Journees d'Analyse Non Lineaire

de Besancon

November, 24-25, 2011

A Multiscale Approach to

Phase Transition Problems in Compressible Media

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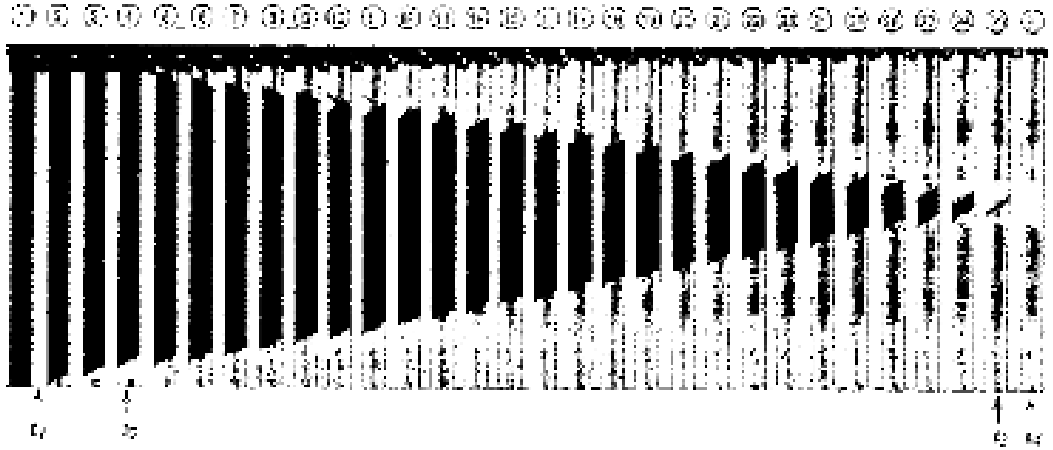
Plan of the Talk

1) Phase Boundaries in Compressible Media
2) Basic Multi-Scale Method
3) Sharp-Interface Models as Micro-Scale Model
4) Diffuse-Interface Model as Micro-Scale Model
5) Summary and Outlook

1) Phase Boundaries in Compressible Media

Uniaxial Motion in Shape Memory Alloys

Experiment with NiTi: (Shaw&Kyriakides '97)



Photographic sequence of stress induced transformation.

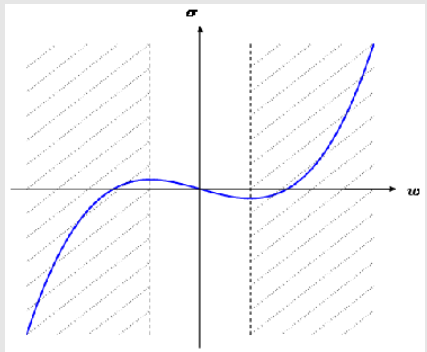
Mathematical Model:

$$\begin{aligned} w_t - v_x &= 0 \\ v_t - \sigma(w)_x &= 0 \end{aligned}$$

Unknowns:

$w = w(x,t) \in (-1,\alpha) \cap (\beta,\infty)$: strain

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



Stress function σ

A **subsonic phase boundary**, i.e., a shock wave with speed $s \in \mathbb{R}$ with end states $w_\pm$ from different phases, that satisfies

$$s^2 < \min\{\sigma'(w_-), \sigma'(w_+)\},$$

is **undercompressive (of degree 1)**.

Kinetic relation: (Abeyaratne&Knowles '91, Truskinovsky '93)

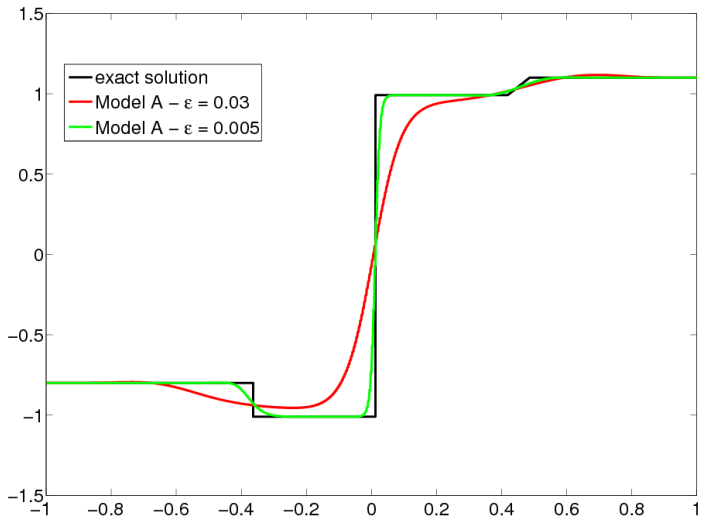
$$[\![\Sigma(w)]\!] - \frac{\sigma(w_-) + \sigma(w_+)}{2}[\![w]\!] = \Psi(s), \qquad \Sigma' = \sigma$$

Note:
The **driving force** Ψ has to be prescribed:

$$s\Psi(s) \geq 0 \Rightarrow \ 2^{\text{nd}} \text{ law of thermodynamics holds.}$$

Viscosity-Capillarity Approximation:
(Slemrod '83, Abeyaratne&Knowles '89,Truskinovsky '82)

$$\begin{aligned} w_t^\varepsilon - v_x^\varepsilon &= 0 \\ v_t^\varepsilon - \sigma(w^\varepsilon)_x &= \varepsilon v_{xx}^\varepsilon - \gamma\varepsilon^2 w_{xxx}^\varepsilon, \quad \gamma > 0 \end{aligned}$$



Numerical result for $\varepsilon = 0.03, 0.005$.

