The use of the Chapman–Jouguet theory for solving the Riemann–problem with vaporization

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Mathématiques Appliquées de Bordeaux

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Overview

1. Thermodynamic of phase transition
2. The Riemann Problem with equilibrium E.O.S
3. The Riemann Problem out of equilibrium
4. Numerical scheme
5. Numerical results

Thermodynamic model (1/3)

- No Van Der Waals (Euler system is not hyperbolic, difficulty to make a difference between metastable and equilibrium state)
- Two equations of state $\varepsilon_l(P,T)$ and $\varepsilon_g(P,T)$
- adimensionned coefficients

$$\gamma = -\frac{\tau}{P}\left(\frac{\partial P}{\partial \tau}\right)_s \qquad \Gamma = -\frac{\tau}{T}\left(\frac{\partial T}{\partial \tau}\right)_s \qquad g = \frac{P\tau}{T^2}\left(\frac{\partial T}{\partial s}\right)_\tau$$

- thermodynamic stability requires that

$$\gamma, g \geq 0 \qquad \gamma g - \Gamma^2 > 0$$

Thermodynamic model (2/3)

- Mixture zone
  - Suppose that fluids are locally non miscible
    $V_l + V_g = V_{\text{tot}}$
  - Optimization of mixture entropy

$\Longrightarrow$ When the mixture is stable

$$P_l = P_g \qquad T_l = T_g \qquad \mu_l = \mu_g$$

Thermodynamic model (2/3)

- Mixture zone

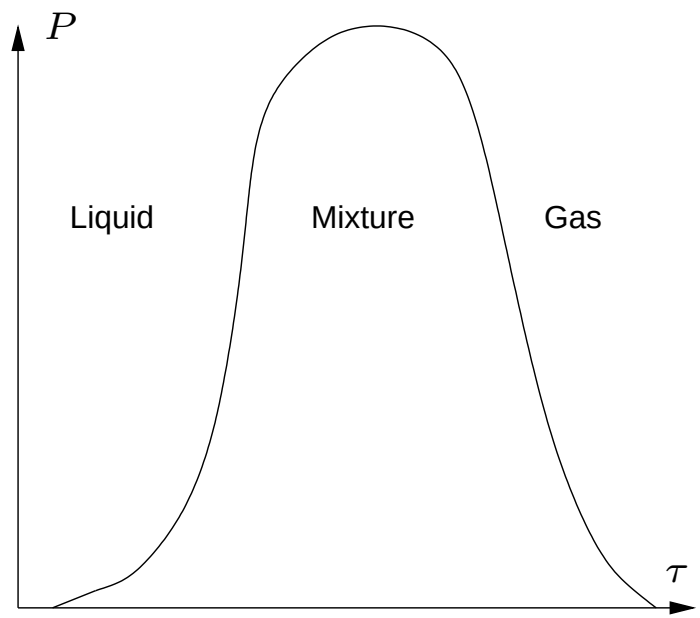
$$P_l = P_g \qquad T_l = T_g \qquad \mu_l = \mu_g$$

- $\mu_l(P,T) = \mu_g(P,T) \implies P = P_{\text{sat}}(T)$

$$\implies \tau_l(T) = \tau_l(P_{\text{sat}}(T), T) \qquad s_l(T) = s_l(P_{\text{sat}}(T), T)$$

Thermodynamic model (2/3)

- Mixture zone



- 3 E.O.S.

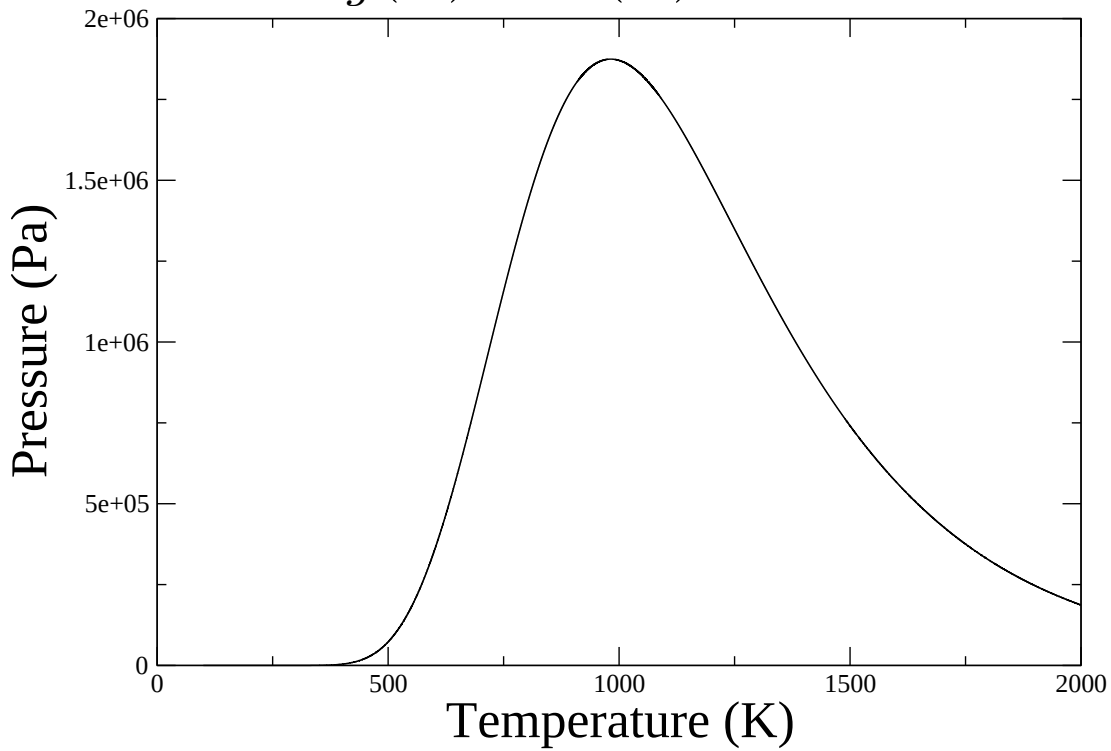
$$\frac{\gamma - \gamma_m}{\gamma_m} = (\gamma g - \Gamma^2) \left(\frac{T}{\tau} \frac{\mathrm{d}s_b}{\mathrm{d}P} \right)^2 > 0$$

Thermodynamic model (3/3)

- Provided $\dfrac{\mathrm{d}P_{\mathrm{sat}}}{\mathrm{d}T} = \dfrac{s_g(T) - s_l(T)}{\tau_g(T) - \tau_l(T)} > 0$
  - $\Phi : \begin{pmatrix} y \\ T \end{pmatrix} \mapsto \begin{pmatrix} y\tau_g(T) + (1-y)\tau_l(T) \\ ys_g(T) + (1-y)s_l(T) \end{pmatrix} = \begin{pmatrix} \tau \\ s \end{pmatrix}$ is a local diffeomorphism
  - The mixture equation of state is convex

Thermodynamic model (3/3)

- Provided $\dfrac{\mathrm{d}P_{\mathrm{sat}}}{\mathrm{d}T} = \dfrac{s_g(T) - s_l(T)}{\tau_g(T) - \tau_l(T)} > 0 \implies$ O.K.



- Dodecane, two stiffened gas, coefficients calculated by Lemétayer et al., Int. J. of Thermal Sciences.

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Equilibrium EOS (1/3)

- Look for undercompressive waves for the Euler system

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + P) = 0 \\ \partial_t(\rho E) + \partial_x((\rho E + P)u) = 0 \end{cases}$$

  - with $E = \varepsilon + \dfrac{1}{2}u^2$
  - ε, P, ρ are linked with an E.O.S.

Equilibrium EOS (1/3)

- Look for undercompressive waves for the Euler system
- Variables are function of $\xi = x/t$

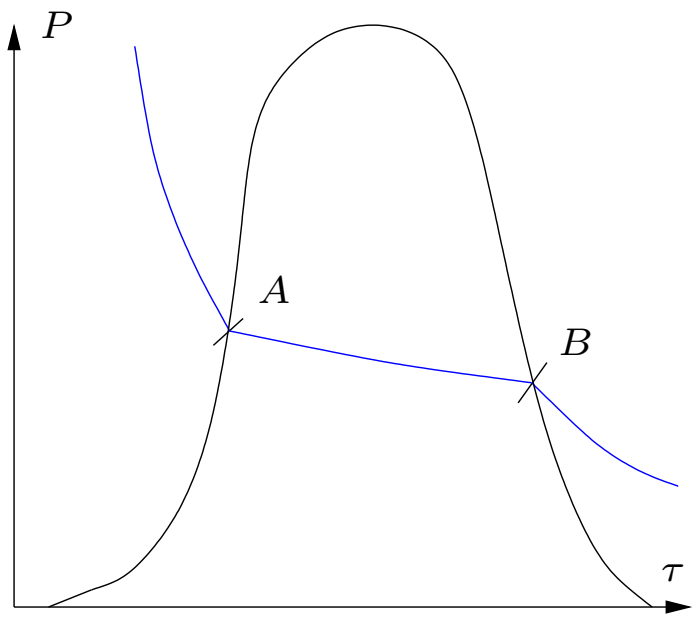
$$\begin{aligned}
&\mp\rho c = \rho(u - \xi) \\
&\mp\rho \mathrm{d}u + \mathrm{d}P = 0 \\
&\mathrm{d}\varepsilon + P\mathrm{d}\tau = 0 \quad \Longrightarrow \quad S = \mathrm{cste}
\end{aligned}$$

- We take P as a parameter, all the thermodynamic is known thanks for P and S. u is obtained by integrating $\mp\rho \mathrm{d}u + \mathrm{d}P = 0$

Is that integration affected by phase transition?

