Second Workshop DFG-CNRS Research Group

Micro-Macro Modelling and Simulation of Liquid-Vapour Flows

Talence, Jan 10–12, 2007

One-Dimensional Wave Patterns in Phase Transition Problems

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Plan of the Talk

1) General Framework

2) The Sharp-Interface Model

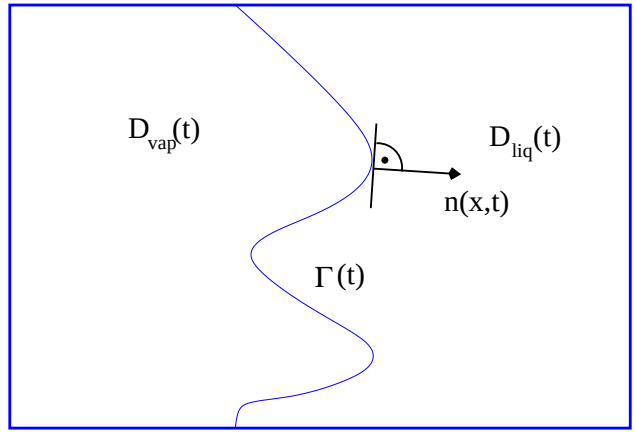
3) The Diffuse-Interface Model

1) General Framework:

Sharp-Interface Model: Euler Equations

$$\begin{aligned} \rho_t + \quad & \mathrm{div}(\rho \mathbf{v}) = 0 \\ (\rho \mathbf{v})_t + \quad & \mathrm{div}(\rho \mathbf{v}\mathbf{v}^T + p(\rho)\mathcal{I}) = 0 \end{aligned} \quad \text{in } D_{\text{vap/liq}}(t)$$

$$\begin{aligned} [\![\rho(\mathbf{v}\cdot\mathbf{n} - s)]\!] &= 0 \\ [\![\rho(\mathbf{v}\cdot\mathbf{n} - s)\mathbf{v} + p\mathbf{n}]\!] &= (d-1)\sigma\kappa\mathbf{n} \end{aligned} \quad \text{in } \Gamma(t)$$



$\rho = \rho(\mathbf{x}, t) > 0$: Density

$\mathbf{v} = \mathbf{v}(\mathbf{x}, t) \in \mathbb{R}^d$: Velocity

$$D = D_{liq}(t) \cup D_{vap}(t) \cup \Gamma(t).$$

Here $\sigma > 0$ is the surface tension and

$s = s(\mathbf{x}, t)$ normal propagation speed of $\Gamma(t)$

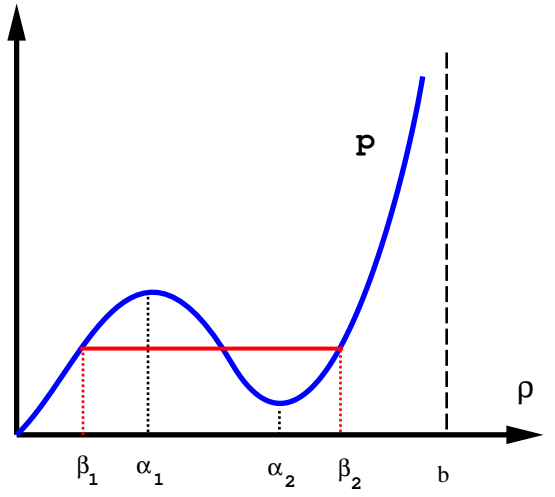
$\kappa = \kappa(\mathbf{x}, t)$ mean curvature of $\Gamma(t)$

Sharp-Interface Model: Euler Equations

$$\begin{aligned} \rho_t + \quad \mathrm{div}(\rho \mathbf{v}) &= 0 \\ (\rho \mathbf{v})_t + \mathrm{div}(\rho \mathbf{v}\mathbf{v}^T + p(\rho)\mathcal{I}) &= 0 \end{aligned} \quad \text{in } D_{\text{vap/liq}}(t)$$

$$\begin{aligned} [\![\rho(\mathbf{v}\cdot\mathbf{n} - s)]\!] &= 0 \\ [\![\rho(\mathbf{v}\cdot\mathbf{n} - s)\mathbf{v} + p\mathbf{n}]\!] &= (d-1)\sigma\kappa\mathbf{n} \quad \text{in } \Gamma(t) \end{aligned}$$

additional jump condition



Pressure: $p'(\rho) = \rho W''(\rho)$.

$\rho = \rho(\mathbf{x}, t) > 0$: Density

$\mathbf{v} = \mathbf{v}(\mathbf{x}, t) \in \mathbb{R}^d$: Velocity

Van-der-Waals pressure:

$$p = p(\rho) = \frac{RT\rho}{1 - d\rho} - a\rho^2$$

Sharp-Interface model: Notes

Wellposedness result for Delhaye-model: Benzoni-Gavage&Freistühler 04

DFG-CNRS research group:
Numerical solution by ghostfluid-approach

(Some) open analytical problems:

(i) thermodynamical consistent modelling of interface conditions

(ii) boundary treatment and contact lines

(iii) multi-dimensional wellposedness for initial value problems

(iv) one-dimensional wellposedness for initial value problems

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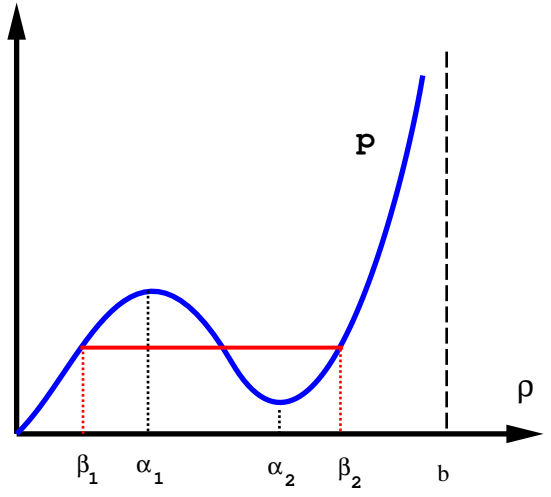
Diffuse Interface Model: Navier-Stokes-Korteweg

$$\begin{aligned} \rho_t &+ \operatorname{div}(\rho \mathbf{v}) &&= 0 \\ (\rho \mathbf{v})_t &+ \operatorname{div}(\rho \mathbf{v}\mathbf{v}^T + p(\rho)\mathcal{I}) &&= \mu \Delta \mathbf{v} + \gamma \rho \nabla D^{\varepsilon}[\rho] \end{aligned}$$

$\rho = \rho(x,t) > 0$: Density

$\mathbf{v} = \mathbf{v}(\mathbf{x},t) \in \mathbb{R}^d$: Velocity



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Diffuse Interface Model: Navier-Stokes-Korteweg

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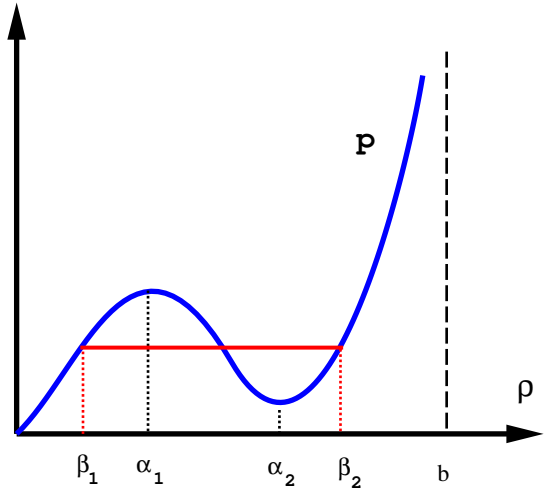

Pressure: $p'(\rho) = \rho W''(\rho)$.