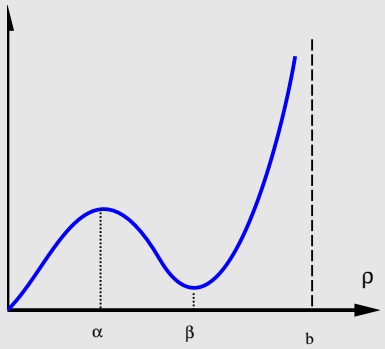
Isothermal Liquid-Vapour Flow

$$\begin{aligned} \rho_t + \operatorname{div}(\rho \mathbf{v}) &= 0 \\ (\rho \mathbf{v})_t + \operatorname{div}(\rho \mathbf{v} \otimes \mathbf{v} + p(\rho)\mathcal{I}) &= 0 \end{aligned}$$

Unknowns:

$\rho = \rho(\mathbf{x}, t) \in (0, \alpha) \cup (\beta, b)$: density

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



Van-der-Waals pressure

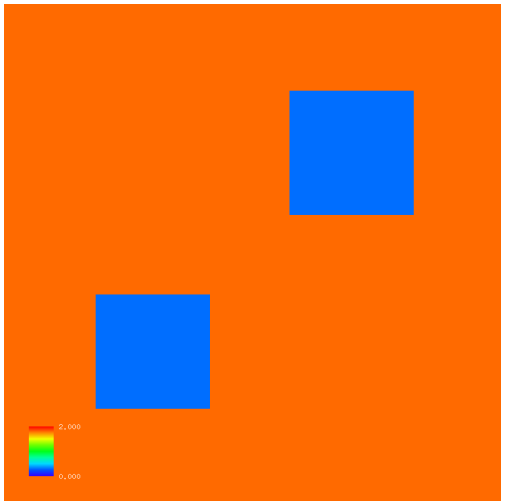
Trace conditions at phase boundary:

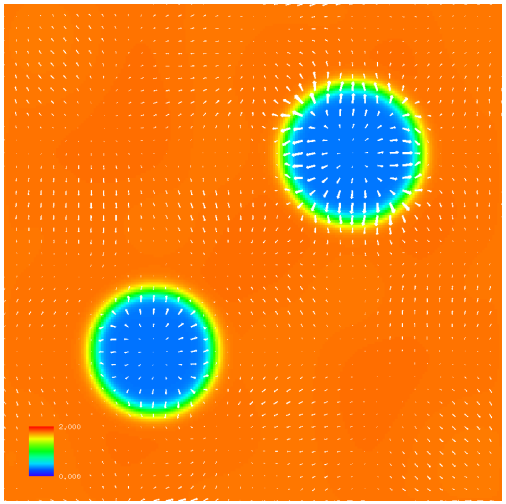
$$\begin{aligned} [\![\rho(\mathbf{v}\cdot\mathbf{n} - s)]\!] &= 0, \\ [\![\rho(\mathbf{v}\cdot\mathbf{n} - s)\mathbf{v} + p\mathbf{n}]\!] &= (d-1)\sigma\kappa\mathbf{n}, \quad \text{surface tension } \sigma > 0 \\ \left[\!\!\left[W'(\rho) + \frac{1}{2}(\mathbf{v}\cdot\mathbf{n} - s)^2 \right]\!\!\right] &= \Psi(j),\ j := \rho_\pm(\mathbf{v}_\pm\cdot\mathbf{n} - s),\ p' = \rho W''. \end{aligned}$$

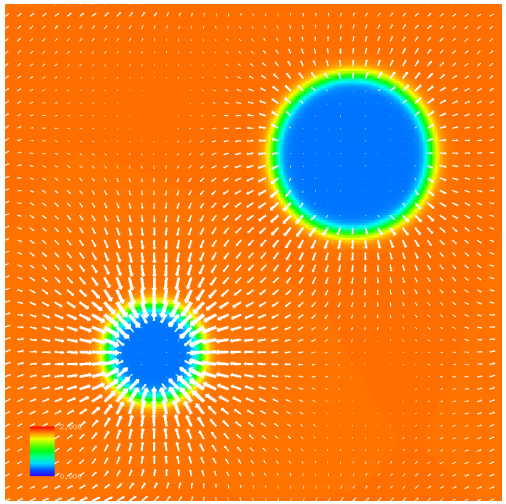
Local Navier-Stokes-Korteweg Model:
(Dunn&Serrin '85, Anderson&McFadden&Wheeler '98)

$$\begin{aligned} \rho^\varepsilon_t + \quad & \operatorname{div}(\rho^\varepsilon \mathbf{v}^\varepsilon) = 0 \\ (\rho^\varepsilon \mathbf{v}^\varepsilon)_t + \operatorname{div}(\rho^\varepsilon \mathbf{v}^\varepsilon \otimes \mathbf{v}^\varepsilon + p(\rho^\varepsilon)\mathcal{I}) &= \varepsilon \operatorname{div}(\mathbf{T}^\varepsilon) + \gamma \varepsilon^2 \rho^\varepsilon \nabla \Delta \rho^\varepsilon \end{aligned}$$

