A numerical scheme for condensation and flash vaporization

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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

- Two equations of state: $\varepsilon_1(P,T)$ and $\varepsilon_2(P,T)$

Thermodynamic model

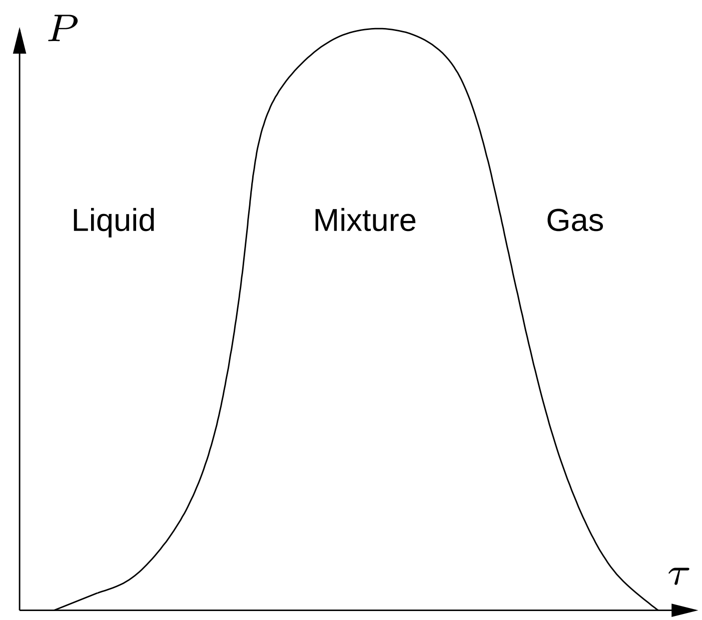
- Two equations of state: $\varepsilon_1(P,T)$ and $\varepsilon_2(P,T)$
- Mixture zone
  - Suppose that fluids are locally non miscible
    $V_1 + V_2 = V_{\text{tot}}$
  - Optimization of mixture entropy

$\Longrightarrow$ When the mixture is stable

$$\mu_1 = \mu_2 \qquad P_1 = P_2 \qquad T_1 = T_2$$

Thermodynamic model

- Two equations of state: $\varepsilon_1(P,T)$ and $\varepsilon_2(P,T)$
- Mixture zone



- 3 convex E.O.S.

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Equilibrium EOS (1/4)

- Look for simple waves for the Euler system

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- Look for simple 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 (1/4)

- Look for simple waves for the Euler system
- Look for self similar solutions

$+$ Entropy criterion

- If P decreases, isentropic regular wave

$$S = \text{cste}$$

Equilibrium EOS (1/4)

- Look for simple waves for the Euler system
- Look for self similar solutions

\+ Entropy criterion

- If P decreases, isentropic regular wave
- If P increases, shock: Rankine–Hugoniot relations

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

Equilibrium EOS (1/4)

- Look for simple waves for the Euler system
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$+$ Entropy criterion

  - If P decreases, isentropic regular wave
  - If P increases, shock: Rankine–Hugoniot relations

- if the E.O.S if globally convex, existence and uniqueness of a solution for the Riemann Problem

Equilibrium EOS (2/4)

- Consequences of the phase transition for Hugoniot Curves

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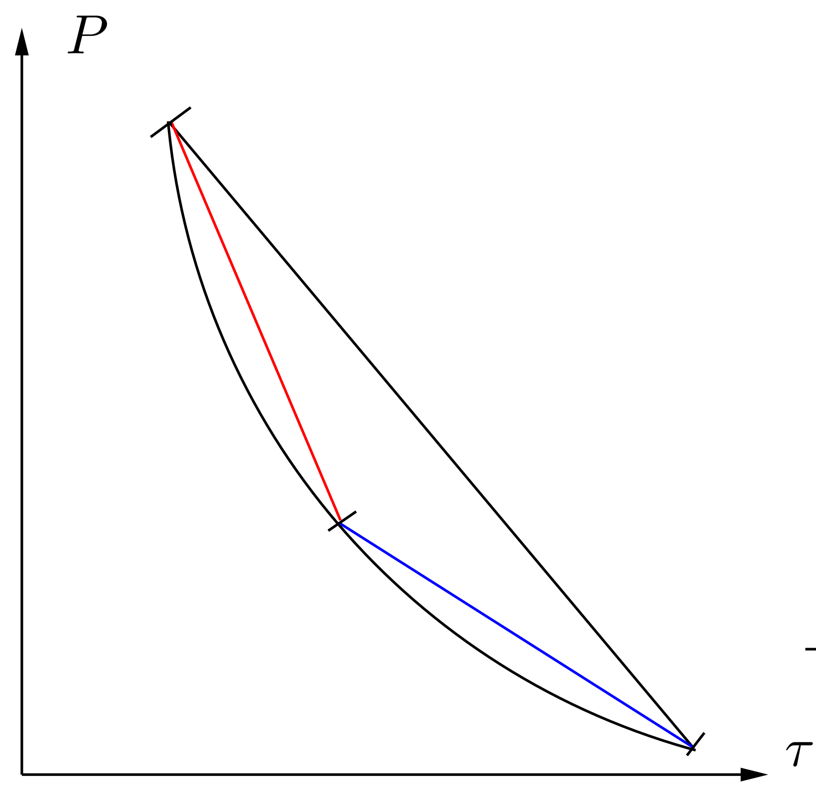
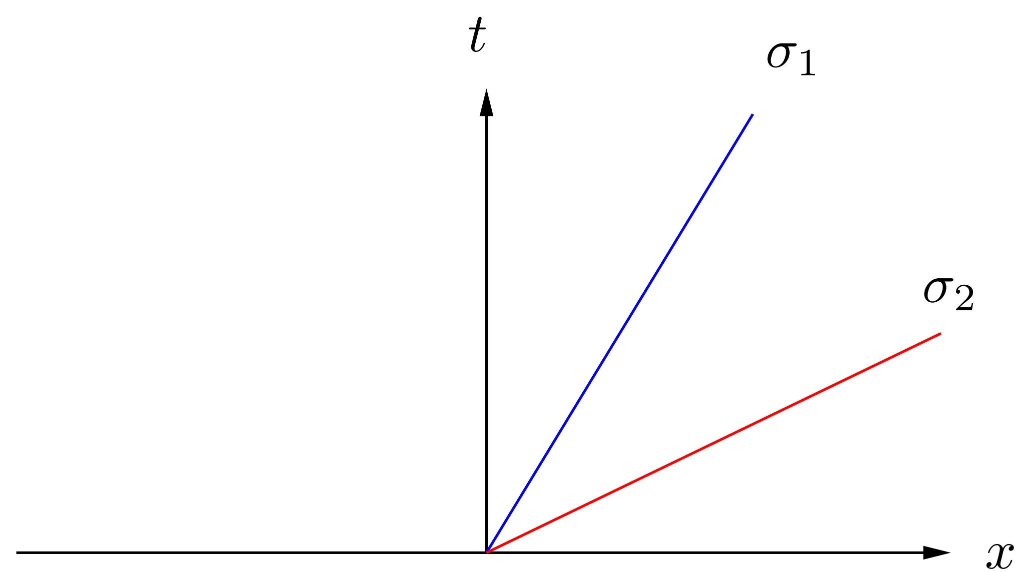
- Consequences of the phase transition for Hugoniot Curves





Equilibrium EOS (2/4)

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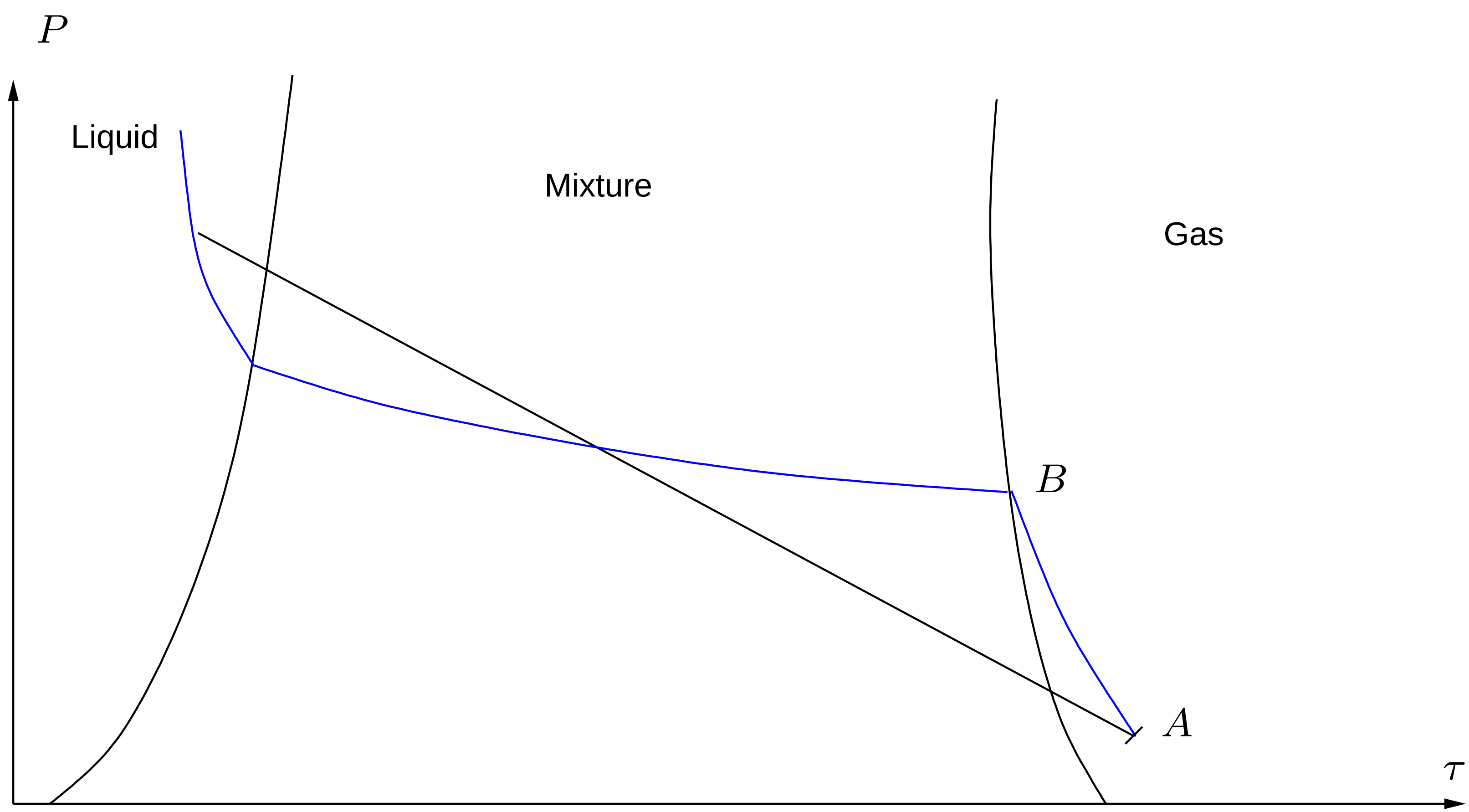