The local version:

$$D^{\varepsilon}_{\text{local}}[\rho] = \varepsilon^2 \Delta \rho$$

The global version:

$$D^{\varepsilon}_{\text{global}}[\rho] = K_{\varepsilon} * \rho - \rho$$

Isentropic Diffuse-Interface Model: Notes

Wellposedness results: local and global existence results for initial value problem

DFG-CNRS research group:
Numerical solution by DG-method $\rightsquigarrow$ Talk by D. Diehl

(Some) open analytical problems:

(i) Sharp-interface limit (Joint work with W. Dreyer, Chr. Kraus)

(ii) Theory for boundary-value problems

(iii) Asymptotic behaviour of weak solutions in multiple space dimensions

(iv) Asymptotic behaviour of weak solutions in 1D

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2) The Sharp-Interface Model

Sharp-Interface Model: Multi-Dimensional Case

$$\begin{aligned} \rho_t &+ \operatorname{div}(\rho\mathbf{v}) &&= 0 \\ (\rho\mathbf{v})_t &+ \operatorname{div}(\rho\mathbf{v}\mathbf{v}^T + p(\rho)\mathcal{I}) &&= 0 \end{aligned} \quad \text{in } D_{\text{vap/liq}}(t)$$

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additional jump condition

Sharp-Interface Model: Planar Front

$$\begin{aligned} \rho_t + \quad \mathrm{div}(\rho\mathbf{v}) &= 0 \\ (\rho\mathbf{v})_t + \mathrm{div}(\rho\mathbf{v}\mathbf{v}^T + p(\rho)\mathcal{I}) &= 0 \end{aligned} \quad \text{in } D_{\text{vap/liq}}(t)$$

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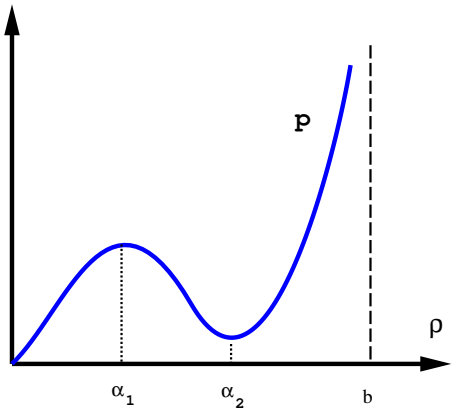
additional jump condition

Analysis: Sharp-Interface Model in 1D

$$\begin{array}{lcll} \rho_t & + & \rho v_x & = 0 \\ (\rho v)_t & + & \left(\rho v^2 + p(\rho)\right)_x & = 0 \end{array} \quad \text{in } \mathbb{R}\times(0,\infty)$$

$\rho = \rho(x,t) > 0$: Density

$v = v(x,t) \in \mathbb{R}$: Velocity



$$p'(\rho) = \rho W''(\rho)$$

Definition: (phases)

A state $(\rho, \rho v)$ is in the **vapour** (**liquid**) phase iff we have

$$\rho \in (0, \alpha_1) \qquad \big(\rho \in (\alpha_2, b)\big).$$

It is called **elliptic** for $\rho \in (\alpha_1, \alpha_2)$.

We define the hyperbolic **state space**

$$\mathcal{U} := (0, b) \setminus (\alpha_1, \alpha_2).$$

Analysis: Sharp-Interface Model in 1D

$$\begin{array}{rcccl} \rho_t & + & \rho v_x & = & 0 \\ (\rho v)_t & + & \left(\rho v^2 + p(\rho)\right)_x & = & 0 \end{array} \quad \text{in } \mathbb{R}\times(0,\infty)$$

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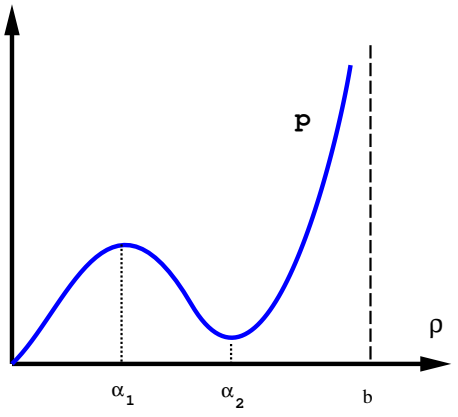


$$p'(\rho) = \rho W''(\rho)$$

Eigenvalues of the Jacobian

$$\lambda_-(\rho,\rho v) = v - \sqrt{p'(\rho)}, \qquad \lambda_+(\rho,\rho v) = v + \sqrt{p'(\rho)}$$

$\rightsquigarrow$ Mixed-type system of conservation laws

Analysis: Weak Solutions, Clausius-Duhem Inequality, Nonuniqueness

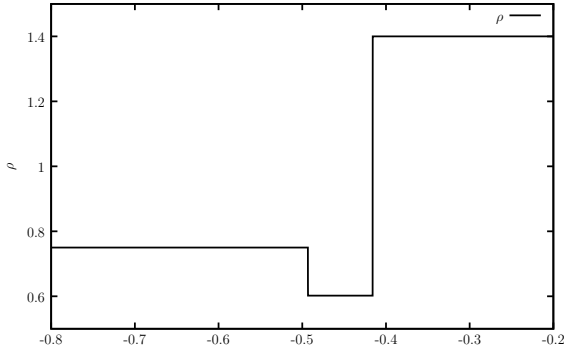
Definition: (Entropy solution)

A weak solution $(\rho, \rho v) \in L^{\infty}_{loc}(\mathbb{R} \times (0, \infty))$ of the SI-model that satisfies

$$\left(W(\rho) + \frac{1}{2}\rho v^2\right)_t + \left(\left(W(\rho) + \frac{1}{2}\rho v^2 + p(\rho)\right)v\right)_x \leq 0$$

in $\mathcal{D}'(\mathbb{R} \times (0, T))$ is called **entropy solution**.

Explicit entropy solutions of 1D-Riemann problem



Density at $t = 0.1$.

Analysis: Weak Solutions, Clausius-Duhem Inequality, Nonuniqueness

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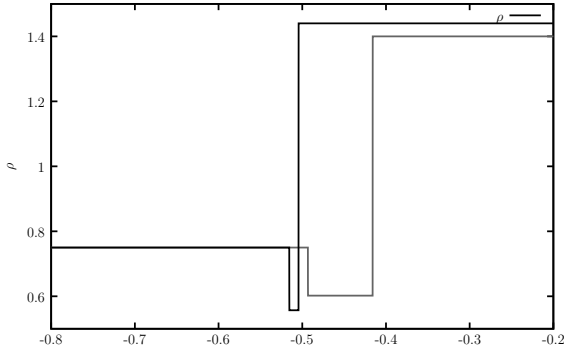

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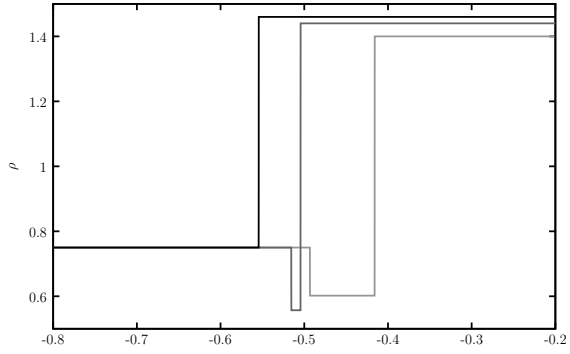


Density at $t = 0.1$.

