Numerical simulation of compressible two-phase flows

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Flows zoology – Position of the topic

- Compressibles
  - Single phase
  - Single velocity
  - Interface problems resolution
  - Two-phase mixtures in mechanical equilibrium

- Incompressibles
  - Multi-phase
  - Multi-velocity
  - Non equilibrium two-phase mixtures
  - General models
Single velocity flows / Interface problems

Single contact interface

Evaporation front

Steam

Liquid

Detonation
Some words about discretisation scales

“Macro” scale: Multi-velocity flow

An averaged model with two velocities is needed

« Micro » scale: Single velocity flow

A reduced model for interface problems is enough
On the choice of the method

- **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

![Diagram showing volume fraction of phase 1](image)

- Zone de mélange = interface
- \( \alpha_{\text{liq}} > 1 - \varepsilon \)
- \( \alpha_{\text{liq}} < \varepsilon \)
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:

$$\frac{\partial \alpha_k}{\partial t} + \tilde{\sigma} \cdot \nabla \alpha_k = \mu (P_k - P_k')$$

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

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

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

$$\tilde{\sigma} = \tilde{u}_2$$ and $$P_1 = P_1$$

Baer & Nunziato (1986)

$$\tilde{\sigma} = \frac{Z_1 \tilde{u}_1 + Z_2 \tilde{u}_2}{Z_1 + Z_2}$$ and $$P_1 = \frac{Z_1 P_2 + Z_2 P_1}{Z_1 + Z_2}$$

Saurel & al. (2003)

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 useless 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:

\[ \lambda, \mu = 1/\varepsilon \rightarrow \infty \quad \text{Relaxation parameters tend to infinity} \]

\[ f = f^0 + \varepsilon f^1 \quad \text{Each flow variable is supporting small variation around an equilibrium state} \]
The diffuse interface model (5-equation model)

\[
\begin{aligned}
\frac{d\alpha_1}{dt} &= \alpha_1 \alpha_2 \left( \frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\alpha_2 \rho_1 c_1^2 + \alpha_1 \rho_2 c_2^2} \right) \frac{\partial u}{\partial x} \\
\rho_1 \frac{\partial \alpha_1 \rho_1}{\partial t} + \rho_1 u \frac{\partial \alpha_1}{\partial x} &= 0 \\
\rho_2 \frac{\partial \alpha_2 \rho_2}{\partial t} + \rho_2 u \frac{\partial \alpha_2}{\partial x} &= 0 \\
\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} &= 0 \\
\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E + p) u}{\partial x} &= 0 \\
\rho e &- \left( \frac{\alpha_1 \gamma_1 p_{\infty,1} + \alpha_2 \gamma_2 p_{\infty,2}}{\gamma_1 - 1 + \frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1}} \right)
\end{aligned}
\]

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 :

\[ p = p(\rho, e, \alpha_k) = \frac{\alpha_1 \gamma_1 p_{\infty,1} + \alpha_2 \gamma_2 p_{\infty,2}}{\gamma_1 - 1 + \frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1}} \]

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

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

Exemple \( K < 0 \)

Liquide : phase 1
Bulles gaz : phase 2

\[ \frac{\partial u}{\partial x} < 0 \implies \alpha_1 \text{ increases} \]

\[ \frac{\partial u}{\partial x} > 0 \implies \alpha_1 \text{ decreases} \]
- 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)

\[
\frac{1}{\rho c_w^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2}
\]
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: \( \frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{u}) = 0 \)
  - Momentum balance: \( \frac{\partial \rho \mathbf{u}}{\partial t} + \text{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \text{grad}(P) = 0 \)
  - Total energy balance: \( \frac{\partial \rho E}{\partial t} + \text{div}((\rho E + P)\mathbf{u}) = 0 \)

- 1D simplification:
  \[
  \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0 \\
  \frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + P}{\partial x} = 0 \\
  \frac{\partial \rho E}{\partial t} + \frac{\partial u(\rho E + P)}{\partial x} = 0
  \]

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = 0 \\
\mathbf{U} = (\rho, \rho u, \rho E)^T \\
\mathbf{F} = (\rho u, \rho u^2 + P, u(\rho E + P))^T
\]
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**

