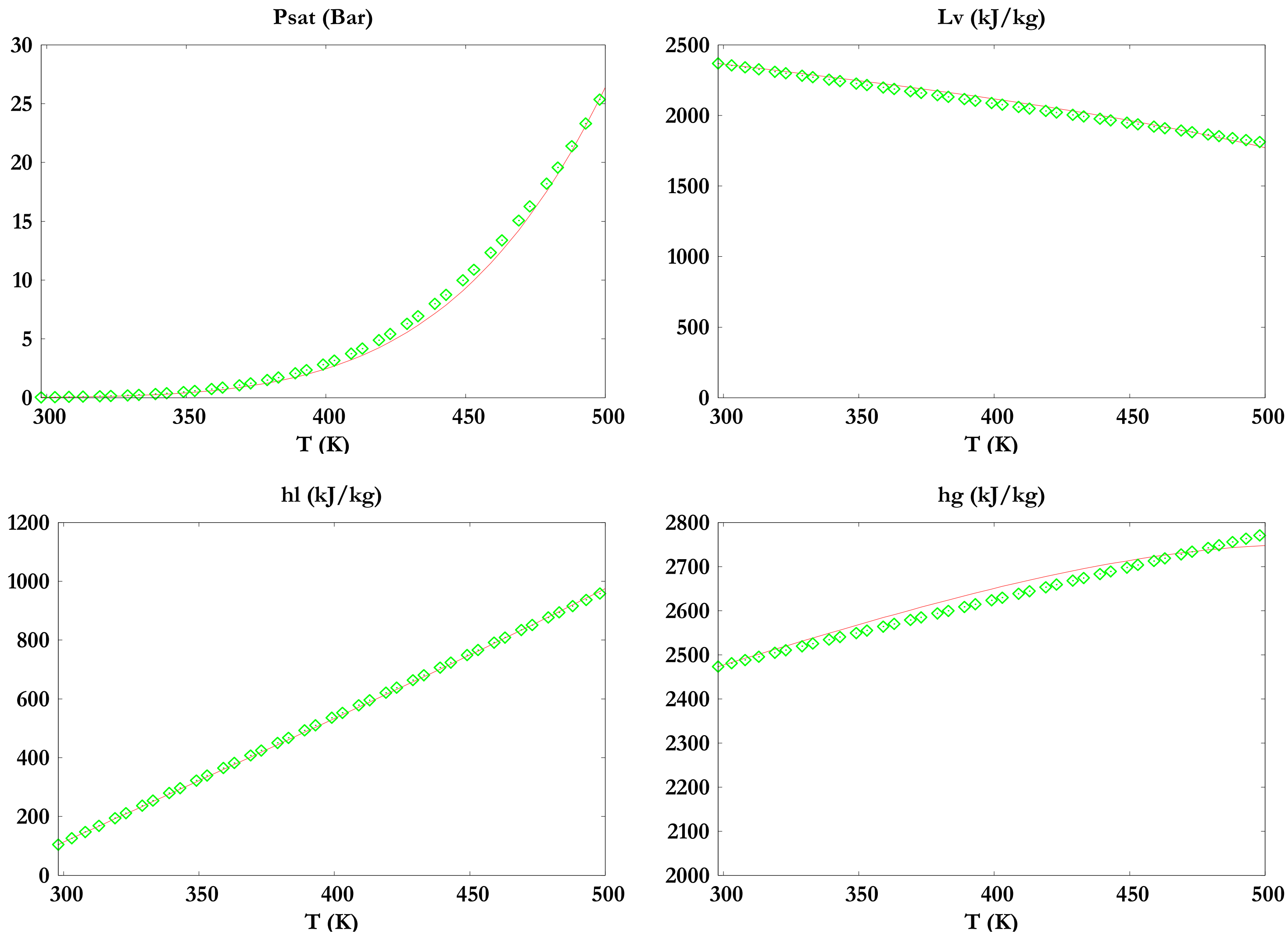
$$h(T) = \gamma C_V T + q$$

$$s(p, T) = C_V \ln \frac{T^\gamma}{(p + p_\infty)^{\gamma - 1}} + q'$$

$$g(p, T) = (\gamma C_V - q')T - C_V T \ln \frac{T^\gamma}{(p + p_\infty)^{\gamma - 1}} + q$$

