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Phase transitions

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Abteilung für Angewandte Mathematik

in collaboration with

- **D. Diehl**[1]
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- **C. Rohde** [3]

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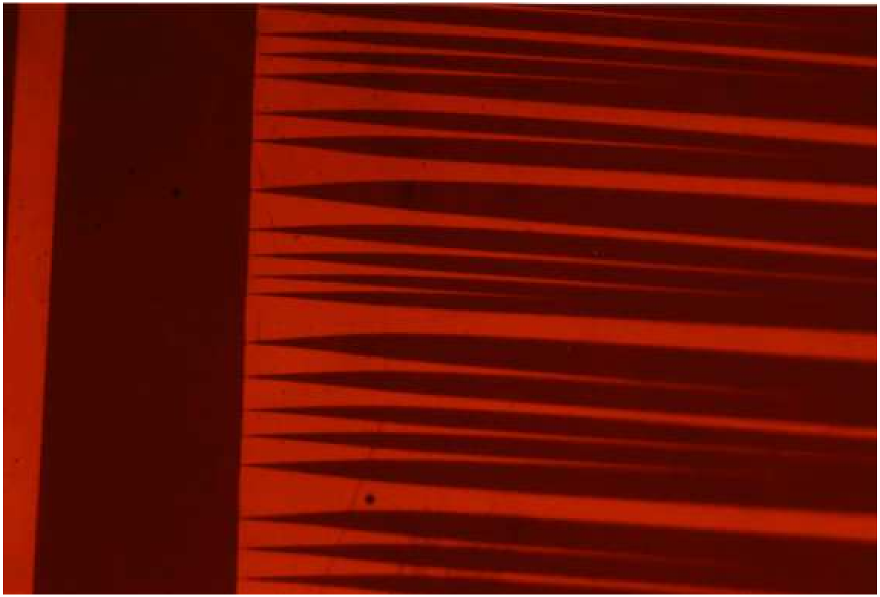
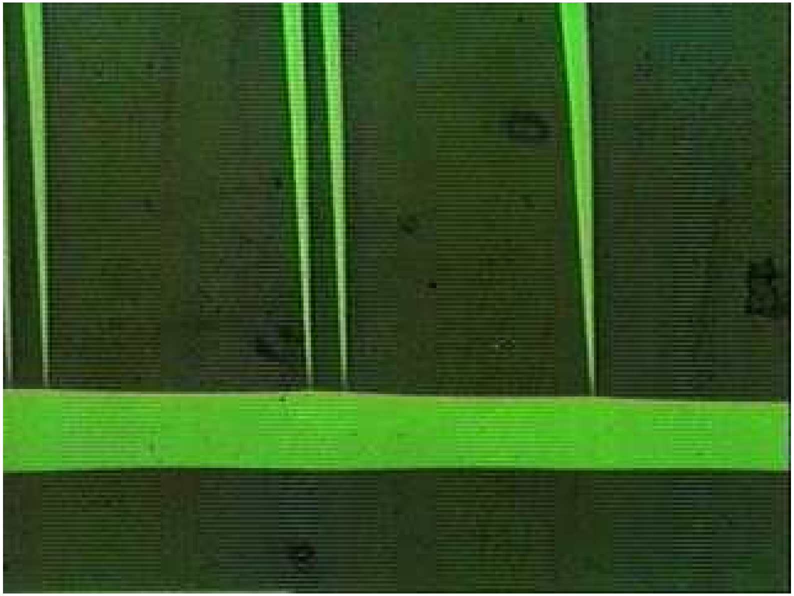
[1] Freiburg, PhD thesis
[2] Freiburg, PhD thesis
[3] University of Bielefeld

Needle Microstructures



R. D. James, R. Kohn, T. W. Shield

Needle Microstructures



R. D. James, R. Kohn, T. W. Shield: mpeg movie

Video

Derivation of the mathematical model [4]

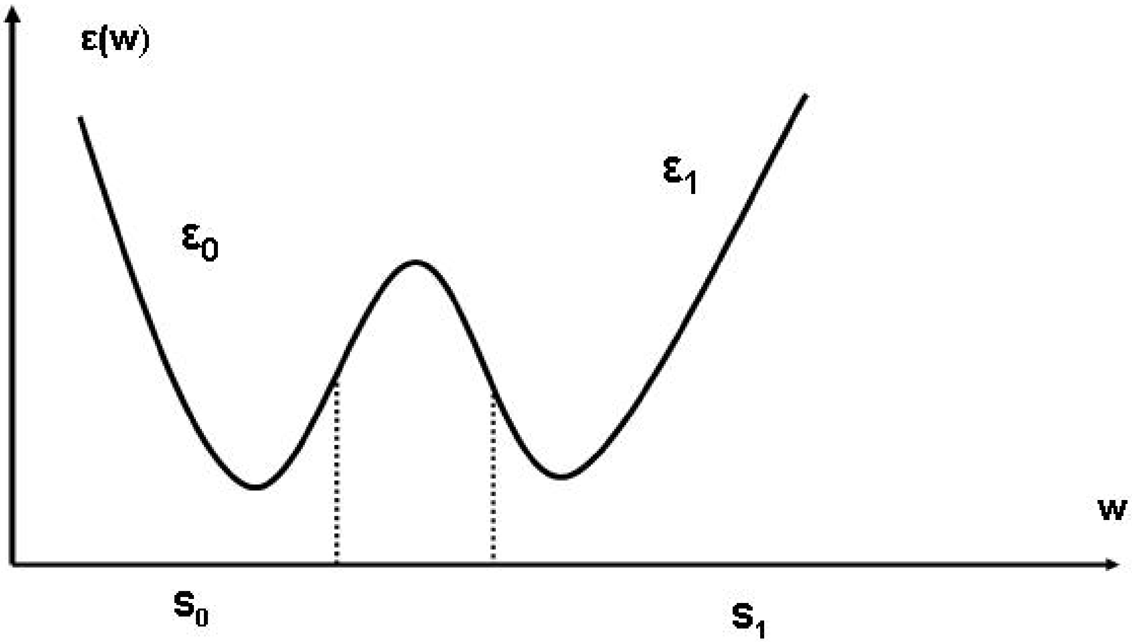
- **Location of the material particle at time t, which was located initially in x:** $y(x,t)$
- **Velocity** $v := \partial_t y$
- **Deformation gradient** $w := \partial_x(y-x)$
- **Internal energy** $e := e(w, \partial_x w) := \bar{e}(\partial_x y, \partial_{xx} y)$

  Standard choice: $e(w, w_x) := \varepsilon(w) + \lambda(w)\frac{w_x^2}{2}$
- **Action functional:** $J(w) := \int_0^T \int_\Omega \left(e(w, \partial_x w) - \frac{v^2}{2} \right) dx\, dt$
- **Euler-Lagrange-equations:**

$$\begin{aligned} \partial_t v - \partial_x \Sigma(w, \partial_x w, \partial_{xx} w) &= 0 \\ \partial_t w - \partial_x v &= 0 \end{aligned}$$

where $\Sigma(w, \partial_x w, \partial_{xx} w) := \partial_w e(w, \partial_x w) - \partial_x \left(\partial_{w_x} e(w, \partial_x w) \right).$

[4] P. LeFloch: Hyperbolioc systems of conservation laws, p. 21



ε(w)
ε1
ε0
w
s0
s1

- $y(x,t)$: **location of of the material particle at time** t**, which was located initially in** x**.**
- **Velocity** $v := \partial_t y$
- **Deformation gradient** $w := \partial_x (y - x)$
- **Internal energy** $e := e(w, \partial_x w) := \bar{e}(\partial_x y, \partial_{xx} y)$

  Standard choice: $e(w, w_x) := \varepsilon(w) + \lambda(w)\frac{w_x^2}{2}$
- **Action functional:** $J(w) := \int_0^T \int_\Omega \left(e(w, \partial_x w) - \frac{v^2}{2} \right) dx\, dt$
- **Euler-Lagrange-equations:**

$$
\begin{aligned}
\partial_t v - \partial_x \Sigma(w, \partial_x w, \partial_{xx} w) &= 0 \\
\partial_t w - \partial_x v &= 0
\end{aligned}
$$

  where $\Sigma(w, \partial_x w, \partial_{xx} w) := \partial_w e(w, \partial_x w) - \partial_x \left(\partial_{w_x} e(w, \partial_x w) \right).$
- **Then we obtain with** $\sigma(w) := \varepsilon'(w)$

$$
\begin{aligned}
\partial_t v - \partial_x \sigma(w) &= \left(\lambda'(w) \frac{w_x^2}{2} - (\lambda(w) w_x)_x \right)_x \\
\partial_t w - \partial_x v &= 0
\end{aligned}
$$

Change of type

$$
\begin{aligned}
\partial_t v - \partial_x \sigma(w) &= \left(\lambda'(w)\frac{w_x^2}{2} - (\lambda(w)w_x)_x\right)_x \\
\partial_t w - \partial_x v &= 0
\end{aligned}
$$