Equilibrium EOS (2/4)

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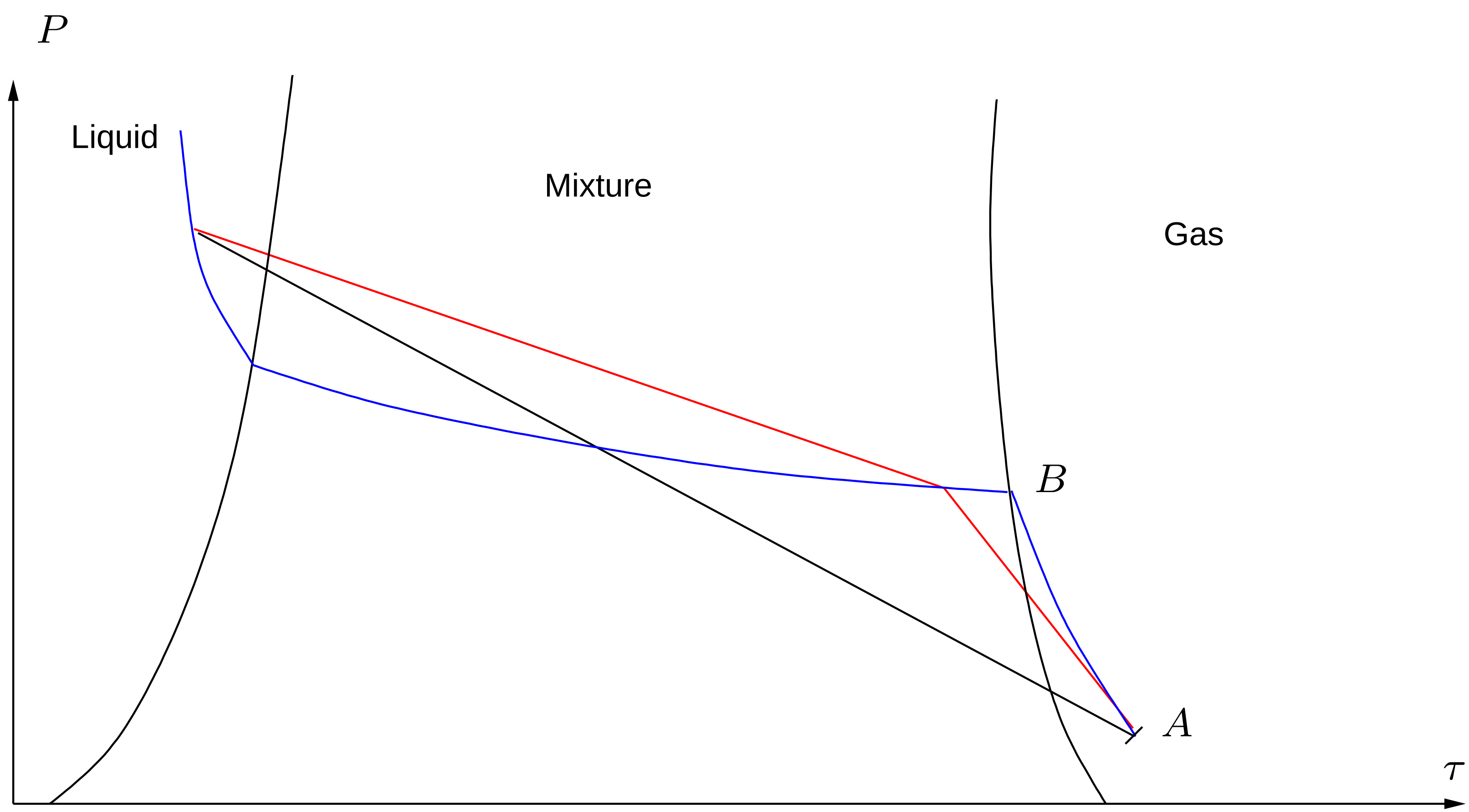


Equilibrium EOS (2/4)

- Consequences of the phase transition for Hugoniot Curves
- Lost the uniqueness of the entropic solution

Equilibrium EOS (2/4)

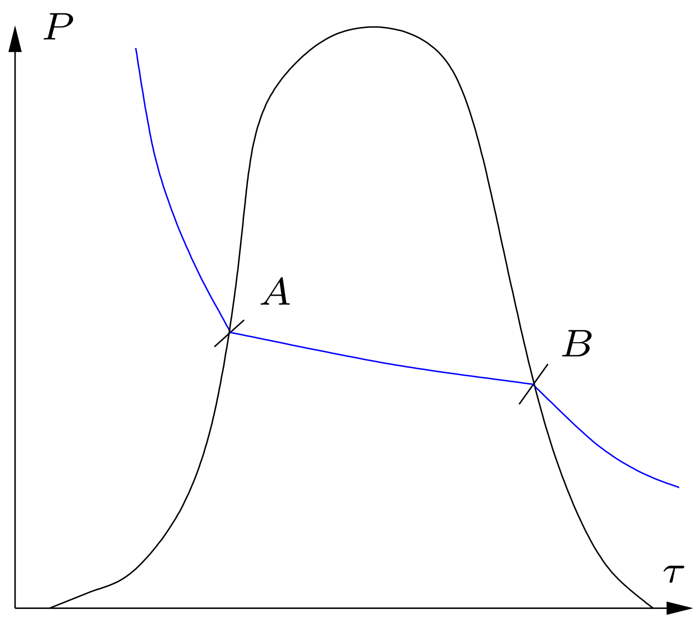
- Consequences of the phase transition for Hugoniot Curves
- Lost the uniqueness of the entropic solution
- Liu (1975) The “ physical” solution is the one with a wave splitting in B

Equilibrium EOS (3/4)

- Consequences for isentropic waves

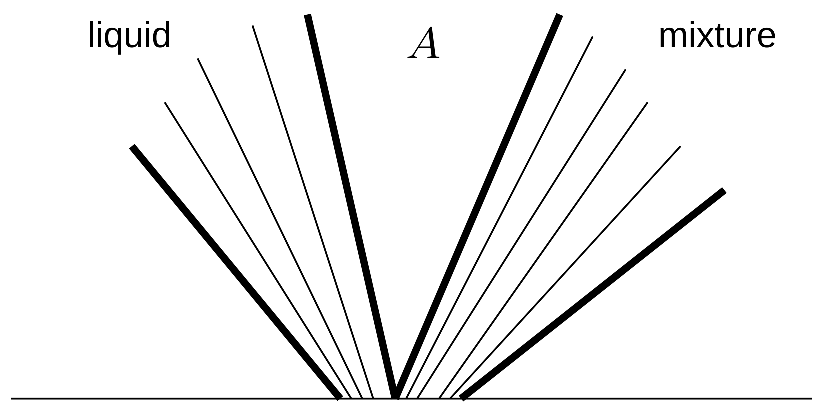
Equilibrium EOS (3/4)

- Consequences for isentropic waves



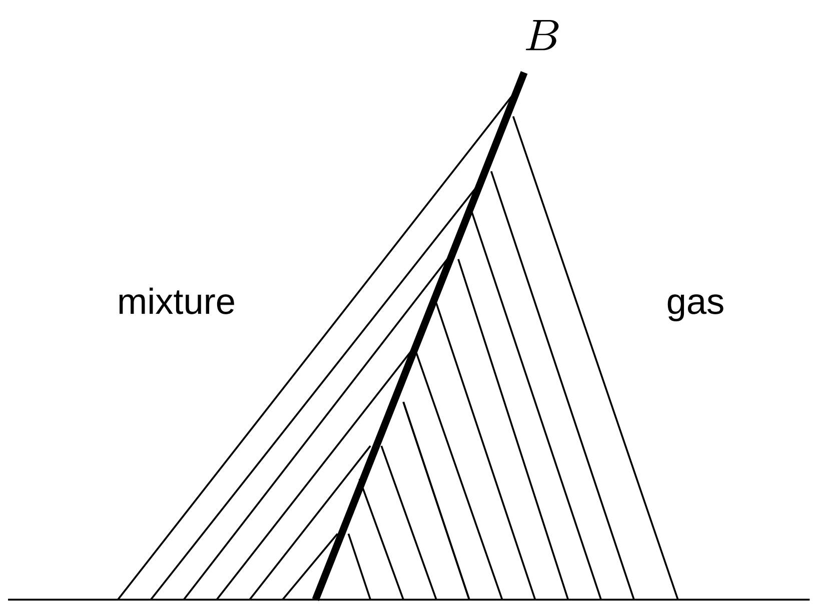
Equilibrium EOS (3/4)

- Consequences for isentropic waves
- Characteristic curves in point A



Equilibrium EOS (3/4)

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



Equilibrium EOS (3/4)

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

Equilibrium EOS (4/4)

- Non uniqueness for compressive waves
  $\Longrightarrow$ difficulties to compute the right solution with approximate solvers (Jaouen Phd Thesis)
- No solution for undercompressive waves
  $\Longrightarrow$ Trash

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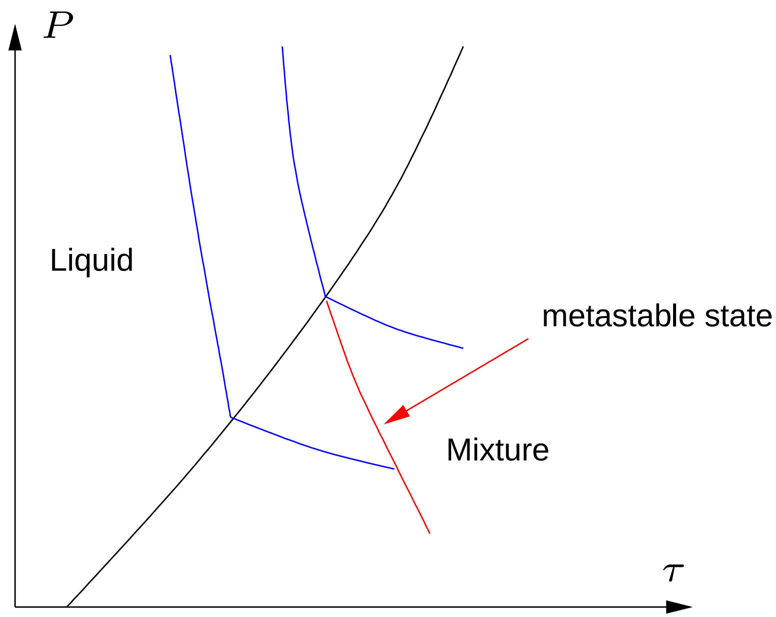
Out of equilibrium Riemann problem (1/3)

- metastable states



$\Longrightarrow$ need for a multiphase code

Out of equilibrium Riemann problem (1/3)

- metastable states
- A phase transition wave is a self–similar discontinuity
  $\Longrightarrow$ Rankine–Hugoniot relations hold