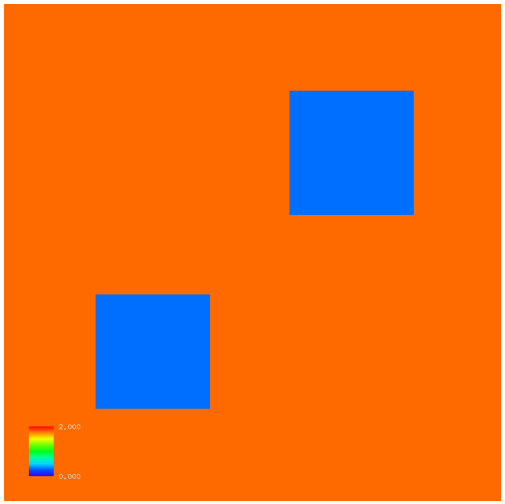
Two Bubbles:

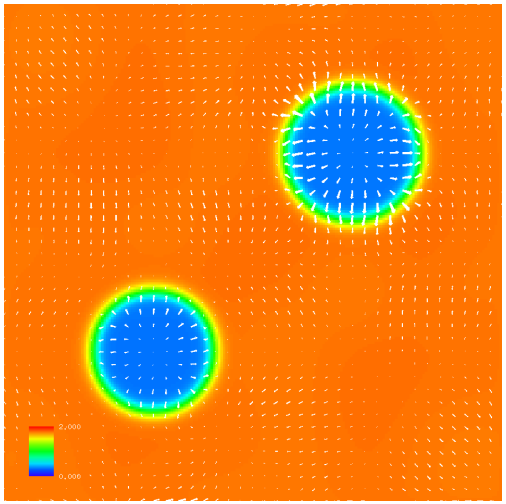


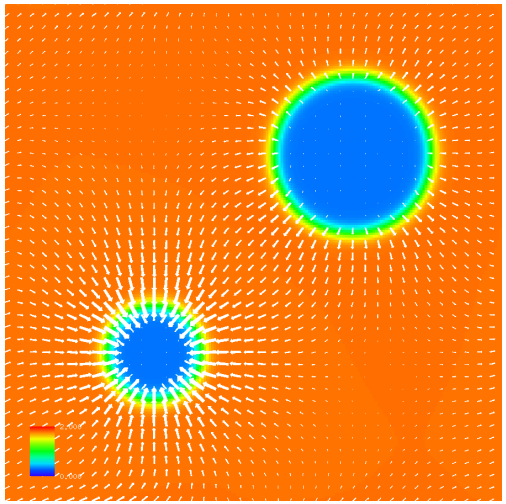


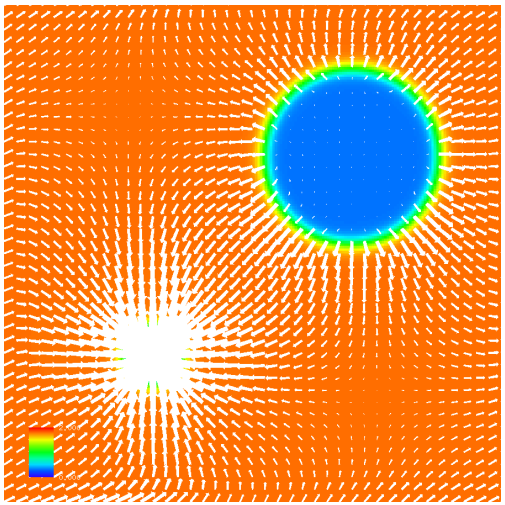


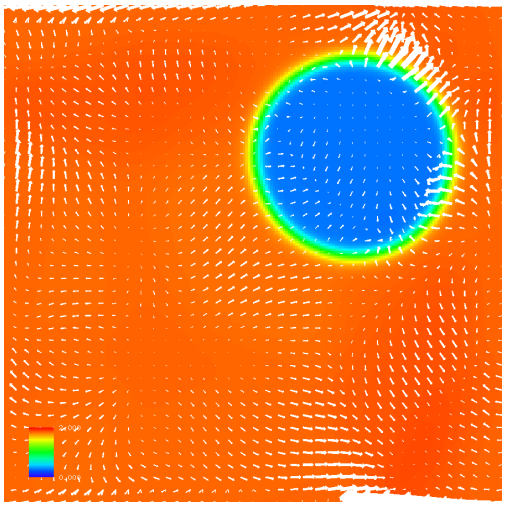
Two Bubbles:

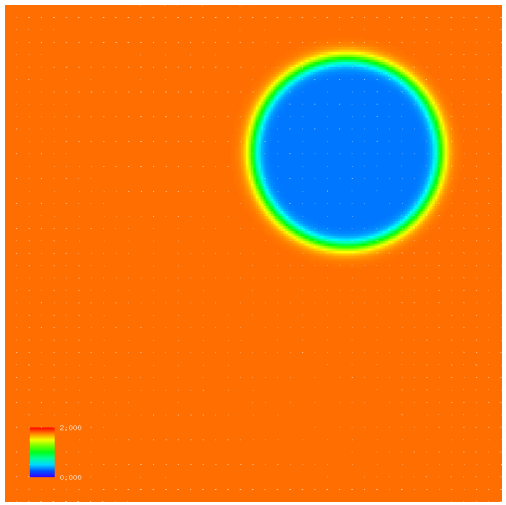












Scaling Obstacle

Scaled Local NSK Model: $(\varepsilon > 0)$

$$\begin{aligned} \rho^\varepsilon_t + \quad & \operatorname{div}(\rho^\varepsilon \mathbf{v}^\varepsilon) = 0 \\ (\rho^\varepsilon \mathbf{v}^\varepsilon)_t + \operatorname{div}(\rho^\varepsilon \mathbf{v}^\varepsilon \otimes \mathbf{v}^\varepsilon + p(\rho^\varepsilon)\mathcal{I}) &= \varepsilon \operatorname{div}(\mathbf{T}^\varepsilon) + \gamma \varepsilon^2 \nabla \Delta \rho^\varepsilon \end{aligned}$$