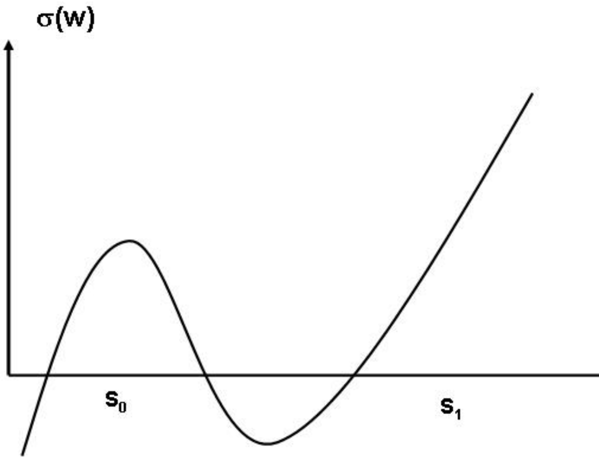
Now use

- **Velocity** $v := \partial_t y$
- **Deformation gradient** $w := \partial_x(y - x)$

and obtain in the main part

$$
\begin{aligned}
\partial_{tt} y - \partial_x \sigma(\partial_x y) &= \cdots \\
\partial_{tt} y - \sigma'(\partial_x y)\partial_{xx} y &= \cdots
\end{aligned}
$$

$$\begin{aligned}\partial_{tt}y - \partial_x\sigma(\partial_x y) &= \cdots \\ \partial_{tt}y - \sigma'(\partial_x y)\partial_{xx}y &= \cdots\end{aligned}$$



Avoid the elliptic region!

$$
\begin{aligned}
\partial_t v - \partial_x \sigma(w) &= \left(\lambda'(w)\frac{w_x^2}{2} - (\lambda(w) w_x)_x\right)_x \\
\partial_t w - \partial_x v &= 0
\end{aligned}
$$

Results for this system [5]

- **Local well-posedness for smooth perturbations of travelling wave profiles.**
- **Generalization to several space dimensions.** [6]**.**

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[5] S. Benzoni-Gavage, R. Danchin, S. Descombes: Well-posedness of one-dimensional Korteweg models, preprint 2004

[6] S. Benzoni-Gavage, R. Danchin, S. Descombes: On the well-posedness for the Euler-Korteweg model in several space dimensions, preprint 2005

Existence of travelling waves

Consider the special case:

$$\begin{aligned}\partial_t w - \partial_x v &= 0\\ \partial_t v - \partial_x \sigma(w) &= \varepsilon \partial_{xx} w - \gamma \varepsilon^2 \partial_{xxx} w\\ v(x,0) &= v_0(x), \quad w(x,0) = w_0(x)\end{aligned}$$

Does there exist a solution of the form

$$\begin{aligned}w_\varepsilon(x,t) &= \bar{w}(\frac{x-st}{\varepsilon})\\ v_\varepsilon(x,t) &= \bar{v}(\frac{x-st}{\varepsilon})\\ \bar{w}(\infty) &= w_l,\ \bar{w}(-\infty) = w_g\\ \bar{v}(\infty) &= v_l,\ \bar{v}(-\infty) = v_g\end{aligned}$$

such that for $\varepsilon \to 0:\ w_\varepsilon(x,t) \to w_1(x,t),\ v_\varepsilon(x,t) \to v_1(x,t)$
and w_1, v_1 **is a shock solution of**

$$\begin{aligned}\partial_t w - \partial_x v &= 0\\ \partial_t v - \partial_x \sigma(w) &= 0\end{aligned}$$

$$v(x,0) = v_0(x), \quad w(x,0) = w_0(x)$$

$$
\begin{aligned}
\partial_t w - \partial_x v &= 0 \\
\partial_t v - \partial_x \sigma(w) &= \varepsilon \partial_{xx} w - \gamma \varepsilon^2 \partial_{xxx} w \\
v(x,0) &= v_0(x), \quad w(x,0) = w_0(x)
\end{aligned}
$$

Theorem 1 [7]

- ***Let*** $\gamma > 0$ ***and*** w_l, v_l ***be given in the phase l. Then there exists a unique state*** w_g, v_g ***in the phase g such that the corresponding travelling wave converges to a shock solution.***
- ***If*** $\gamma = 0$ ***then there does not exist a state*** w_g, v_g ***in the phase g such that the corresponding travelling wave converges to a shock solution.***

[7] M. Slemrod: Admissibility criteria for propagating phase boundaries in a van der Waals fluid. Arch. Ration. Mech. Anal. 81 (1983), 302-315.

Main problem:

$$\begin{aligned}
\partial_t w - \partial_x v &= 0 \\
\partial_t v - \partial_x \sigma(w) &= \varepsilon \partial_{xx} w - \delta \partial_{xxx} w \\
v(x,0) &= v_0(x), \quad w(x,0) = w_0(x)
\end{aligned}$$

For the limit $\varepsilon, \delta \to 0$ the limit will in general depend on $\frac{\delta}{\varepsilon^2}$.

Model problem

$$\begin{aligned} \partial_t u^\varepsilon + \partial_x f(u^\varepsilon) &= \varepsilon \partial_{xx} u^\varepsilon + \delta \partial_{xxx} u^\varepsilon, \ f(u) = u^3 \\ u^\varepsilon(.,0) &= u_0 \end{aligned} \tag{1}$$

Results for the model problem

- **If $|\delta| << \varepsilon^2$ then the limit for ε, $\delta \to 0$ is the same as for the viscosity limit in (??)[8].**
- **If $|\delta| >> \varepsilon^2$ then there is no convergence to a weak solution of the conservation law for ε, $\delta \to 0$.** [9]
- **If $\delta = \mu\varepsilon^2$ then**
  - **For $\varepsilon > 0$ there exists a unique classical solution $u^\varepsilon \in C^{2,1}(\mathbb{R} \times [0,T])$ of (??) and a weak solution $u \in L^1(\mathbb{R} \times [0,T])$ of the limit problem such that**

    $$\lim_{\varepsilon\to 0} ||u^\varepsilon - u||_{L^1(\mathbb{R}\times[0,T])} = 0^{10}.$$
  - **The limit for ε, $\delta \to 0$ will depend on $\mu := \frac{\delta}{\varepsilon^2}$.**

[8] LeFloch: Hyperbolic conservation laws 2002, p. 23
[9] LeFloch, Archive Rational Mech. Anal. 139, 1997, p.4
[10] Hayes, LeFloch 1998

$$\partial_t u^\varepsilon + \partial_x f(u^\varepsilon) \;=\; \varepsilon \partial_{xx} u^\varepsilon + \delta \partial_{xxx} u^\varepsilon,\; f(u) = u^3 \tag{2}$$

- **If $\delta = \mu\varepsilon^2$ then**
  - **For $\varepsilon > 0$ there exists a unique classical solution $u^\varepsilon \in C^{2,1}(\mathbb{R} \times [0,T])$ of (??) and a weak solution $u \in L^1(\mathbb{R} \times [0,T])$ of the limit problem such that**

    $$\mathbf{lim}_{\varepsilon \to 0} ||u^\varepsilon - u||_{L^1(\mathrm{R}\times[0,T])} = 0^{11}.$$
  - **The limit for ε, $\delta \to 0$ will depend on $\mu := \frac{\delta}{\varepsilon^2}$.**
  - **The limit is a weak solution of $\partial_t u + \partial_x f(u) = 0$ which satisfies**

    $$\partial_t U(u) + \partial_x F(u) \leq 0$$

    for a single strictly convex entropy pair (U, F) (depending on μ) but in general it will not satisfy the Oleinik entropy condition .
  - **Repeat:**

    For viscous approximations and convex f the limit satisfies

    $$\partial_t U(u) + \partial_x F(u) \leq 0$$

    for a all strictly convex entropy pairs (U, F) and the Oleinik entropy condition.
  - **Obtain uniqueness of the limit problem by additional conditions: Kinetic relation and nucleation criterion.** [12]

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[11] Hayes, LeFloch 1998

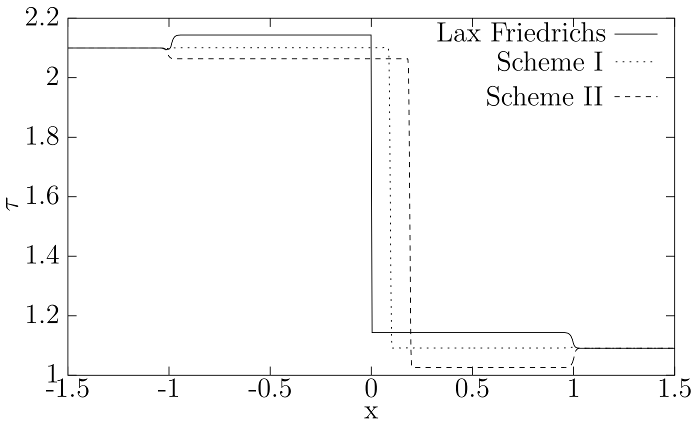
[12] LeFloch, Archive Rational Mech. Anal. 139, 1997, p.34

$$\begin{aligned} \partial_t w - \partial_x v &= 0 \\ \partial_t v - \partial_x \sigma(w) &= 0 \\ v(x,0) &= v_0(x), \quad w(x,0) = w_0(x). \end{aligned} \tag{3}$$

* **Choose initial data in different phases.**
* **Solve with three different numerical schemes, which corresponds to different choices of ε, δ.**

$$
\begin{aligned}
\partial_t w - \partial_x v &= 0 \\
\partial_t v - \partial_x \sigma(w) &= \varepsilon \partial_{xx} w - \gamma \varepsilon^2 \partial_{xxx} w \\
v(x,0) &= v_0(x), \quad w(x,0) = w_0(x)
\end{aligned}
\tag{4}
$$

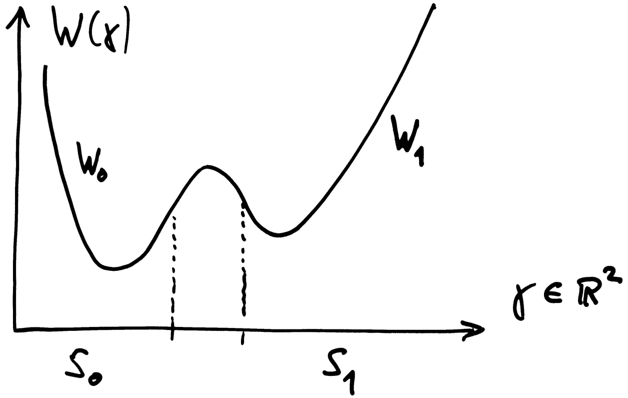
* **Choose initial data in different phases.**
* **Solve with three different numerical schemes, which corresponds to different choices of ε, δ.**
* **All solutions are weak and entropy solutions of (??).**