Analysis: Uniqueness by Kinetic Relations:
(Abeyaratne&Knowles, Truskinovsky, LeFloch et al.)
A (subsonic) phase transition

$$(\rho, \rho v)(x,t) = \begin{cases} (\rho_-, \rho_- v_-) & : \quad x - st < 0 \\ (\rho_+, \rho_+ v_+) & : \quad x - st > 0 \end{cases}$$

is called **admissible** iff it satisfies the RH-conditions and the **kinetic relation**

$$s[\![W(\rho) + \frac{1}{2}\rho v^2]\!] - [\![\big(W(\rho) + \frac{1}{2}\rho v^2 + p(\rho)\big)v]\!] = jG(j),\ j = \rho_-(v_- - s).$$

Example:

$$G(j) = -j \ (\Rightarrow \text{ Phase transition is entropy solution.})$$

Note The kinetic relation can be written in the form

$$\rho_l = \Psi(\rho_r), \Psi : (0,\infty) \to (0,\infty).$$

Analysis: The Riemann Problem

Define $u := (\rho, \rho v)$.

For $u_l, u_r \in \mathcal{U}$ we consider the SI-model for the inital datum

$$u(x,0) = \begin{cases} u_l : x < 0 \\ u_r : x > 0 \end{cases}$$

Theorem: (Merkle&R. 06)

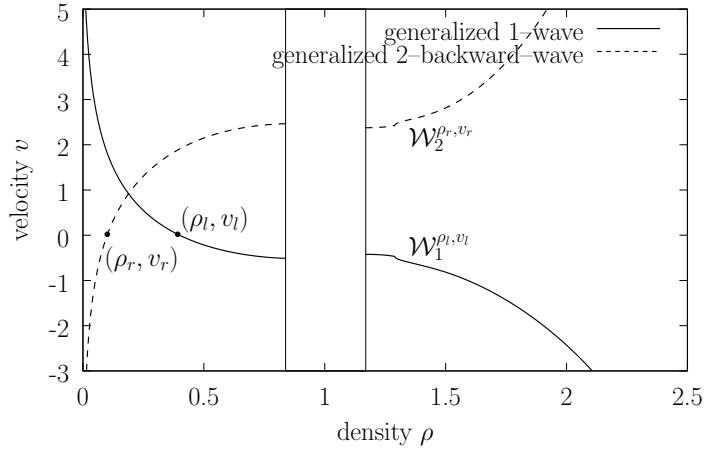
Under appropriate assumptions on $\Psi : (0,\infty) \to (0,\infty)$ we have

(i) The Riemann problem admits a weak solution $u : \mathbb{R} \times [0,\infty) \to \mathcal{U}$ in the class of self-similar functions consisting of Laxian shock waves, admissible phase transitions, attached and rarefaction waves.

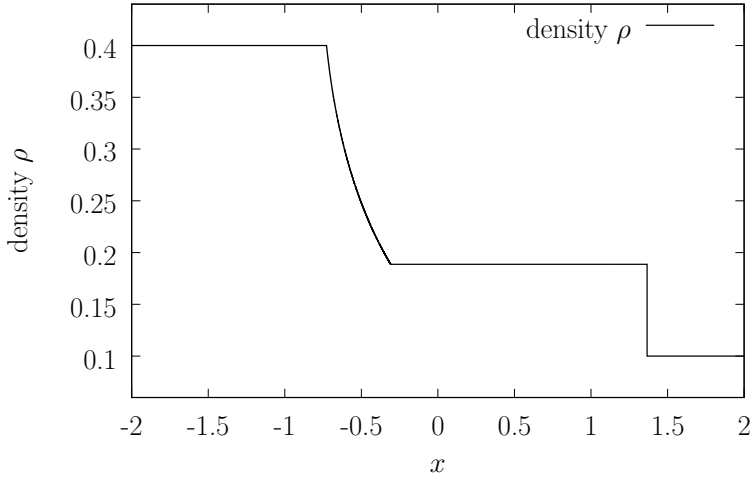
(ii) It is unique in this class if it satisfies the following properties.

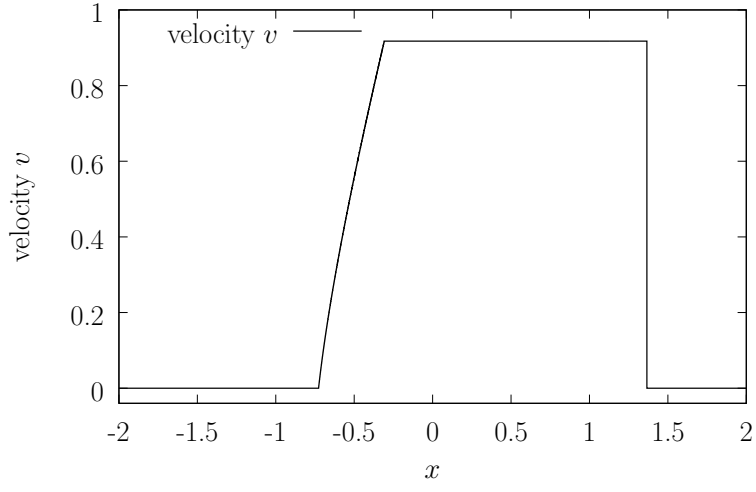
1. phase transitions connecting states with the same pressure connect Maxwell–states,
2. a one-phase solution is used whenever it exists.

Analysis: Wave Curves and Solution for a One-Phase Case



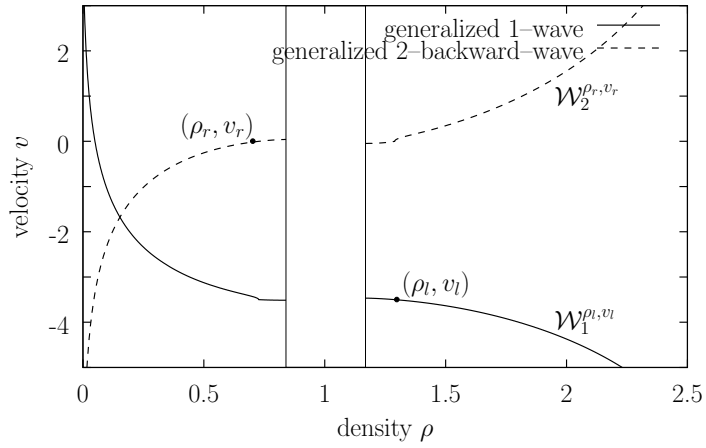
Generalized one-forward and two-backward curves