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The Scaling Obstacle:

The parameter ε controls interfacial width **and** surface tension

Static solution: $\quad [\![p(\rho)]\!] = \sigma(\varepsilon)\kappa, \quad \sigma = \mathcal{O}(\varepsilon).$

This means $\varepsilon < 10^{-16}$ for water system...

2) Basic Multi-Scale Method and Macro-Scale Solver

The Heterogeneous Multi-Scale Method in 1D:
(E&Engquist '03, Kissling&R. '10)

System of conservation laws as macro-scale model:

$$u_t + f(u)_x = 0$$

Micro-scale model:

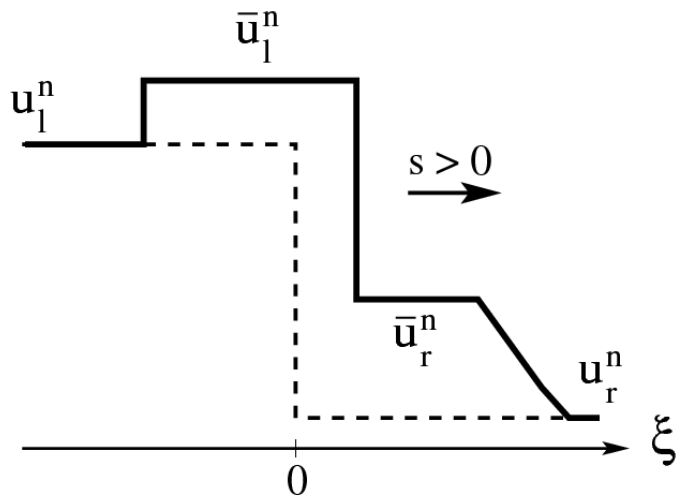
(SI) Exact Riemann solver for given kinetic relation

(DI) Approximation of form $u_t^\varepsilon + f(u^\varepsilon)_x = R[u;\varepsilon]$ for some $\varepsilon > 0$.

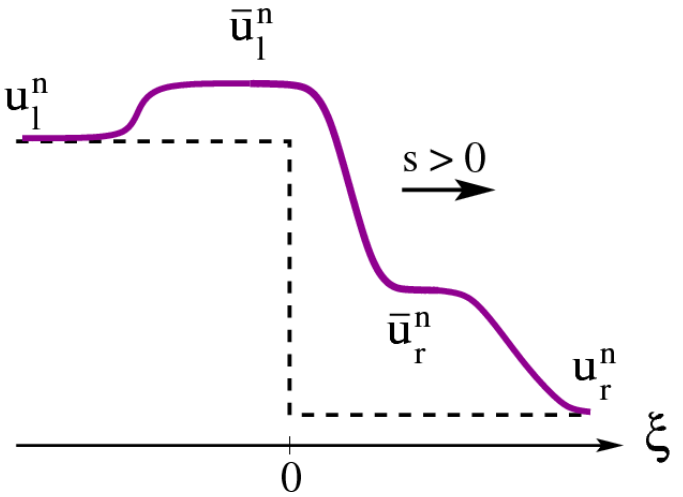
Prototype HMM macro time-step $T^n \to T^{n+1}$**:**

Given: $\{u_j^n\}_{j\in\mathbb{Z}}$ macro-scale approximation on macro-grid with grid size $\Delta X > 0$ and front location X_Γ^n

Step 1: Solve the micro-scale model for Riemann-initial data at X_Γ^n.



SI-micro-scale model



DI-micro-scale model **on micro-scale domain** with micro-grid size $\delta x > 0$

Prototype HMM macro time-step $T^n \to T^{n+1}$:

Given: $\{u_j^n\}_{j\in\mathbb{Z}}$ macro-scale approximation on macro-grid with grid size $\Delta X > 0$ and front location X_Γ^n

Step 2: Extract adjecent states of phase boundary $\bar{u}_{l/r}^n$ and phase boundary speed s

Step 3: Solve the macro-scale model in the two macro-scale bulk domains using extracted states at phase boundary with any (finite-volume) scheme in cells away from X_Γ^n

$$\rightsquigarrow \{u_j^{n+1}\}_{j\in\mathbb{Z}} \text{ and } X_\Gamma^{n+1}$$

3) SI-Micro-Scale Models: Riemann Solvers

(Joint work with Ch. Chalons, F. Coquel, P. Engel)

Uniaxial Motion in Shape Memory Alloys

Macro-Scale Model:

$$\begin{aligned} w_t - v_x &= 0 \\ v_t - \sigma(w)_x &= 0 \end{aligned}$$

Micro-Scale Model:

Exact Riemann solver using given kinetic relation in the (equivalent) form

$$w_\pm = \varphi(w_\mp).$$

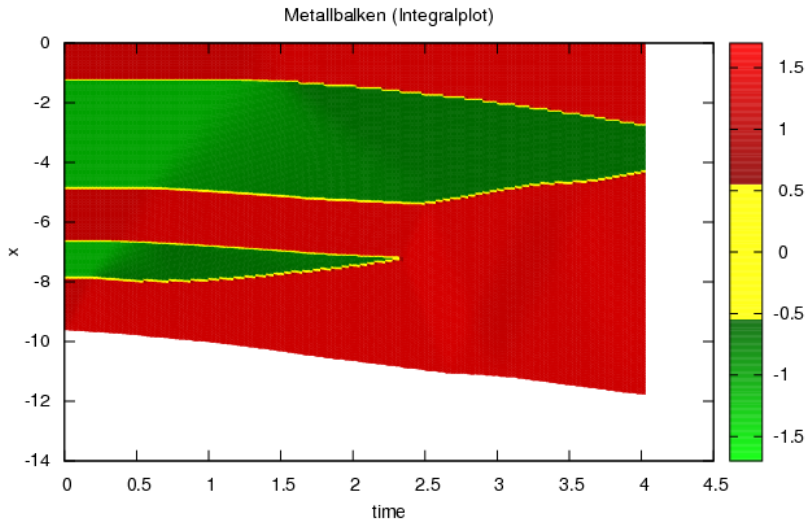
Exact Riemann solvers: Abeyaratne&Knowles '91, Shearer&Yang '95, Hattori '98, Colombo&Corli '99, **Lefloch&Thanh '02**, Mercier&Piccoli '02,...

Numerical experiment: (pull-motion)

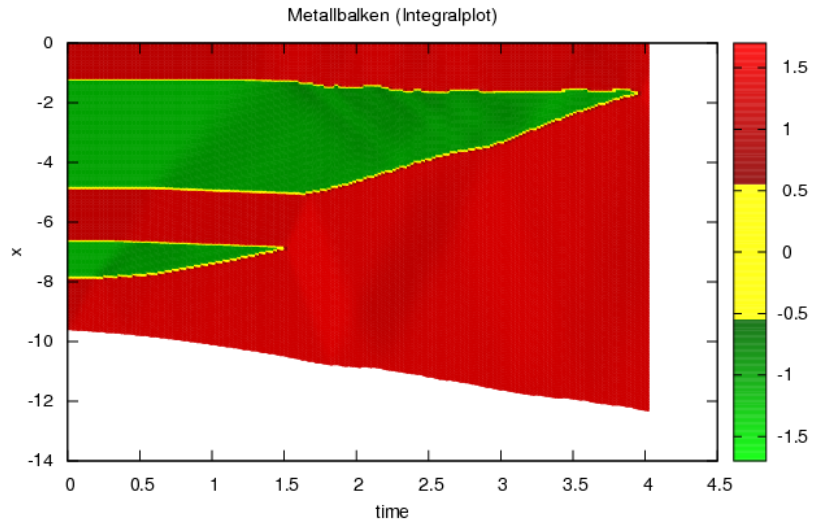
Initial and boundary data:

$$w(x,0)=\begin{cases} -1 : x \in (-0.8, 0.1) \cup (0.4, 0.7) \\ \quad 1 : \text{elsewhere in } (-1,1) \end{cases} \qquad \begin{aligned} v(-1) &= 0, \\ \sigma(w(1)) &= 0.5 \end{aligned}$$

$$v(.,0) \equiv 0 \text{ in } (-1,1)$$



Kinetic relation: $\varphi(w) = -0.5w$.



Kinetic relation: $\varphi(w) = -0.75w$.

Isothermal Liquid-Vapour Flow

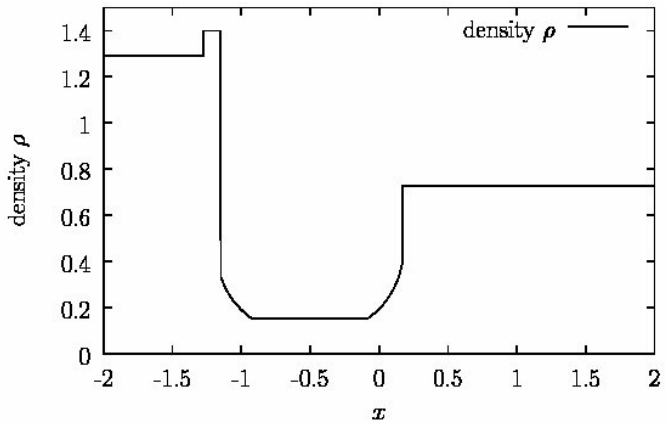
Mathematical model:

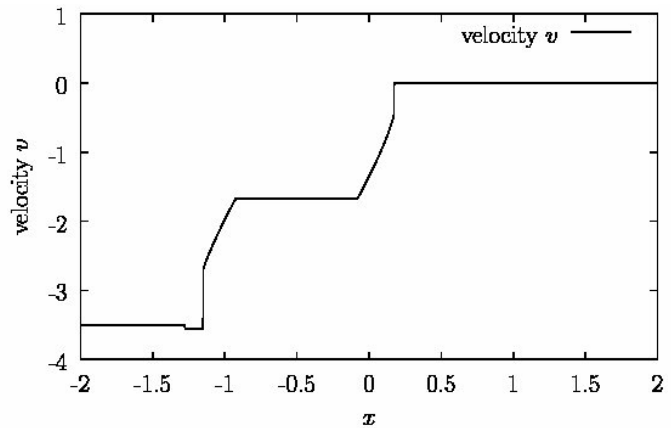
$$\begin{aligned} \rho_t + (\rho v)_x &= 0 \\ (\rho v)_t + (\rho v^2 + p(\rho))_x &= 0 \end{aligned}$$