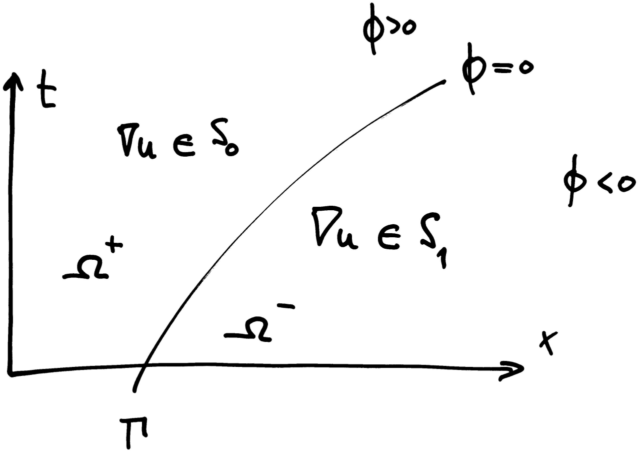
Nonlinear elastodynamics and phase transitions in 2D [13]

- $u(x,t)$: **displacement**
- $\sigma(\nabla u)$: **shear stress**
  - $\sigma(s) = \frac{\partial W}{\partial \gamma}$
  - **W: nonconvex, two well potential**
    - $W(\gamma) = W_0(\gamma)$ **in the low strain phase, i.e.** $\gamma \in S_0$
    - $W(\gamma) = W_1(\gamma)$ **in the high strain phase, i.e.** $\gamma \in S_1$
    - W_i **are convex**
    - **Physics: no strains in the nonconvex parts of** W

[13] **T.Y. Hou, P. Rosakis, Ph. LeFloch, Merkle**



$W(\gamma)$
W_0
W_1
$\gamma \in \mathbb{R}^2$
S_0
S_1



t
$\phi > 0$
$\phi = 0$
$\nabla u \in S_0$
$\phi < 0$
$\nabla u \in S_1$
Ω^+
Ω^-
x
Γ

Mathematical model (simplified):

$$\partial_t^2 u - \nabla \cdot \sigma(\nabla u) = 0 \;\; \textbf{in} \;\; \Omega - \Gamma_t$$

$$\textbf{and jump condition on } \Gamma_t$$

Levelset formulation: $\partial_t \phi - V|\nabla\phi| = 0$ **in** Ω

Use ϕ to meet only the convex parts of W.

$$W(\gamma, \phi) = W_0(\gamma) + H(\phi)(W_1(\gamma) - W_0(\gamma))$$

$$W_\varepsilon(\gamma, \phi) = W_0(\gamma) + H_\varepsilon(\phi)(W_1(\gamma) - W_0(\gamma))$$

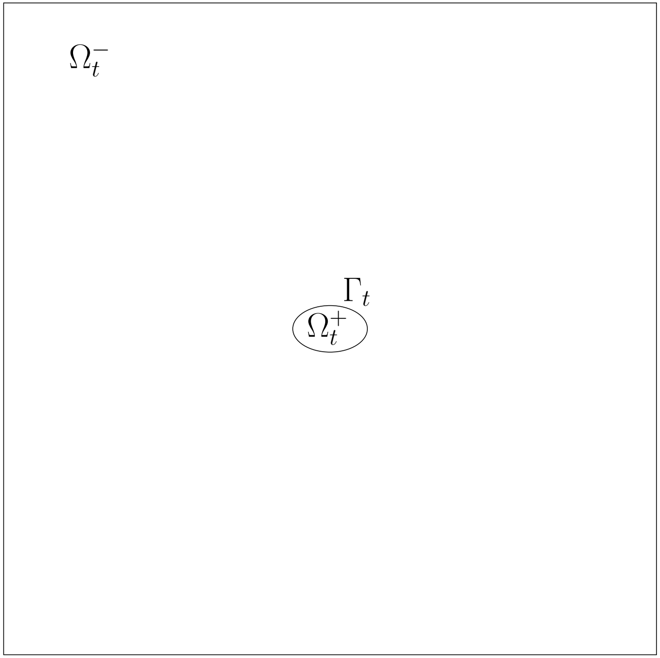
$$\sigma_\varepsilon = \frac{\partial W_\varepsilon}{\partial \gamma}$$

$$\partial_t^2 u - \nabla \cdot \sigma_\varepsilon(\nabla u, \phi) = 0 \;\; \textbf{in} \;\; \Omega$$

V is given by a kinetic relation (Abeyaratne, Knowles):

$$V = g(f, n), \;\; f = [|W|] + [|\nabla u|](\sigma^+ + \sigma^-)$$

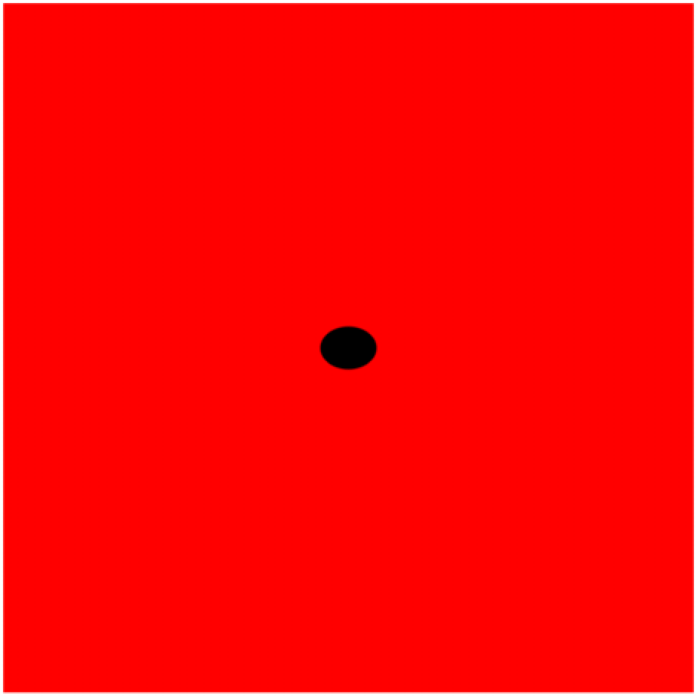
Twinning

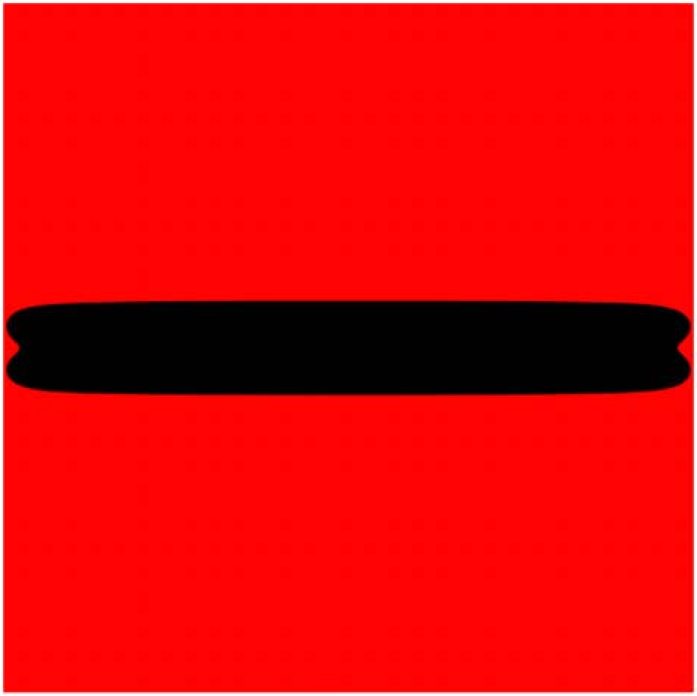


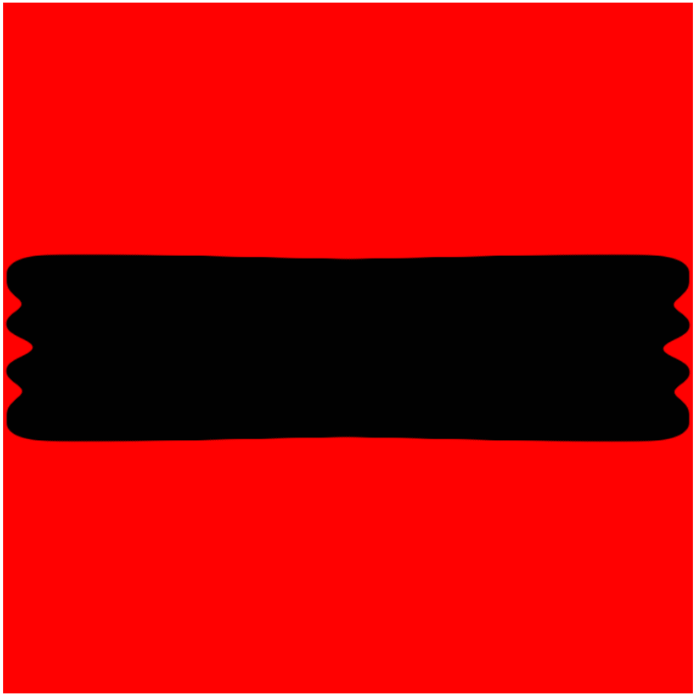
Boundary:

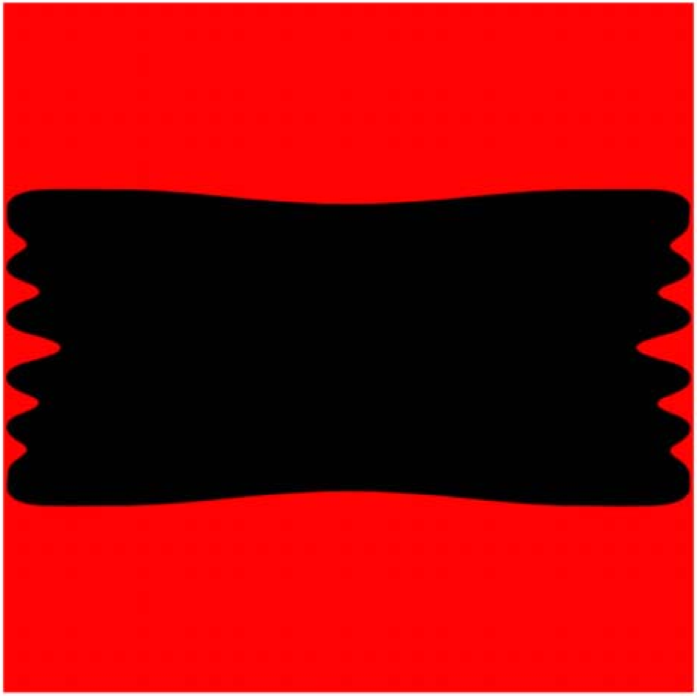
$$\mathbf{u}(x, y, t) = ky.$$

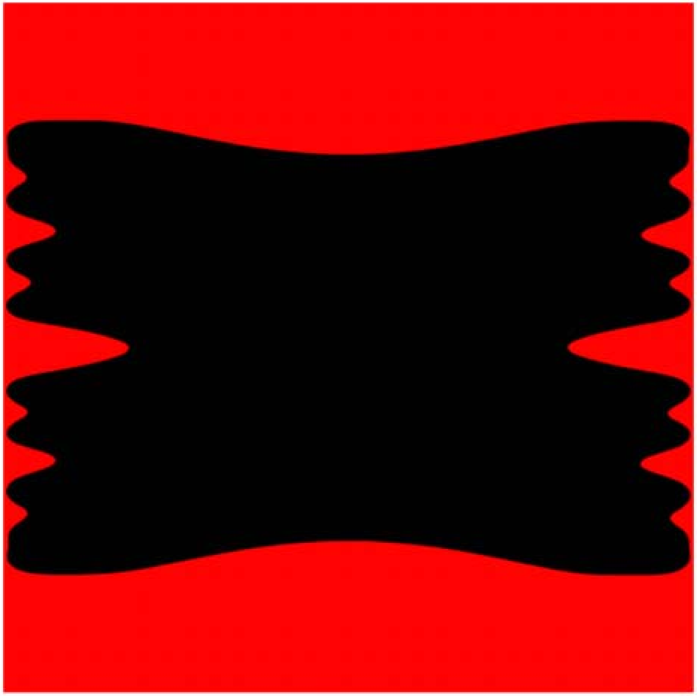
$$g(f, \mathbf{n}) = M_1 f + M_2 |\mathbf{n}_1| f$$