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

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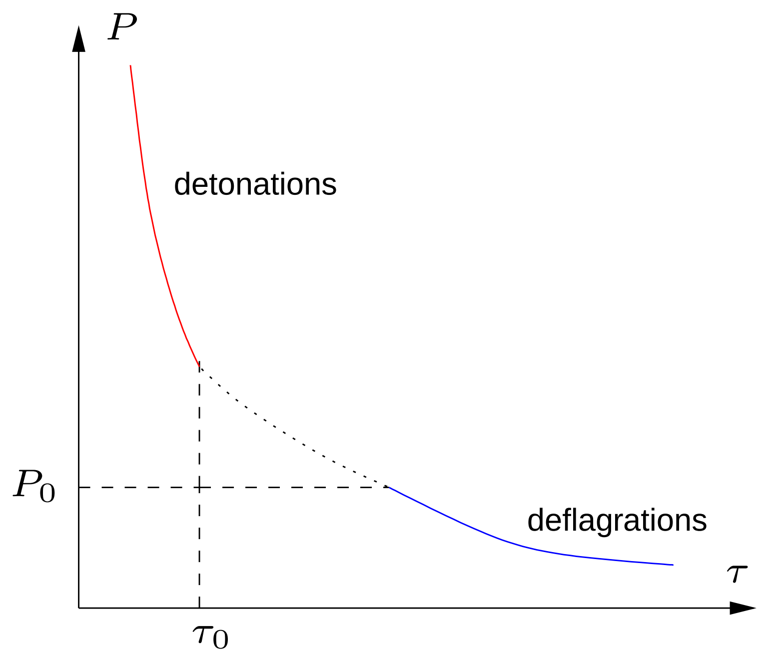
beware! ε_1 == E.O.S of the liquid
ε_2 == E.O.S of the mixture or the gas

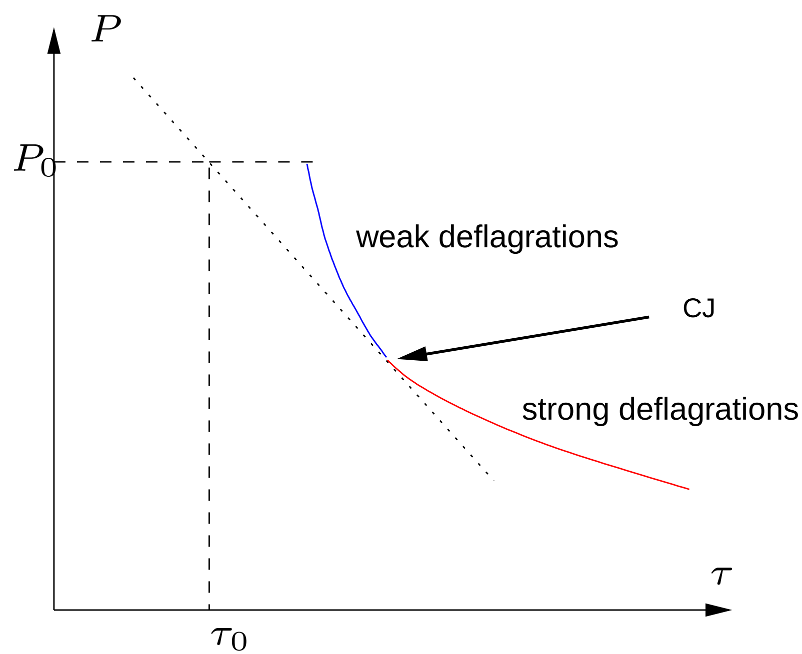
Out of equilibrium Riemann problem (2/3)

- upstream state $\notin$ the set of the downstream states



Out of equilibrium Riemann problem (2/3)

- upstream state $\notin$ the set of the downstream states
- τ increases $\Longrightarrow$ deflagration



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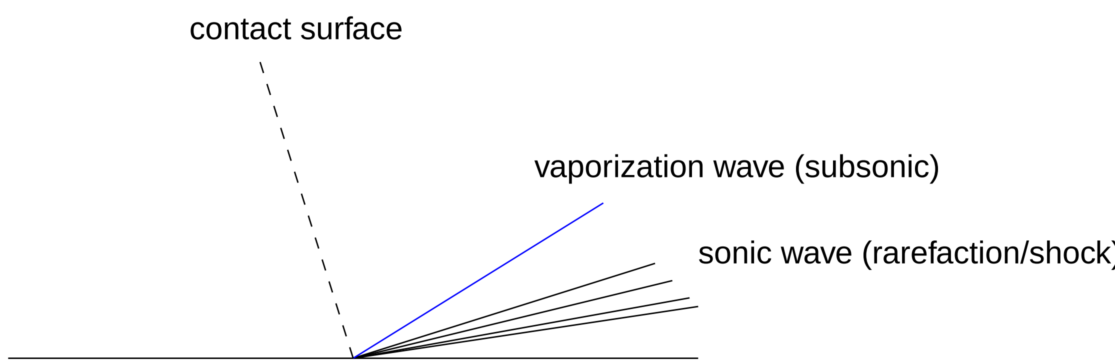
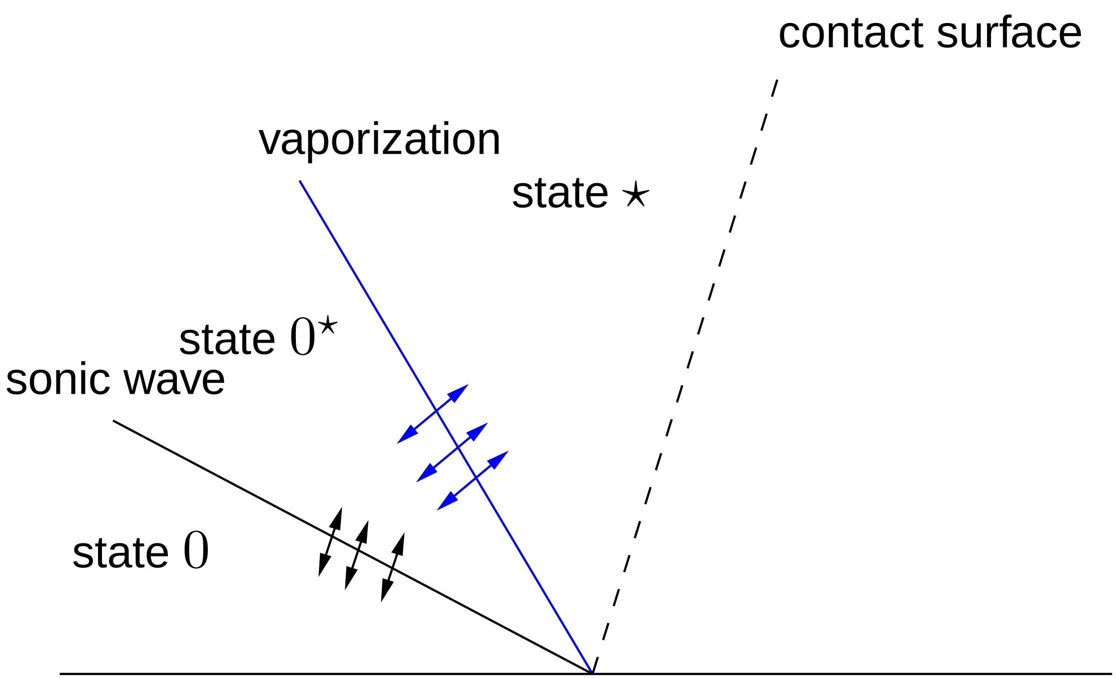


Out of equilibrium Riemann problem (2/3)

- upstream state $\notin$ the set of the downstream states
- τ increases $\Longrightarrow$ deflagration
- No strong deflagrations (Lax characteristic condition) $\Longrightarrow$ subsonic wave
- entropy growth is ensured for all the downstream states of weak deflagration

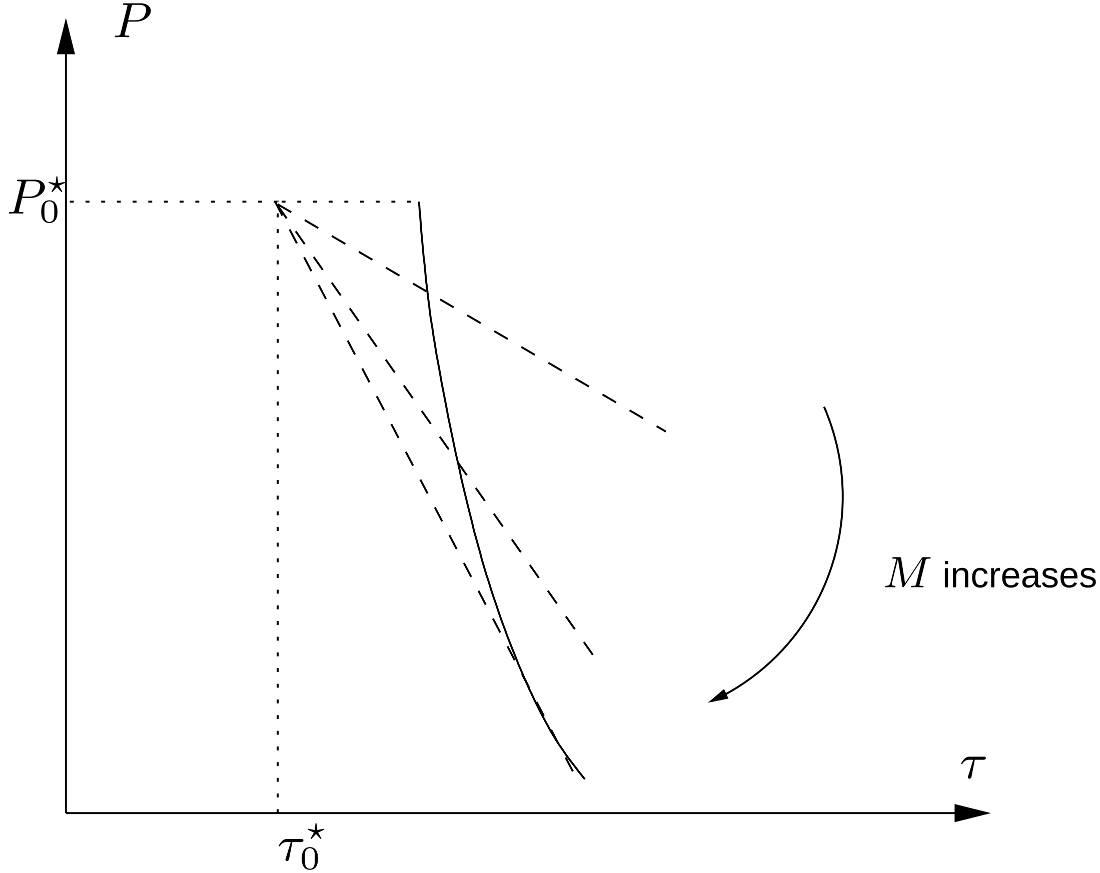
Out of equilibrium Riemann problem (3/3)

- one indeterminate



Out of equilibrium Riemann problem (3/3)

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



Out of equilibrium Riemann problem (3/3)