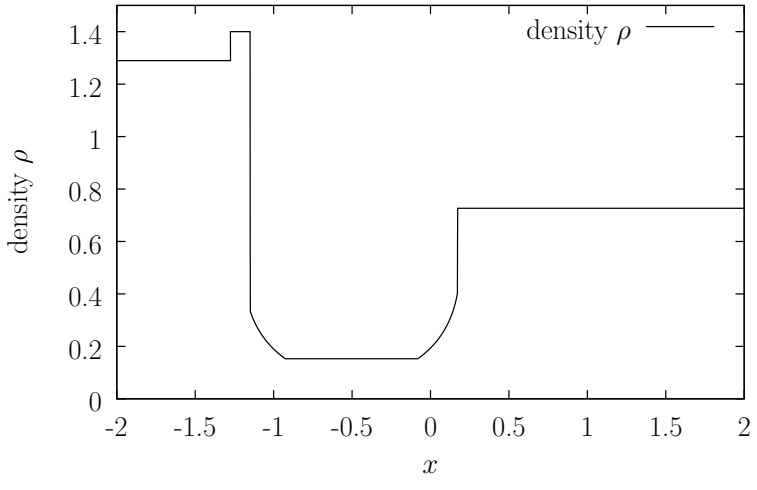


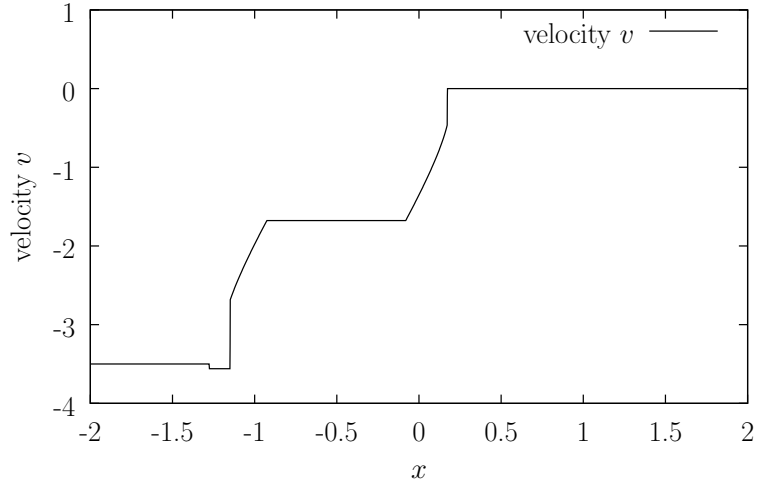
Graphs for density and velocity.

Analysis: Wave Curves and Solution for a Two-Phase Case



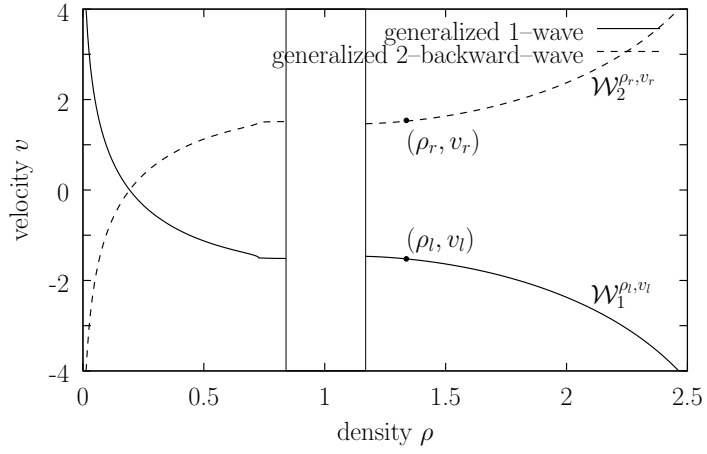
Generalized one-forward and two-backward curves



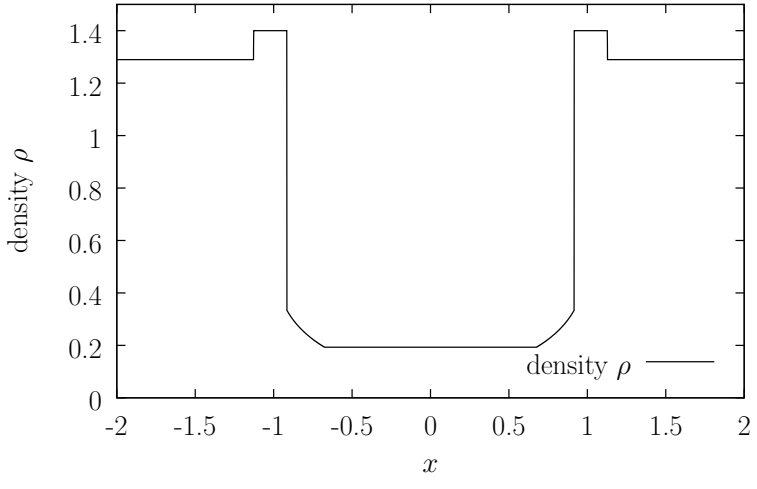


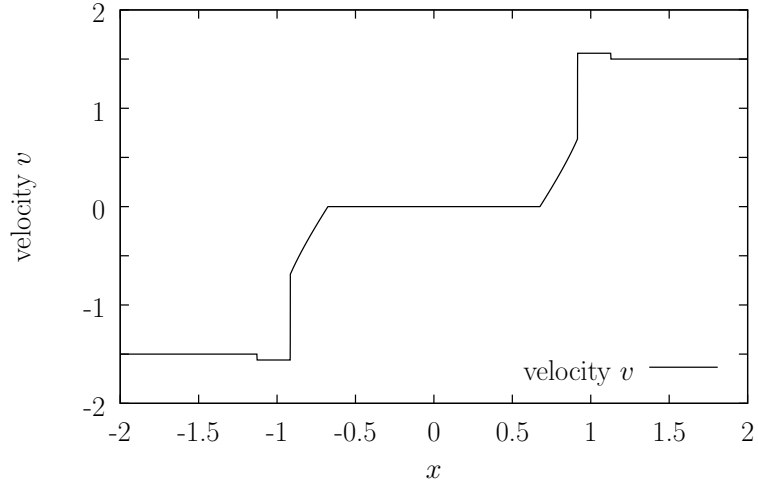
Graphs for density and velocity.

Analysis: Wave Curves and Solution for a Nucleation Case



Generalized one-forward and two-backward curves





Graphs for density and velocity.

Numerics: Some Methods for Undercompressive Waves/Mixed-Type Systems

- Lax-Friedrichs type schemes
- Hou&Rosakis&LeFloch ‘99, Merkle&R.’06: level-set appoach for (trilinear) pressure function,
- LeFloch, Hayes, Mercier, R. ’98-’01: artificial dissipation approach for scalar equations,
- Abgrall&Saurel ‘03, Le Metayer&Massoni& Saurel 05: discrete equations method for evaporation fronts,
- Chalons ’06: transport-equilibrium approach

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$\rightsquigarrow$ Keep phase boundary sharp (whatever it costs)

$\rightsquigarrow$ Do not use (hidden) phase field coupling

Numerics: Riemann Solver Based Ghostfluid Approach (Merkle&R. 06)

Step 0: (data initialization)

For $t^0 := 0$ we define

$$u_j^0 := (\rho_j^0, m_j^0) := \frac{1}{h} \int_{I_j} (\rho_0, \rho_0 v_0)(x)\, dx \qquad (j \in \mathbb{Z}).$$

Assume that for time $t^n > 0$ the sequence

$$u_j^n := \{(\rho_j^n, m_j^n)\}_{j \in \mathbb{Z}} \subset \mathcal{U}$$

is given.