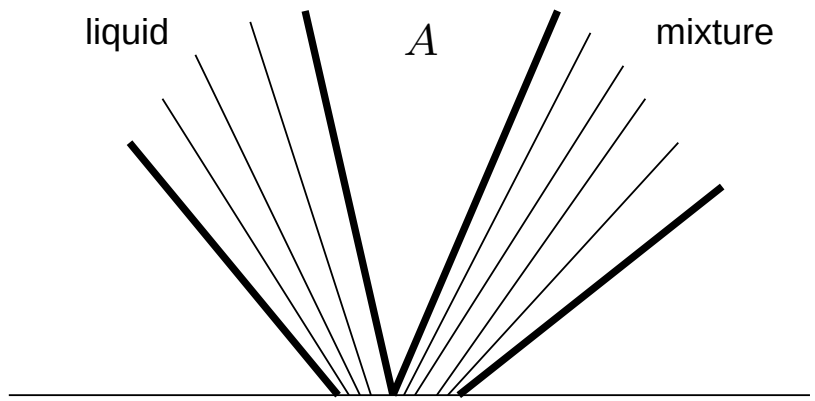
Equilibrium EOS (2/3)

- Consequences for characteristic curves



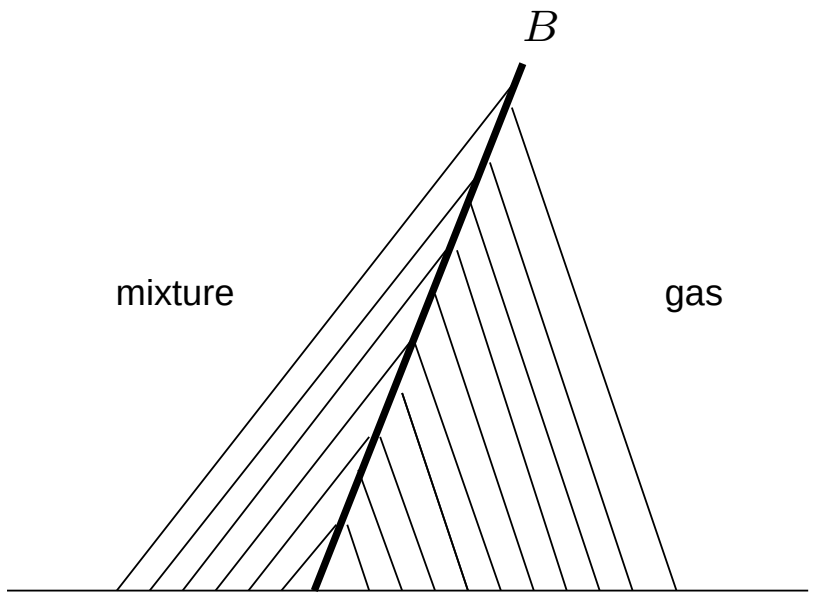
Equilibrium EOS (2/3)

- Consequences for characteristic curves
- Characteristic curves in point A



Equilibrium EOS (2/3)

- Consequences for characteristic curves
- Characteristic curves in point A
  $\Longrightarrow$ OK
- Characteristic curves in point B



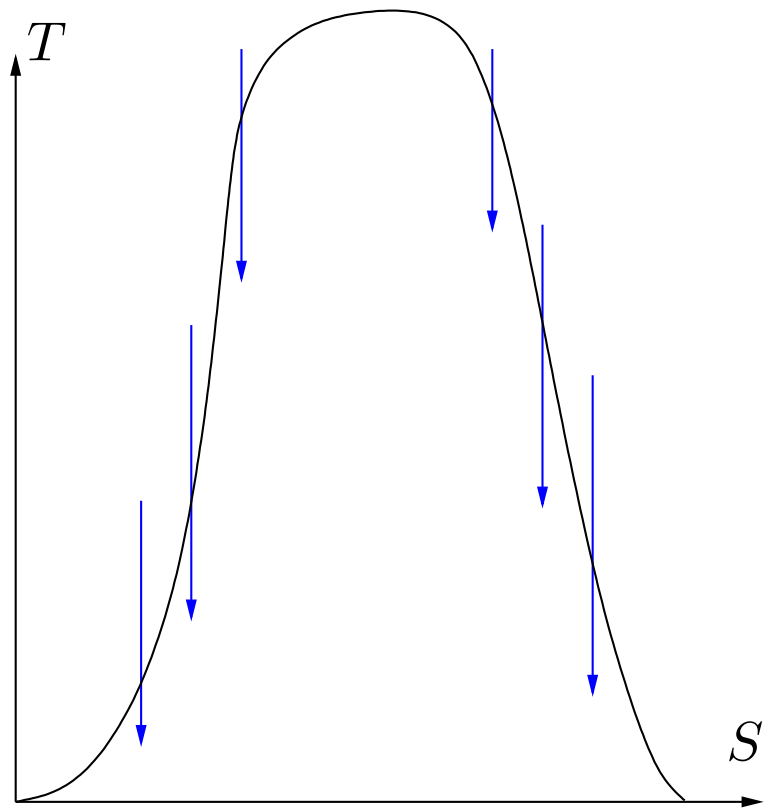
Equilibrium EOS (2/3)

- Consequences for characteristic curves
- Characteristic curves in point A
  $\Longrightarrow$ OK
- Characteristic curves in point B
  $\Longrightarrow$ non regular wave ???

But do A and B really exist?

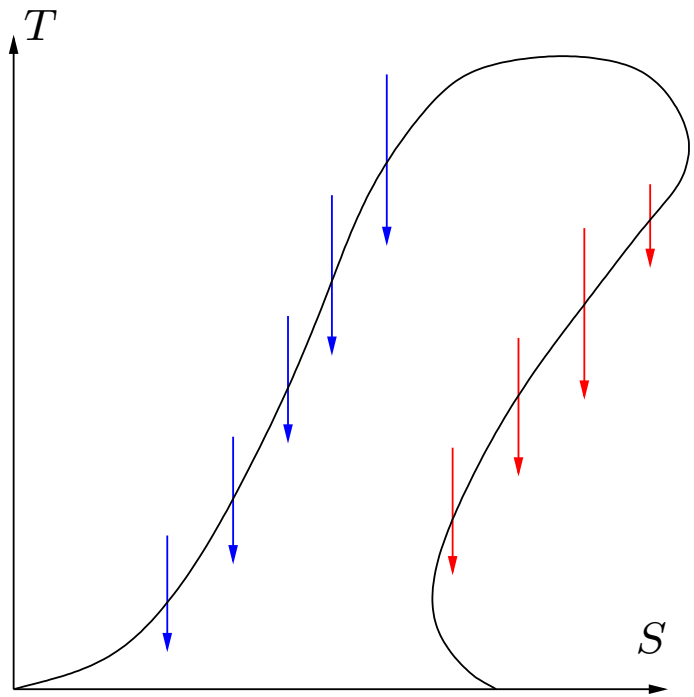
Equilibrium EOS (3/3)

- Existence of A and B depends on the behaviour of isentrope near the saturation curves.
  - Regular fluid :



Equilibrium EOS (3/3)

- Existence of A and B depends on the behaviour of isentrope near the saturation curves.
  - Regular fluid : Isentropes cross the saturation curve from the pure phase to the mixture
  - Retrograde fluid :



Equilibrium EOS (3/3)

- Existence of A and B depends on the behaviour of isentrope near the saturation curves.
  - Regular fluid : Isentropes cross the saturation curve from the pure phase to the mixture
  - Retrograde fluid : Isentropes cross the saturation curve from the mixture to the pure phase
- Liquid saturation curve is always regular. Vapor saturation curve exhibits often at least one retrograde part.

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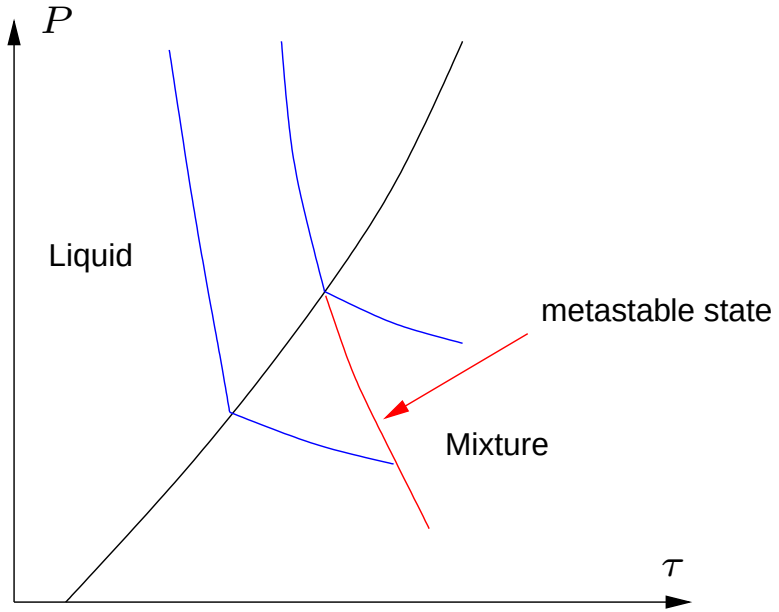
Out of equilibrium Riemann problem (1/4)

- metastable states (Thomson et al., JFM 1986 and 1988; Simoes-Moreira, JFM 1999)



$\Longrightarrow$ need for a multiphase code

Out of equilibrium Riemann problem (1/4)