<table>
<thead>
<tr>
<th></th>
<th>(i-1)</th>
<th>(i)</th>
<th>(i+1)</th>
<th>(i+2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i-1/2)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(i+1/2)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Integration on cell \(i\) over time:

\[
\int_{\Delta t} \nabla \left[ \frac{\partial U}{\partial t} + \text{div}(F) \right] dV dt = 0
\]

\[
U_{i}^{n+1} = U_{i}^{n} - \frac{\Delta t}{\Delta x} \left( F_{i+1/2}^{*} - F_{i-1/2}^{*} \right)
\]

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

At $t=0$

- The initial data are known at a given time and are constant on the right and left side.
- A discontinuity connects the two states.
- Question: How does the solution evolve at $t>0$?
The Riemann problem solution (advection)

The two possible solutions are:

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

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

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} &= 0 \\
\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + P}{\partial x} &= 0 \\
\frac{\partial \rho E}{\partial t} + \frac{\partial u(\rho E + P)}{\partial x} &= 0
\end{align*}
\]

\[
\begin{equation}
\frac{\partial W}{\partial t} + A(W) \frac{\partial W}{\partial x} = 0 \quad \text{analogue of} \quad \frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = 0
\end{equation}
\]

\[
W = (\rho, u, P)^T
\]

\[
A(W) = \begin{pmatrix}
u & \rho & 0 \\
0 & u & 1/\rho \\
0 & \rho c^2 & u
\end{pmatrix}
\]

Plays the role of a propagation velocity

The eigenvalues of A are the waves speeds:

\[
\lambda^+ = u + c \quad , \quad \lambda^- = u - c \quad , \quad \lambda^0 = u
\]
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

\[
\begin{align*}
  u^* &= \frac{p_L - p_R + Z_R u_R + Z_L u_L}{Z_R + Z_L} \\
  p^* &= \frac{Z_R p_L + Z_L p_R + Z_R Z_L (u_L - u_R)}{Z_R + Z_L} \\
  \rho_R^* &= \rho_R + \frac{p^* - p_R}{c_R^2} \\
  \rho_L^* &= \rho_L + \frac{p^* - p_L}{c_L^2}
\end{align*}
\]
Example: shock tube

P=10 000 bars
u=0 m/s
ρ=10 kg/m³

P=1 bar
u=0 m/s
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:
  Springer Verlag
The diffuse interface model (5-equation model)

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

4 conservative equations

Equilibration
t mechanics

\[ u_1 = u_2 = u \]
\[ p_1 = p_2 = p \]

Variables of mixture:

\[ \rho = \alpha_1 \rho_1 + \alpha_2 \rho_2 \]
\[ \rho E = \alpha_1 \rho_1 E_1 + \alpha_2 \rho_2 E_2 \]

\[ p = p(\rho, e, \alpha_k) = \frac{\frac{\alpha_1 \gamma_1 P_{\infty,1}}{\gamma_1 - 1} + \frac{\alpha_2 \gamma_2 P_{\infty,2}}{\gamma_2 - 1}}{\alpha_1 \gamma_1 - 1 + \alpha_2 \gamma_2 - 1} \]

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?

\[
\frac{\partial \alpha_1}{\partial t} + \vec{u} \cdot \nabla \alpha_1 = \frac{(\rho_2 c_2^2 - \rho_1 c_1^2)}{\rho_1 c_1^2 + \rho_2 c_2^2} \nabla \cdot \vec{u}
\]

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

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

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

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

\[
\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + (\alpha_1 \rho_1 + \alpha_2 \rho_2)}{\partial x} = 0
\]

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

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

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

\[
\frac{\partial \rho (Y_1 e_1 + Y_2 e_2 + \frac{1}{2} u^2)}{\partial t} + \frac{\partial \left( \rho (Y_1 e_1 + Y_2 e_2 + \frac{1}{2} u^2) + (\alpha_1 \rho_1 + \alpha_2 \rho_2) \right)}{\partial x} = 0
\]

- 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 \((\mu=0)\).
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:

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

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

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

\[ \frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + (\alpha_1 \rho_1 + \alpha_2 \rho_2)}{\partial x} = 0 \]

\[ \frac{\partial \alpha_1 \rho_1 e_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 e_1 u}{\partial t} + \alpha_1 \rho_1 \frac{\partial u}{\partial x} = 0 \]

\[ \frac{\partial \alpha_2 \rho_2 e_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 e_2 u}{\partial t} + \alpha_2 \rho_2 \frac{\partial u}{\partial x} = 0 \]