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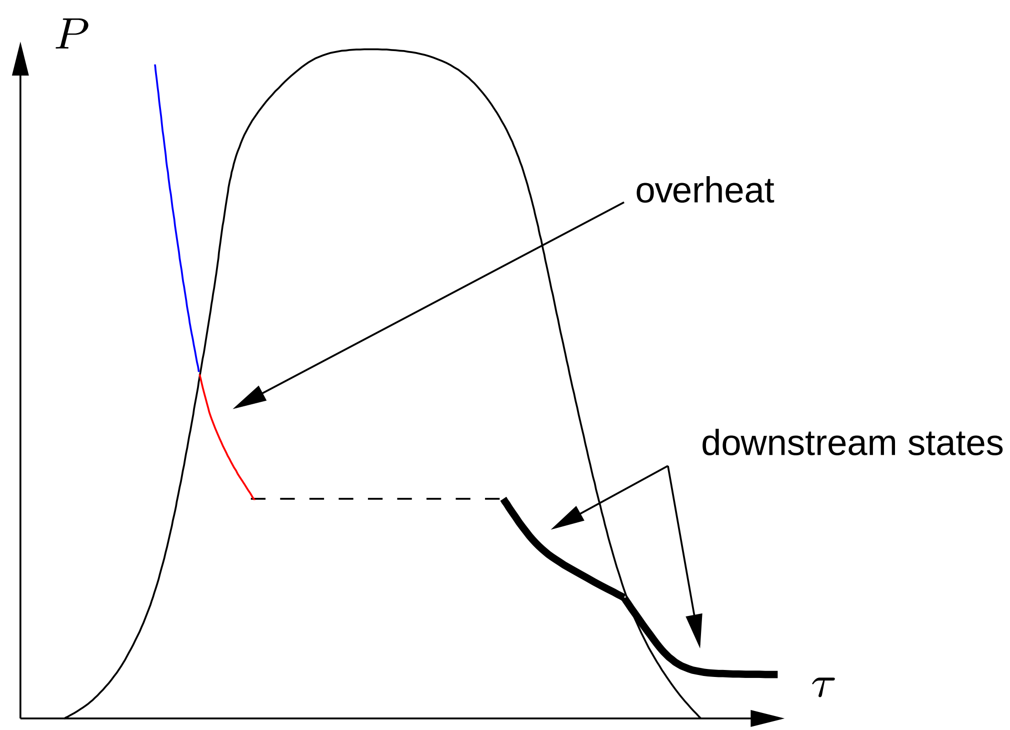
- ... leads to an ill posed problem!!!



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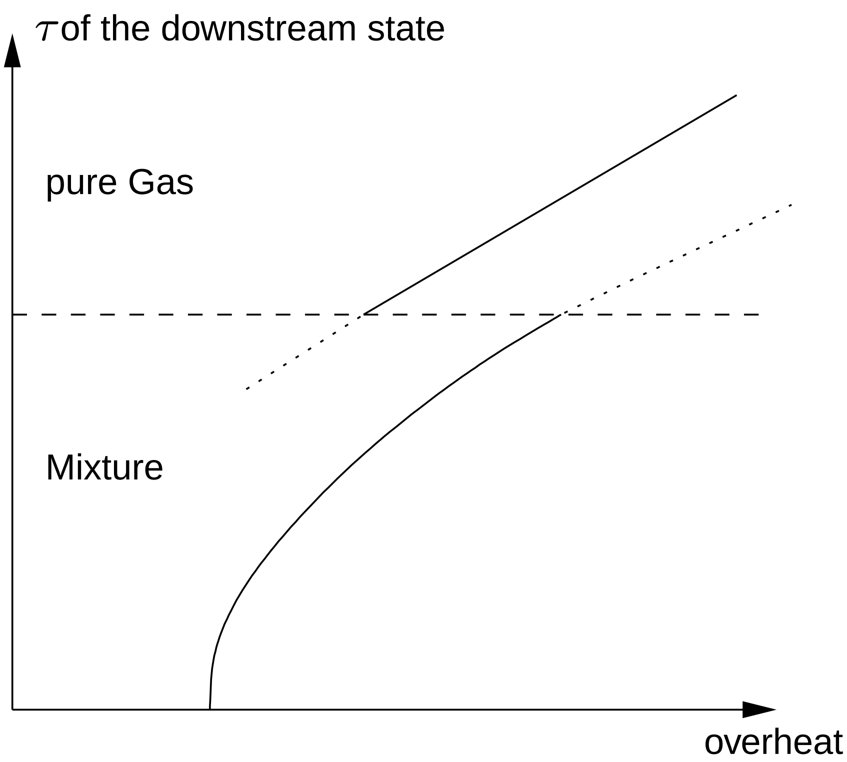

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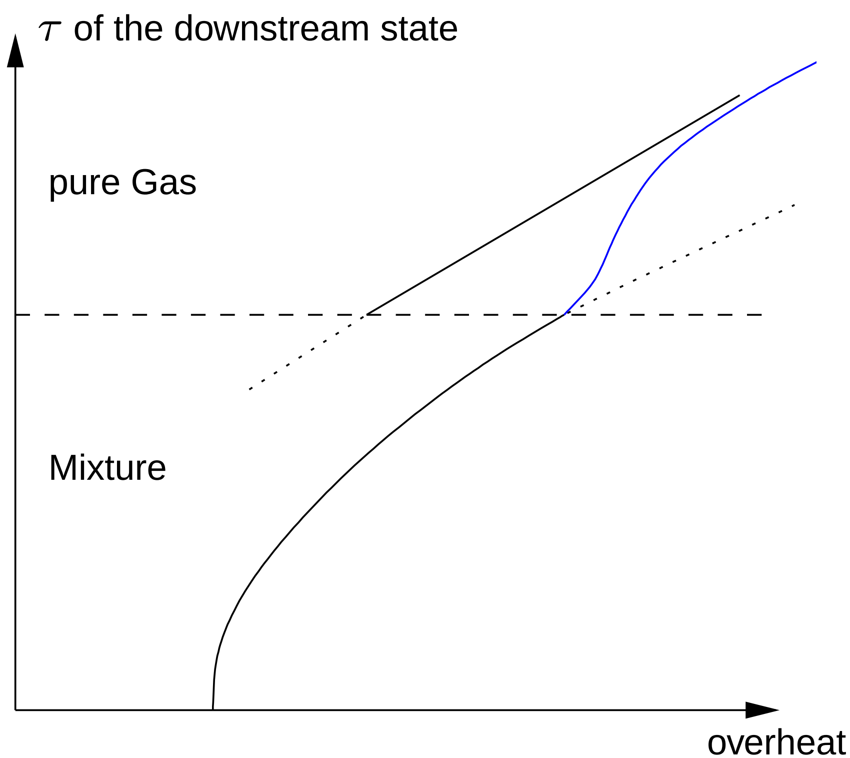

Overview

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Numerical method (Continuous model)

- Multiphase model

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

- problems
  - How to choose u_I, p_I ? modelisation 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**

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

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

Numerical method (Continuous model)

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

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

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

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

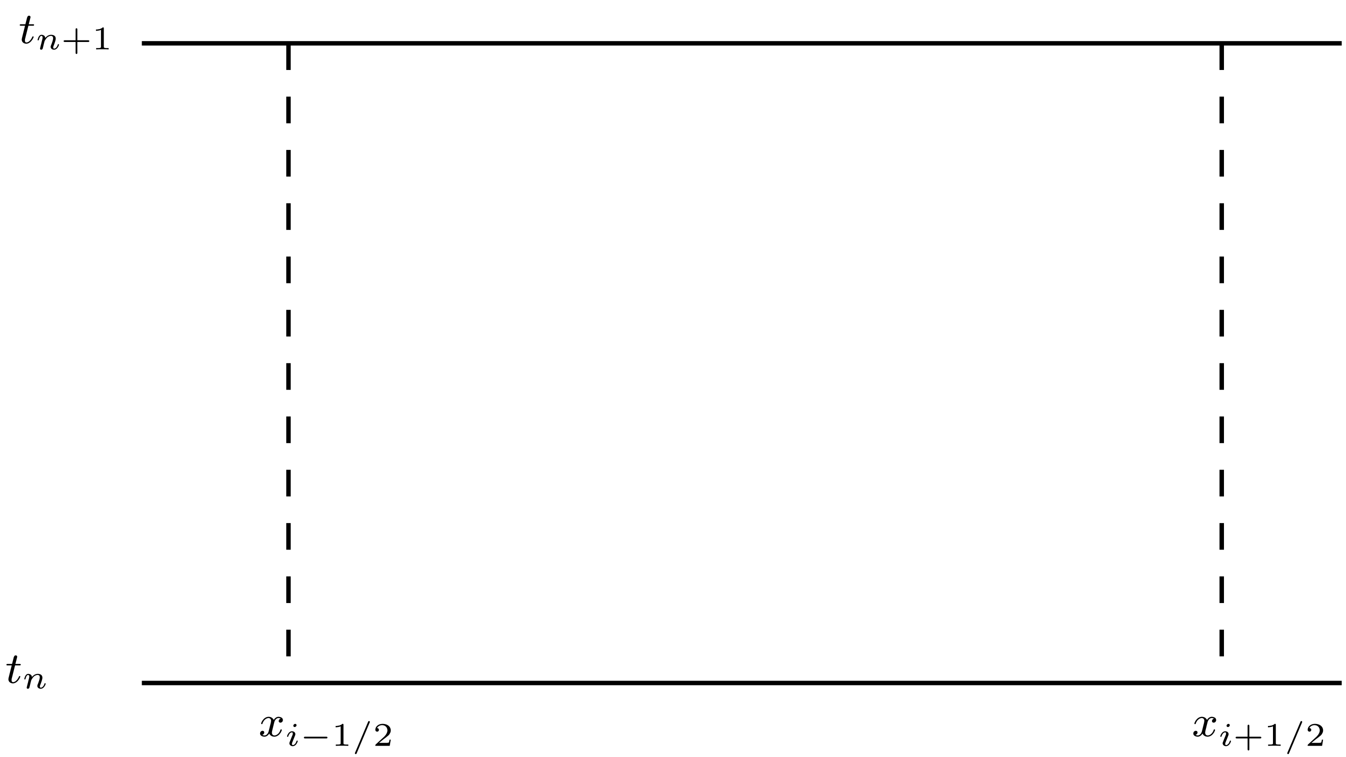
$$\mathcal{E}\left(\sigma \cdot \nabla \chi_k\right) = \mathbf{u}_I \nabla \alpha_k$$

Numerical method (Continuous model)