- metastable states (Thomson et al., JFM 1986 and 1988; Simoes-Moreira, JFM 1999)
- A phase transition wave is a self–similar discontinuity
  $\Longrightarrow$ Rankine–Hugoniot relations hold

$$\begin{cases} M = \dfrac{u_2 - u_1}{\tau_2 - \tau_1} \\ M^2 = -\dfrac{p_2 - p_1}{\tau_2 - \tau_1} \\ \varepsilon_2 - \varepsilon_1 + \dfrac{1}{2}(p_2 + p_1)(\tau_2 - \tau_1) = 0 \end{cases}$$

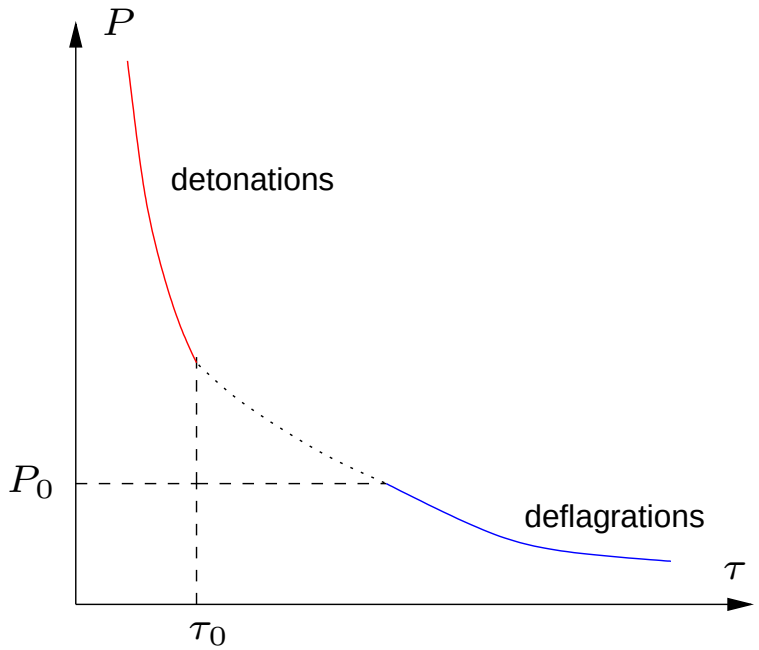
beware! ε_1 == E.O.S of the liquid

ε_2 == E.O.S of the mixture or the gas

$\Longrightarrow$ Chapman–Jouguet (CJ) theory

Out of equilibrium Riemann problem (2/4)

- Assumptions for the use of the CJ theory:
  - EOS are convex
  - $\varepsilon_2(P,\tau) - \varepsilon_1(P,\tau) < 0$
- upstream state $\notin$ the set of the downstream states



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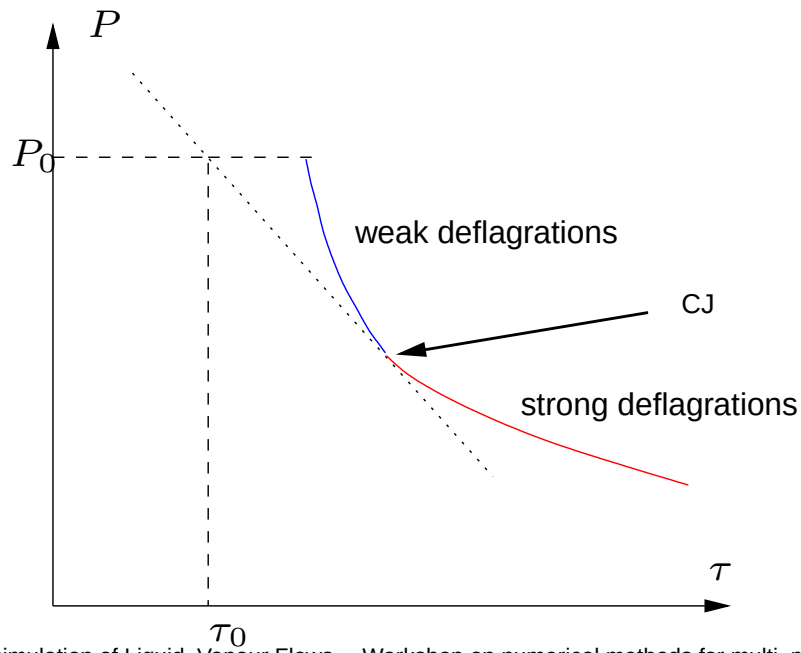
- τ increases $\Longrightarrow$ deflagration



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- No strong deflagrations $\Longrightarrow$ subsonic wave

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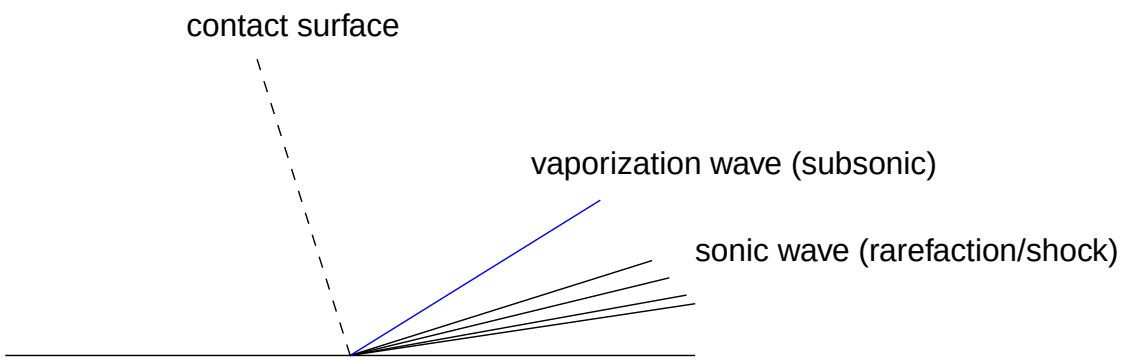

Out of equilibrium Riemann problem (3/4)

- $$\begin{aligned}\delta\varepsilon(y_l) = y_l\varepsilon_l(P,\tau_l(P)) + (1-y_l)\varepsilon_g(P,\tau_g(P)) \\ -\varepsilon_l(P, y_l\tau_l(P) + (1-y_l)\tau_g(P))\end{aligned} < 0$$

$$\frac{\mathrm{d}\delta\varepsilon}{\mathrm{d}T}(y_l) = (\tau_g - \tau_l)\,\frac{T^2}{\tau}\,\frac{\gamma g - \Gamma^2}{\Gamma}\frac{\mathrm{d}s_l}{\mathrm{d}T}$$

Out of equilibrium Riemann problem (3/4)

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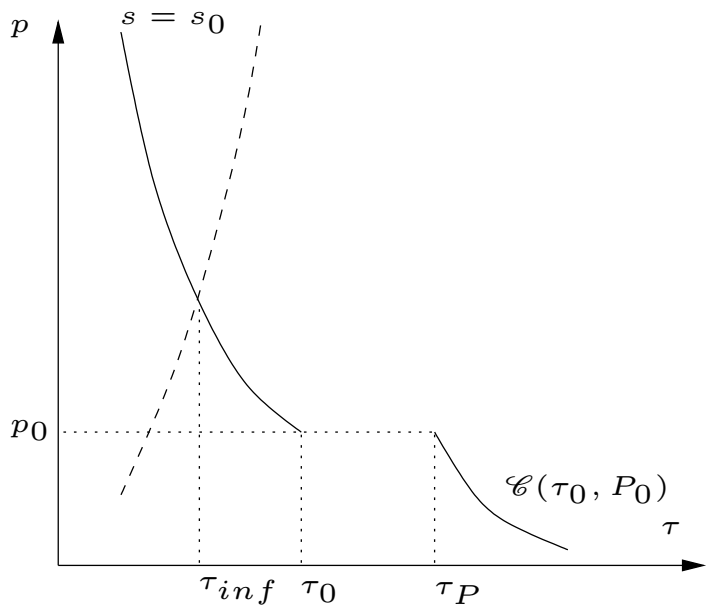
- entropy growth criterion



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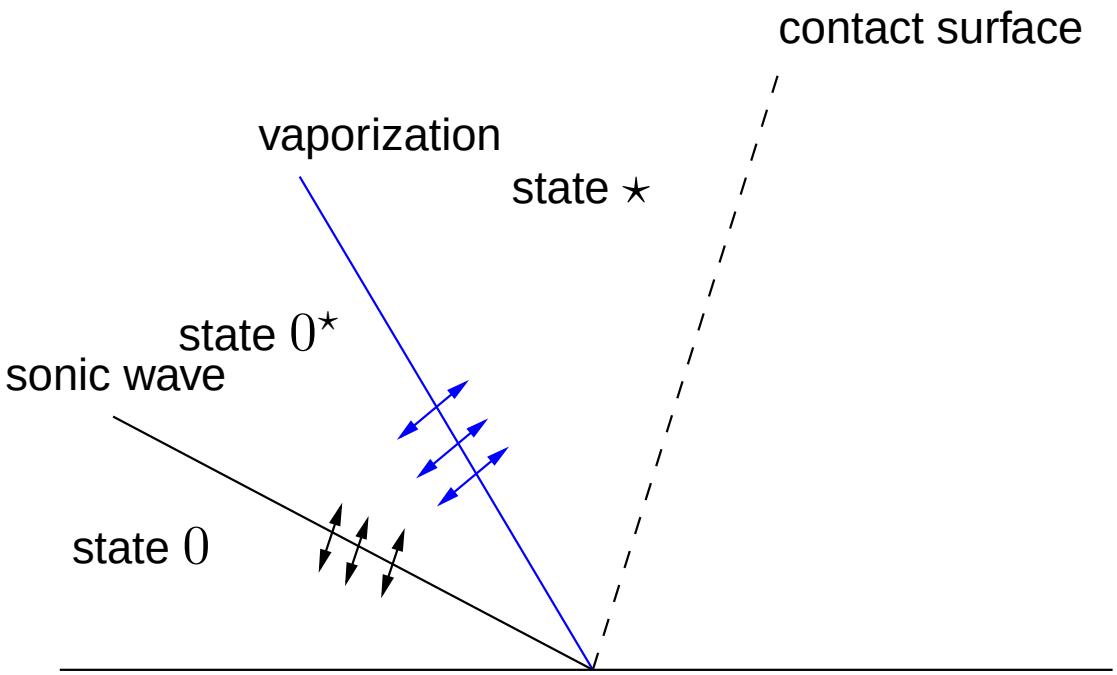
- entropy growth criterion

$$\frac{\mathrm{d}s}{\mathrm{d}\tau_0} = \frac{\gamma_m P_0}{T\Gamma_m}\left(\frac{\gamma_l\Gamma_m}{\gamma_m}\left(\frac{\tau_P}{\tau_0}-1\right) + \frac{\tau_P}{\tau_0}\left(\frac{\gamma_l}{\gamma_m}-1\right)\right)$$