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

\[ U = (\alpha \rho)_1, \quad (\alpha \rho)_2, \quad \rho u, \quad \rho E)^r \]

\[ F = (\alpha \rho)_1 u, \quad (\alpha \rho)_2 u, \quad \rho u^2 + p, \quad (\rho E + p)u]^r \]

+ A non conservative one

\[ \frac{\partial \alpha_1 \rho_1 e_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 e_1 u}{\partial t} + \alpha_1 \rho_1 \frac{\partial u}{\partial x} = 0 \]

\[ \frac{\partial \alpha_2 \rho_2 e_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 e_2 u}{\partial t} + \alpha_2 \rho_2 \frac{\partial u}{\partial x} = 0 \]
1st step: Godunov-type scheme

Godunov scheme for advection equation
\[
\frac{\partial \alpha_1}{\partial t} + u \frac{\partial \alpha_1}{\partial x} = 0
\]
\[
\alpha_{i+1}^n = \alpha_i^n - \frac{\Delta t}{\Delta x} \left( (u \alpha_i^*)_{i+1/2} - (u \alpha_i^*)_{i-1/2} - \alpha_i^n (u_{i+1/2}^* - u_{i-1/2}^*) \right)
\]

Godunov scheme for conservative equations
\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0
\]
\[
U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x} \left( F(U_i^n, U_{i+1}^n) - F(U_{i-1}^n, U_i^n) \right)
\]
with
\[
U = ((\alpha \rho)_1, \ (\alpha \rho)_2, \ \rho u, \ \rho E)^T
\]
\[
F = ((\alpha \rho)_1 u, \ (\alpha \rho)_2 u, \ \rho u^2 + p, \ (\rho E + p)u)^T
\]

A non conventional scheme for non conservative internal energies equations
\[
\frac{\partial \alpha_1 \rho_1 e_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 e_1 u}{\partial t} + \alpha_1 \rho_1 \frac{\partial u}{\partial x} = 0
\]
\[
\frac{\partial \alpha_2 \rho_2 e_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 e_2 u}{\partial t} + \alpha_2 \rho_2 \frac{\partial u}{\partial x} = 0
\]
\[
(\alpha \rho e)_{ki}^{n+1} = (\alpha \rho e)_{ki}^n
\]
\[
- \frac{\Delta t}{\Delta x} \left( (\alpha \rho e u)_{k+i+1/2}^* - (\alpha \rho e u)_{k-i-1/2}^* + (\alpha \rho p)_{ki} (u_{i+1/2}^* - u_{i-1/2}^*) \right)
\]
Riemann solver

\[
\begin{align*}
\frac{\partial \alpha_1}{\partial t} + u \frac{\partial \alpha_1}{\partial x} &= 0 \\
\frac{\partial \alpha_1 \rho_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 u}{\partial x} &= 0 \\
\frac{\partial \alpha_2 \rho_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 u}{\partial x} &= 0 \\
\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + (\alpha_1 \rho_1 + \alpha_2 \rho_2)}{\partial x} &= 0 \\
\frac{\partial \alpha_1 \rho_1 e_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 e_1 u}{\partial t} + \alpha_1 \rho_1 \frac{\partial u}{\partial x} &= 0 \\
\frac{\partial \alpha_2 \rho_2 e_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 e_2 u}{\partial t} + \alpha_2 \rho_2 \frac{\partial u}{\partial x} &= 0 \\
\rho &= \rho_1 - \rho_2 \\
\rho &= \rho_1 e_{1}^2 u \\
\rho &= \rho_2 e_{2}^2 u \\
\frac{\partial W}{\partial t} + A(W) \frac{\partial W}{\partial x} &= 0 \\
W &= (\alpha_1, s_1, s_2, u, p_1, p_2)^T \\
A(W) &= \begin{pmatrix}
\alpha_1 & \alpha_2 \\
0 & 0 & u & 0 & 0 \\
0 & 0 & 0 & u & 0 \\
0 & 0 & 0 & \rho & \rho \\
0 & 0 & 0 & \rho & 0 \\
0 & 0 & 0 & \rho & u \\
\end{pmatrix}
\end{align*}
\]

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

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

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

\[ \alpha_{kL}^* = \alpha_{kL} \]

\[ \alpha_{kR}^* = \alpha_{kR} \]

\[ S_{kR}^* = S_{kR} \]

\[ S_{kL}^* = S_{kL} \]

