On a simple model of isothermal phase transition

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Micro-Macro Modelling and Simulation of Liquid-Vapour Flows

Bordeaux

Outline of the talk

- **Modelling of isothermal phase transition**
  - Optimization of the entropy
  - The Homogeneous Relaxation Model (HRM)
  - The Homogeneous Equilibrium Model (HEM)
  - The zero-relaxation limit
- **The Riemann problem for the HEM**
  - Multiple waves and the Liu entropy condition
  - Main results : existence, uniqueness and $\mathbf{L}^1_{\mathrm{loc}}$-continuity
- **Numerical tests**
  - Some shock tubes
  - Two-dimensional cavitation
- **Conclusion**

Context of this study

Collaboration between the **Laboratoire Jacques-Louis Lions**

C. Chalons, F. Coquel, E. Godlewski, F. Lagoutière, P.-A. Raviart, N. Seguin

and the **CEA Saclay**

A. Ambroso, S. Kokh , J. Segré.

Goal: Interfacial coupling of thermohydraulic models

- ▷ Hyperbolic systems
- ▷ Theory and numerics
- ▷ Two-phase flows

Bifluid model and entropy optimization

See [Barberon, Helluy '04], [Helluy, Seguin '06] and [Allaire, Faccanoni, Kokh '06].
(and [Coquel, Perthame '98], [Jaouen '01], [Chanteperdrix, Villedieu, Vila '02]...)

- Classical **Euler equations** for the mixture

$$\begin{cases} \partial_t \rho + \partial_x \rho u = 0 \\ \partial_t \rho u + \partial_x (\rho u^2 + p) = 0 \\ \partial_t \rho E + \partial_x ((\rho E + p) u) = 0 \\ \partial_t Y + u \partial_x Y = \lambda (Y_{eq} - Y) \end{cases}$$

  where Y is the vector of fractions of volume, mass and energy

- **Thermodynamical behaviour**
  - Mixture laws for thermodynamical variables (ρ, p, T, s...)
  - Thermodynamical equilibrium defined by entropy optimization w.r.t. Y:

$$Y_{eq}(\tau, \varepsilon) = \max_{Y \in [0,1]^3} s(\tau, \varepsilon, Y)$$

The isothermal Homogeneous Relaxation Model

The **isothermal HRM** we consider here is (in Lagrangian coordinates “(t, x)”)

$$\begin{cases} \partial_t \tau - \partial_x u = 0 \\ \partial_t u + \partial_x \mathscr{P}_R(\tau, \alpha) = 0 \\ \partial_t \alpha = \lambda(\alpha_{eq}(\tau) - \alpha) \end{cases}$$

where α is the mass fraction.

The equilibrium α_{eq} is given by the equality of chemical potentials.

Proposition
The HRM model is strictly hyperbolic. Its eigenvalues are

$$-\sqrt{-\partial_\tau \mathscr{P}_R(\tau, \alpha)}, 0, \sqrt{-\partial_\tau \mathscr{P}_R(\tau, \alpha)}.$$

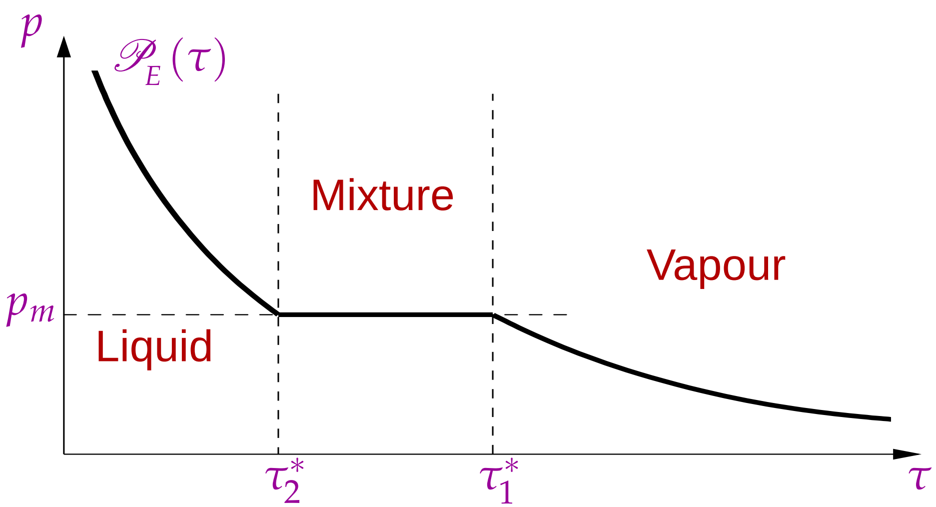
The isothermal Homogeneous Equilibrium Model