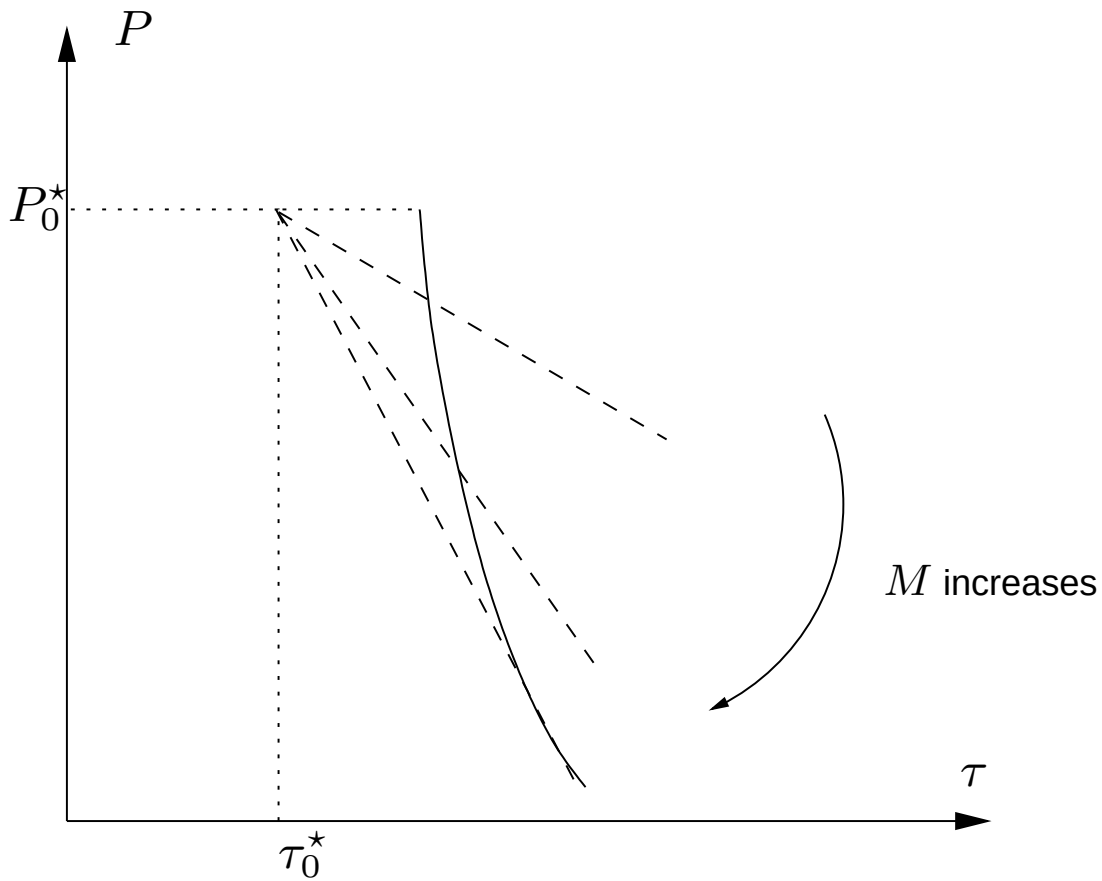
Out of equilibrium Riemann problem (4/4)

- one indeterminate



Out of equilibrium Riemann problem (4/4)

- one indeterminate
- A “physical” closure (Lemétayer et al, JCP 2005)



Out of equilibrium Riemann problem (4/4)

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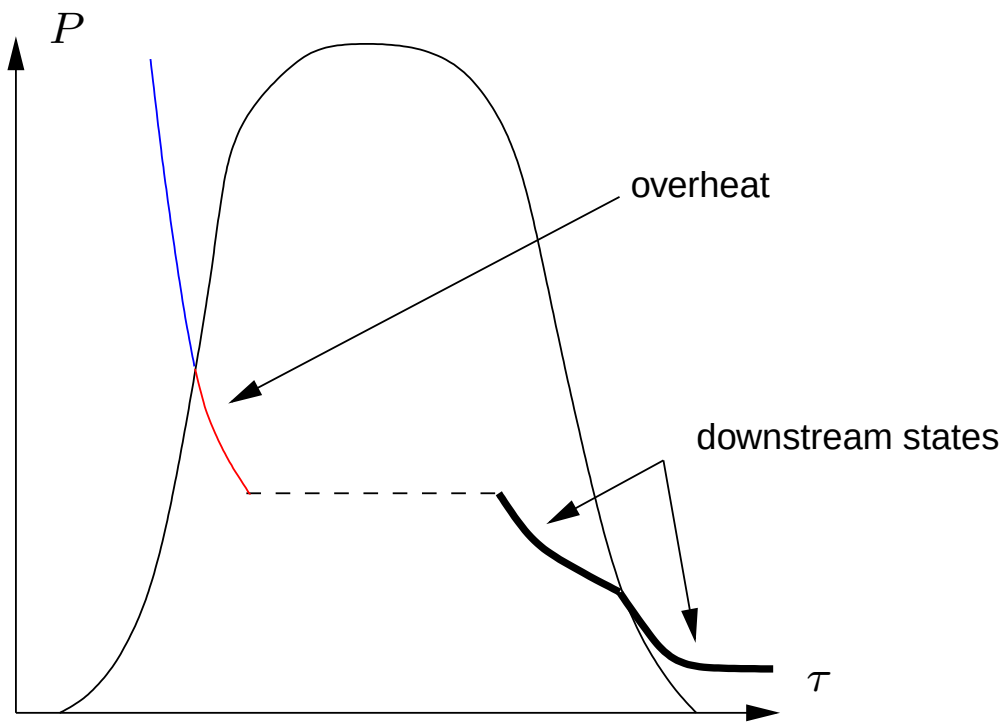
- ... leads to a solution that is not continuous with respect to its initial data!!!



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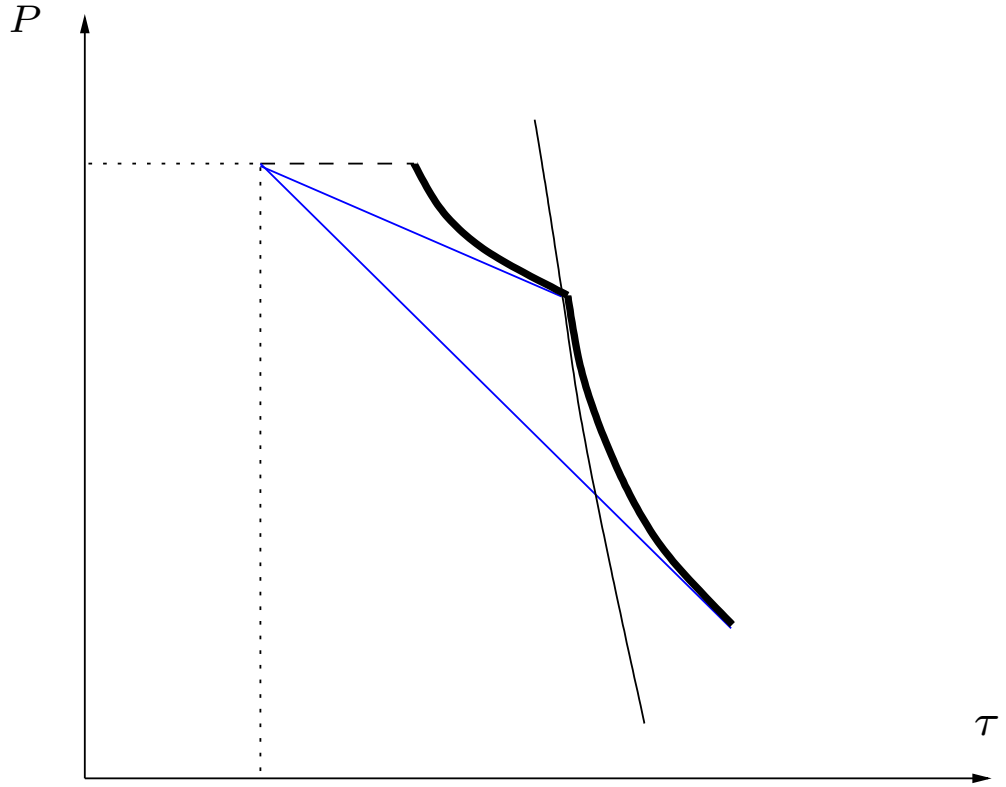