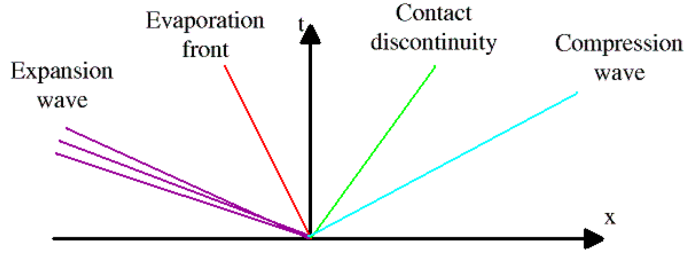
For each fluid EOS : 5 parameters to determine : $\gamma, P_\infty, C_V, q, q'$

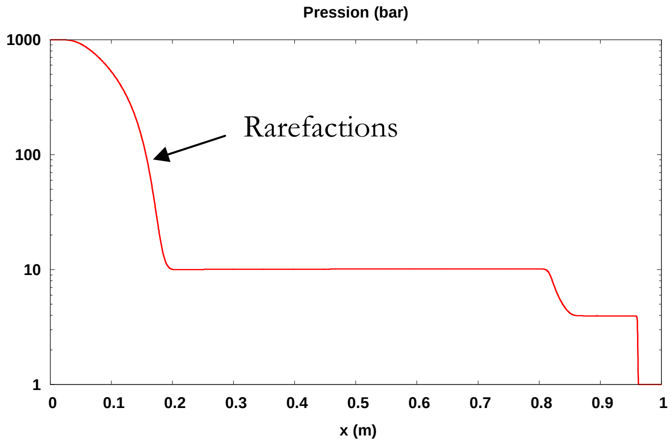
Saturation curves for liquid water and vapor water

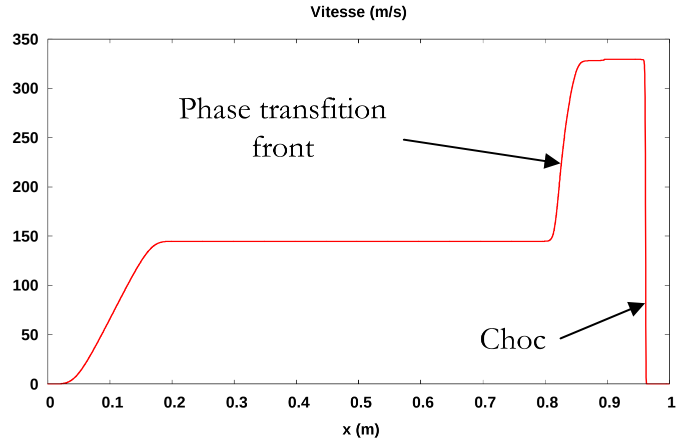


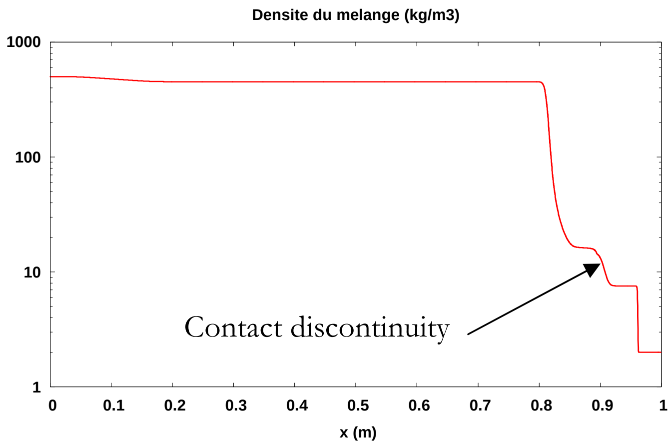
Le Métayer et al., Int. Journal of Thermal Sciences, 2004

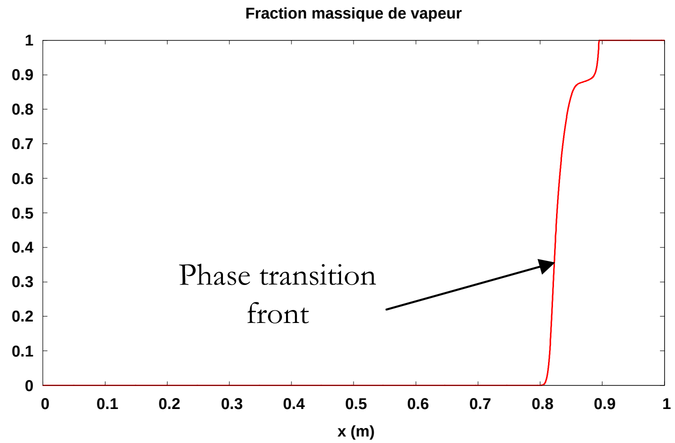
Dodécane liquide	Dodécane vapeur
$P_{liquide}$ = 1 000 bar $\rho_{liquide}$ = 500 kg/m^3	P_{vapeur} = 1 bar ρ_{vapeur} = 2 kg/m^3