Numerics: Riemann Solver Based Ghostfluid Approach (Merkle&R. 06)

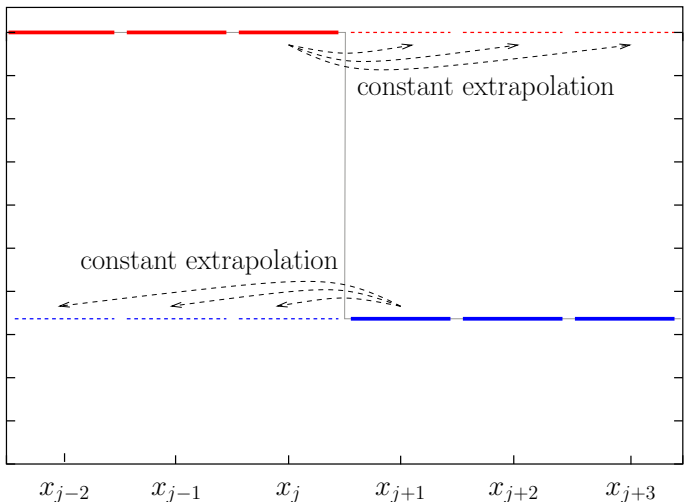
Step 1: (Construction of two preliminary one-phase data sets)

For $j \in \mathbb{Z}$ define the **vapour data set** $\{u_{vap}{}_j^n\}_{j\in\mathbb{Z}}$ at $t = t^n$ by

$$u_{vap}{}_j^n := \begin{cases} u_j^n & : \quad u_j^n \text{ is vapour state,} \\ u_{k(j)}^n & : \quad u_j^n \text{ is liquid state.} \end{cases}$$

Here $u_{k(j)}^n$ denotes the values of the vapour state in the cell $I_{k(j)}$ which is most close to the cell I_j.

The **liquid data set** $\{u_{liq}{}_j^n\}_{j\in\mathbb{Z}}$ at $t = t^n$ is defined analogously.

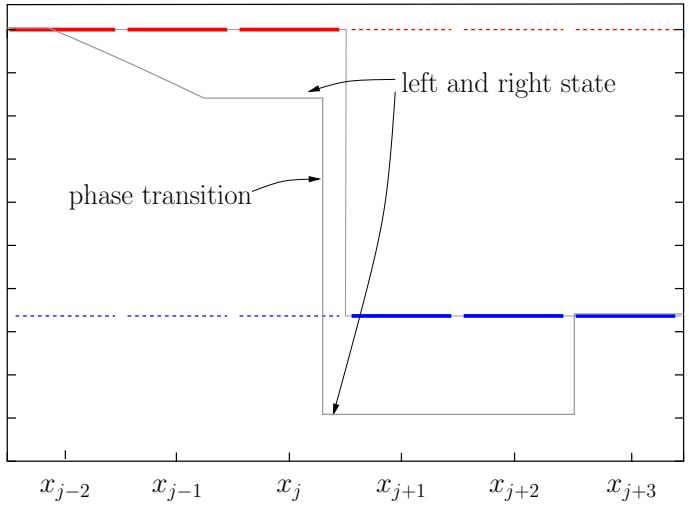


Numerics: Riemann Solver Based Ghostfluid Approach (Merkle&R. 06)

Step 2: (Solution of Riemann problems)

For $j \in \mathbb{Z}$ determine the unique weak solution $u^{(j,n)} : \mathbb{R} \times [0, \infty) \to \mathcal{U}$ of the Riemann problem with initial data

$$u^{(j,n)}(x,0) := \begin{cases} \begin{cases} u_{liq}{}_j^n & : \quad x < 0 \\ u_{vap}{}_j^n & : \quad x > 0 \end{cases} & (u_{vap}{}_j^n = u_j^n), \\ \begin{cases} u_{vap}{}_j^n & : \quad x < 0 \\ u_{liq}{}_j^n & : \quad x > 0 \end{cases} & (u_{liq}{}_j^n = u_j^n). \end{cases}$$



$p_{liq}{}_j^n$: liquid state at phase boundary

$p_{vap}{}_j^n$: vapour state at phase boundar

s_j^n : speed of phase boundary

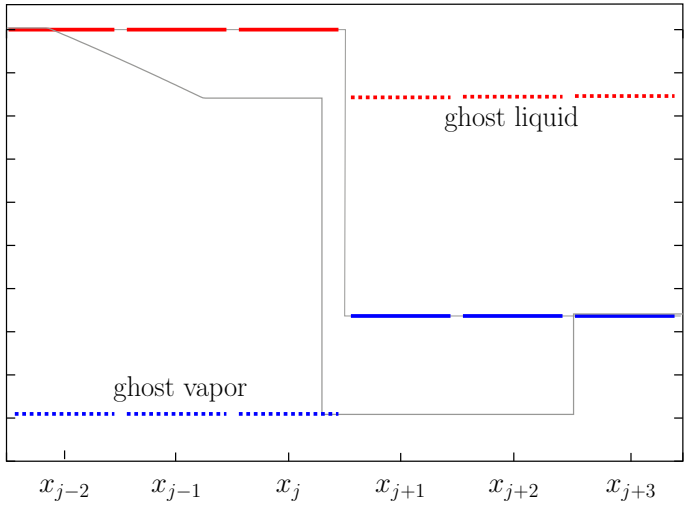
Numerics: Riemann Solver Based Ghostfluid Approach (Merkle&R. 06)

Step 3: (Construction of two final one-phase data sets)

Define the **final vapour data set** $\{u\,\mathbf{vap}_j^n\}_{j\in\mathbb{Z}}$ at $t = t^n$ by

$$u\mathbf{vap}_j^n := \begin{cases} u_j^n & : \quad u_j^n \text{ is vapour state} \\ p_{vap}{}_j^n & : \quad u_j^n \text{ is liquid state} \end{cases} \qquad (j \in \mathbb{Z})$$

The **final liquid data set** $\{u\mathbf{liq}_j^n\}_{j\in\mathbb{Z}}$ is defined analogously.



Numerics: Riemann Solver Based Ghostfluid Approach (Merkle&R. 06)

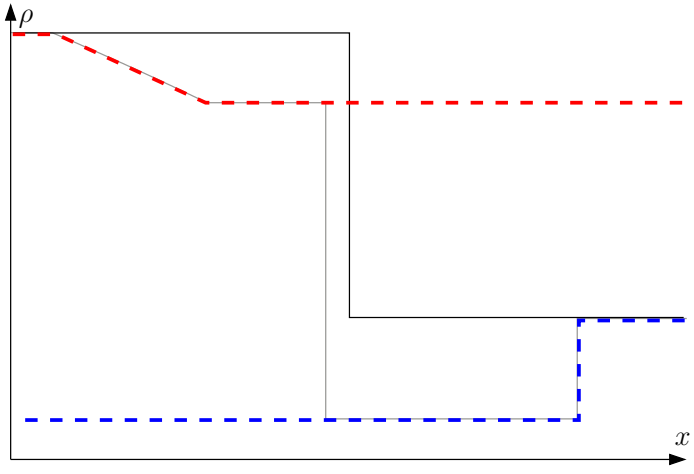
Step 4: (Time evolution)

For $j \in \mathbb{Z}$ define $\{u_{\textbf{liq}}{}_j^{n+1}\}_{j\in\mathbb{Z}}$

$$u_{\textbf{liq}}{}_j^{n+1} := u_{\textbf{liq}}{}_j^{n} - \frac{\Delta t^n}{h}\left[g(u_{\textbf{liq}}{}_j^{n}, u_{\textbf{liq}}{}_{j+1}^{n}) - g(u_{\textbf{liq}}{}_{j-1}^{n}, u_{\textbf{liq}}{}_j^{n})\right]$$

Here $g : \mathcal{U}^2 \longrightarrow \mathbb{R}^2$ is a standard numerical flux function for the Euler equations.