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

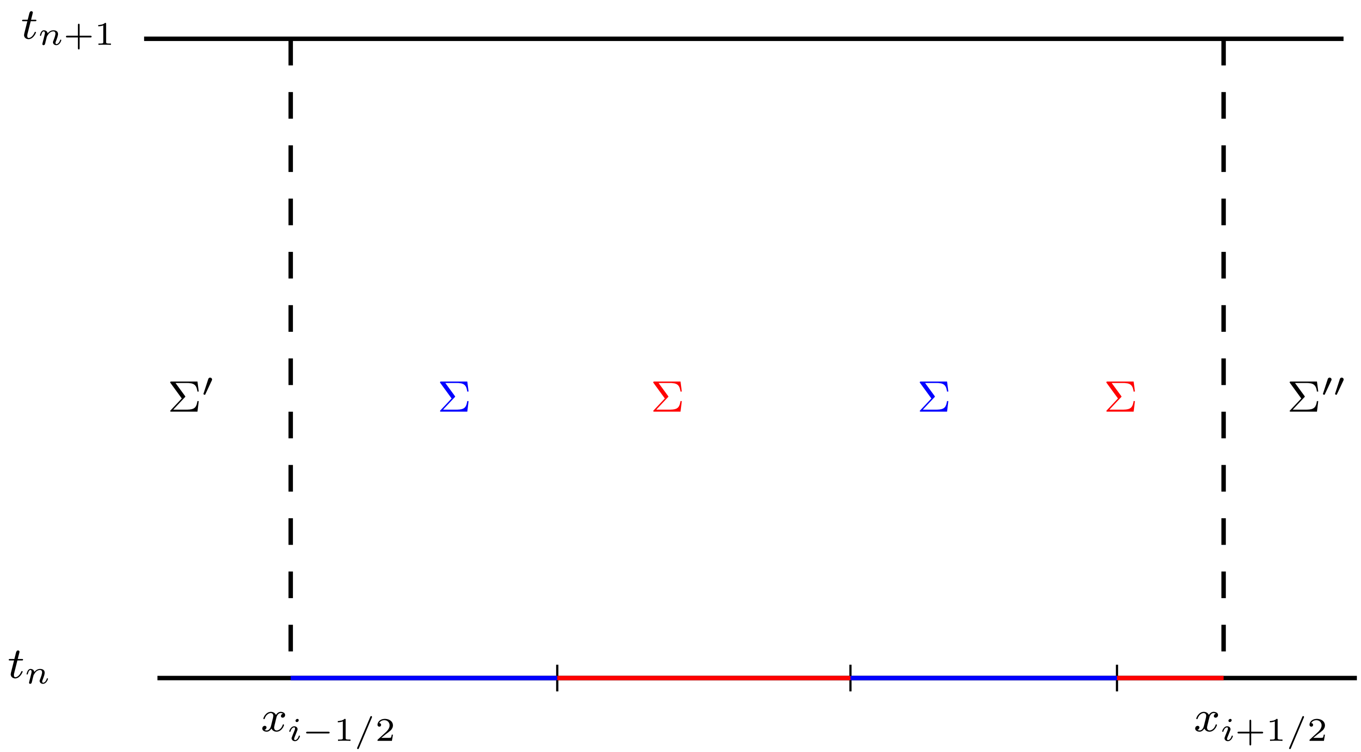
1. **Equations for each phase**
   Euler $+$ Topological equation for the interface
2. **Average**
   Closure Problems
3. **Modelling**
   Non conservative Products+ Closure Pbs

Numerical method



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

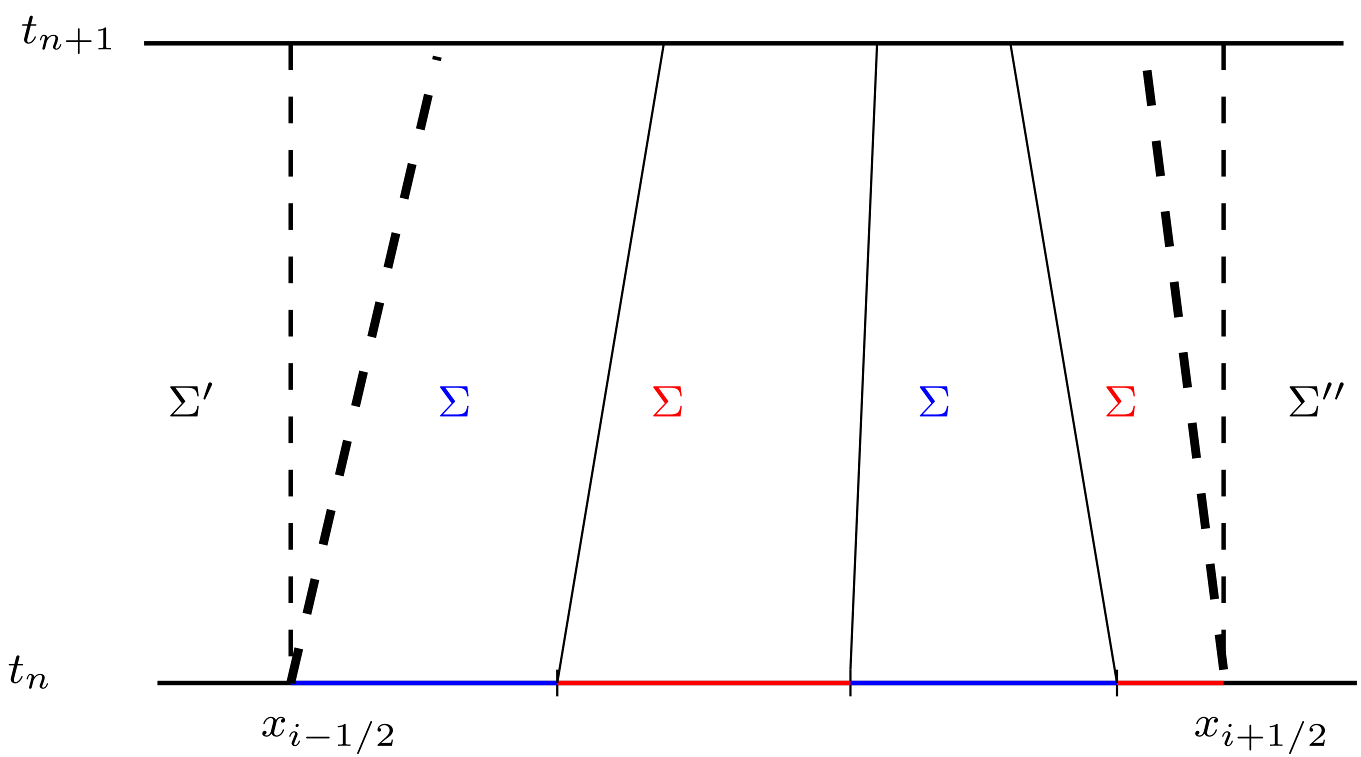
Numerical method



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

  do the same for the neighbours cells

Numerical method



- Evolution in time

Numerical method

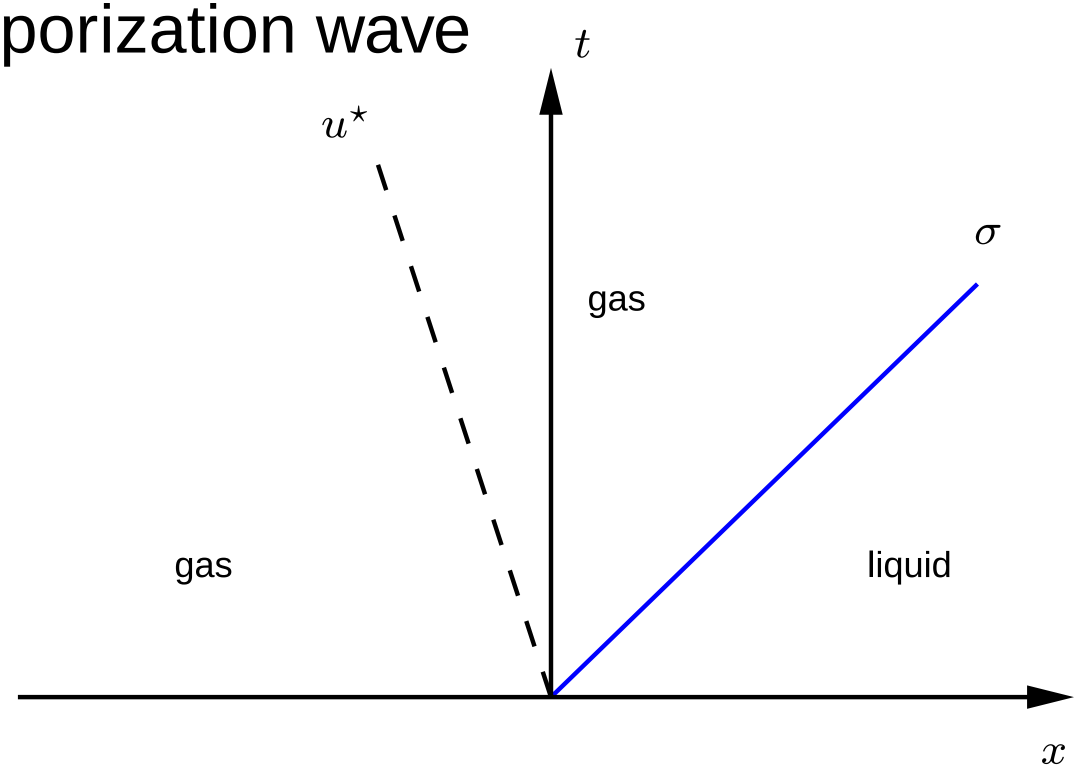
- Averaging procedure
- Probability in the boundary of the cell:

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

- see Abgrall/Saurel, JCP, 2003

Numerical method

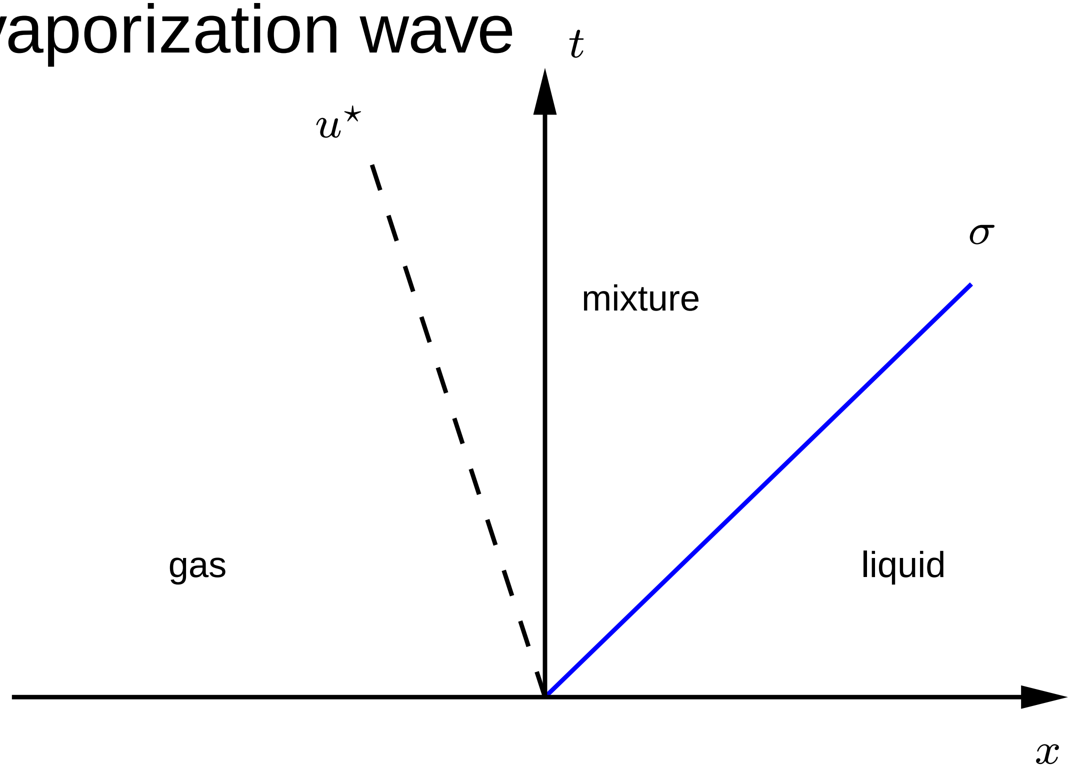
- extension to reactive flux
- Total vaporization wave