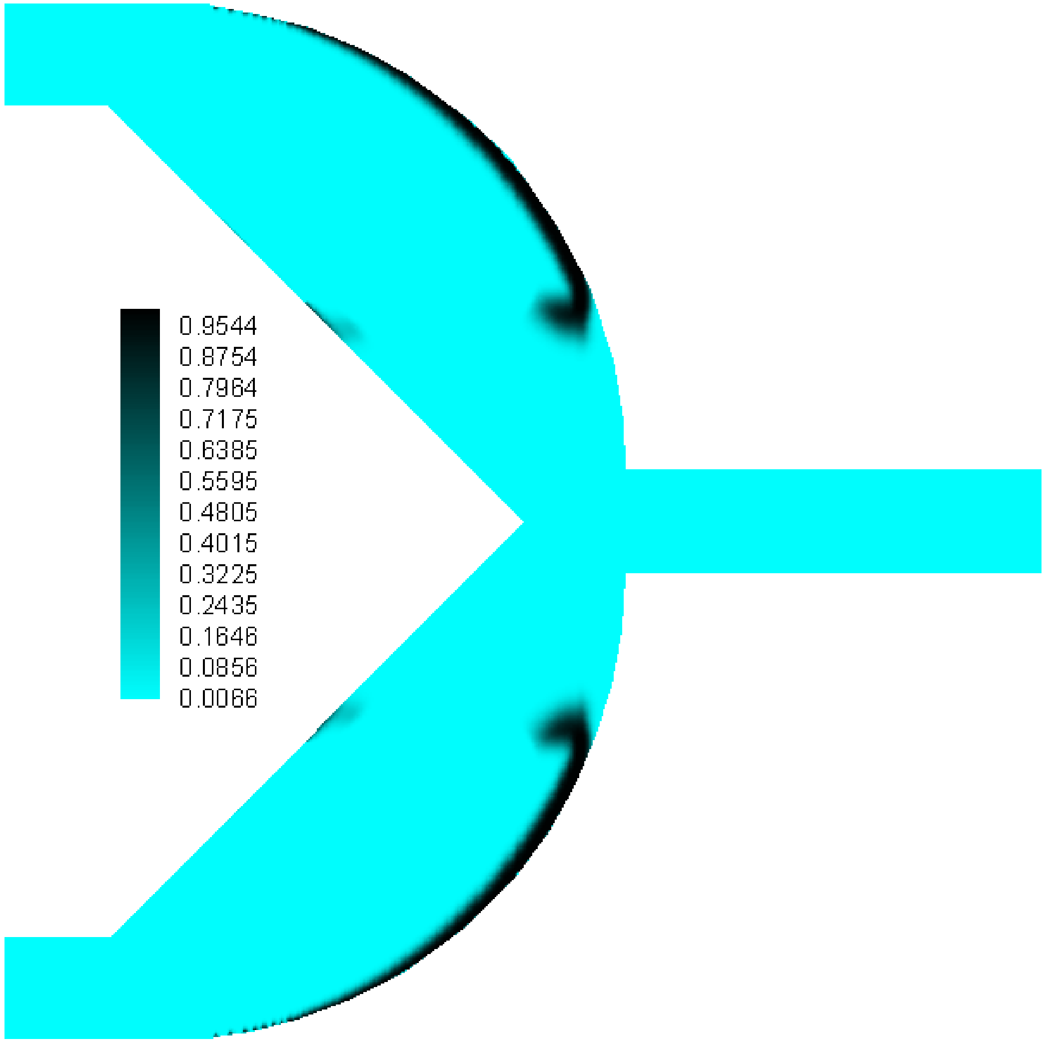




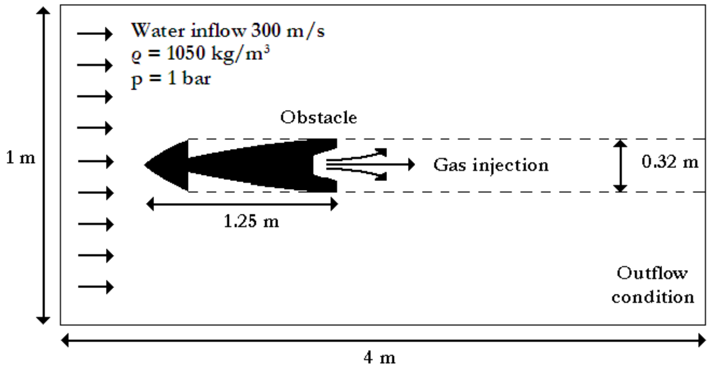


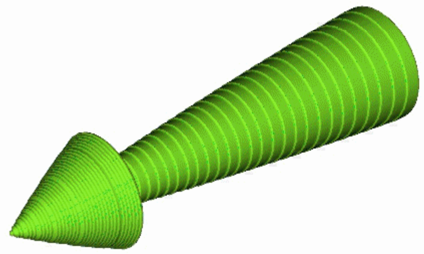
Saurel, Petitpas & Abgrall, JFM, 2008

High pressure diesel injector



High speed motion under water