The data set $\{u_{\textbf{vap}}{}_j^{n+1}\}_{j\in\mathbb{Z}}$ is defined analogously.



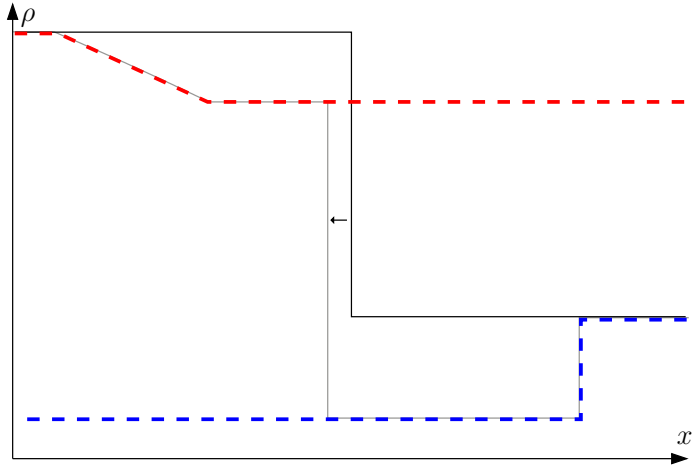
Numerics: Riemann Solver Based Ghostfluid Approach (Merkle&R. 06)

Step 5: (Finalization)

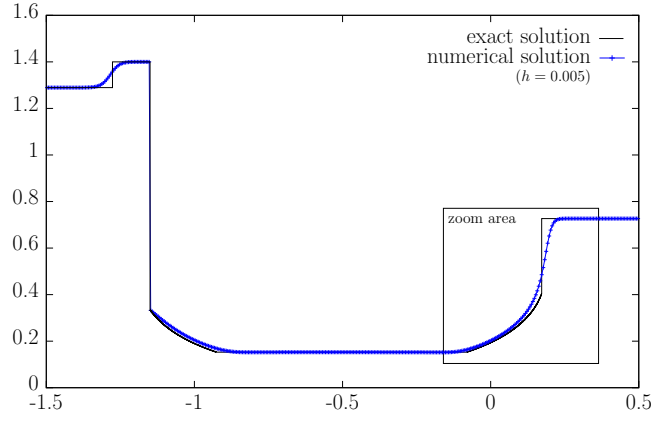
Determine from $\{u_j^n\}_{j\in\mathbb{Z}}$ and $\{s_j^n\}_{j\in\mathbb{Z}}$ a new phase distribution.

For $j \in \mathbb{Z}$ define $\{u_j^{n+1}\}_{j\in\mathbb{Z}}$ by

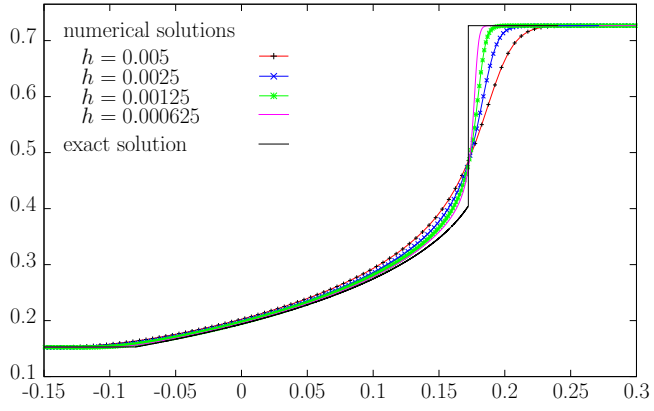
$$u_j^{n+1} := \begin{cases} u_{\mathbf{vap}}{}_j^{n+1} & : \quad \text{state in } I_j \text{ is vapour state} \\ u_{\mathbf{liq}}{}_j^{n+1} & : \quad \text{state in } I_j \text{ is liquid state} \end{cases}$$



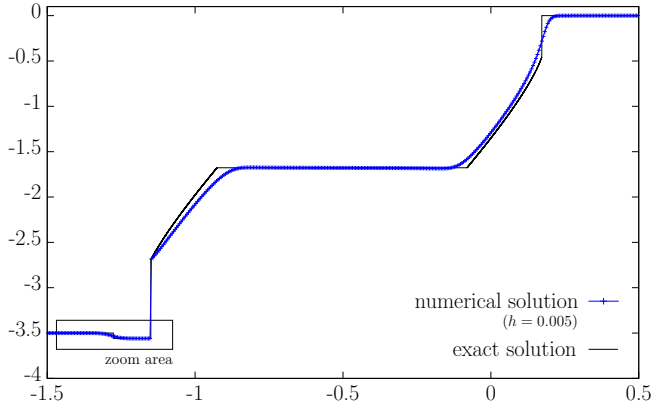
Numerics: an experiment



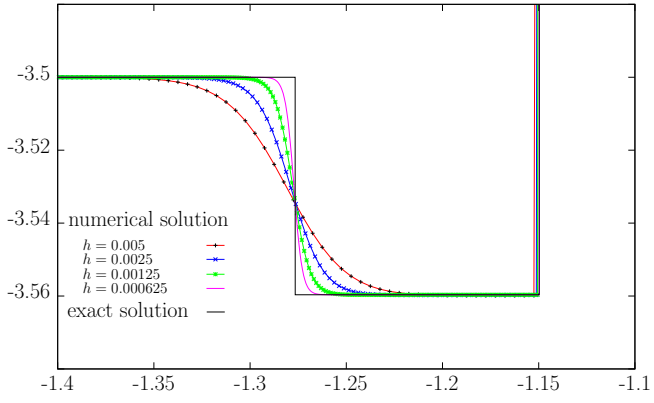
Density



Density: Detailed view.



Velocity



Velocity: Detailed view.

Numerics: an experiment

grid size	L^1–error of ρ	EOC	L^1–error of v	EOC
0.04	0.08953370		0.22612267	
		0.85		1.03
0.02	0.04975303		0.11056125	
		0.48		0.39
0.01	0.03562381		0.08429837	
		0.75		0.84
0.005	0.02126755		0.04722471	
		0.77		0.88
0.0025	0.01247926		0.02572075	
		0.79		0.90
0.00125	0.00721779		0.01378924	
		0.83		0.97
0.000625	0.00406572		0.00702086	
		0.87		1.08
0.0003125	0.00222163		0.00332194	
		0.77		0.77
0.00015625	0.00130720		0.00195002	
		0.77		0.75
0.000078125	0.00076604		0.00115614	
		0.76		0.70
0.0000390625	0.00045315		0.00071321	
		0.85		0.89
0.00001953125	0.00025183		0.00038543	

L^1–error and EOC rate for subsequent refinement levels of the grid.