The **equilibrium pressure** is given by

$$\mathscr{P}_E(\tau) = \mathscr{P}_R(\tau, \alpha_{eq}(\tau)), \quad \tau > 0,$$

and the **isothermal HEM** is

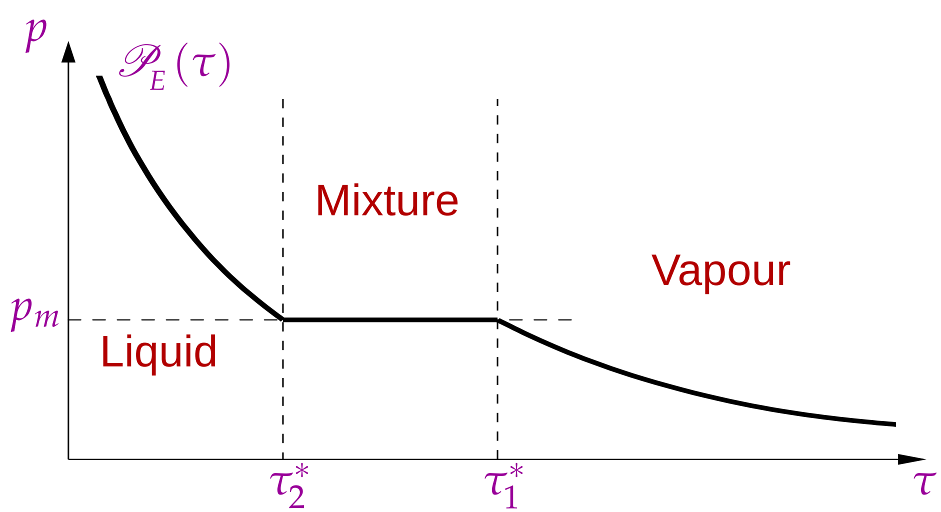
$$\begin{cases} \partial_t \tau - \partial_x u = 0, \\ \partial_t u + \partial_x \mathscr{P}_E(\tau) = 0. \end{cases}$$



The isothermal Homogeneous Equilibrium Model

Proposition
In $\Omega_p = ((0, \tau_2^*) \cup (\tau_1^*, \infty)) \times \mathbb{R}$,
the HEM is strictly hyperbolic ($\lambda_\pm(\mathbf{u}) = \pm\sqrt{-\mathscr{P}_E'(\tau)}$).

In $\Omega_m = [\tau_2^*, \tau_1^*] \times \mathbb{R}$,
the HEM is nonstrictly hyperbolic ($\lambda_-(\mathbf{u}) = \lambda_+(\mathbf{u})$ and loss of basis).
The model locally becomes the system of pressureless gases.



From HRM to HEM

Since **HEM is not strictly hyperbolic**, it does not enter in classical frameworks. ([Liu '87], [Chen, Liu, Levermore '94], [Hanouzet, Natalini '03], [Yong '04]...)

Study of **relaxation shock profiles** [Yong, Zumbrun '04]:

- Take two states (τ_L, u_L) and (τ_R, u_R) and a speed σ satisfying the Rankine-Hugoniot jump relations:

$$\begin{cases} -\sigma(\tau_R - \tau_L) - (u_R - u_L) = 0, \\ -\sigma(u_R - u_L) + (\mathscr{P}_E(\tau_R) - \mathscr{P}_E(\tau_L)) = 0. \end{cases}$$

- Parametrize the solutions of HRM by $\xi = \lambda(x - \sigma t)$: $\tau(\xi)$, $u(\xi)$, $\alpha(\xi)$.
- Solve the system of ODE with $(\tau_L, u_L, \alpha_{eq}(\tau_L))$ for $\xi = -\infty$ and $(\tau_R, u_R, \alpha_{eq}(\tau_R))$ for $\xi = +\infty$.

From HRM to HEM

Relaxation shock profiles [Kokh, Seguin '07]:

- **First case:** if $\alpha_{eq}(\tau_L) = \alpha_{eq}(\tau_R)$ ($= 0$ or 1), the relaxation term is inactive.
  $\Longrightarrow$ Use of the Lax entropy condition
- **Second case:** $\alpha_{eq}(\tau_L) \neq \alpha_{eq}(\tau_R)$
  We have to solve the 2×2 ODE system

$$\begin{cases} \sigma^2 \tau'(\xi) + \mathrm{d}_\xi \mathscr{P}_R(\tau(\xi), \alpha(\xi)) = 0, \\ \alpha'(\xi) = (\alpha_{eq}(\tau(\xi)) - \alpha(\xi)). \end{cases}$$

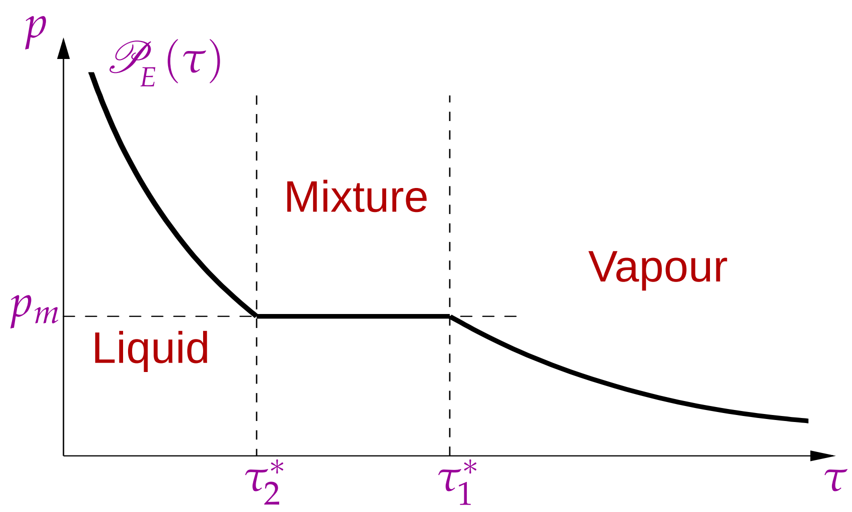
If the equations of state of each phase are perfect gas pressure laws:

> **Proposition**
> A relaxation shock profile exists for the discontinuity
> $\Longleftrightarrow$
> The discontinuity statisfies the Liu entropy condition

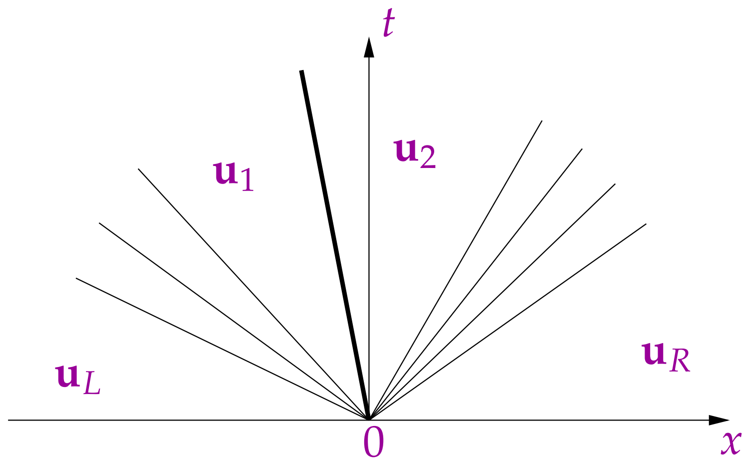
The Riemann problem for HEM

The Riemann problem for HEM:
[Godlewski, Seguin '06]

$$\partial_t \tau - \partial_x u = 0,$$
$$\partial_t u + \partial_x \mathscr{P}_E(\tau) = 0,$$
$$(\tau, u)(0, x) = \begin{cases} (\tau_L, u_L) & \text{if } x < 0, \\ (\tau_R, u_R) & \text{if } x > 0. \end{cases}$$



We consider self-similar solutions $\mathbf{u}(x, t) = \mathbf{u}(x/t)$.



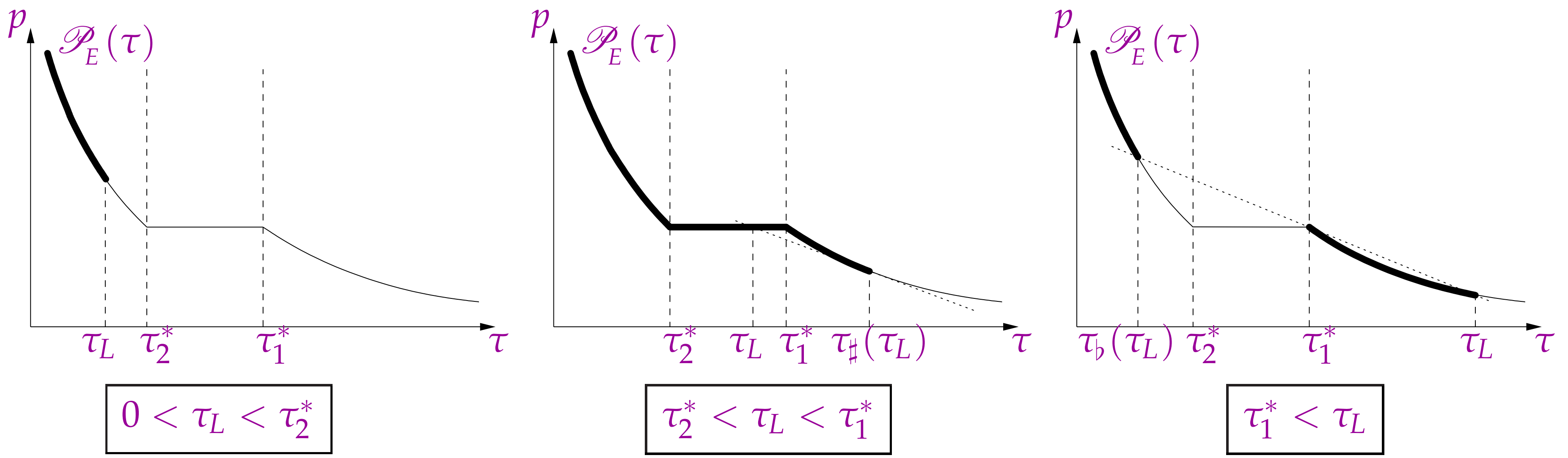
The Riemann problem for HEM

A discontinuity is admissible if it satisfies the Liu entropy condition:

$$\sigma(\mathbf{u}_l, \mathbf{u}_r) \leq \sigma(\mathbf{u}_l, \mathbf{u})$$

for all $\mathbf{u} \in \mathscr{S}(\mathbf{u}_l)$ with $\tau \in (\min(\tau_l, \tau_r), \max(\tau_l, \tau_r))$.

The speed of an admissible discontinuity is smaller than the speed of any discontinuity included in it.