Kinetic relation can be equivalenty rewritten in form

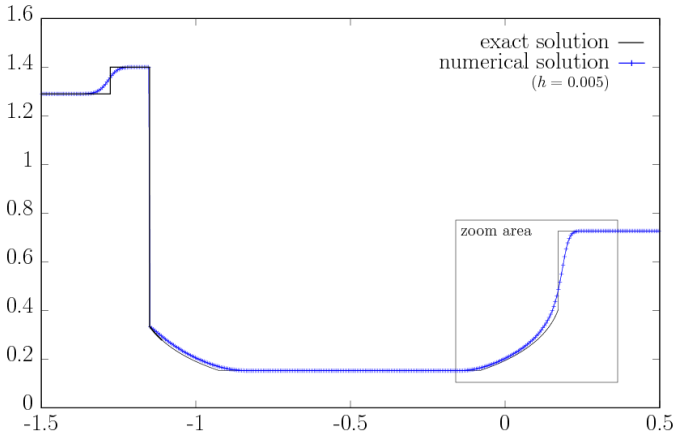
$$\rho_\pm = \varphi(\rho_\mp) \rightsquigarrow \text{artificial choice}$$

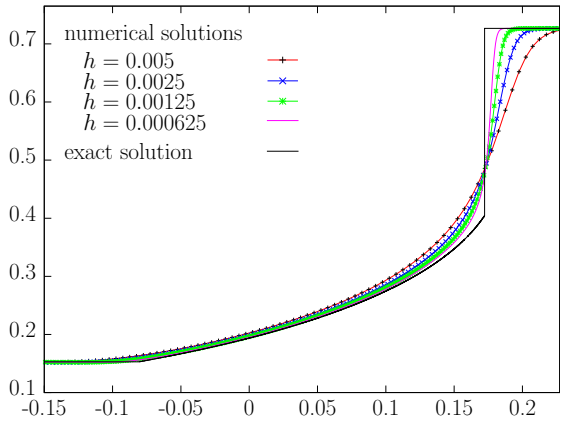
An exact Riemann solution: (Merkle&R. '08)





Numerical experiment for Riemann problem:





Density (left) and detailed view.

grid size	L^1–error	EOC
0.04	0.08953370	
		0.48
0.01	0.03562381	
		0.77
0.0025	0.01247926	
		0.83
0.000625	0.00406572	
		0.77
0.00015625	0.00130720	
		0.76
0.0000390625	0.00045315	

Limitations of the exact Riemann solver

1. **Exact Riemann solvers are computationally expensive.**
   - More than 80 percent of computing time used for Riemann solutions

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2. **Useful exact Riemann solvers are rarely available.**
   - Slight change of flux has impact on Riemann structure
   - Each change of kinetic relation has impact on Riemann problem

Limitations of the exact Riemann solver

1. **Exact Riemann solvers are computationally expensive.**
   - More than 80 percent of computing time used for Riemann solutions
2. **Useful exact Riemann solvers are rarely available.**
   - Slight change of flux has impact on Riemann structure
   - Each change of kinetic relation has impact on Riemann problem
3. *Theory of (analytic) kinetic relations seems to be limited.*
   - *correct interface speed requires Atomistic2Continuum bridging*

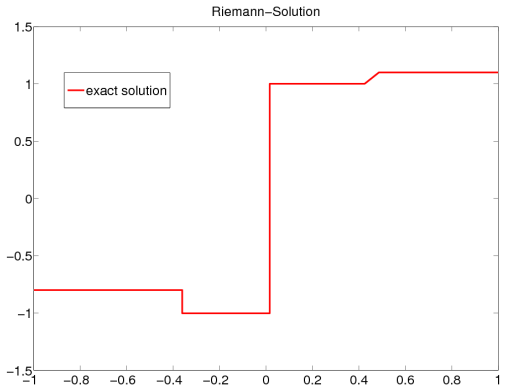
A Relaxation Solver

The original system:

$$\begin{aligned} w_t - v_x &= 0 \\ v_t - \sigma(w)_x &= 0 \end{aligned}$$

Trace conditions at phase boundary

$$\begin{aligned} -s[\![w]\!] &= [\![v]\!] \\ -s[\![v]\!] &= [\![\sigma(w)]\!] \\ w_- &= \varphi(w_+) \end{aligned}$$



Exact solution.

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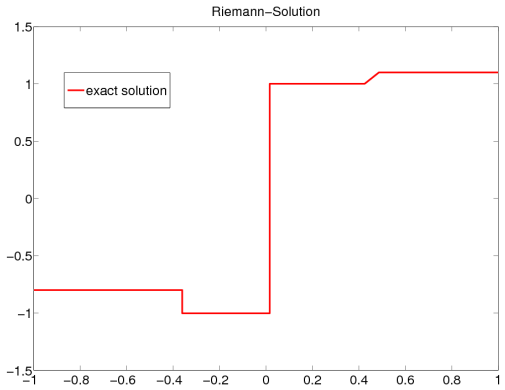


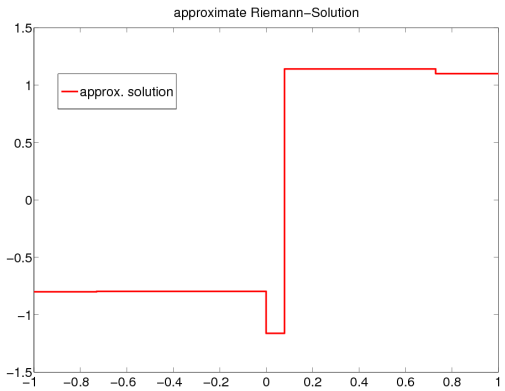
Exact solution.