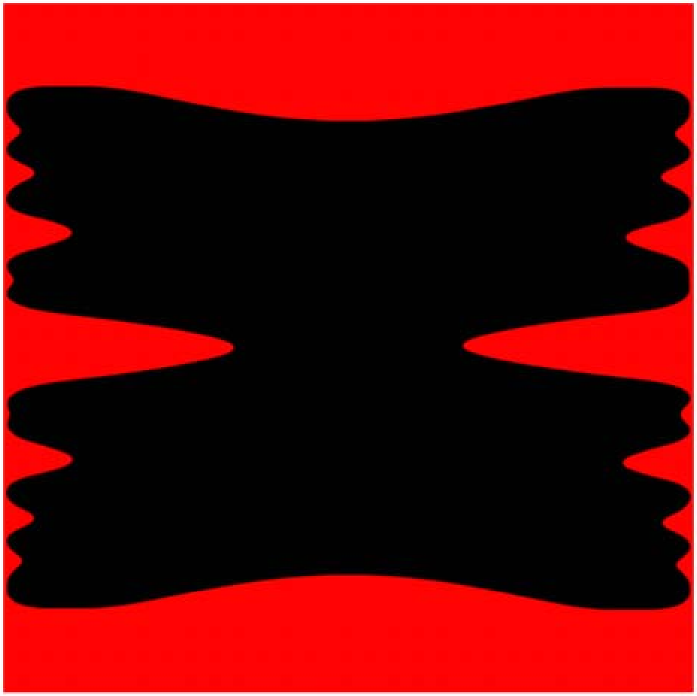


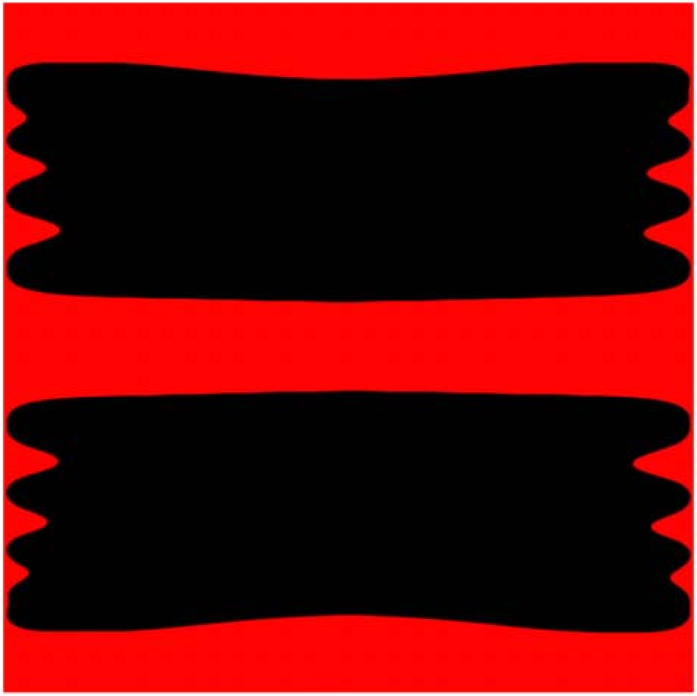


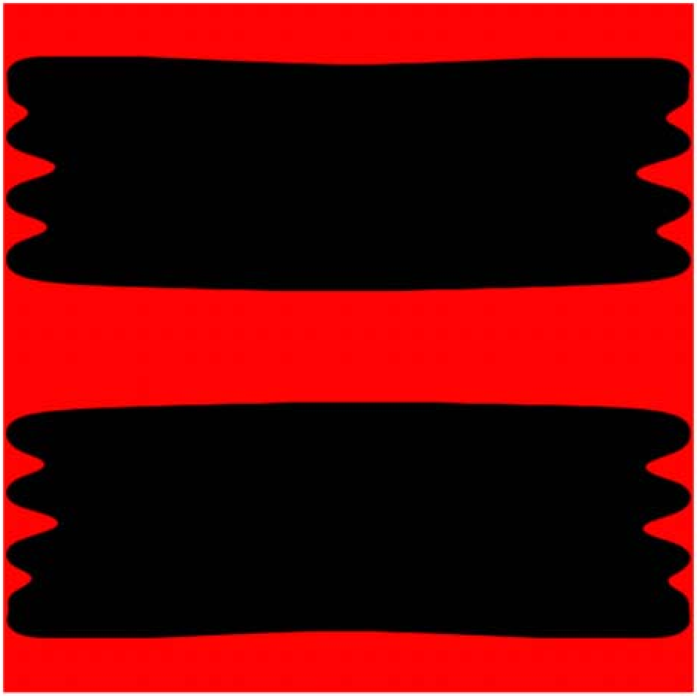


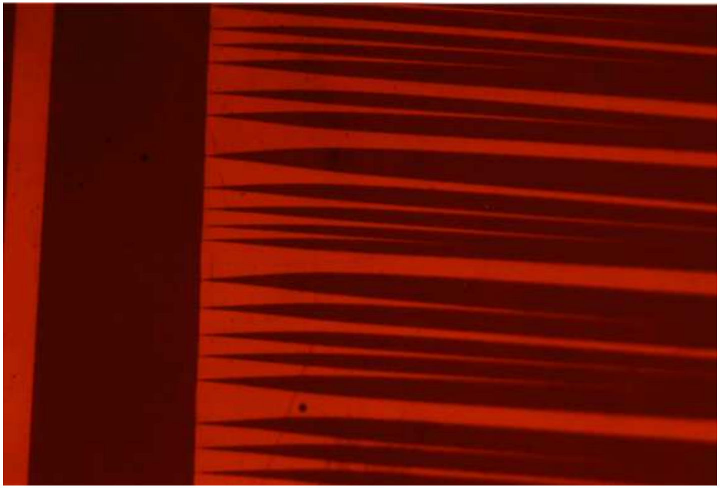


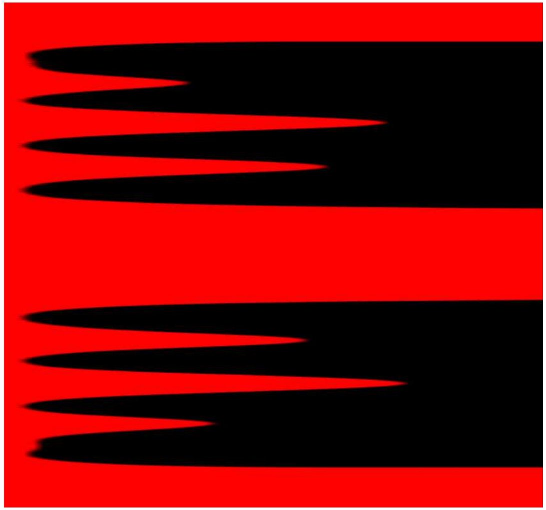












The original system is of the form

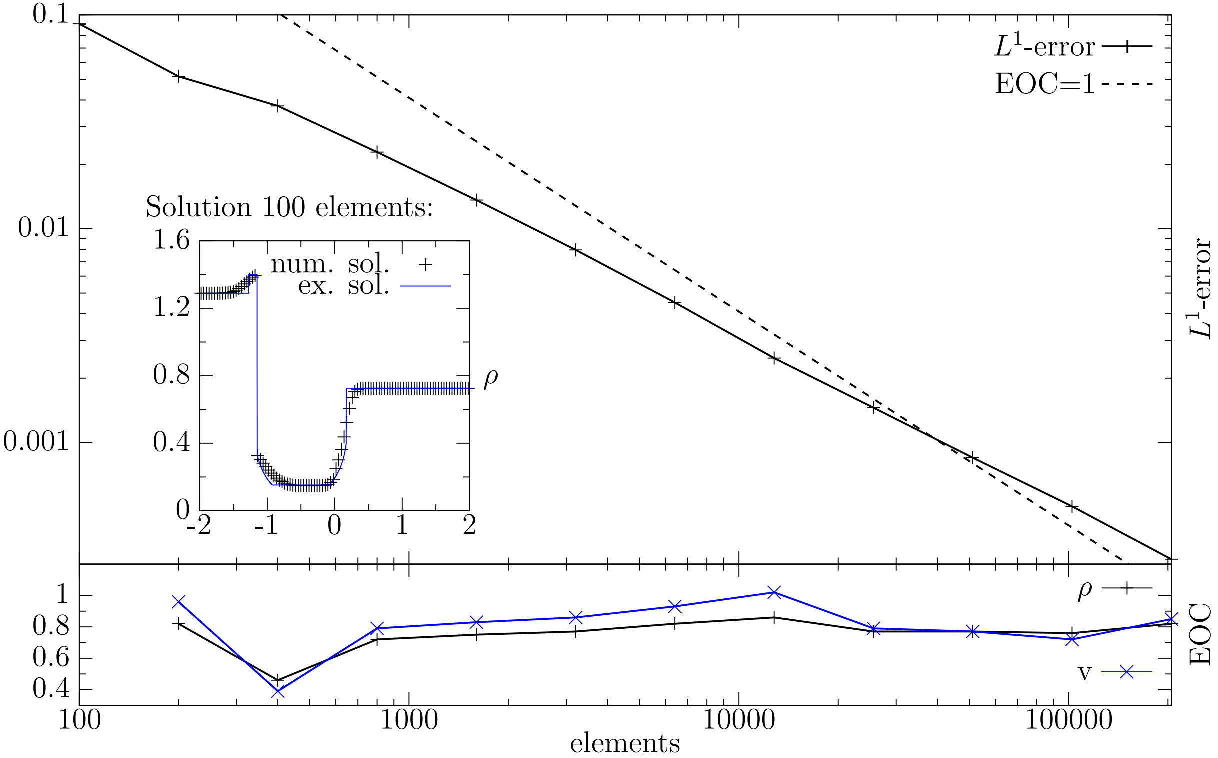
$$\begin{aligned} \partial_t w - \partial_x v &= 0 \\ \partial_t v - \partial_x \sigma(w) &= 0 \\ v(x,0) &= v_0(x), \quad w(x,0) = w_0(x). \end{aligned} \tag{5}$$

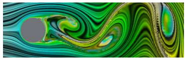
Question: Do there exist Riemann solvers, for treating

- **(??) with non monotone σ**
- **or Euler equations with van der Waals equation of state [14].**

[14] Merkle PhD thesis 2005

Numerical results I





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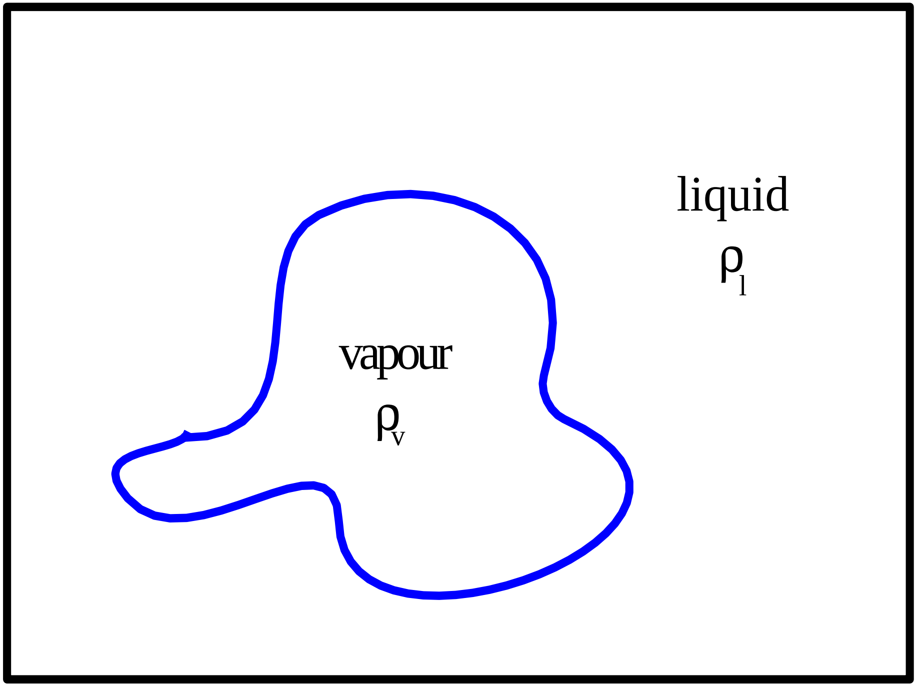
Fluids and phase transitions

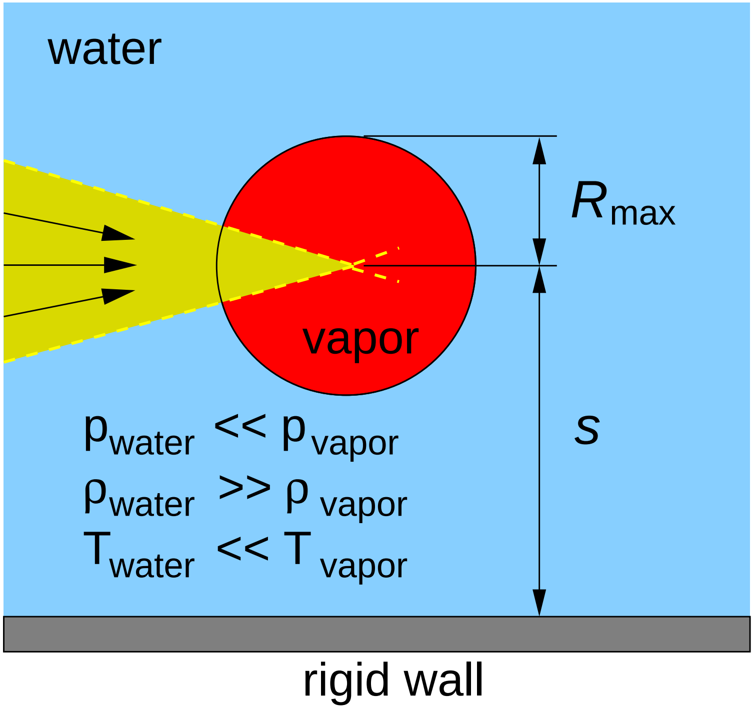
The physical problem of phase transition



Experiments:

Lauterborn, Göttingen

2^{nd} **Experiment (fast time scale): Laser produced bubbles and bubble shock interaction (B1)**:

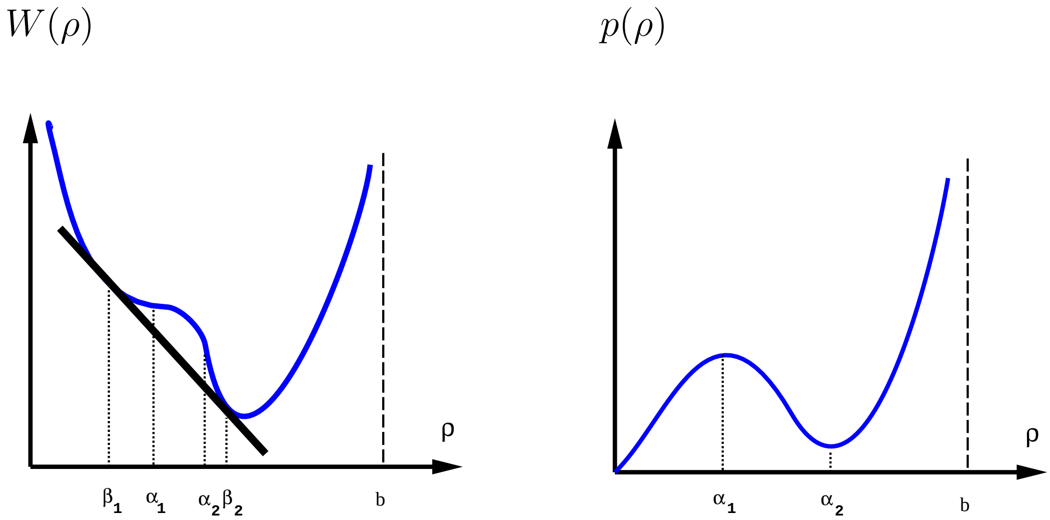


Mathematical model for the static case $v = 0$

Notations

$$\begin{aligned}
\rho \quad &: \quad \textbf{density of the fluid} \\
v \quad &: \quad \textbf{velocity of the fluid} \\
W(\rho) \quad &: \quad \textbf{free energy density (double well)} \\
E(\rho) \quad &: \quad \textbf{total energy} \\
E(\rho) \quad &= \int_\Omega W(\rho)\, dx \\
\textbf{Constraint} \quad &: \int_\Omega \rho \ \mathbf{dx} = M \quad \textbf{(conservation of mass)}
\end{aligned}$$