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

Numerical method

- extension to reactive flux
- Partial vaporization wave



Numerical method

- extension to reactive flux
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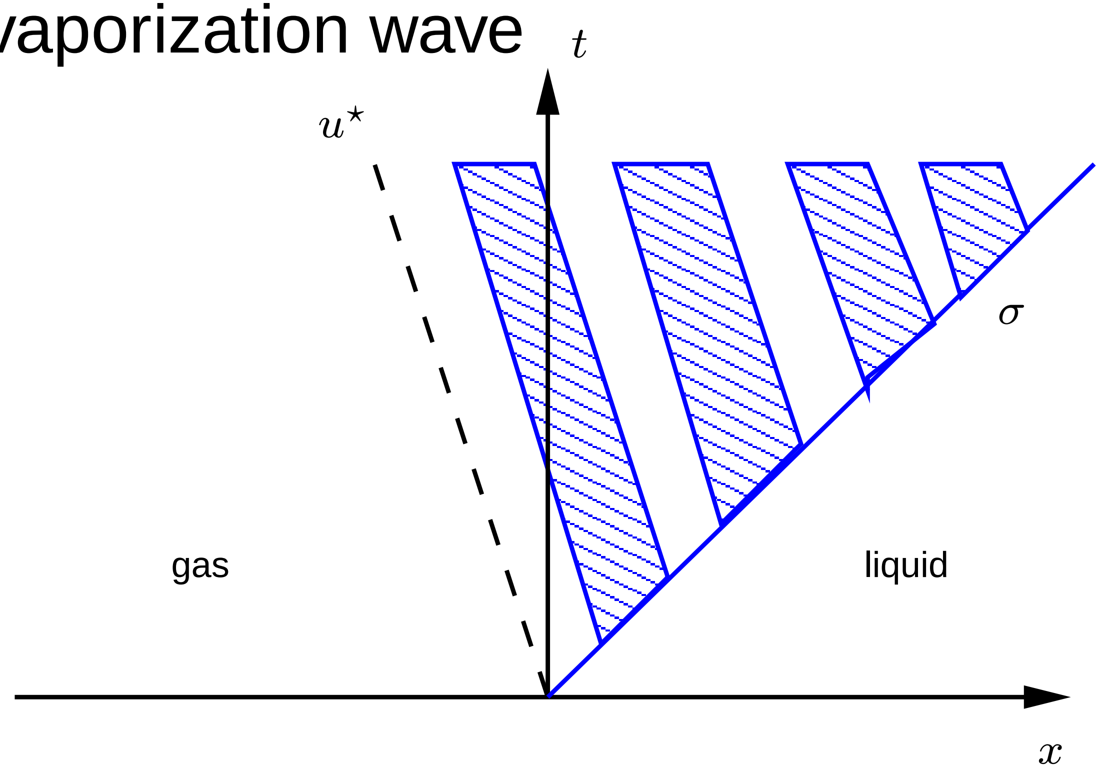

$\Longrightarrow$ Average of total and partial vaporization wave

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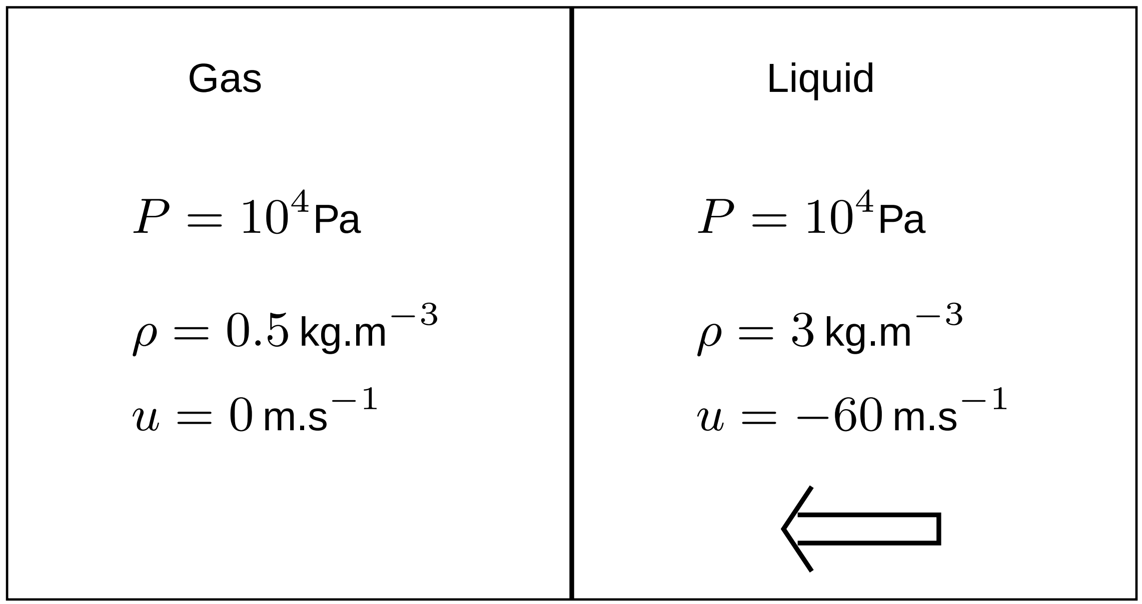
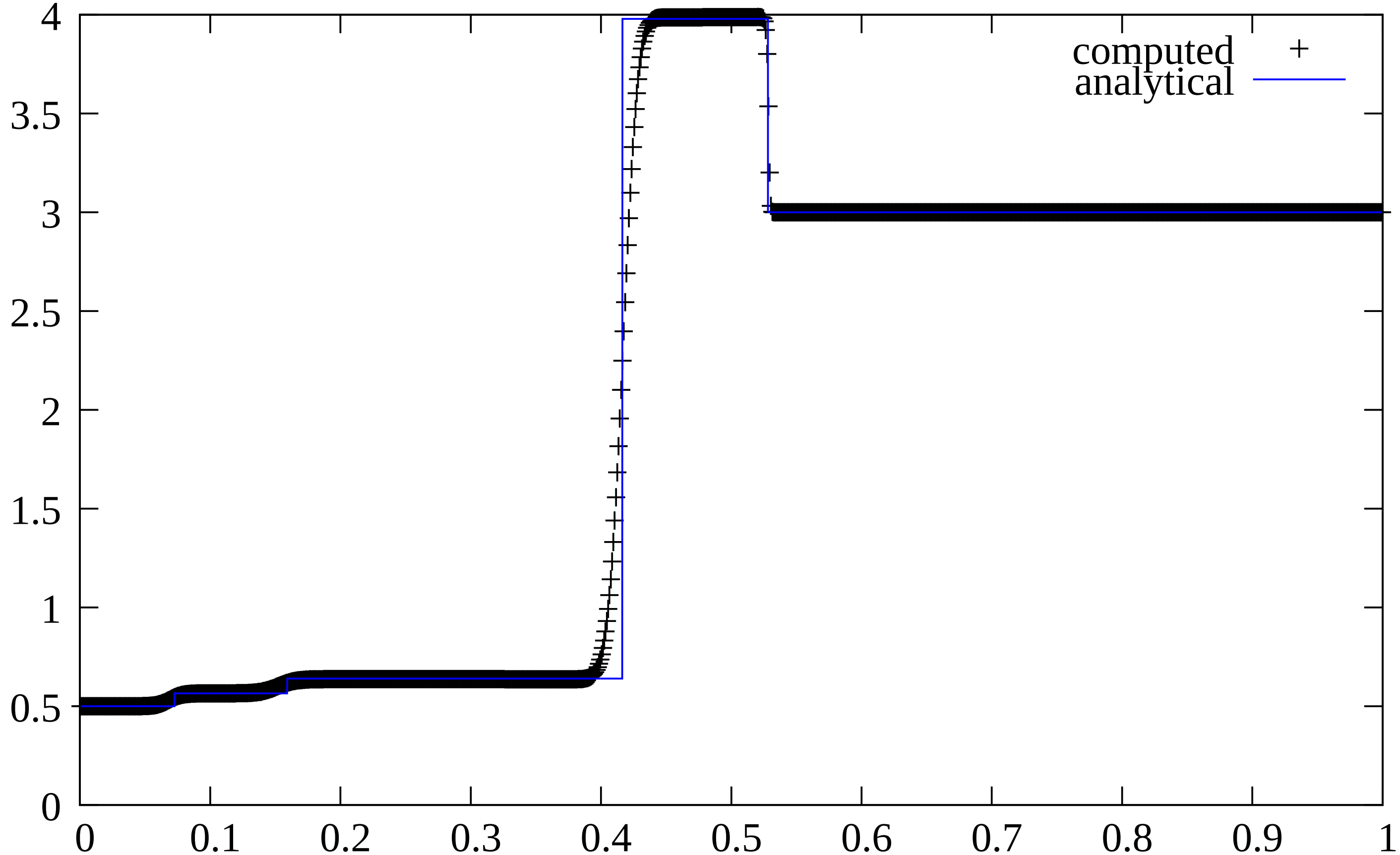
Liquefaction