Relaxation approximation:

$$\begin{aligned} w_t - v_x &= 0 \\ v_t - \Pi_x &= 0 \\ \Pi_t - a^2 v_x &= \frac{\sigma(w)-\Pi}{\delta} \end{aligned}$$

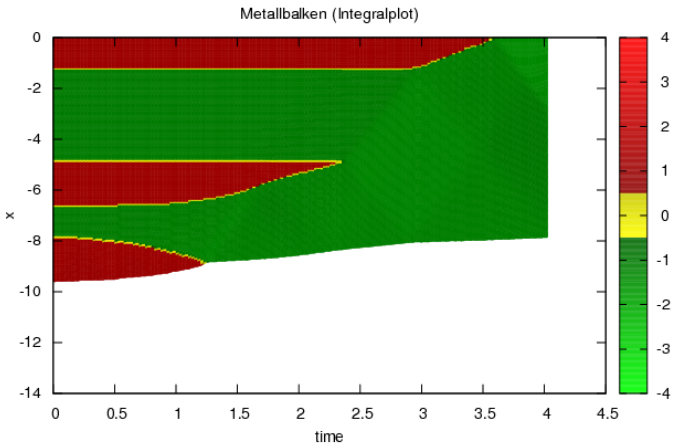
Trace conditions at phase boundary

$$\begin{aligned} -s[\![w]\!] &= [\![v]\!] \\ -s[\![v]\!] &= [\![\Pi]\!] \\ -s[\![\Pi]\!] &= [\![a^2 v]\!] \\ w_- &= \varphi(w_+) \end{aligned}$$

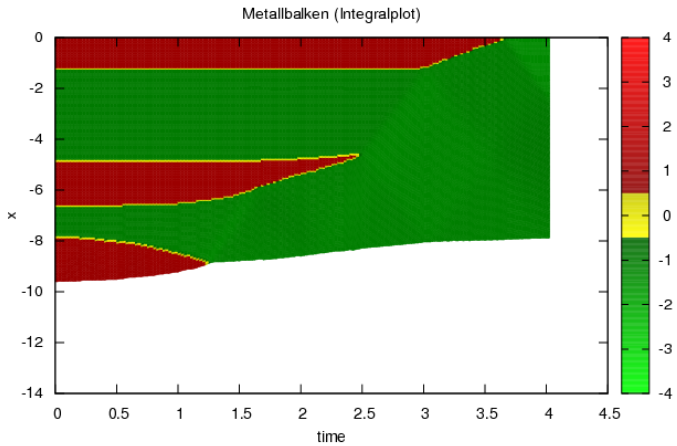


Approximate solution.

Unaxial Motion in Shape Memory Alloys

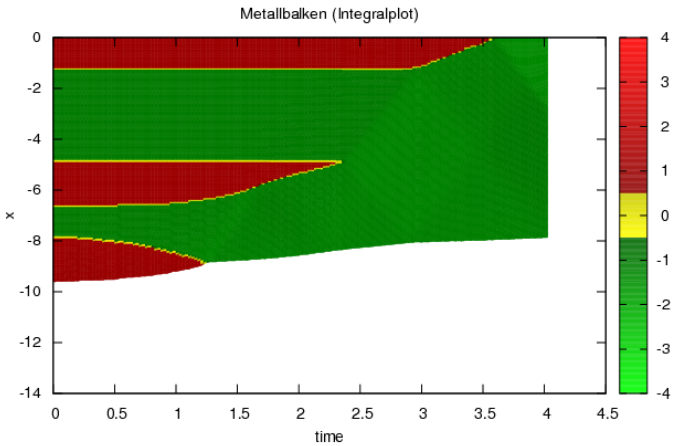


Exact Riemann solver.



Relaxation solver.