Similar to Euler Riemann solver

with

\[ p = \alpha_1 p_1 + \alpha_2 p_2 \]

\[ \rho = \alpha_1 \rho_1 + \alpha_2 \rho_2 \]

\[ Z = \rho c \]

\[ c_f^2 = Y_1 c_1^2 + Y_2 c_2^2 \]
2nd step: Pressure relaxation

Already solved by the 1st step

\[
\begin{align*}
\frac{\partial \alpha_1}{\partial t} + u \frac{\partial \alpha_1}{\partial x} & = & \\
\frac{\partial \alpha_1 \rho_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 u}{\partial x} & = & 0 \\
\frac{\partial \alpha_2 \rho_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 u}{\partial x} & = & 0 \\
\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} + (\alpha_1 \rho_1 + \alpha_2 \rho_2) & = & 0 \\
\frac{\partial \alpha_1 \rho_1 e_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 e_1 u}{\partial t} + \alpha_1 \rho_1 \frac{\partial u}{\partial x} & = & -p_1 \mu(p_1 - p_2) \\
\frac{\partial \alpha_2 \rho_2 e_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 e_2 u}{\partial t} + \alpha_2 \rho_2 \frac{\partial u}{\partial x} & = & p_1 \mu(p_1 - p_2)
\end{align*}
\]

Relaxation system

\[
\begin{align*}
\frac{\partial \alpha_1}{\partial t} & = \mu(p_1 - p_2) \\
\frac{\partial \alpha_1 \rho_1 e_1}{\partial t} & = -p_1 \mu(p_1 - p_2) \\
\frac{\partial \alpha_2 \rho_2 e_2}{\partial t} & = p_1 \mu(p_1 - p_2) \\
\frac{\partial \alpha_1 \rho_1}{\partial t} & = 0 \\
\frac{\partial \alpha_2 \rho_2}{\partial t} & = 0 \\
\frac{\partial \rho u}{\partial t} & = 0 \\
\frac{\partial \rho E}{\partial t} & = 0
\end{align*}
\]
2nd step: Pressure relaxation

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

\[ \left\{ \begin{align*}
\frac{\text{de}_1}{\text{dt}} + p_1 \frac{\text{dv}_1}{\text{dt}} &= 0 \\
\frac{\text{de}_2}{\text{dt}} + p_1 \frac{\text{dv}_2}{\text{dt}} &= 0 
\end{align*} \right. \]

Time integration:

\[ e_k - e_0^k + \hat{p}_{lk}(v_k - v_k^0) = 0 \]

\[ \hat{p}_{lk} = \frac{1}{v_k - v_k^0} \int_{v_k^0}^{v_k} \frac{\text{dv}_k}{\text{dt}} \text{d}t = 0 \]

\[ \sum_k \Rightarrow Y_1 e_1 - Y_1 e_1^0 + Y_2 e_2 - Y_2 e_2^0 + \hat{p}_{l1}(Y_1 v_1 - Y_1 v_1^0) + \hat{p}_{l2}(Y_2 v_2 - Y_2 v_2^0) = 0 \]

\[ e - e^0 + (\hat{p}_{l1} - \hat{p}_{l2})(Y_1 v_1 - Y_1 v_1^0) = 0 \]

Possible choice \[ \hat{p}_{l1} = \hat{p}_{l2} = \hat{p}_l \]

Using mass equations

Entropy inequality is verified
2\textsuperscript{nd} step: Pressure relaxation

Using EOS:

\[
\begin{align*}
e_1(p, v_1) - e_1^0(p_1^0, v_1^0) + p(v_1 - v_1^0) &= 0 \\
e_2(p, v_2) - e_2^0(p_2^0, v_2^0) + p(v_2 - v_2^0) &= 0
\end{align*}
\]

\[
\begin{cases}
v_1 = v_1(p) \\
v_2 = v_2(p)
\end{cases}
\]

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

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

Then, we determine: \( p \to v_k(p) \to \alpha_k = (\alpha \rho)_k v_k \)
3\textsuperscript{th} step: Internal energy reset

- We have in the 2\textsuperscript{nd} step determined: \( p, v_k, \alpha_k \)
- We forget the relaxed pressure but keep volume fractions:

\[ p \rightarrow \alpha_k \]

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

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

- Phasic EOS permits to reset internal energies:

\[ e_k = e_k(p_{\text{new}}, \alpha_k \rho_k, \alpha_k) \]