Free energy density [15]



$$p(\rho) := \rho\, W'(\rho) - W(\rho)$$

[15] Coquel, Diehl, Merkle, Rohde

Diffusive interface approach

- **van der Waals** [16] **has recognized first the non-uniqueness problem of this approach.**
- **He proposed to penalize the occurence of free boundaries between the phases by**

$$\int_\Omega \gamma\varepsilon^2 \frac{|\nabla\rho|^2}{2}\,dx$$

and to consider

$$\begin{aligned} E(\rho) &: \quad \textbf{total energy} \\ E(\rho) &= \int_\Omega \left(W(\rho) + \gamma\varepsilon^2 \frac{|\nabla\rho|^2}{2} \right) dx, \;\; \bar{E}(\rho) = \int_\Omega W(\rho)\,dx \\ \textbf{Constraint} &: \int_\Omega \rho\;\mathbf{dx} = M \quad \textbf{(conservation of mass)} \end{aligned} \tag{6}$$

Let ρ_ε be a minimizer of E and ρ_0 be a minimizer of $\bar{E}$, then

$$\lim_{\varepsilon\to 0} ||\rho_0 - \rho_\varepsilon||_{L^1} = 0.$$ [17]

[16] J.D. van der Waals: Thermodynamische Theorie der Kapillarität unter Voraussetzung stetiger Dichteänderung. Z. Phys. Chem. 1894.
[17] L. Modica: The gradient theory of phase transitions and the minimal interface criterion. Arch. Ration. Mech. Anal. 98 (1987)

Mathematical model for the dynamical case $\partial_t v \neq 0$

- **Lagrangian:** $L(\rho, v) := \frac{1}{2}\rho|v|^2 - W(\rho) - \frac{\gamma}{2}|\nabla\rho|^2$
- **Minimize the action functional:** $\int_0^T \int_{\mathrm{R}^3} L(\rho(x,t), v(x,t))\, dx\, dt$
- **Obtain the Euler-Lagrange-equations:**

$$\partial_t v + v\nabla v = \nabla\left(-W'(\rho) + \gamma\varepsilon^2\Delta\rho\right).$$

- **Using** $p'(\rho) = \rho W''(\rho)$ **and conservation of mass we get**

$$\partial_t(\rho v) + \nabla\cdot(\rho v v^t + p(\rho)I) = \gamma\varepsilon^2\nabla\Delta v\rho$$ [18] [19]

.

- **Add some scaled viscosity and obtain**

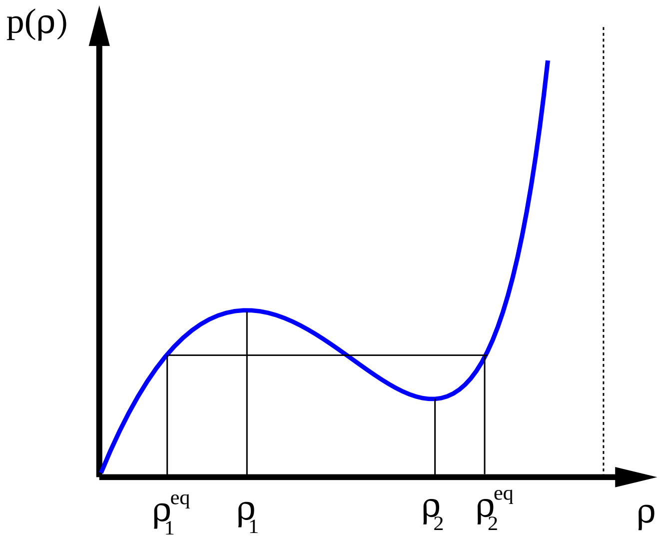
$$\begin{aligned}\partial_t\rho + \nabla\cdot(\rho v) &= 0\\ \partial_t(\rho v) + \nabla\cdot(\rho v v^t + p(\rho))I) &= \varepsilon\alpha\Delta v + \gamma\varepsilon^2\rho\nabla\Delta\rho\end{aligned}$$

[18] S. Benzoni-Gavage, R. Danchin, S. Descombes: On the well-posedness for the Euler-Korteweg model in several space dimensions, preprint 2005

[19] J.E. Dunn, J. Serrin: On the thermodynamics of interstitial working. Arch. Ration. Mech. Anal. 88 (1985), 95,133.

Basic model
(Navier-Stokes-Korteweg model, isothermal case):

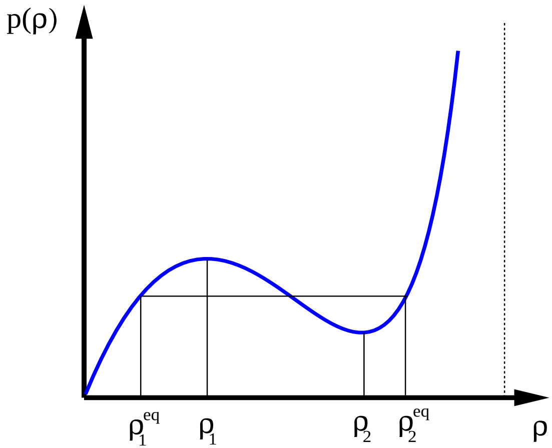
$$\begin{aligned} \partial_t \rho + \mathrm{div}(\rho\, u) &= 0 \\ \partial_t(\rho\, u) + \mathrm{div}(\rho\, u \otimes u) + \nabla p(\rho) &= \mu \Delta u + \lambda \rho \nabla \Delta \rho \end{aligned}$$



Van-der-Waals equation of state (low temperature)

Known results:

$$
\begin{aligned}
\partial_t \rho + \mathrm{div}(\rho\, u) &= 0 \\
\partial_t(\rho\, u) + \mathrm{div}(\rho\, u \otimes u) + \nabla p(\rho) &= \mu \Delta u + \lambda \rho \nabla \Delta \rho
\end{aligned}
$$



Danchin, Desjardin [20]**:**

– **Global existence result for initial data close to stable equilibrium, d=2,3;**

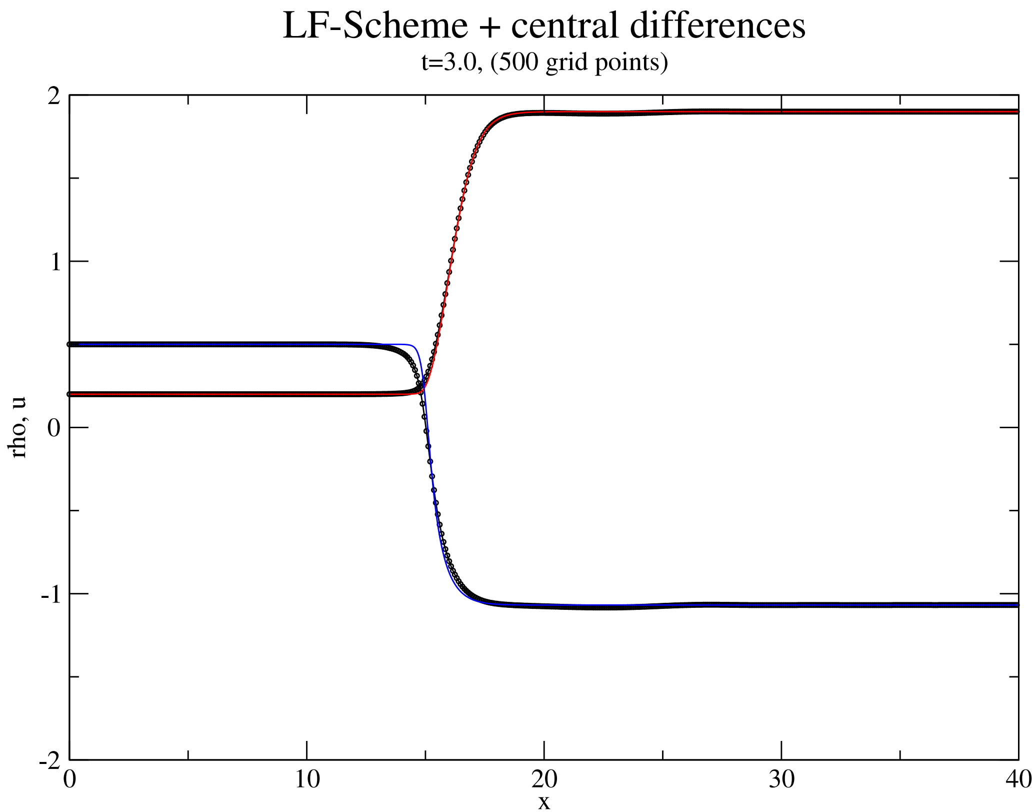
– **local in time existence for** $\rho_0 \geq c > 0$.