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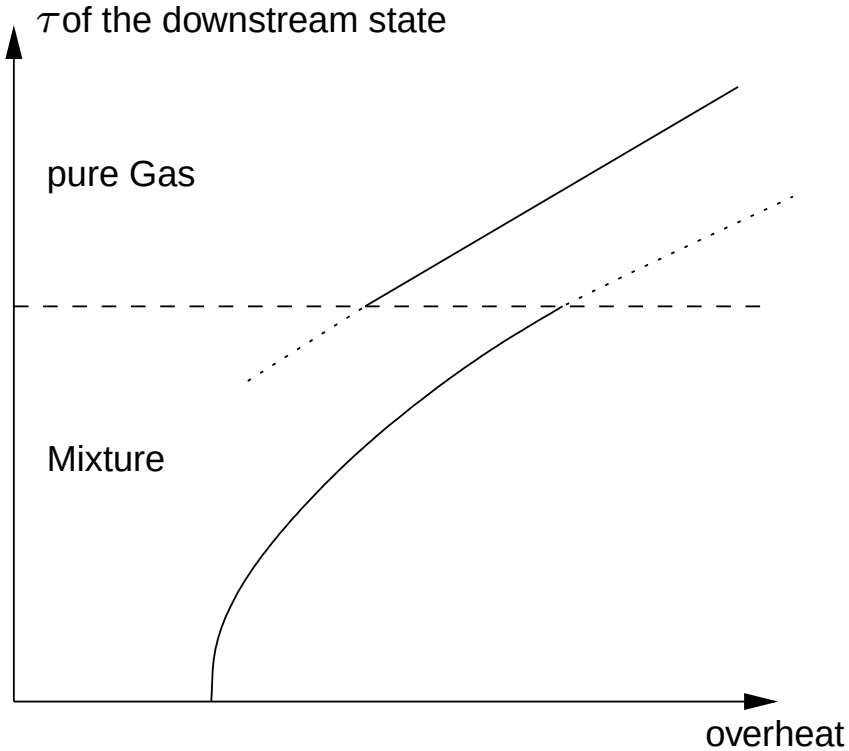

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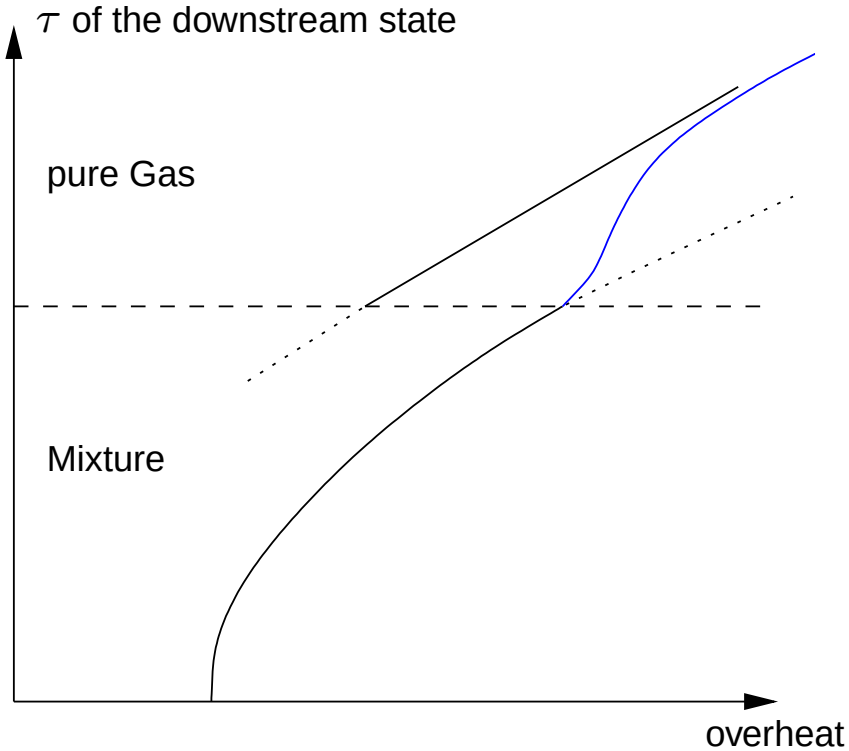

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Numerical method (Continuous model)

- Multiphase model

$$
\begin{array}{lcll}
\dfrac{\partial \alpha_k}{\partial t} & + & u_I \dfrac{\partial \alpha_k}{\partial x} & = 0 \\
\dfrac{\partial \alpha_k \rho_k}{\partial t} & + & \dfrac{\partial \alpha_k \rho u_k}{\partial x} & = 0 \\
\dfrac{\partial \alpha_k \rho_k u_k}{\partial t} & + & \dfrac{\partial \alpha_k \left(\rho_k u_k^2 + p_k\right)}{\partial x} & = p_I \dfrac{\partial \alpha_k}{\partial x} \\
\dfrac{\partial \alpha_k \rho_k E_k}{\partial t} & + & \dfrac{\partial \alpha_k u_k \left(\rho_k E_k + p_k\right)}{\partial x} & = u_I p_I \dfrac{\partial \alpha_k}{\partial x}
\end{array}
$$

- problems
  - How to choose u_I, p_I ? modelling problem
  - non conservative products

Numerical method (Continuous model)

Reference : Drew–Passman, Theory of multicomponent fluids, *Applied Math. Sciences*, **135**, Springer, 1998

Assumptions

1. Location of bubbles, size, micro-scale details of the flow are unknown
2. Given a set of initial and boundary condition, we consider one experiment as a realisation of this flow.
3. What we expect to observe/compute is an <u>ensemble average</u> of these experiments

Numerical method (Continuous model)

Reference : Drew–Passman, Theory of multicomponent fluids, *Applied Math. Sciences*, **135**, Springer, 1998

1. **Equations for each phase**
   Euler

$$\chi_k \left(\partial_t U_k + \partial_x F_k(U_k)\right) = 0$$

$+$ Topological equation for the interface

$$\partial_t \chi_k + \sigma \partial_x \chi_k = 0$$

Numerical method (Continuous model)

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1. **Equations for each phase**
   Euler $+$ Topological equation for the interface
2. **Average**

$$
\begin{aligned}
&\partial_t \alpha_k \rho_k + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = \mathcal{E}\left(\rho\left(\mathbf{u}_k - \sigma\right) \cdot \nabla \chi_k\right) \\
&\partial_t \alpha_k \rho_k \mathbf{u}_k + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \otimes \mathbf{u}_k + \alpha_k P_k) \\
&\qquad = \mathcal{E}\left(\left(\rho_k \mathbf{u}_k (\mathbf{u}_k - \sigma) + P_k\right) \cdot \nabla \chi_k\right) \\
&\partial_t \alpha_k \rho_k E_k + \nabla \cdot (\alpha_k \rho_k E_k \mathbf{u}_k + \alpha_k P_k \mathbf{u}_k) \\
&\qquad = \mathcal{E}\left(\left(\rho_k E_k (\mathbf{u}_k - \sigma) + P_k \mathbf{u}_k\right) \cdot \nabla \chi_k\right)
\end{aligned}
$$

$$
\partial_t \alpha_k + \mathcal{E}\left(\sigma \cdot \partial_x \chi_k\right) = 0
$$

Numerical method (Continuous model)

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1. **Equations for each phase**
   Euler $+$ Topological equation for the interface
2. **Average**
3. **Modelling**

$$\mathcal{E}\left(P_k \nabla \chi_k\right) = P_I \nabla \alpha_k$$

$$\mathcal{E}\left(\left(P_k \mathbf{u}\right) \cdot \nabla \chi_k\right) = P_I \mathbf{u}_I \nabla \alpha_k$$

$$\mathcal{E}\left(\sigma \cdot \nabla \chi_k\right) = \mathbf{u}_I \nabla \alpha_k$$

Numerical method (Continuous model)