Towards Multiple Space Dimensions

$$\begin{aligned} \rho_t &+ \operatorname{div}(\rho \mathbf{v}) &= 0 \\ (\rho\mathbf{v})_t &+ \operatorname{div}(\rho\mathbf{v}\mathbf{v}^T + p(\rho)\mathcal{I}) &= 0 \end{aligned} \quad \text{in } D_{\text{vap/liq}}(t)$$

$$\begin{aligned} [\![\rho(\mathbf{v}\cdot\mathbf{n} - s)]\!] &= 0 \\ [\![\rho(\mathbf{v}\cdot\mathbf{n} - s)\mathbf{v} + p\mathbf{n}]\!] &= (d-1)\sigma\kappa\mathbf{n} \quad \text{in } \Gamma(t) \end{aligned}$$

+ additional jump condition

Without curvature ($\kappa = 0$) : transfer ghostfluid idea to multiple space dimensions
solve 1D-Riemann problem over Γ-edges

With curvature : transfer ghostfluid idea to multiple space dimensions
determine curvature of approximate phase boundary
solve generalized 1D-Riemann problem over Γ-edges

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Joint Work with Chr. Chalons, P.G. Lefloch (for next period)

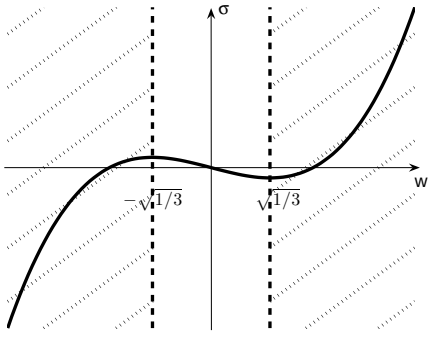
3) The Diffuse-Interface Model

The Non-Local Equations in 1D (Lagrangian coordinates)

$$
\begin{aligned}
w_t - v_x &= 0 \\
v_t - \sigma(w)_x &= \alpha\varepsilon v_{xx} - (K_\varepsilon * w - w)_x
\end{aligned}
$$

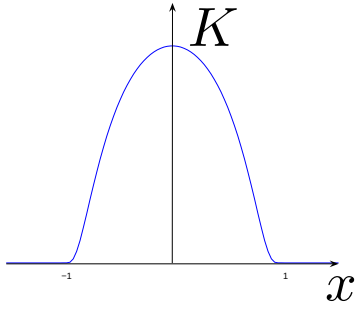
$w = w(x,t) > 0$: Strain

$v = v(x,t) \in \mathbb{R}$: Velocity

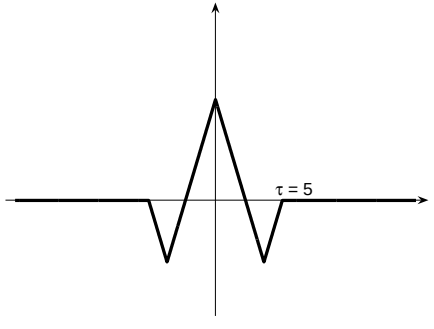


Stress-strain relation: $\sigma = \sigma(w)$

Choices for the kernel function K for $K_\varepsilon(x) = K(x/\varepsilon)/\varepsilon$:



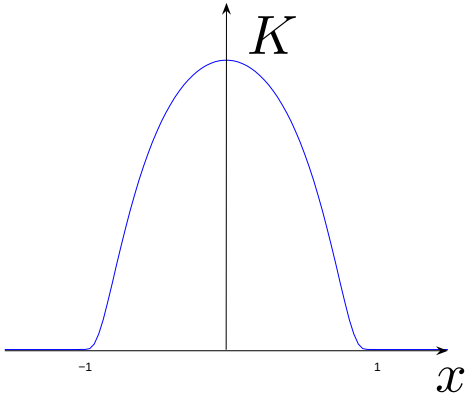
Purely repelling kernel

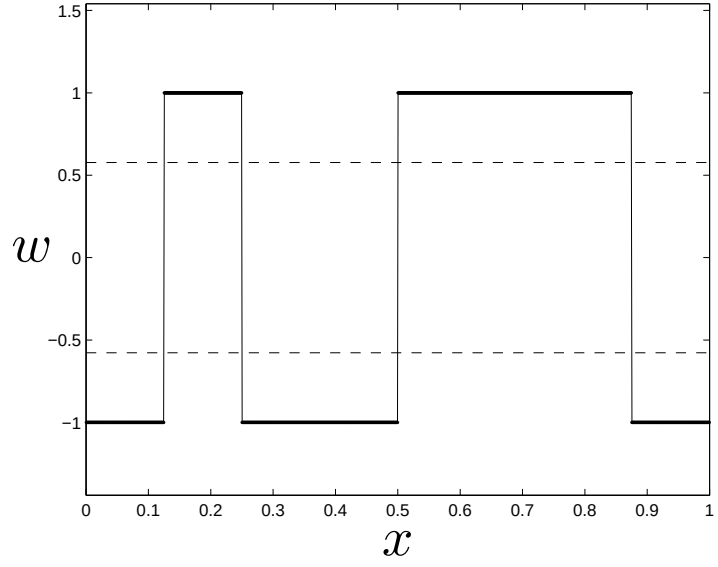


Attracting-repelling kernel

Numerical Experiments for the Elasticity System I: (Haink 05)

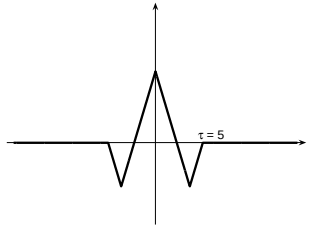
$$w_0(x) = \begin{cases} 1 : x \in \left[\frac{1}{8}, \frac{1}{4}\right] \cup \left[\frac{1}{2}, \frac{7}{8}\right], \\ -1 : \text{elsewhere} \end{cases} \quad v_0(x) \equiv 0.$$

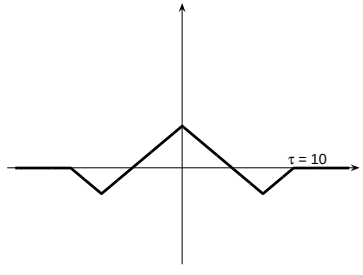


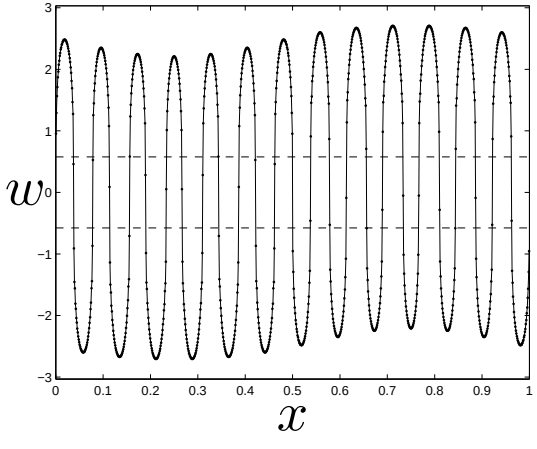


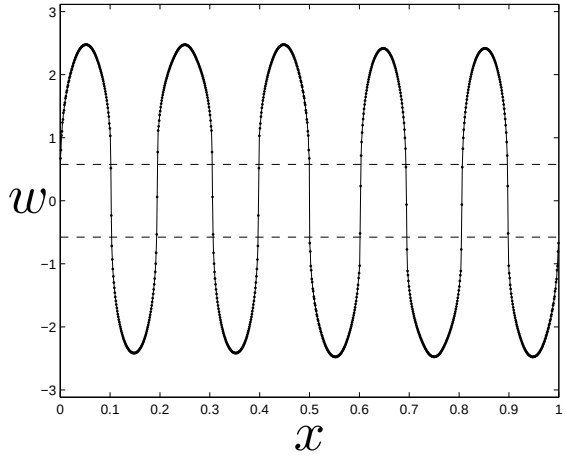
Numerical Experiments for the Elasticity System II: (Haink 05)

$$w_0(x) = \begin{cases} 1.2 : x \in \left[0, \frac{1}{2}\right] \\ -1.2 : \text{elsewhere} \end{cases}, \quad v_0(x) \equiv 0.$$