- double shock



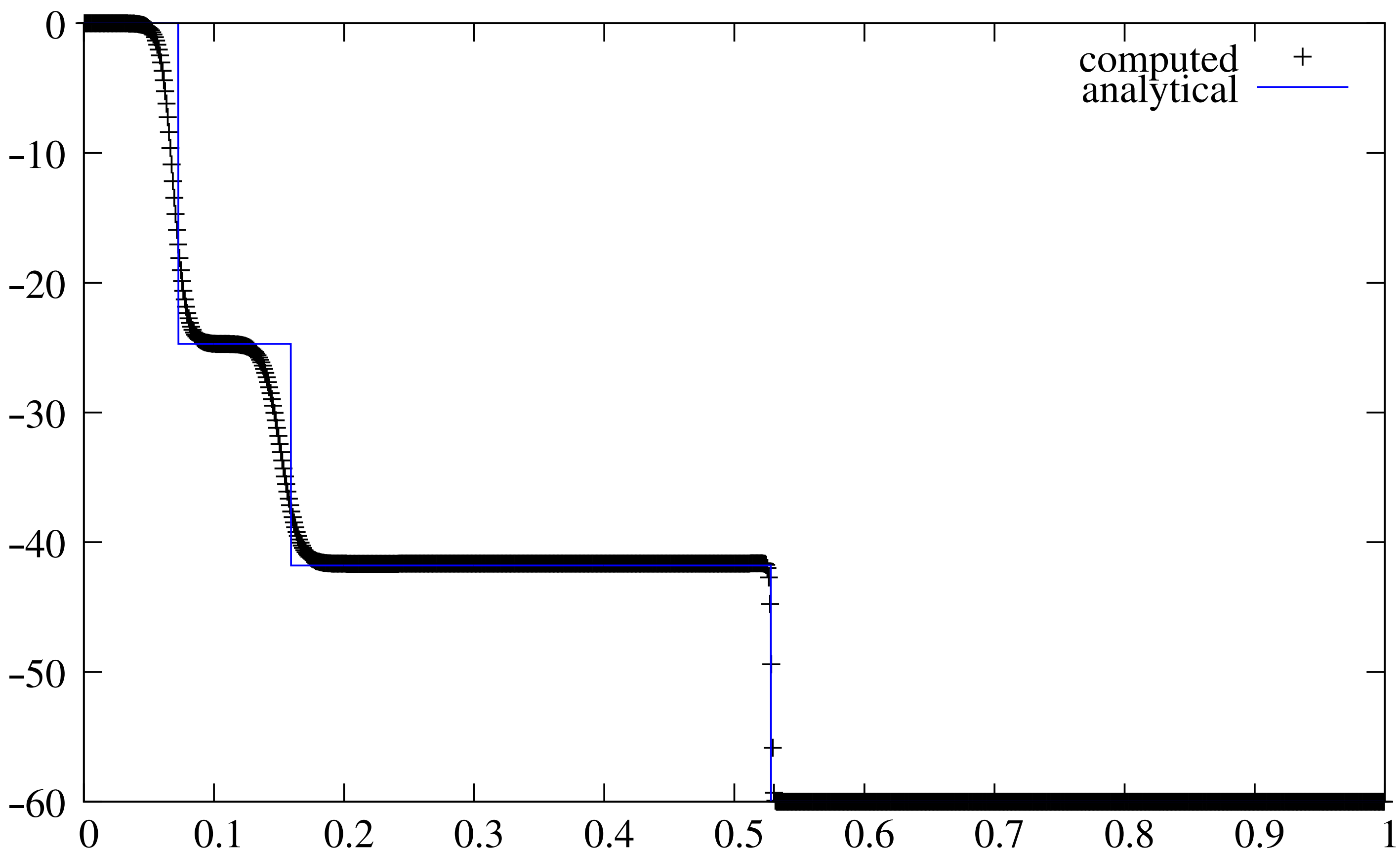
Liquefaction

- Density



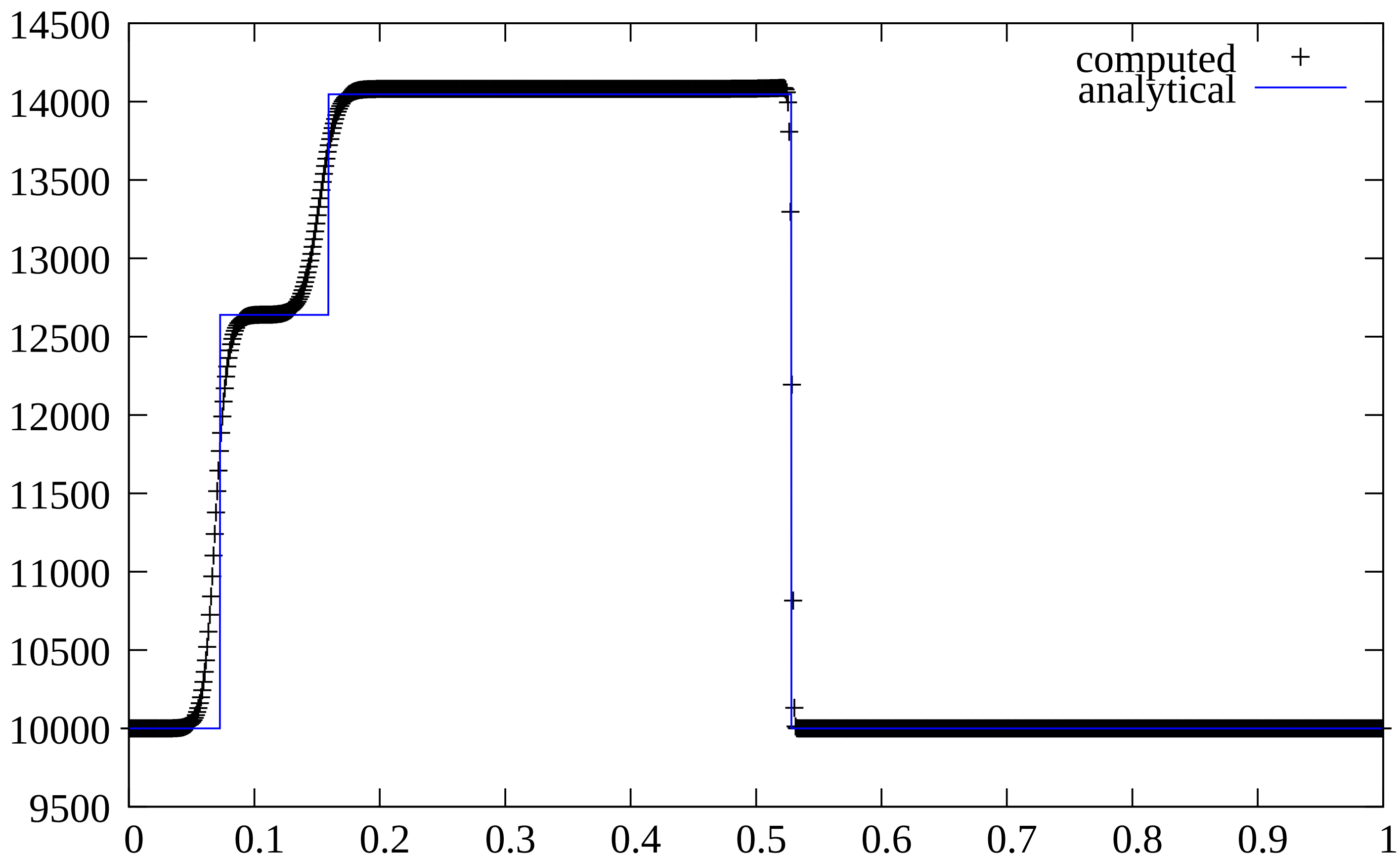
Liquefaction

- Velocity



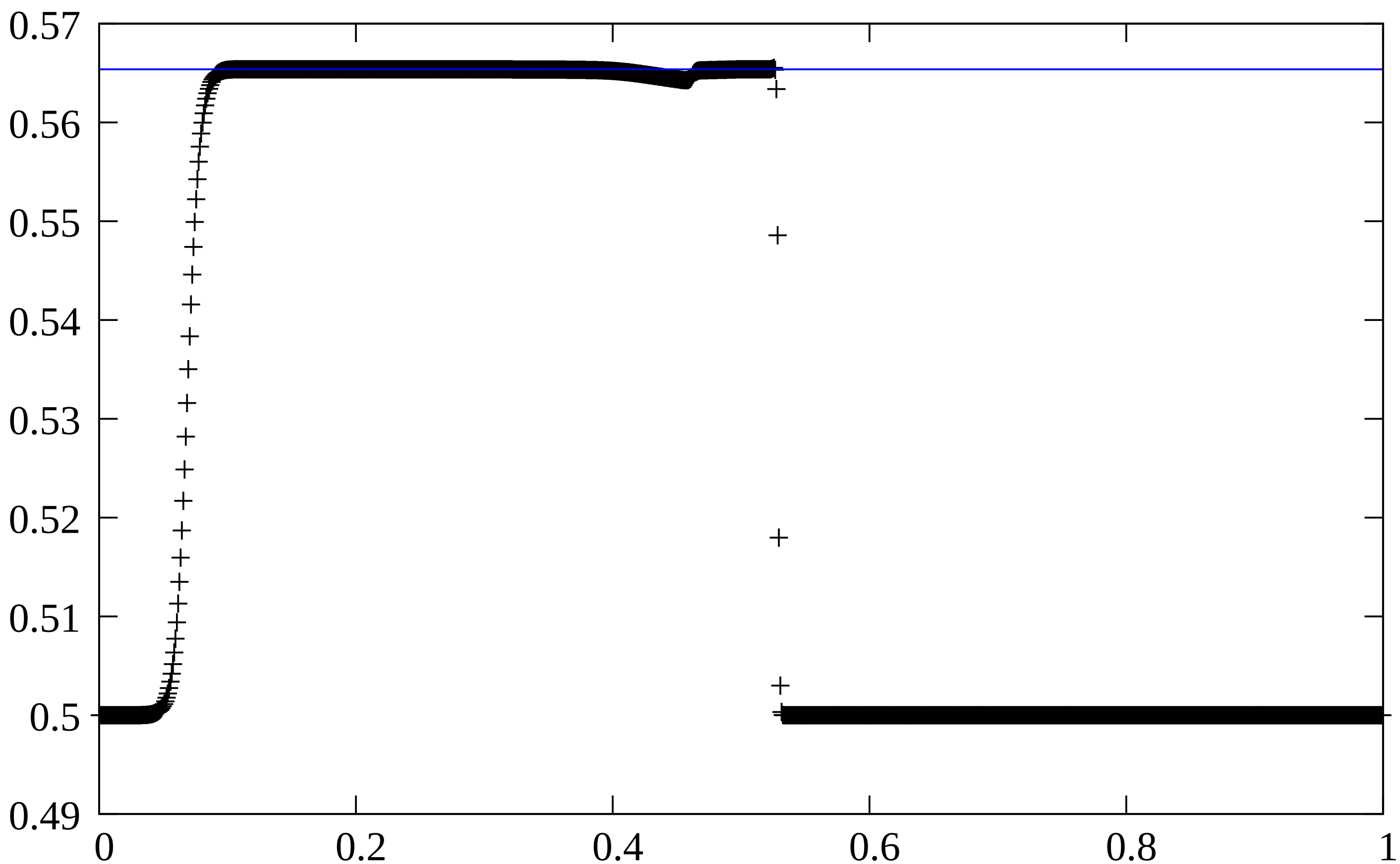
Liquefaction

- Pressure



Liquefaction

- Liquid Density



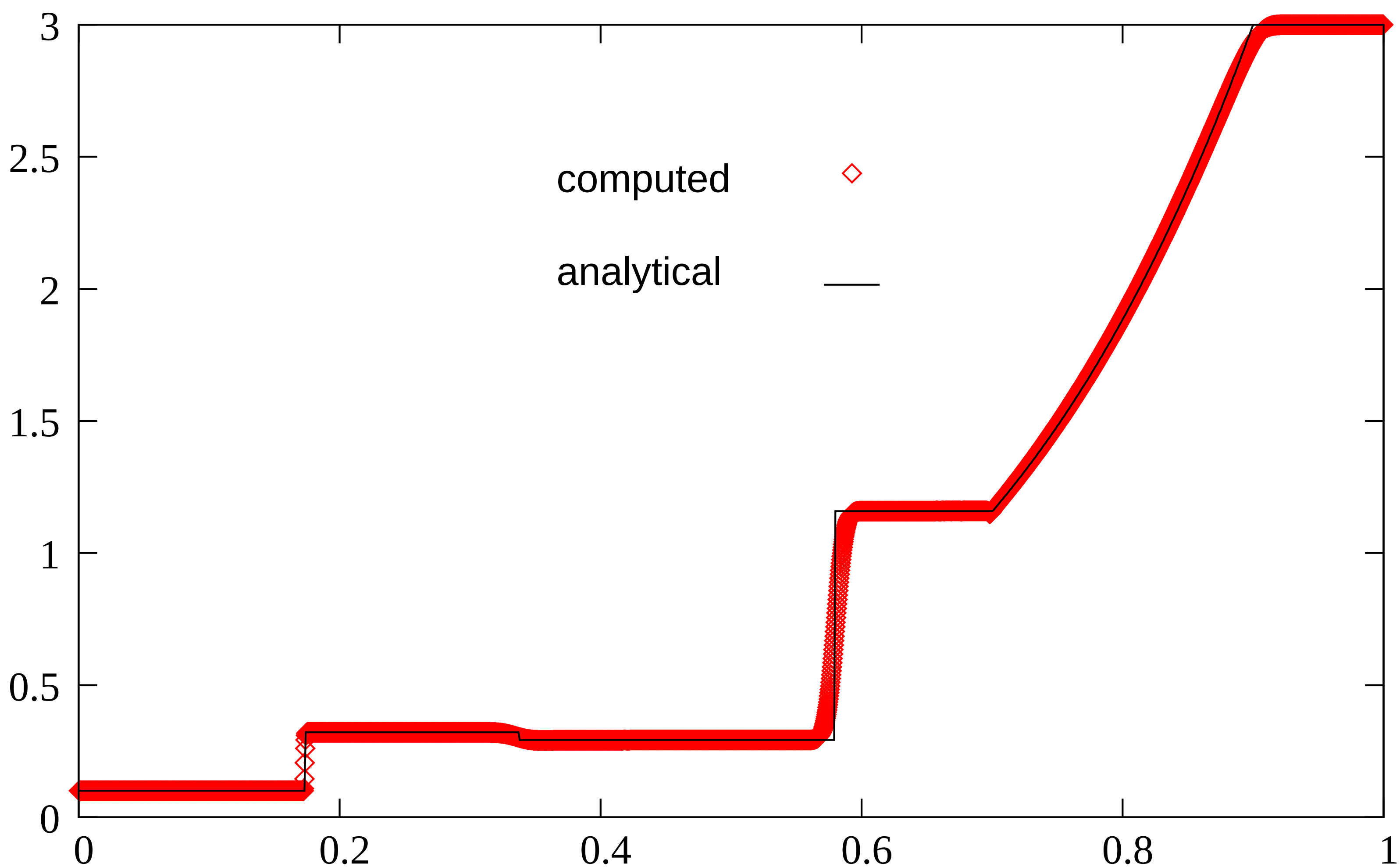
Vaporisation

- Shock tube