Main results

Theorem 1
For all $\mathbf{u}_L, \mathbf{u}_R \in \Omega$, the self-similar solution of the Riemann problem exists and is unique, allowing the occurrence of vacuum $\{\tau = +\infty\}$ when necessary.

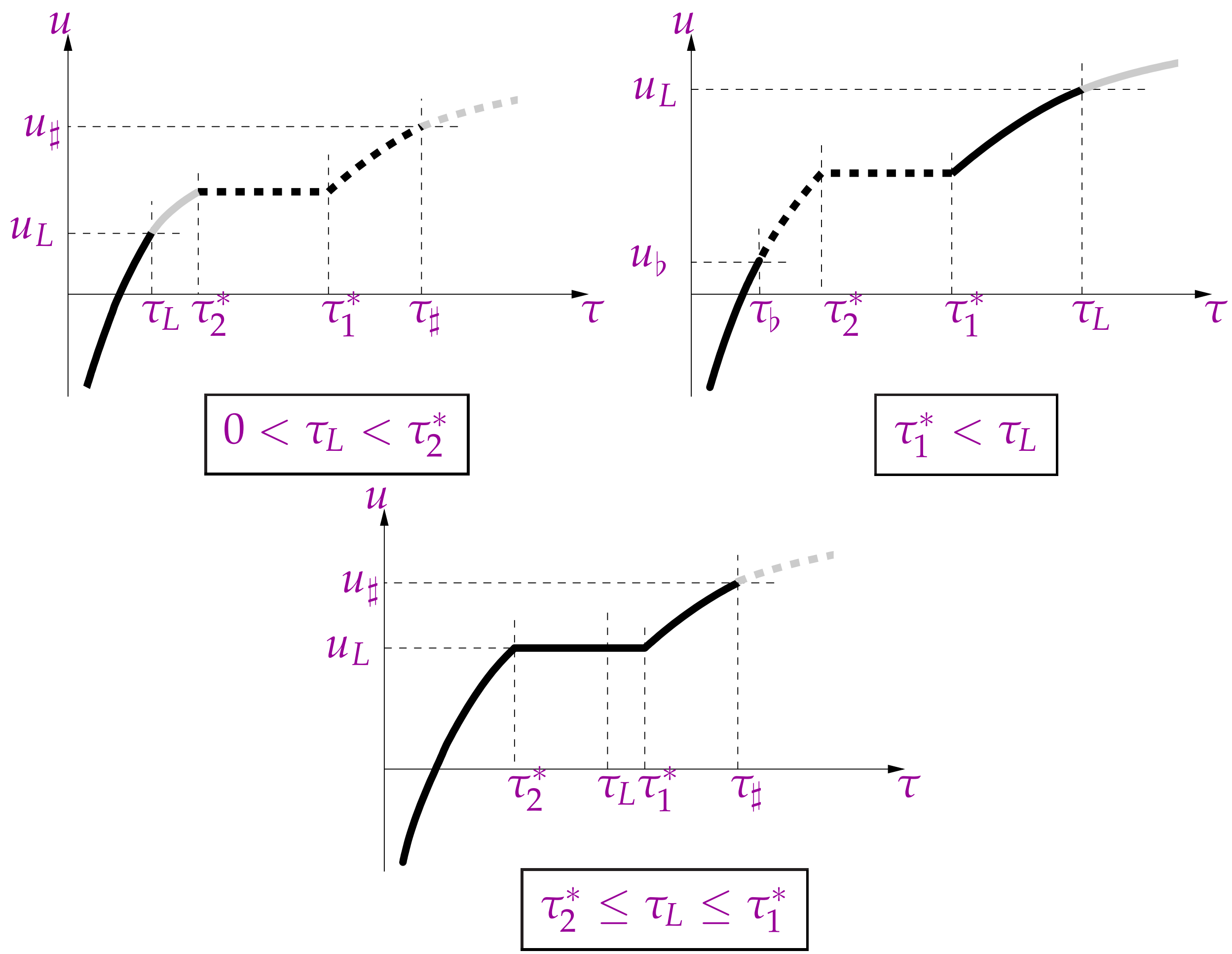
Theorem 2
Let $\mathscr{W}(x/t; \mathbf{u}_L, \mathbf{u}_R)$ be the self-similar solution of the Riemann problem. For any $L > 0$ and initial data $(\mathbf{u}_L, \mathbf{u}_R), (\mathbf{v}_L, \mathbf{v}_R) \in \Omega^2$, there exists a constant $C > 0$ such that

$$\int_{-L}^{L} |\mathscr{W}(\xi; \mathbf{u}_L, \mathbf{u}_R) - \mathscr{W}(\xi; \mathbf{v}_L, \mathbf{v}_R)| d\xi \leq C(|\mathbf{u}_L - \mathbf{v}_L| + |\mathbf{u}_R - \mathbf{v}_R|)$$

where $|\cdot|$ stands for the Euclidean norm of $\mathbb{R}^2$.

Nonpositive multiple waves

Nonpositive multiple waves are given as a succession of nonpositive rarefaction waves and admissible discontinuities (geometric interpretation) $\Longrightarrow \mathscr{U}(\mathbf{u}_L)$.