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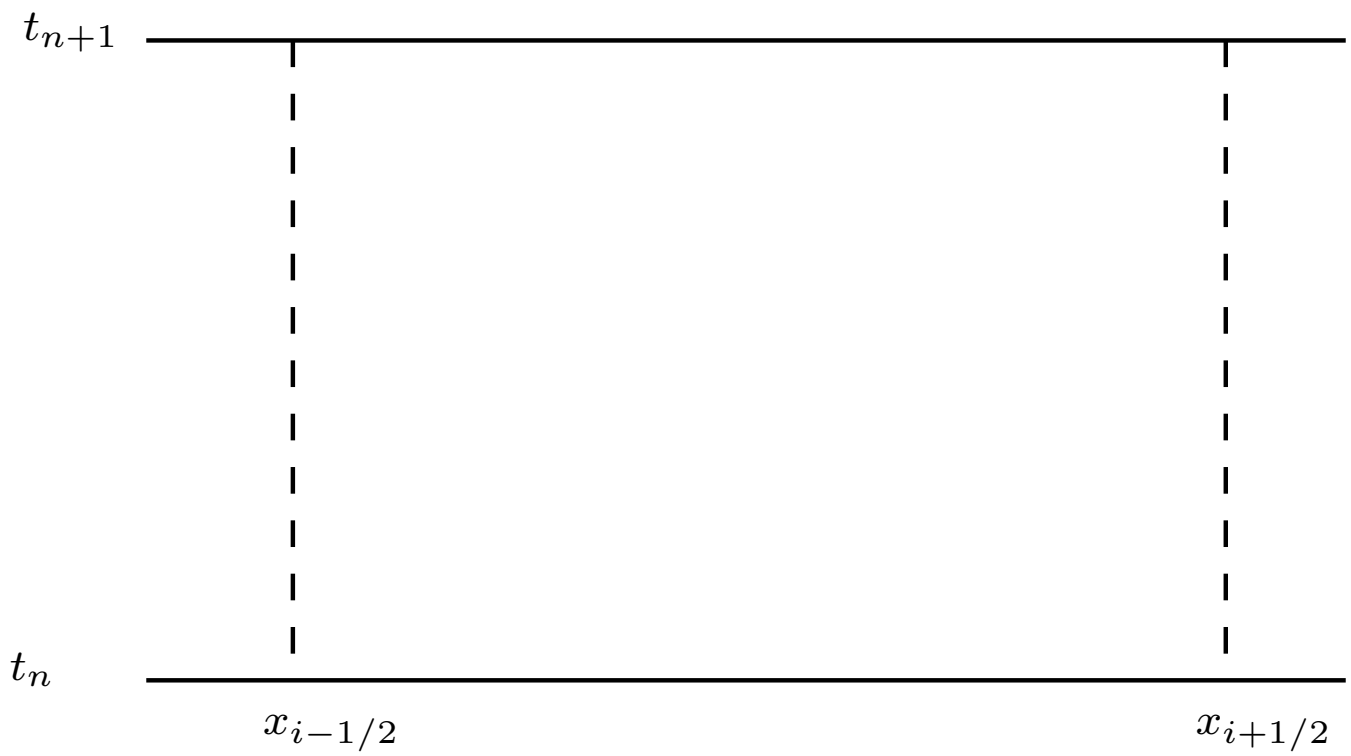
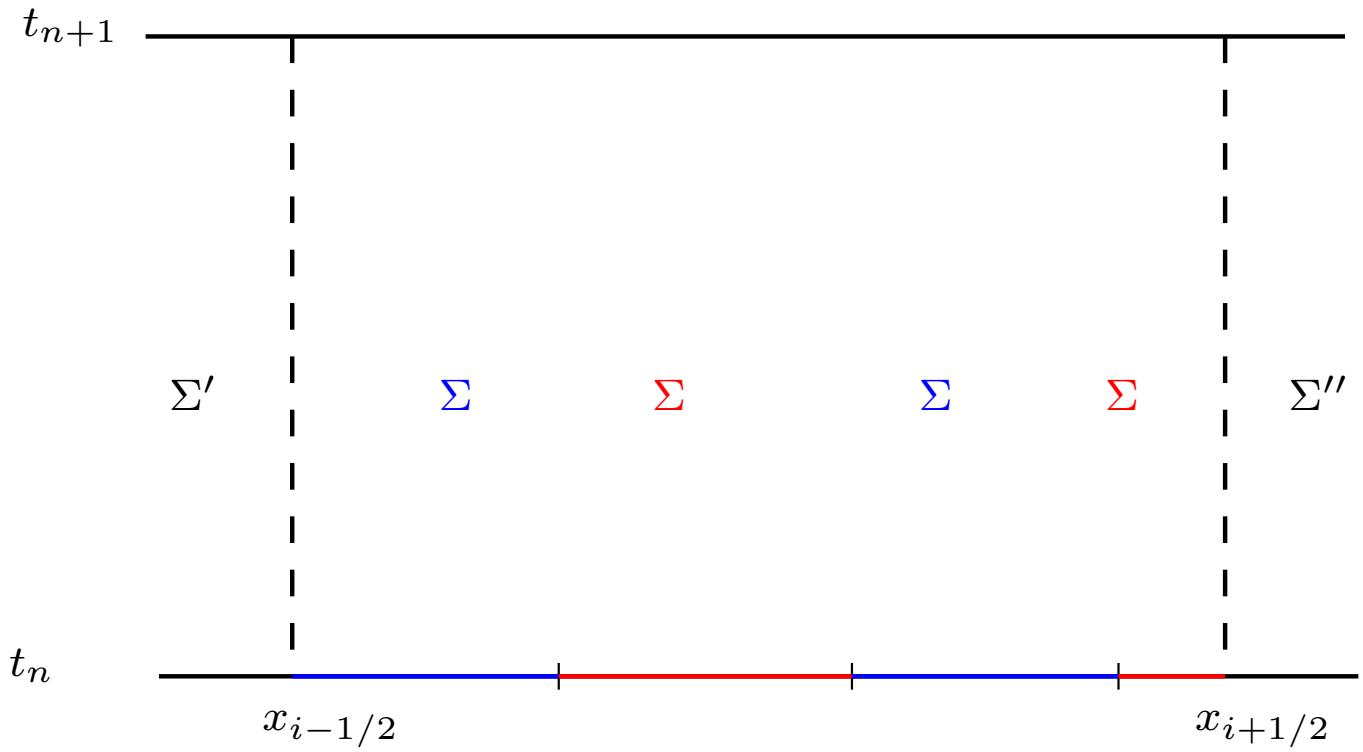
1. **Equations for each phase**
   Euler $+$ Topological equation for the interface
2. **Average**
   Closure Problems
3. **Modelling**
   Non conservative Products+ Closure Pbs

Numerical method



- a Cell of the mesh. We know (α, ρ, u, P) in each cell

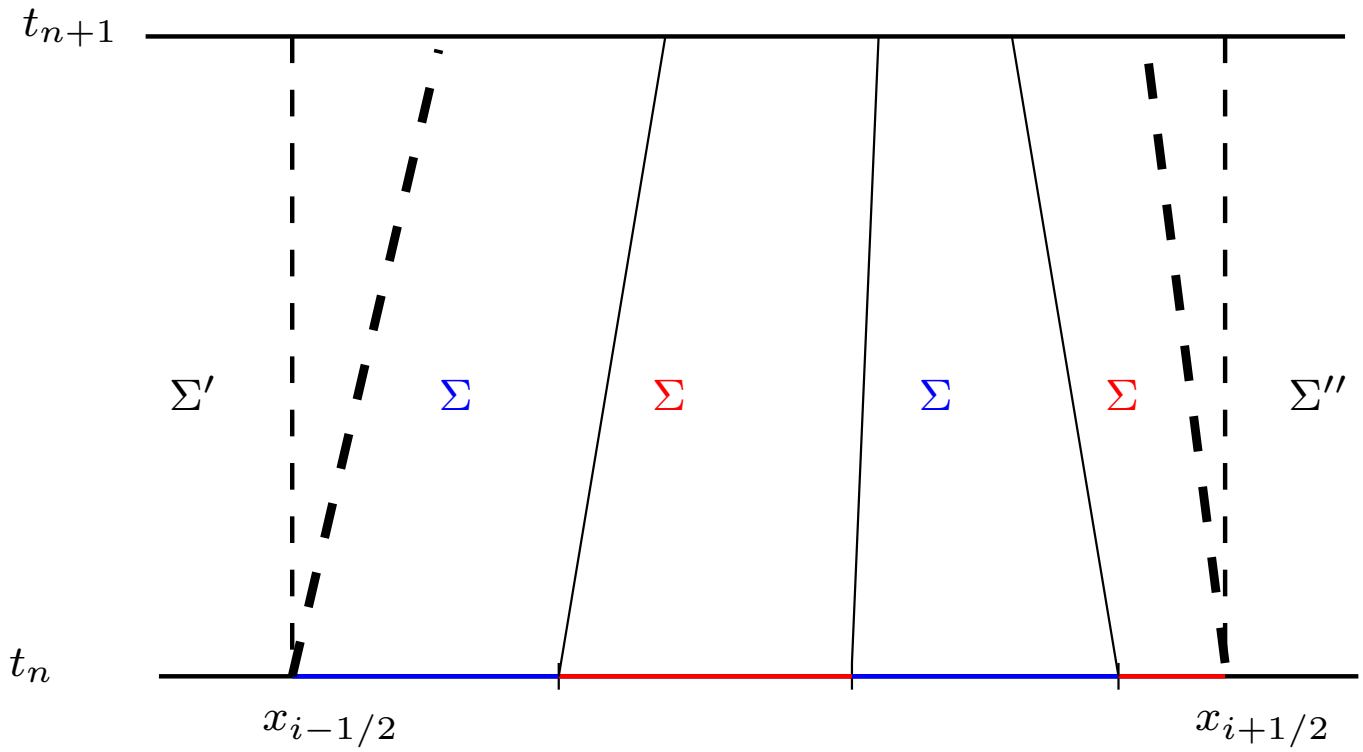
Numerical method



- cut the cell into subcells, taking care of $\displaystyle\int_{\Delta x} X = \alpha$

  do the same for the neighbours cells

Numerical method



- Evolution in time

Numerical method

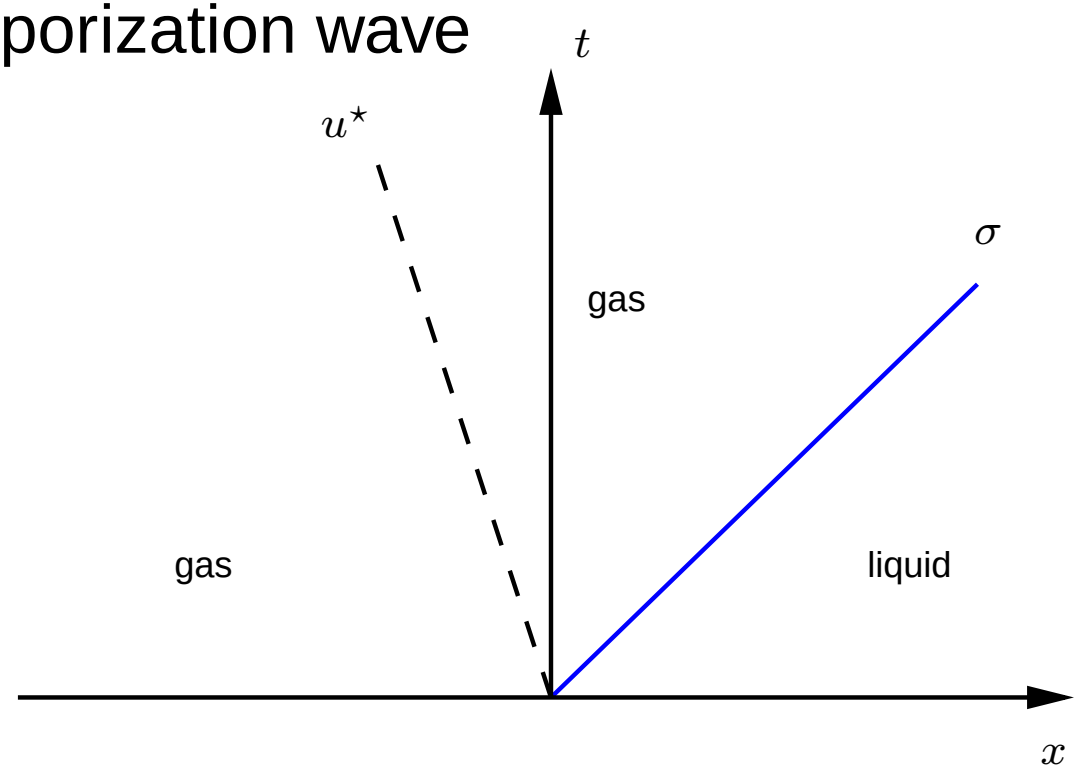
- Averaging procedure
- Probability in the boundary of the cell:

$$\mathcal{P}_{i+1/2}(\Sigma_1, \Sigma_1) = \min(\alpha_i^{(1)}, \alpha_{i+1}^{(1)})$$
$$\mathcal{P}_{i+1/2}(\Sigma_1, \Sigma_2) = \max(0, \alpha_i^{(1)} - \alpha_{i+1}^{(1)})$$

- see Abgrall/Saurel, JCP, 2003

Numerical method

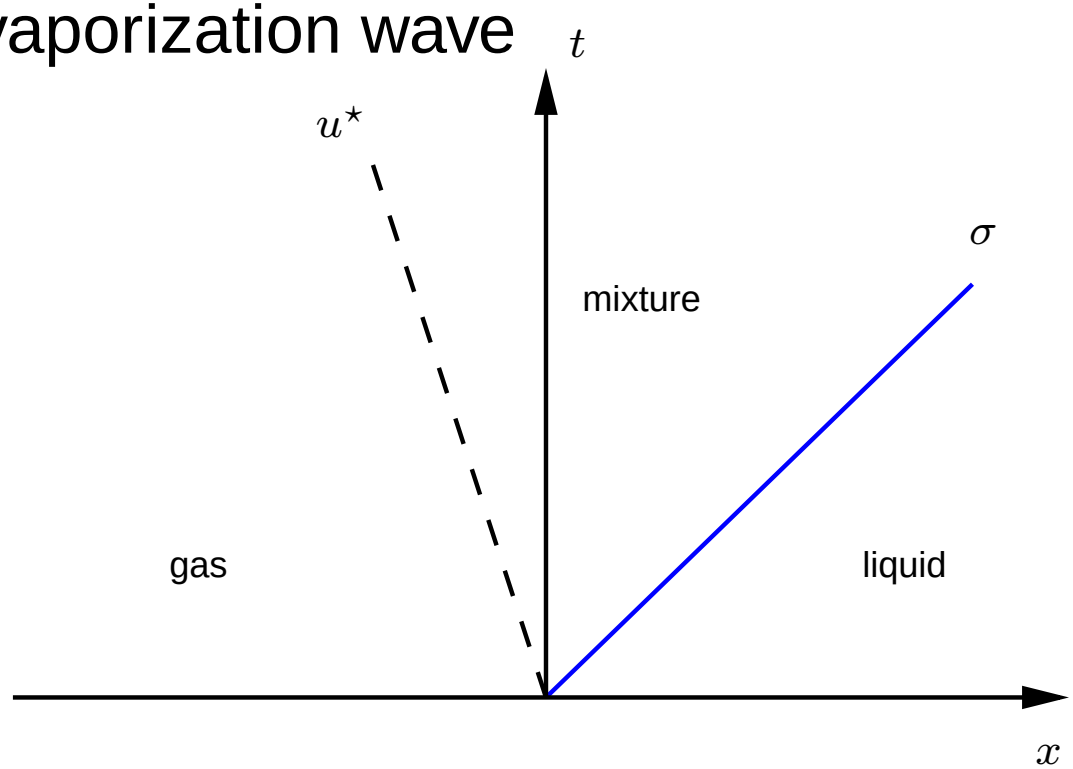
- extension to reactive flux
- Total vaporization wave



$\Longrightarrow$ replace the contact discontinuity by the vaporization wave

Numerical method

- extension to reactive flux
- Partial vaporization wave



Numerical method

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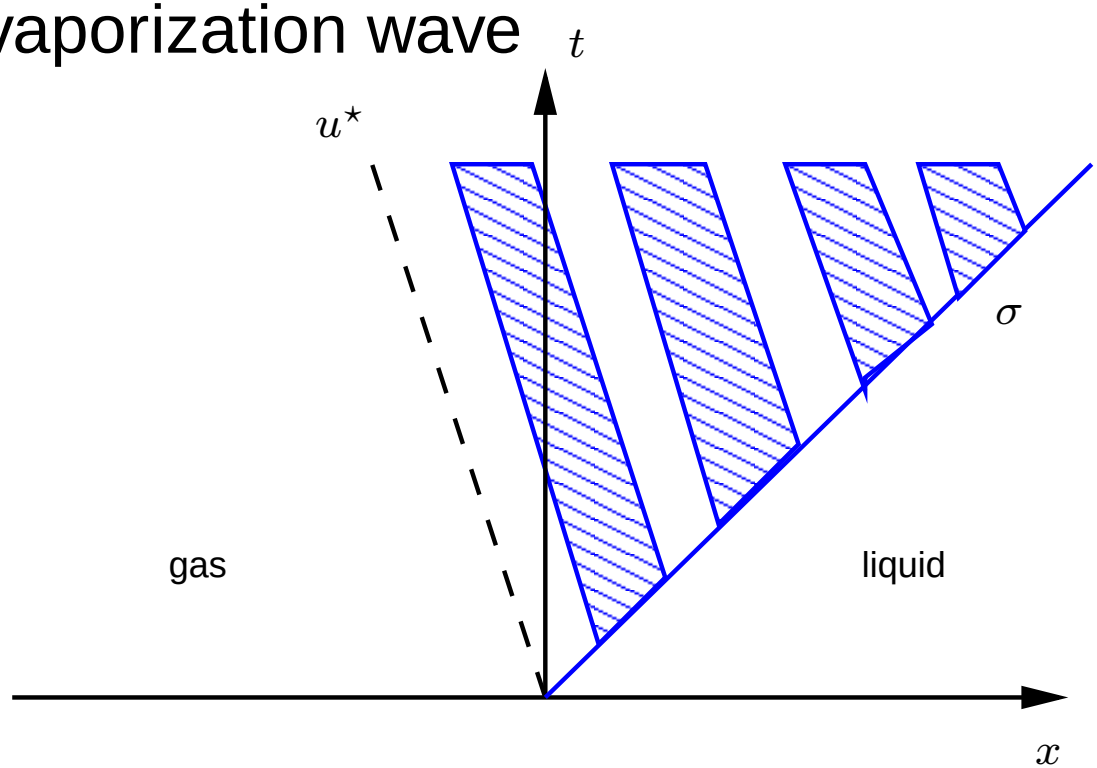

$\Longrightarrow$ Average of total and partial vaporization wave

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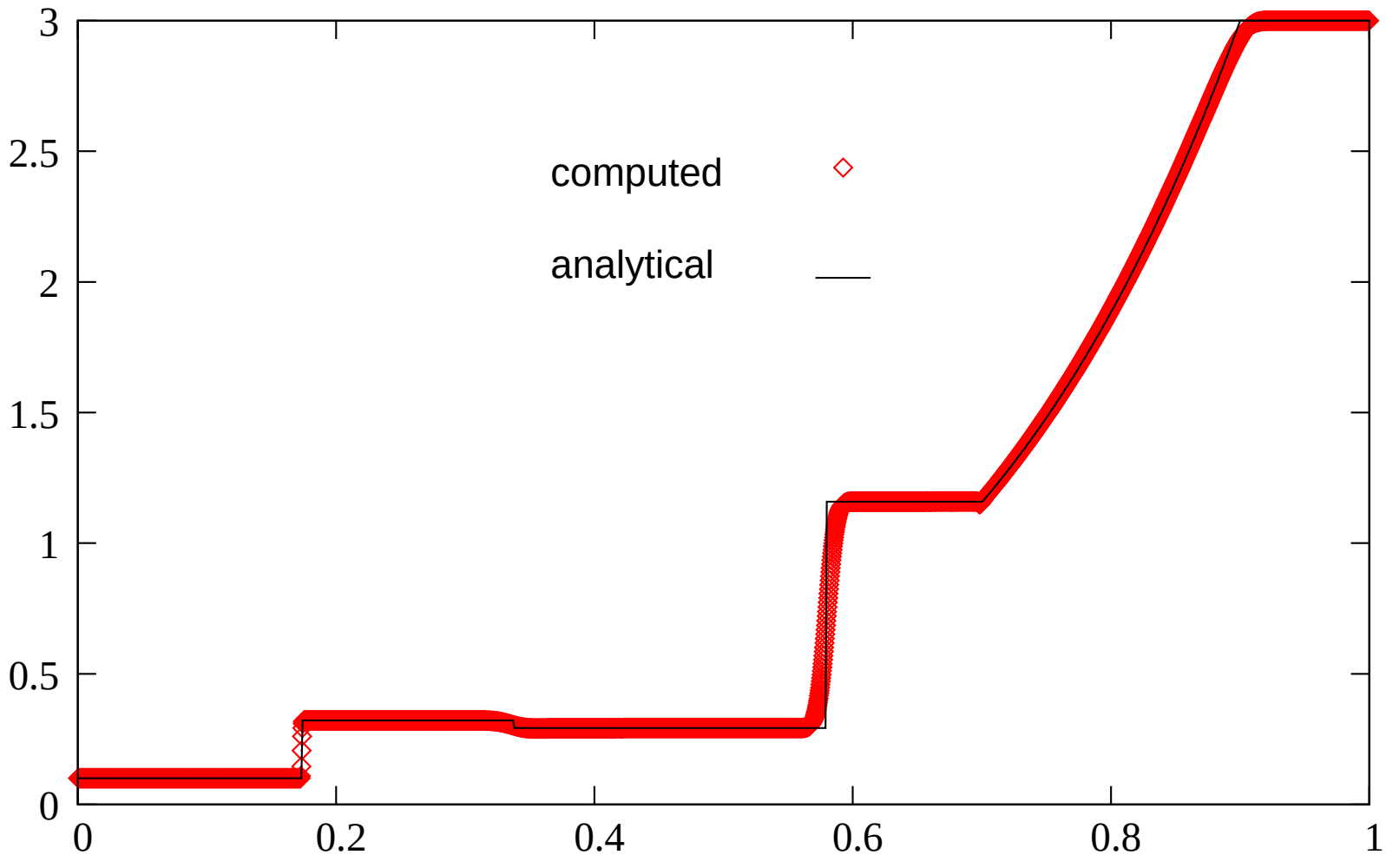
Vaporisation