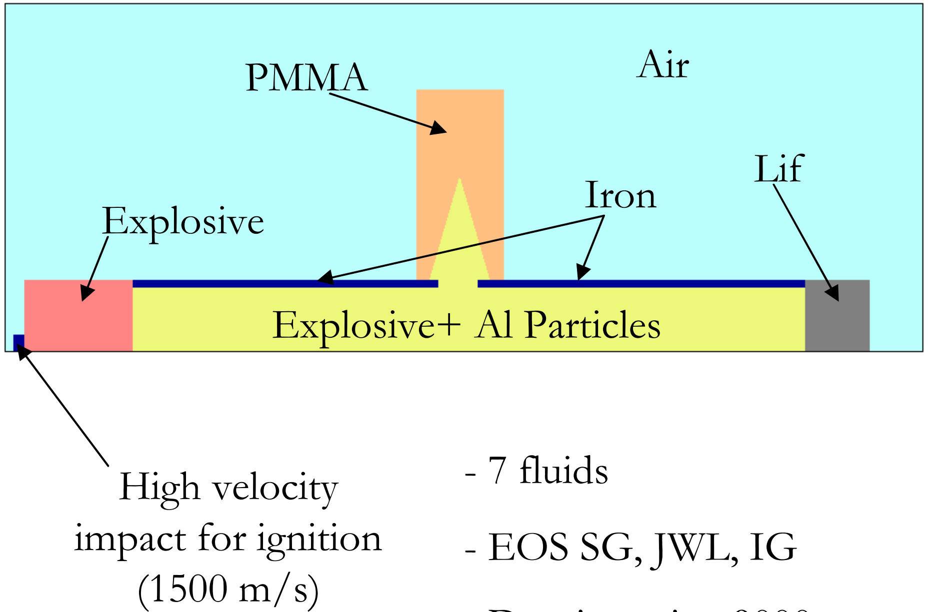


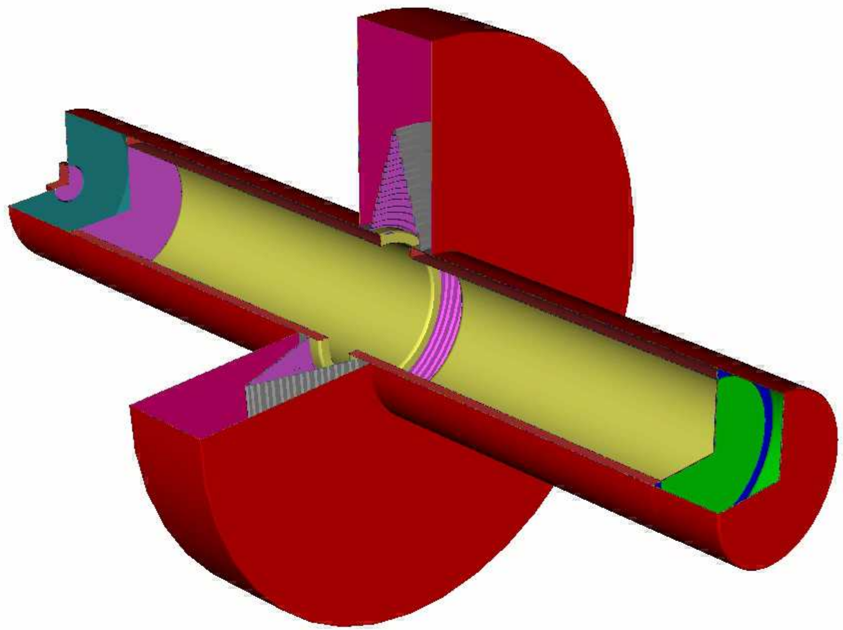
Topic 4 : Some possible extensions

- Capillary effects (Perigaud & Saurel, 2005)
- Detonation (Petitpas et al. 2009)
- Gravity, heat conduction, viscosity, turbulence, etc.