Theorem for Time-Asymptotic Behaviour

$$\begin{aligned} w_t - v_x &= 0 \\ v_t - \sigma(w)_x &= \alpha\varepsilon v_{xx} - (K_\varepsilon * w - w)_x \end{aligned} \qquad \text{in } I \times (0,\infty),\ I = (0,1)$$

$$w(.,0) = w_0,\ v(.,0) = v_0$$

$$u(0,t) = u(1,t) = 0, \quad u(x,t) := \int_0^x w(y,t)\,dy$$

Theorem: (Dressel&R.06)
Let $w_0, v_0 \in L^2(I)$ and σ be global Lipschitz.

(i) There is unique weak solution $(w,v) \in C([0,\infty), L^2(I))$ with

$$\|(w,v)\|_{L^2(I)} < C(\|(w_0,v_0)\|_{L^2(I)}), \quad v \in L^2((0,\infty); H^1(I)).$$

(ii) We have $v(.,t) \overset{*}{\rightharpoonup} 0, \quad w(.,t) \overset{*}{\rightharpoonup} \bar{w}$ for $t \to \infty$.
Thereby $\bar{w} : I \to \mathbb{R}$ is a weak solution of

$$\sigma(w) + K_\varepsilon * w - w = 0.$$

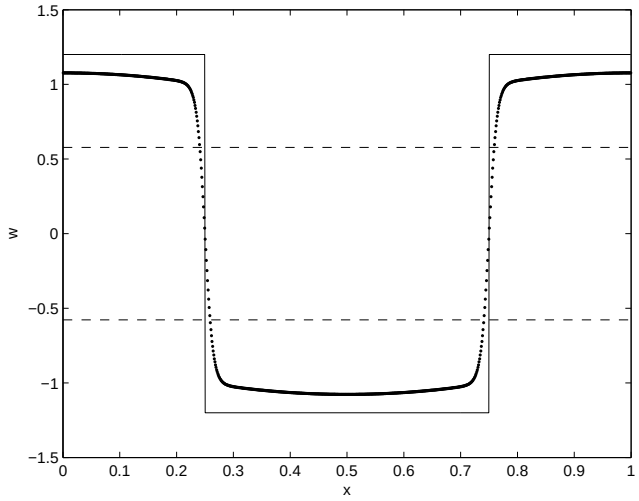
Notes on the theorem:

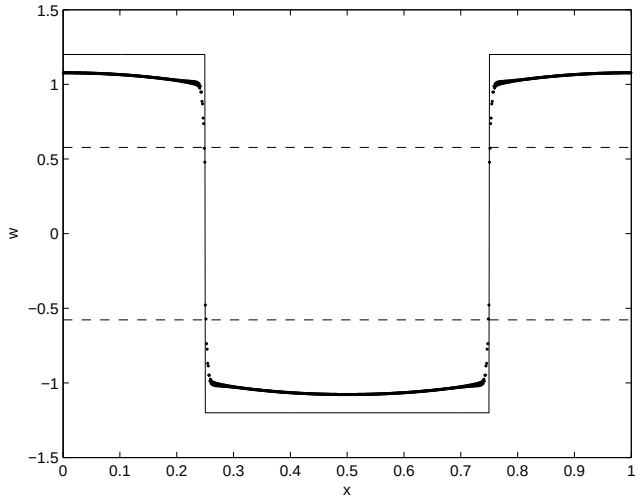
(i) Almost(!) same result as by Andrews&Ball ’83 for local model

(ii) Solutions of the stationary (integral) equation

$$\sigma(w) + K_\varepsilon * w - w = 0.$$

are not smooth in general.





Local versus global approach

Analytical Entropy/Energy Inequality:

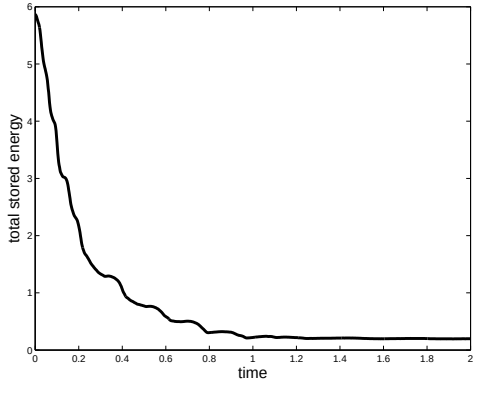
For $w, v : I \to \mathbb{R}$ define the energy

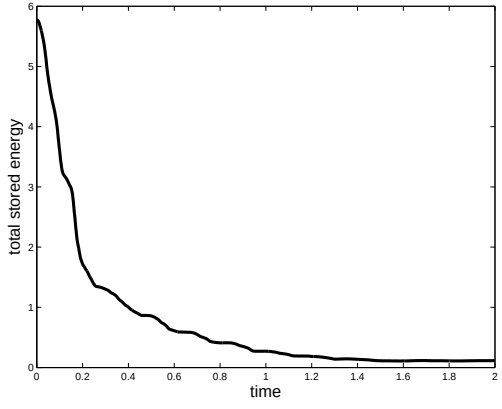
$$E[w,v] = \int_0^1 W(w(x)) + \frac{1}{2}v^2(x)\,dx + \int_0^1 \int_0^1 K_\varepsilon(x-y)(w(x)-w(y))^2\,dydx$$

A weak solution $(w,v) \in C([0,\infty), L^2(I))$ satisfies

$$E[w(.,t), v(.,t)] < E[w(.,s), v(.,s)] \quad (0 < s < t).$$

Discrete Entropy/Energy Decay for LDG-Scheme (Haink 06):





Energy versus time for two different kernels K_ε.

Towards Convergence for the LDG-scheme:

$$\begin{aligned} w_t - v_x &= 0 \\ v_t - \big(\sigma(w) - \alpha\varepsilon p + (K_\varepsilon * w - w)\big)_x &= 0 \quad \text{in } I \times (0,\infty) \\ p - v_x &= 0 \end{aligned}$$

Theorem: (Haink&R.07)
The approximate solution (w_h, v_h) of a semi-discrete LDG-scheme on a uniform mesh satisfies

$$\frac{d}{dt} E_h[w_h(.,t), v_h(.,t)] \leq 0.$$

Thereby we have

$$E_h[w,v] = \int_0^1 W(w(x)) + \frac{1}{2} v^2(x)\, dx + \int_0^1 \int_0^1 K_{\varepsilon,h}(x-y)(w(x)-w(y))^2\, .dydx$$