- Shock tube

Gas	Liquid
$P = 10^5$Pa	$P = 10^9$Pa
$\rho = 0.1$kg.m^{-3}	$\rho = 3$kg.m^{-3}
$u = 0$	$u = 0$

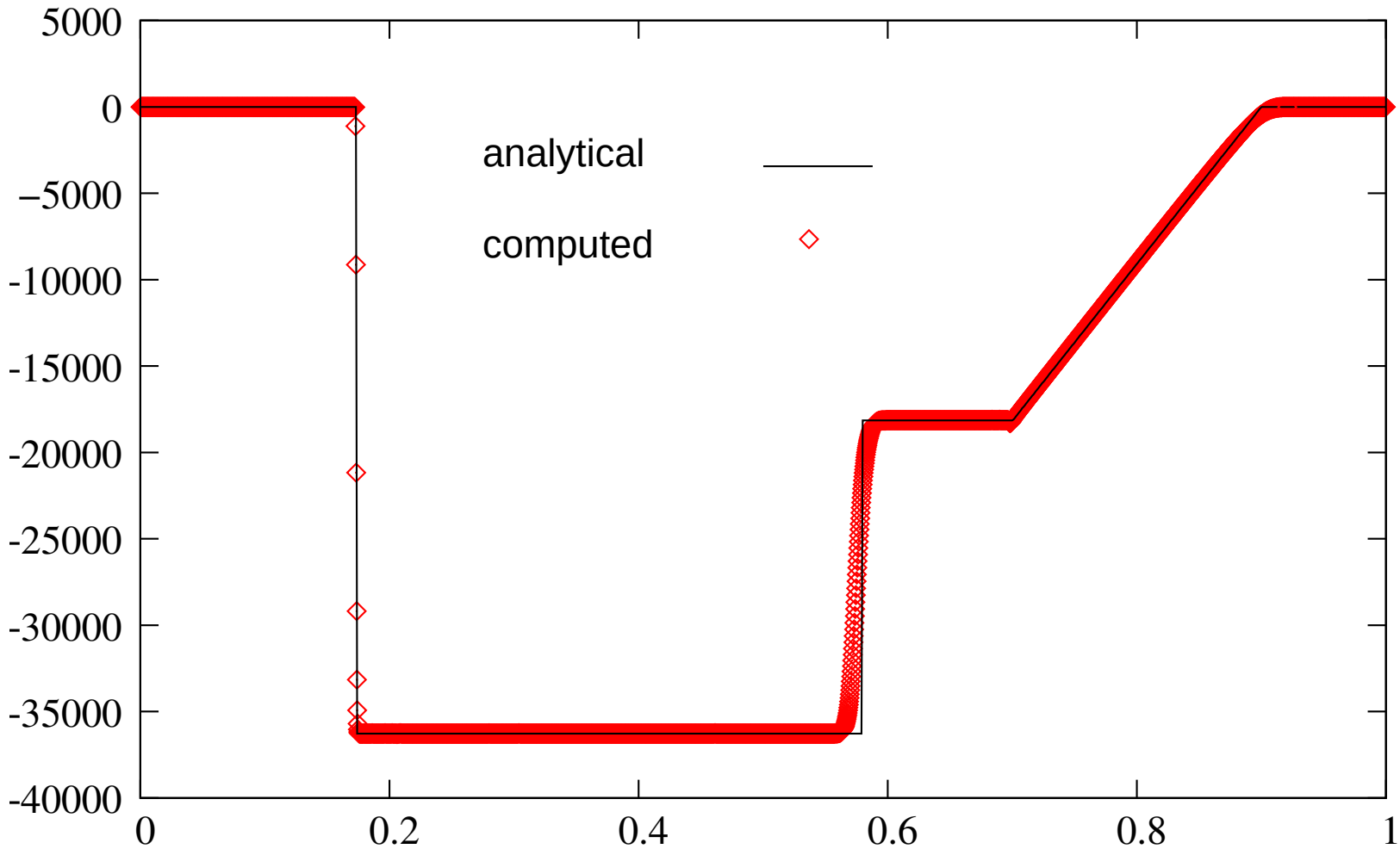
Vaporisation

- Density



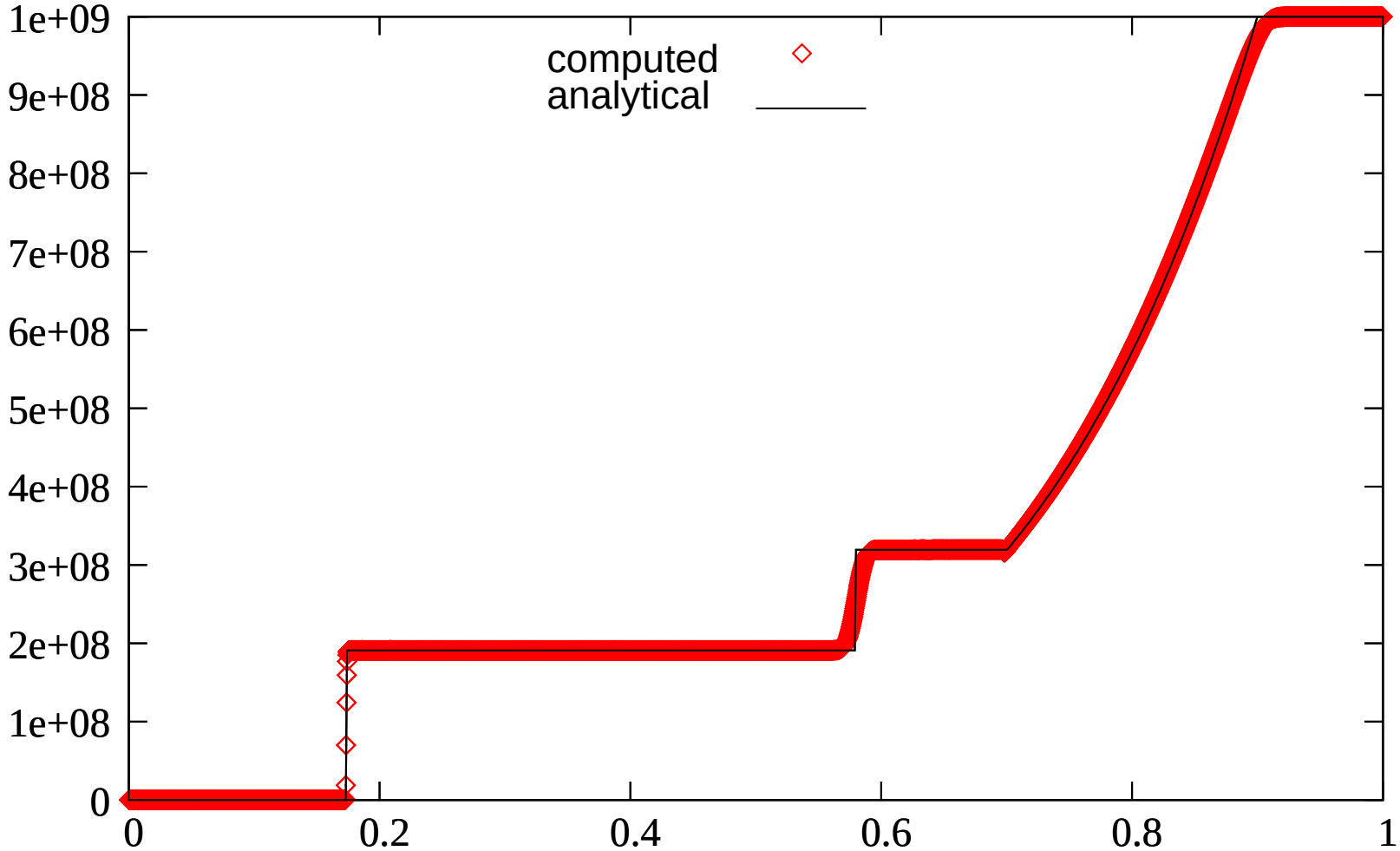
Vaporisation

- Velocity



Vaporisation

- Pressure



Conclusion

- contruction of a solution for the Riemann problem with phase transition
  - entropy growth condition
  - continuity of the intermediates states with respect to the initial states
- easy computation thanks for the discrete equation method (right and left states of the Riemann problems are always pure fluids)

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Thank you!

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