Detonation problems

Russian experiences done for the DGA

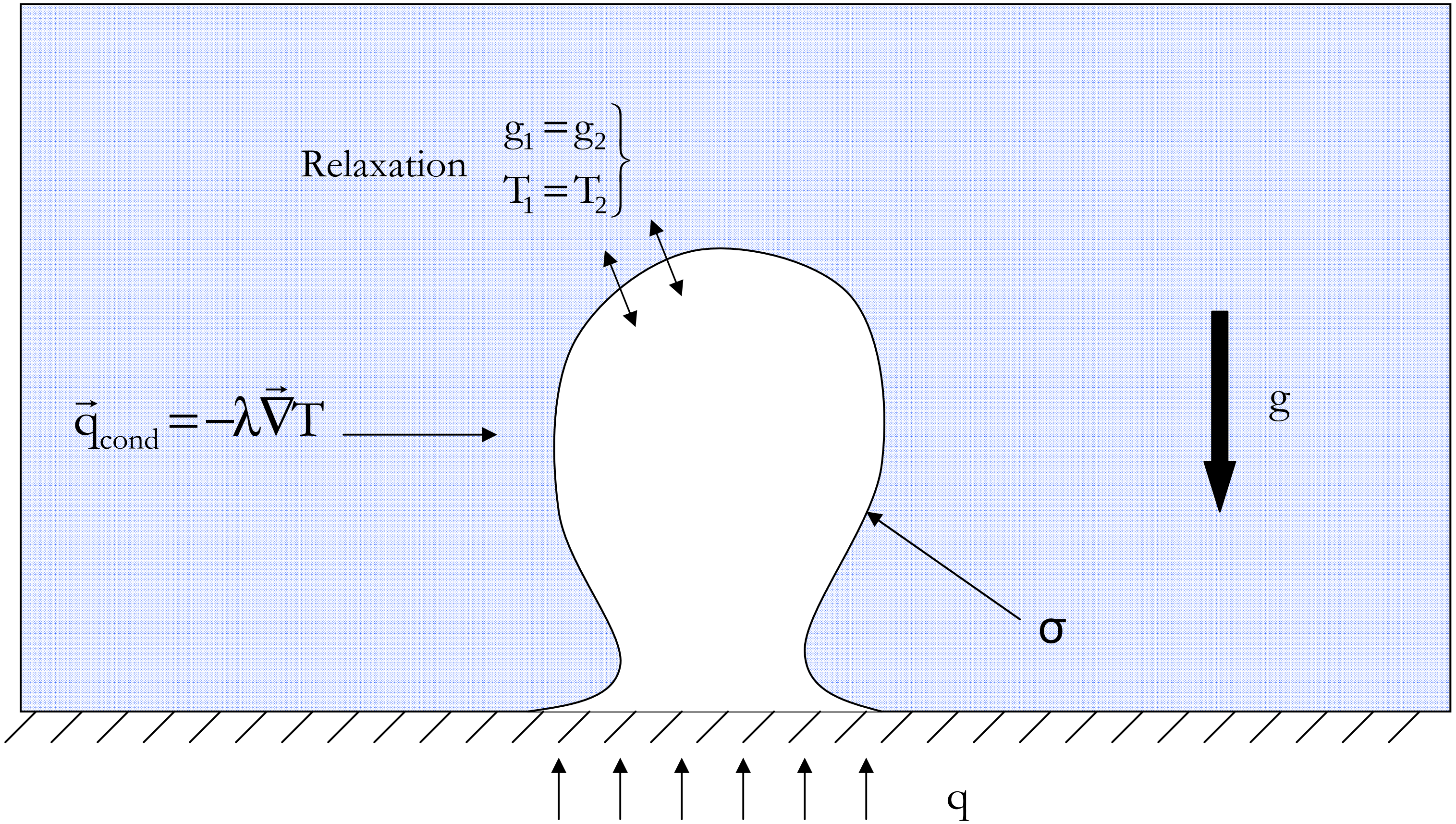




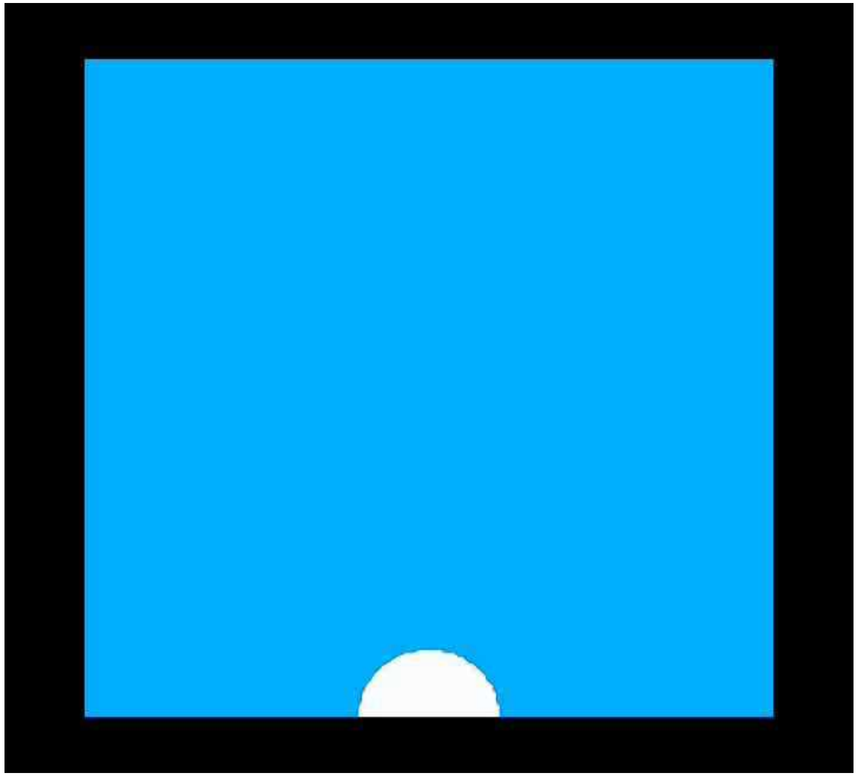
- 7 fluids
- EOS SG, JWL, IG