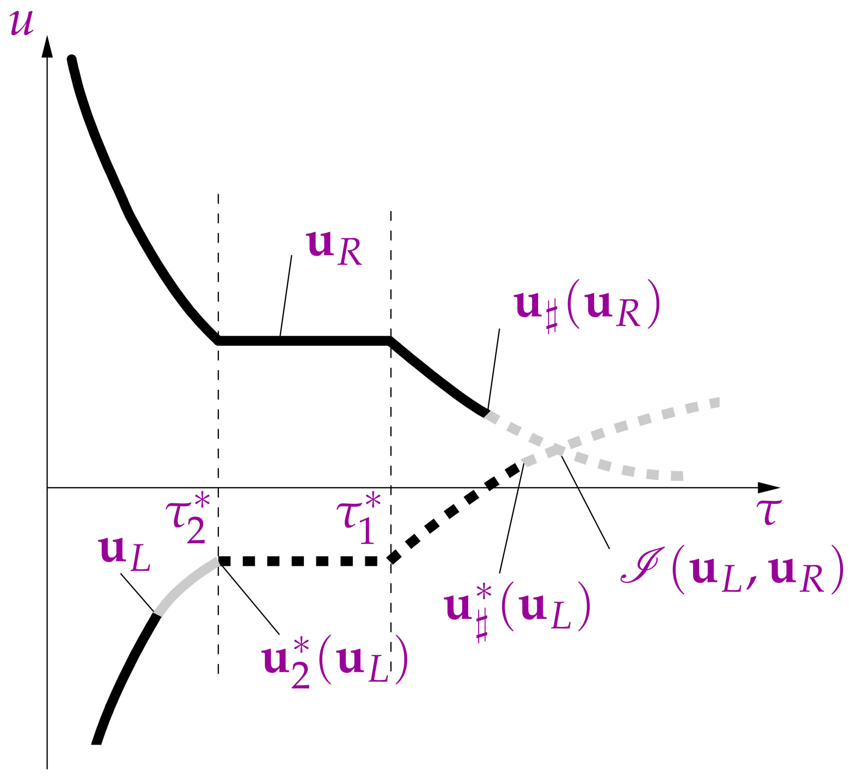


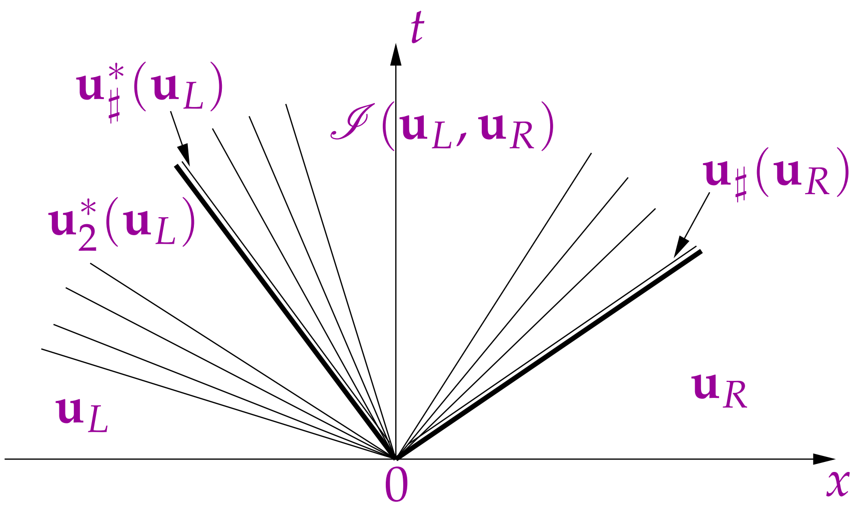
An example of Riemann solution

Construction (by symmetry) of $\mathscr{U}(\mathbf{u}_R)$ and find the intersection

$$\mathscr{I}(\mathbf{u}_L, \mathbf{u}_R) = \mathscr{U}_-(\mathbf{u}_L) \cap \mathscr{U}_+(\mathbf{u}_R).$$

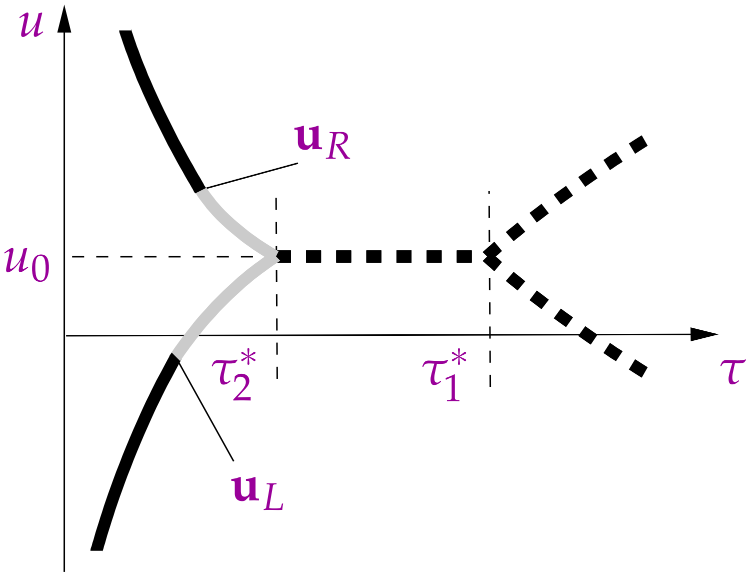
A solution with multiple waves:

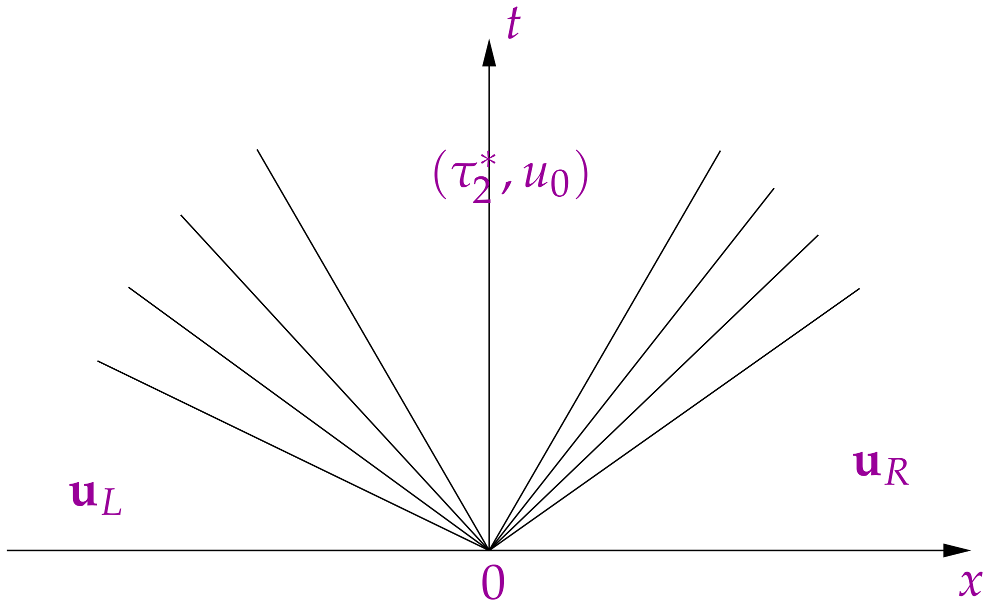




Uniqueness of the Riemann solution

The uniqueness is given if $\mathscr{I}(\mathbf{u}_L, \mathbf{u}_R) = \mathscr{U}_-(\mathbf{u}_L) \cap \mathscr{U}_+(\mathbf{u}_R)$ is a singleton.





Some properties of the exact solution

Remark
If two states are separated by a phase transition discontinuity, at least one of them is at **saturation**.

Remark
If the initial data is composed only by **pure phases**, no mixture zone can occur in the solution.

Remark
The Cauchy problem can be **ill-posed** if the initial data is in the mixture zone. [Lagoutière]

$\Longrightarrow$ Instable behaviour of the mixture zone

Numerical schemes

Any classical Finite Volume scheme can be used.

Two approaches:

- ▷ Compute HRM + instantaneous equilibrium $\alpha = \alpha_{eq}$ after each time step
- ▷ Directly compute HEM

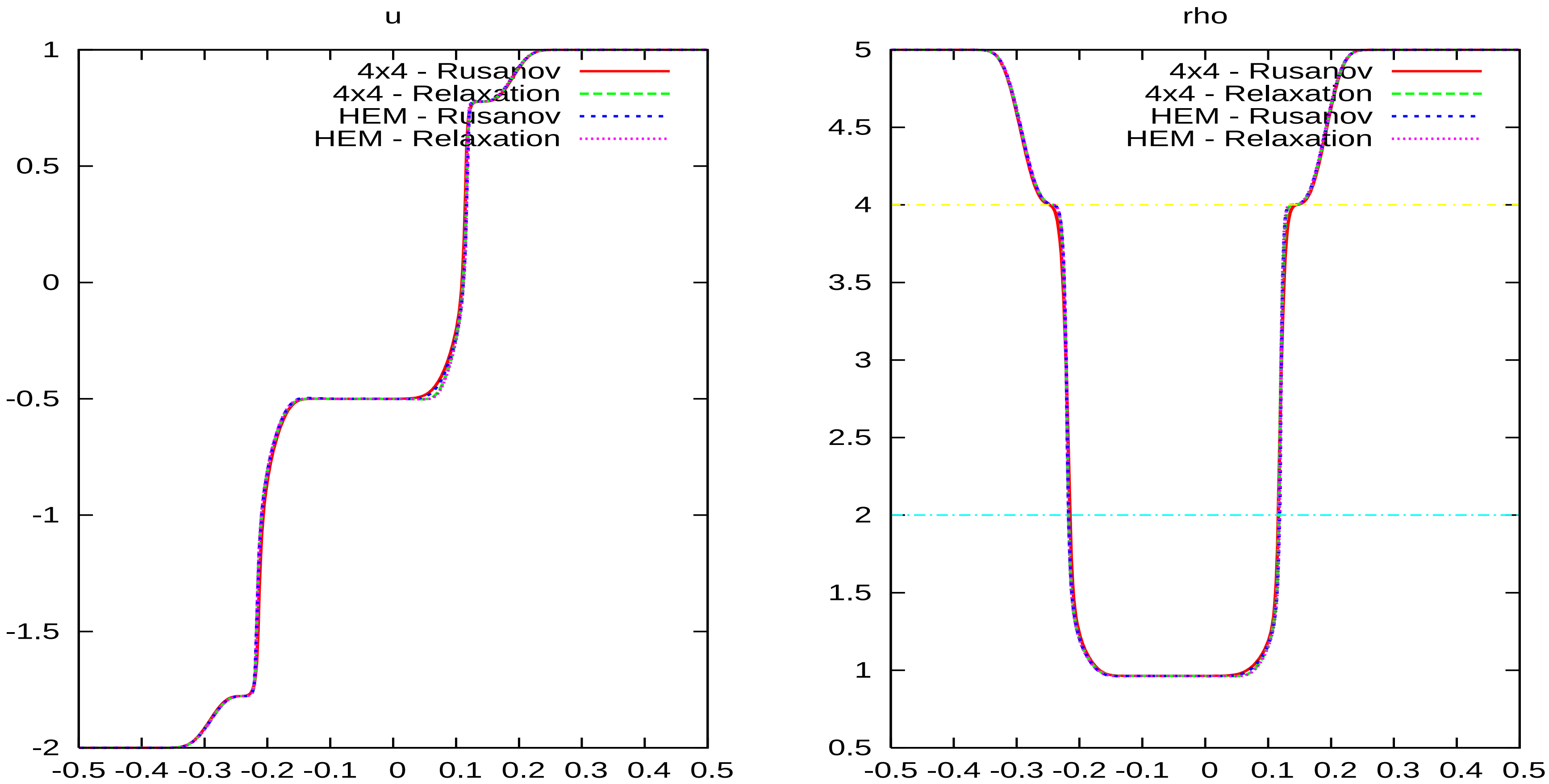
Here, we used two different numerical schemes:

- ▷ Suliciu's relaxation method ([Coquel *et al.* '99], [Bouchut '04])
- ▷ The Rusanov scheme

1D and 2D tests in the Eulerian setting.

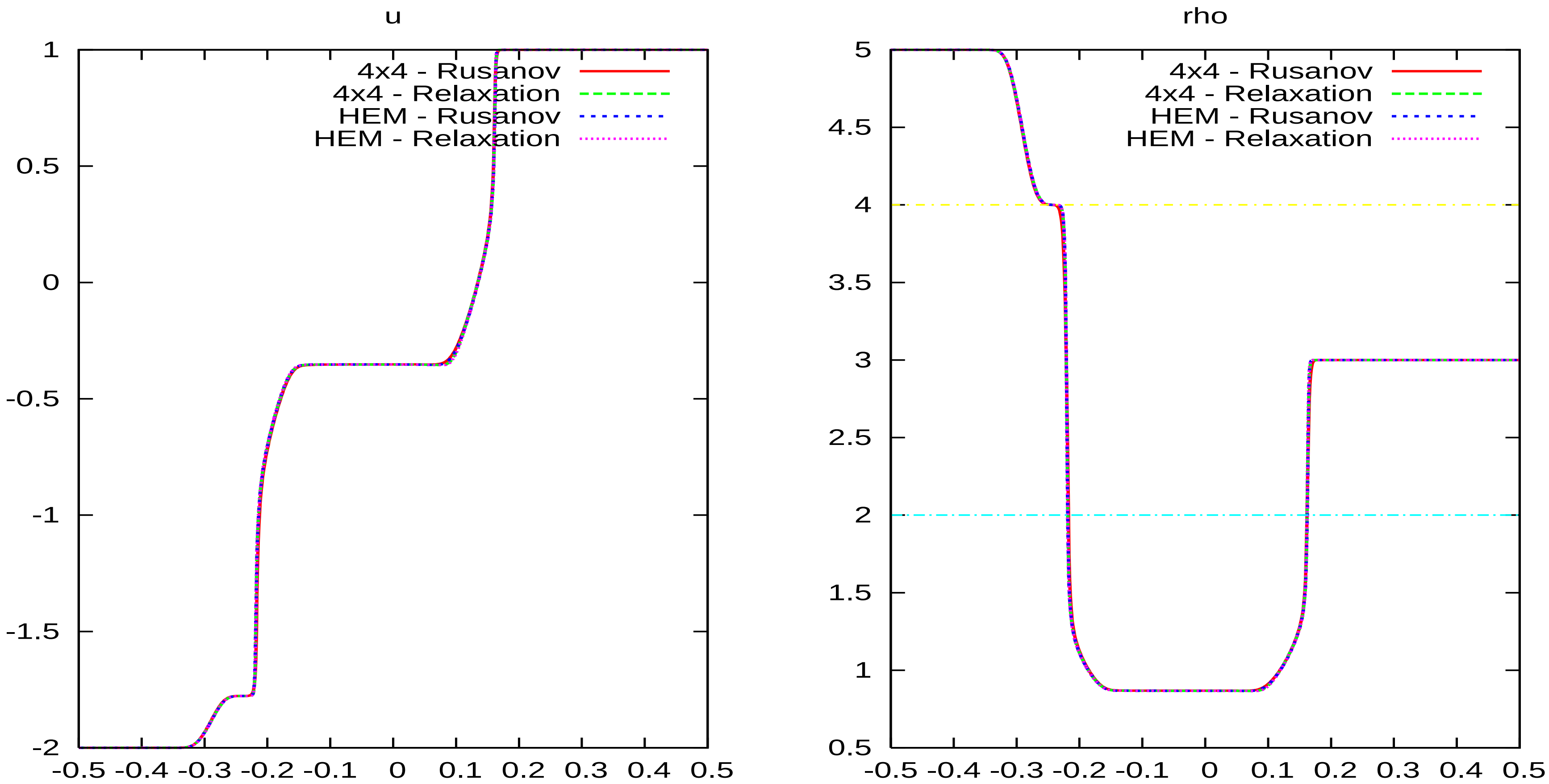
Numerical tests

Two rarefaction waves in the “liquid” with occurence of “vapor”



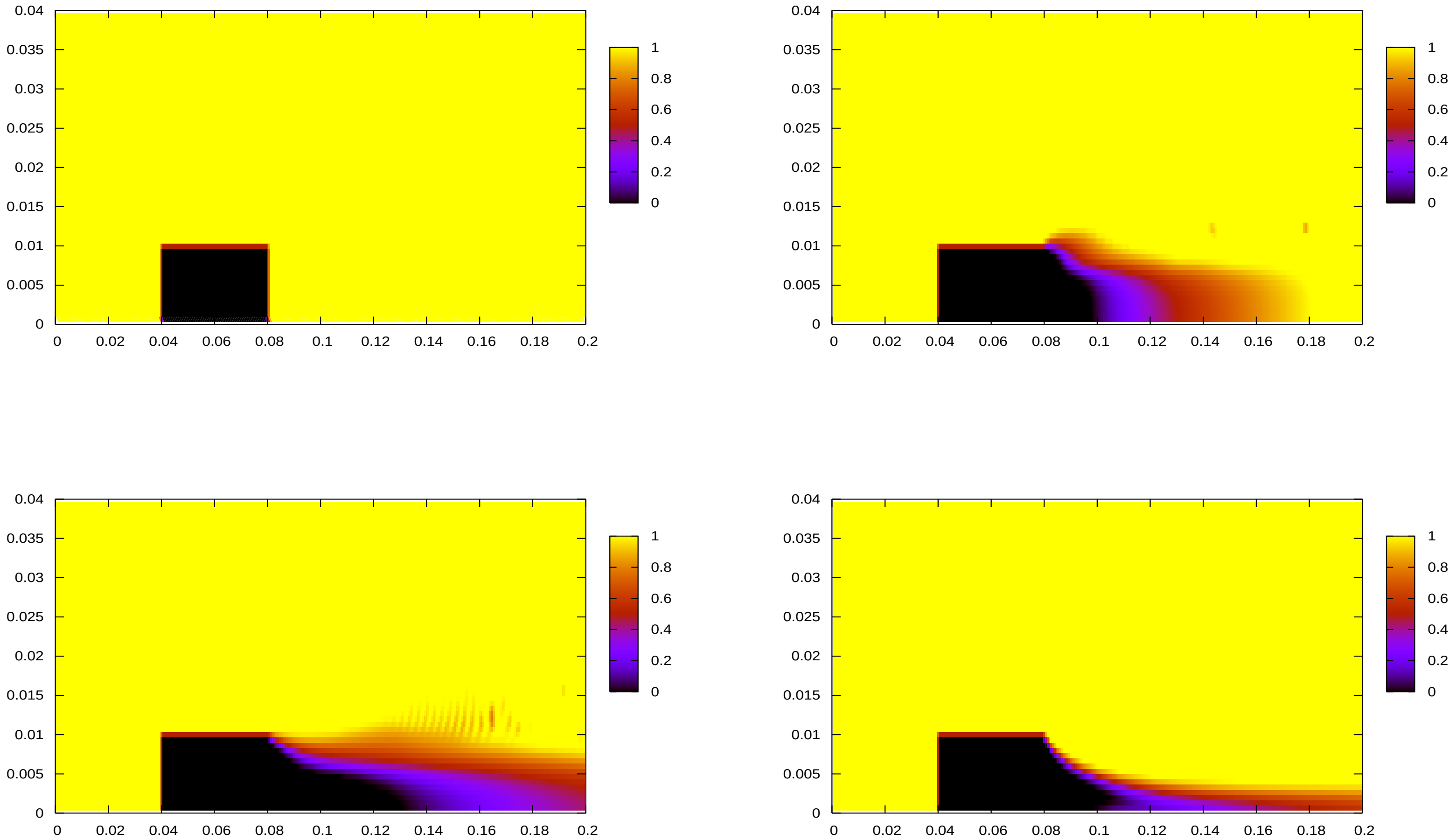
Numerical tests

Two rarefaction waves with one state in the “liquid” and the other in the mixture



Numerical tests

Box in a hypervelocity “liquid” flow (mesh: 300x60)



Conclusion

- Study of a model of isothermal phase change
  - Relaxation
  - Riemann problem
  - Numerical approximations
- Remaining points
  - Zero-relaxation limit for rarefaction waves and smooth solutions
  - The Cauchy problem
  - More numerical tests
- More complex modelling
  - Realistic equations of state
  - More complex phase change