Conservative and good treatment of wave dynamics from both sides of the interface
1D example: Water-Air shock tube

\( P_{\text{eau}} = 10 \ 000 \ \text{bar} \)
\( \rho_{\text{eau}} = 1000 \ \text{kg/m}^3 \)

EAU

\( P_{\text{air}} = 1 \ \text{bar} \)
\( \rho_{\text{air}} = 1 \ \text{kg/m}^3 \)

AIR

Solution exacte

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

Shock wave propagation

\[ t = 134\mu s \]
\[ t = 274\mu s \]
\[ t = 344\mu s \]
\[ t = 554\mu s \]

\[ t = 137\mu s \]
\[ t = 291\mu s \]
\[ t = 350\mu s \]
\[ t = 577\mu s \]
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

\[ c^2 = -v^2 \frac{\partial p}{\partial v} \bigg|_{s=\text{cte}} < 0 \]

Hyperbolicity is lost into the phase diagram

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

Liquid and Vapor isentropes are linked by a kinetic process

Hyperbolicity is preserved in the entire domain
Phase transition modeling

1) Mass transfer modifies mass equations:

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

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

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:

\[ \frac{d\alpha_1}{dt} = K \text{div}(\vec{u}) + AQ_1 + \frac{\dot{m}_1}{\rho_1} \]

This « interfacial » density has to be determined in order to close the model.
Two-phase model for interface problems with phase transition

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

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

\[ \frac{\partial \rho \vec{u}}{\partial t} + \text{div}(\rho \vec{u} \otimes \vec{u}) + \nabla(p) = 0 \]

\[ \frac{\partial \rho E}{\partial t} + \text{div}((\rho E + p) \vec{u}) = 0 \]

\[ \frac{\partial \alpha_1}{\partial t} + \vec{u} \cdot \nabla(\alpha_1) = \frac{\rho_1 c_1^2 - \rho_2 c_2^2}{\rho_1 c_1^2 + \rho_2 c_2^2} \text{div}(\vec{u}) + \rho \nu (g_2 - g_1) \frac{\alpha_1}{\alpha_1 + \alpha_2} \frac{c_1^2}{c_1^2 + c_2^2} + H(T_2 - T_1) \frac{\alpha_1}{\alpha_1 + \alpha_2} \frac{c_1^2}{c_1^2 + c_2^2} + \frac{\alpha_2}{\alpha_1 + \alpha_2} \frac{c_2^2}{c_1^2 + c_2^2} \]

Entropy analysis for each phase and for the mixture

Mechanical relaxation
Mass transfer
Heat transfer

Lois d’état :

\[ e_1(\rho_1, p) = \frac{p + \gamma_1 p_{\infty 1}}{(\gamma_1 - 1) \rho_1} + e_{0,1} \quad \text{For the liquid} \]

\[ e_2(\rho_2, p) = \frac{p}{(\gamma_2 - 1) \rho_2} + e_{0,2} \quad \text{For vapor} \]

\[ \rho e = \alpha_1 \rho_1 e_1 + \alpha_2 \rho_2 e_2 \]

\[ p(\rho, e, \alpha_1, \alpha_2) = \frac{\rho e - \gamma_1 \rho_1 p_{\infty 1}}{\gamma_1 - 1} + \frac{\alpha_2 \gamma_2 p_{\infty 2}}{\gamma_2 - 1} \frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1} \]

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

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

\[ p(\rho, e) = (\gamma - 1) \rho (e - q) - \gamma p_\infty \]

- 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

\[ P_{\text{liquide}} = 1\,000 \text{ bar} \]
\[ \rho_{\text{liquide}} = 500 \text{ kg/m}^3 \]

Dodécane vapeur

\[ P_{\text{vapeur}} = 1 \text{ bar} \]
\[ \rho_{\text{vapeur}} = 2 \text{ kg/m}^3 \]

Saurel, Petitpas & Abgrall, JFM, 2008
High pressure diesel injector
High speed motion under water

Water inflow 300 m/s

\( \rho = 1050 \text{ kg/m}^3 \)

\( p = 1 \text{ bar} \)

1 m

Obstacle

Gas injection

Outflow condition

0.32 m

1.25 m

4 m
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

\[ \bar{q}_{\text{cond}} = -\lambda \vec{\nabla}T \]
Bubble growth