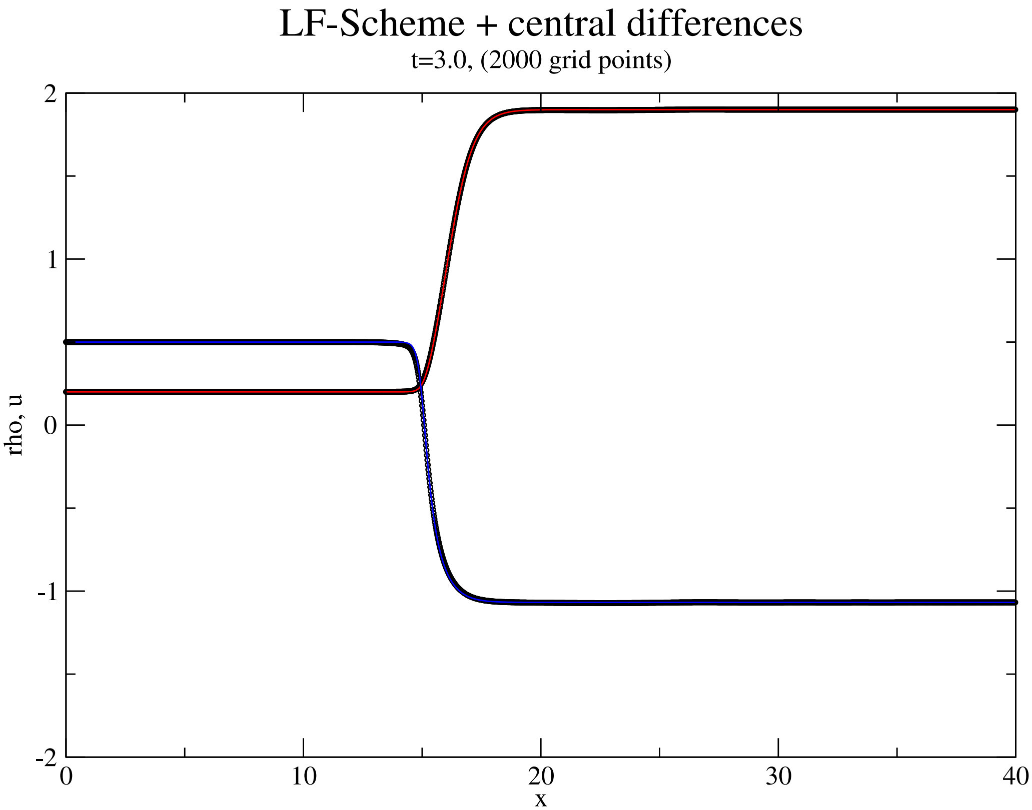
[20] R. Danchin, B. Desjardin, : Existence of solutions for compressible fluid models of korteweg type. Annales de l'IHP, Analyse non lineaire, 18,(2001), 97-133.

Numerical scheme

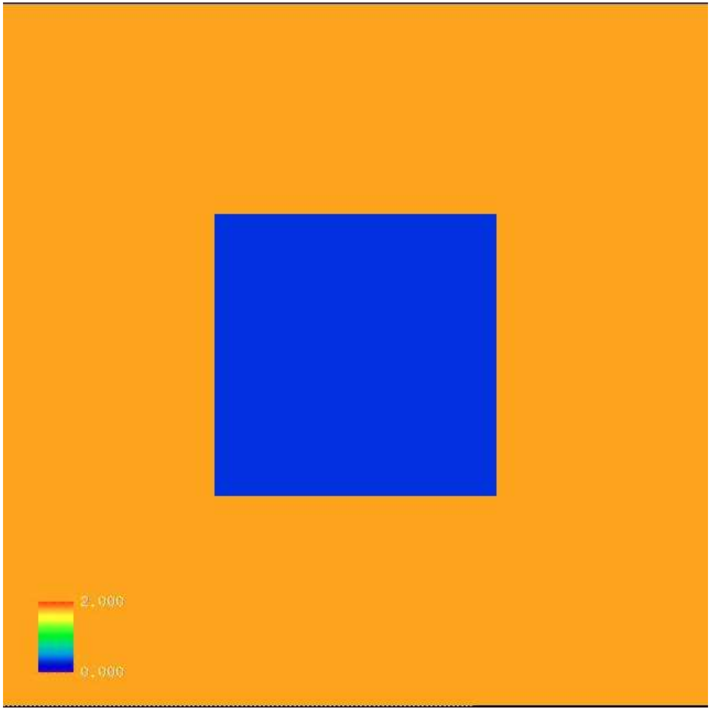
- **Lax-Friedrichs scheme for solving**

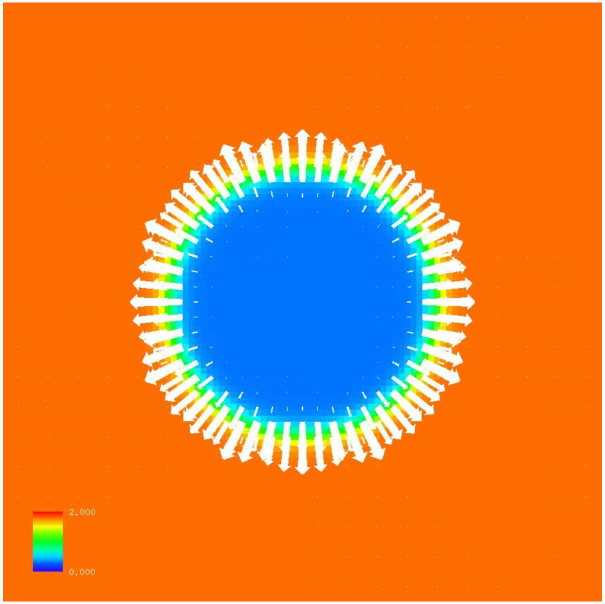
$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho v) &= \alpha \Delta \rho \\
\partial_t (\rho v) + \nabla \cdot (\rho v v^t + p(\rho)) I) &= \varepsilon \alpha \Delta v + \gamma \varepsilon^2 \rho \nabla \Delta \rho
\end{aligned}
\tag{7}
$$


LF-Scheme + central differences
t=3.0, (500 grid points)
rho, u
x
2
1
0
-1
-2
0
10
20
30
40



- **But the scheme has poor convergence properties, in particular for stationary solutions.**

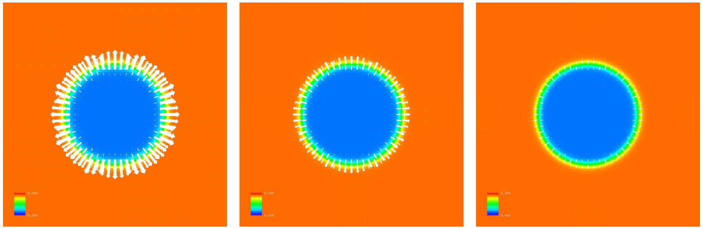

2.000
0.000


2.000
0.000

$$\begin{aligned} \partial_t \rho + \nabla \cdot (\rho v) &= \alpha \Delta \rho \\ \partial_t(\rho v) + \nabla \cdot (\rho v v^t + p(\rho)) I) &= \varepsilon \alpha \Delta v + \gamma \varepsilon^2 \rho \nabla \Delta \rho \end{aligned} \tag{8}$$

$$\begin{aligned} \partial_t \rho + \nabla \cdot (\rho v - \alpha \nabla \rho) &= 0 \\ \alpha &= O(h) \\ \partial_t(\rho v) + \nabla \cdot (\rho v v^t + p(\rho)) I) &= \varepsilon \alpha \Delta v + \gamma \varepsilon^2 \rho \nabla \Delta \rho \end{aligned} \tag{9}$$

- The scheme converges to the exact solution
- It gives poor results at static equilibrium



- The Energy does not decrease monotonically

$$
\begin{aligned}
E(\rho) &: \quad \textbf{total energy} \\
E(\rho) &= \int_\Omega \left(W(\rho) + \gamma\varepsilon^2 \frac{|\nabla\rho|^2}{2} \right) dx \\
\textbf{Constraint} &: \int_\Omega \rho \, \mathbf{dx} = M \quad \textbf{(conservation of mass)} \\
\textbf{Euler Lagrange equations} &: -W'(\rho) + \gamma\varepsilon^2 \Delta\rho = constant
\end{aligned}
$$

$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho v) &= \alpha \Delta \rho \\
\partial_t (\rho v) + \nabla \cdot (\rho v v^t + p(\rho)) I) &= \varepsilon \alpha \Delta v + \gamma \varepsilon^2 \rho \nabla \Delta \rho
\end{aligned}
$$

$$
\textbf{Euler Lagrange equations} \; : \; \kappa(\rho) := -W'(\rho) + \gamma\varepsilon^2 \Delta\rho = constant
$$

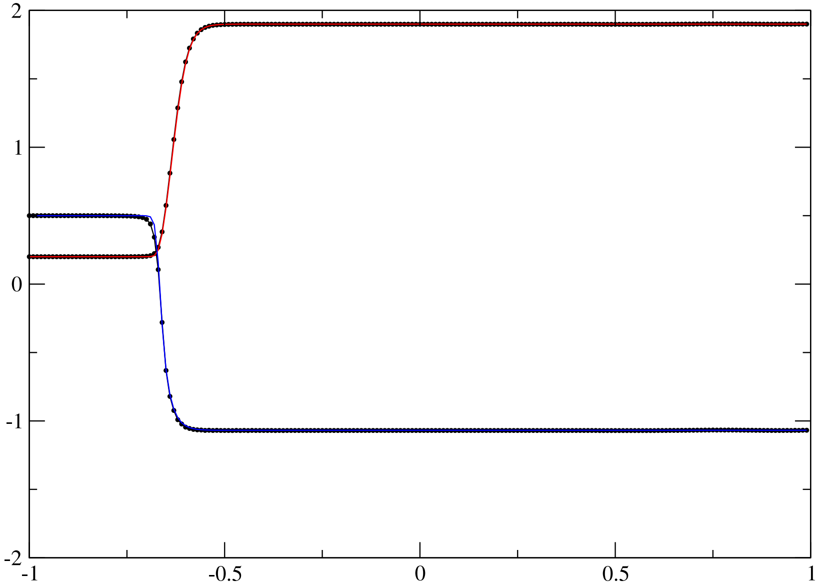
$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho v) &= \alpha \Delta \kappa \\
\partial_t (\rho v) + \nabla \cdot \rho v v^t + \rho \nabla \kappa(\rho) &= \varepsilon \alpha \Delta v
\end{aligned}
$$