- Density ratio : 9000

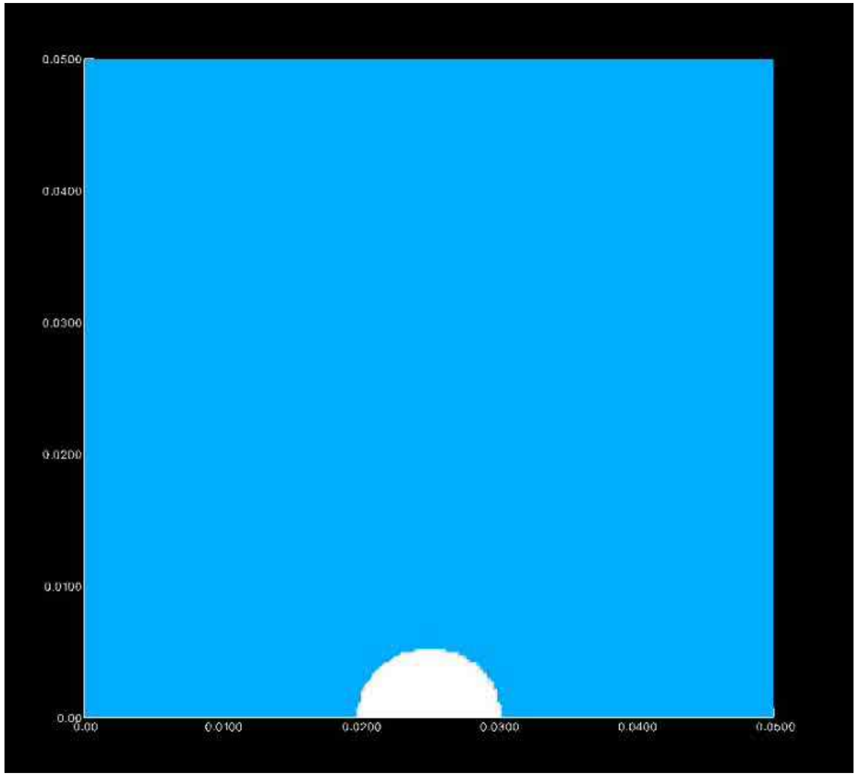
Ebullition crisis simulation

Many physical ingredients are required



Bubble growth






THE
END