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

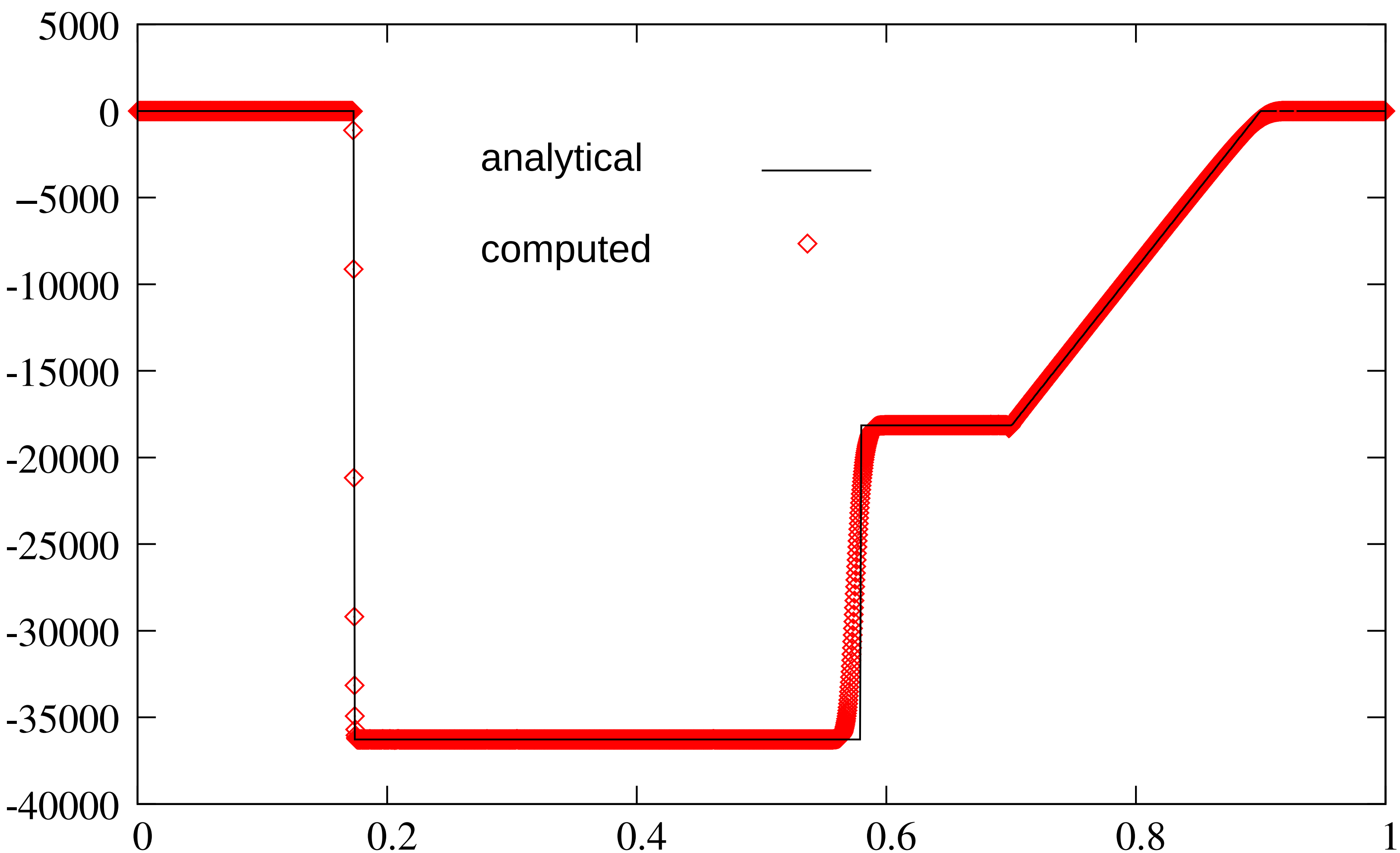
Vaporisation

- Density



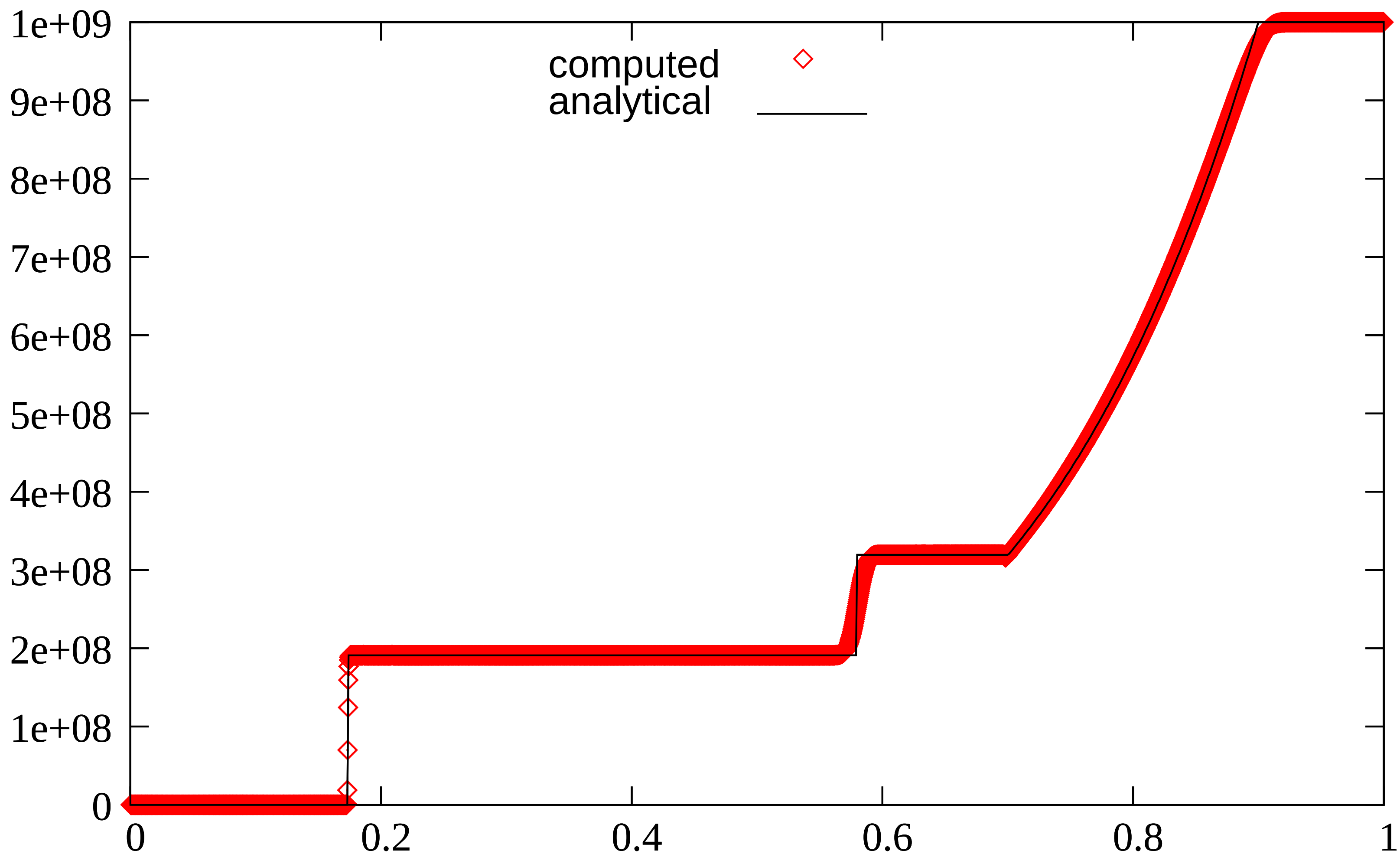
Vaporisation

- Velocity



Vaporisation

- Pressure



Conclusion

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

...

Thank you!

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