- **Well balanced scheme [21]: central differences in space, explicit Euler in time .**

[21] D. Kröner, M.D. Thanh, SINUM 2005, M. Nolte, D. Kröner, Preprint 2005

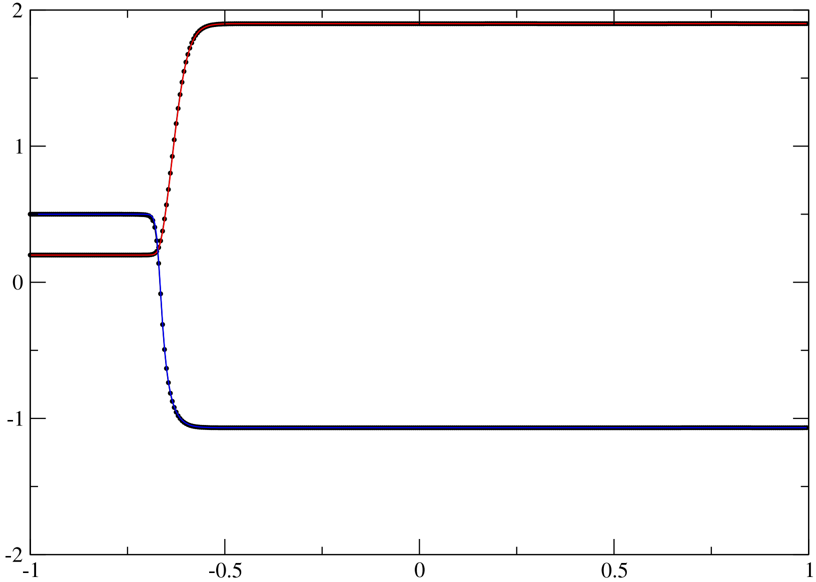
Non-Conservative 1st Order Scheme

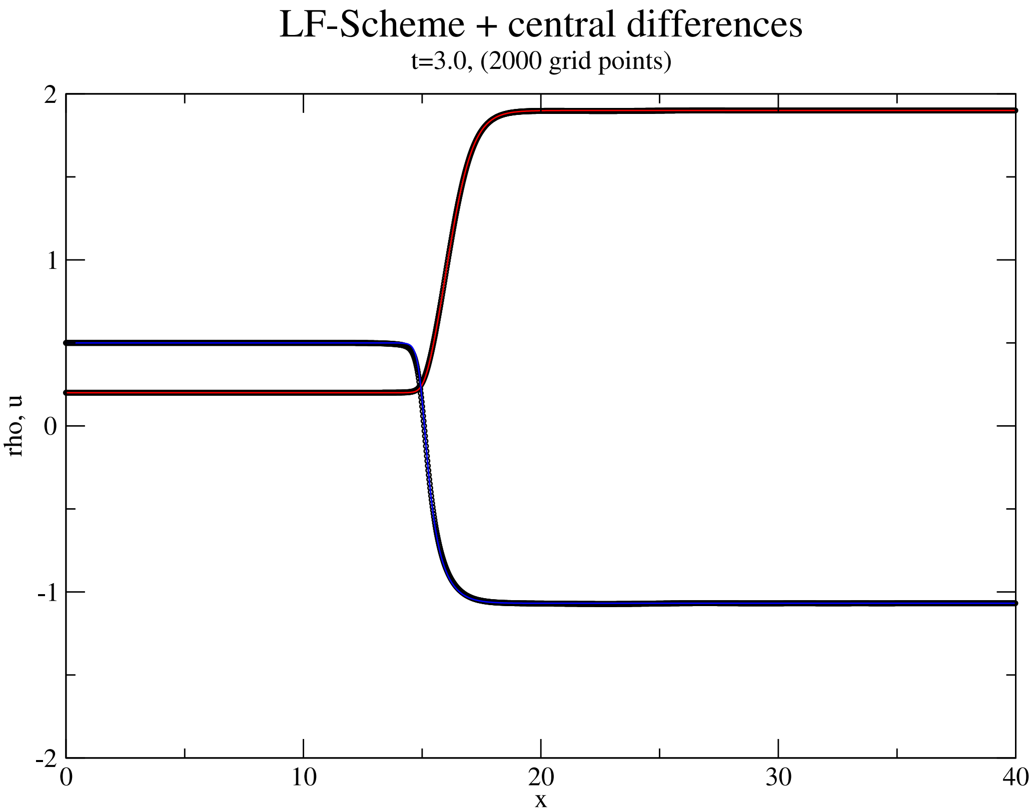
t=0.5, (200 grid points)



Non-Conservative 1st Order Scheme

t=0.5, (400 grid points)



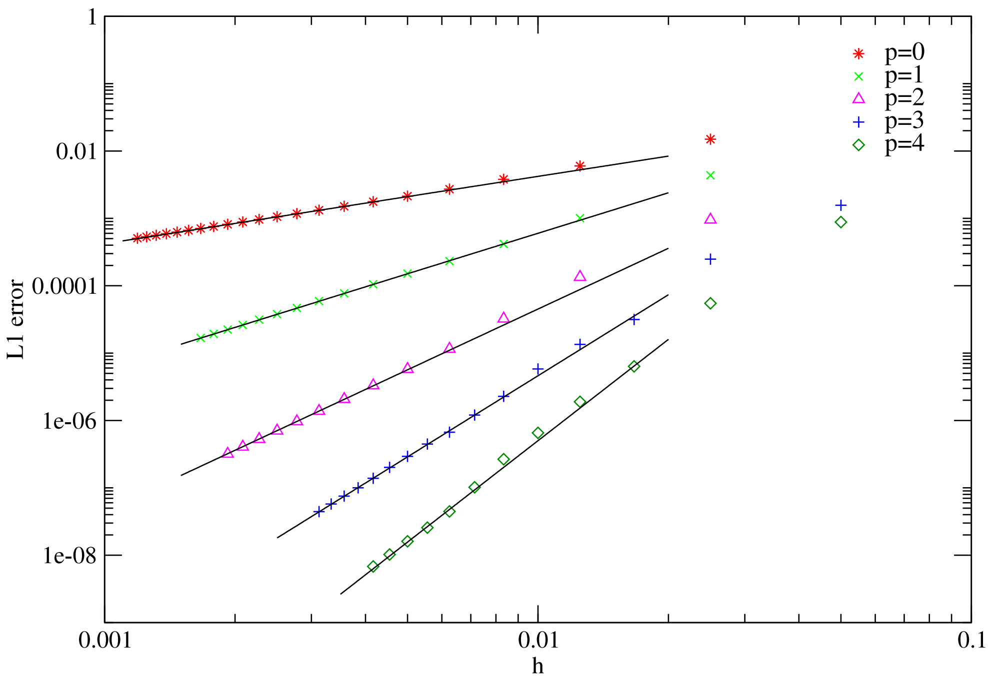


- The scheme converges to the exact solution

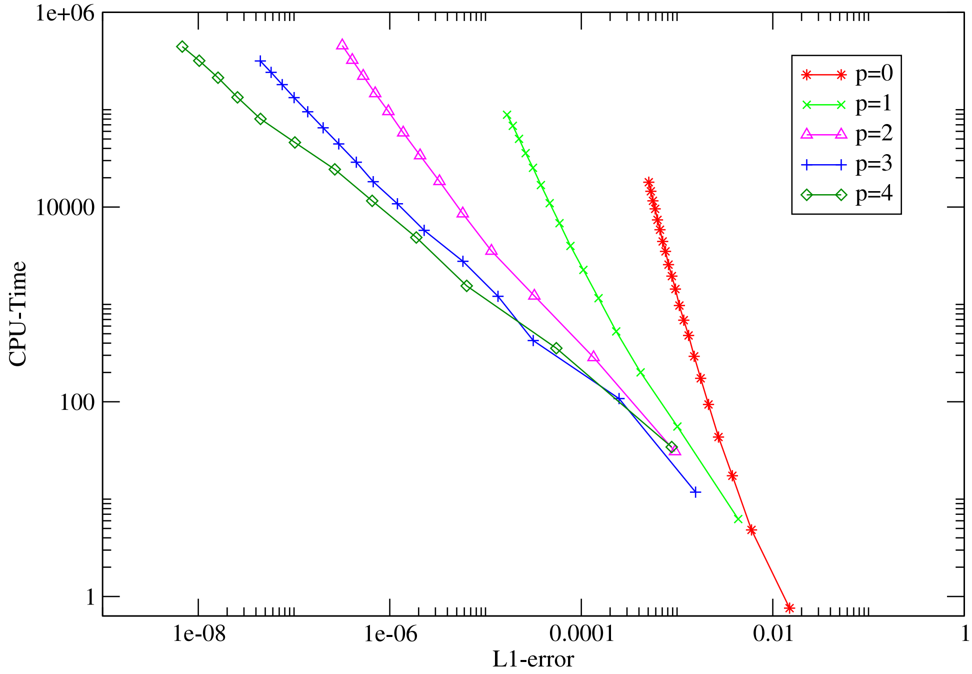
- **Discontinuous Galerkin schemes** [22]
  - **2D triangular nonconform and conform meshes**
  - **adaptive mesh refinement**
  - **conservative and nonconservative schemes**
  - **accuracy in space: 1,2,...,6,...**
  - **implicit and explicit Runge Kutta methods, accuracy in time: 1,...4**

[22] N. Besse, D. Kröner, M^2AN 2005

Discontinuous Galerkin Schemes



Discontinuous Galerkin Schemes



merging bubbles

- third order Discontinuous Galerkin scheme
- second order implicit Runge-Kutta method
- adaptive refined nonconform triangular mesh

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