Unaxial Motion in Shape Memory Alloys



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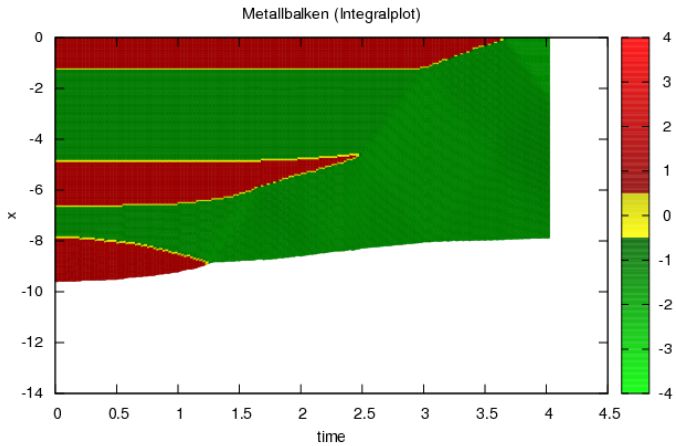
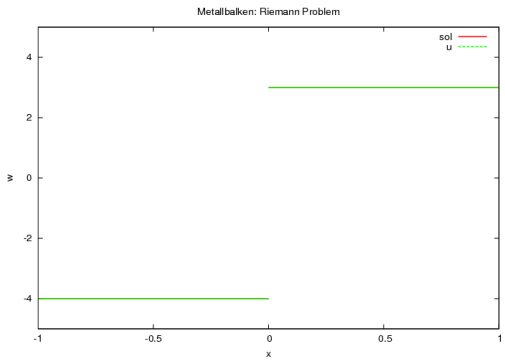
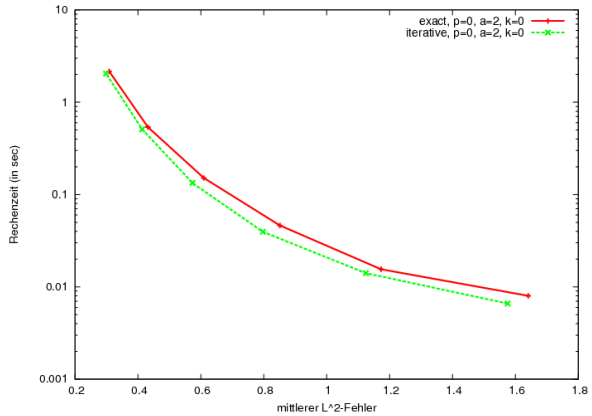


Relaxation solver.

Numerical Experiment: (Convergence and Efficiency)



Initial stress.

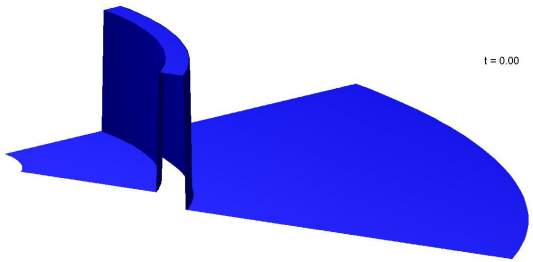


Error versus runtime.

Isothermal Liquid-Vapour Flow with Surface Tension

Mathematical Model:
(in spherical coordinates)

$$\begin{aligned} \rho_t + (\rho v)_r &= -2\frac{\rho v}{r} \\ (\rho v)_t + (\rho v^2 + p(\rho))_r &= -2\frac{\rho v^2}{r} \end{aligned}$$



Initial density,
volume-weighted total mass
in vapour phase

Traces at interface:

$$\begin{aligned} [\![\rho(v-s)]\!] &= 0, \\ [\![\rho(v-s)v + p]\!] &= 2\sigma\tfrac{1}{r}, \\ \rho_\pm &= \varphi(\rho_\mp) \end{aligned}$$

Exact Riemann solver: ??

3) DI-Micro-Scale Models:

(Joint work with A.Corli, P. Engel, A. Viorel)

Uniaxal Motion in Shape Memory Alloys

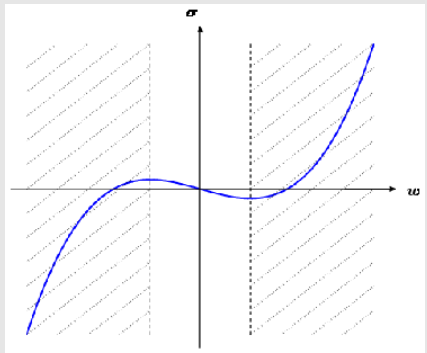
Macro-Scale Mathematical Model:

$$\begin{aligned} w_t - v_x &= 0 \\ v_t - \sigma(w)_x &= 0 \end{aligned} \qquad (P_0)$$

Unknowns:

$w = w(x,t) \in (-1,\alpha) \cup (\beta,\infty)$: strain

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



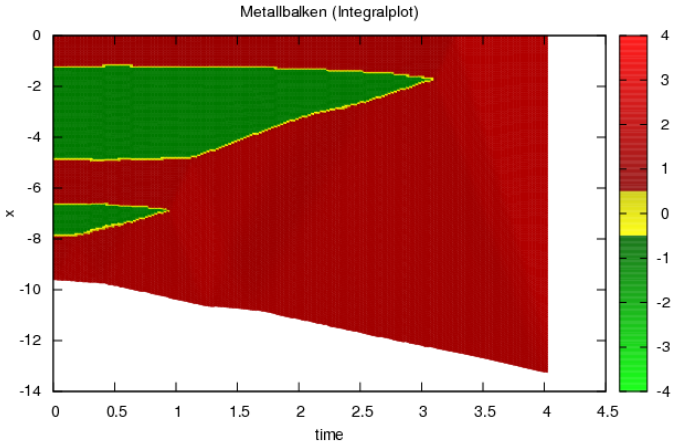
Stress function σ

Micro-Scale Mathematical Model:

$$\begin{aligned} w^\varepsilon_t - v^\varepsilon_x &= 0 \\ v^\varepsilon_t - \sigma(w^\varepsilon)_x &= \varepsilon v^\varepsilon_{xx} - \gamma\varepsilon^2 w^\varepsilon_{xxx} \end{aligned} \qquad (P_\varepsilon)$$

Performance for DI-Micro-Scale Model

Test: Pull Motion in Shape Memory Alloys



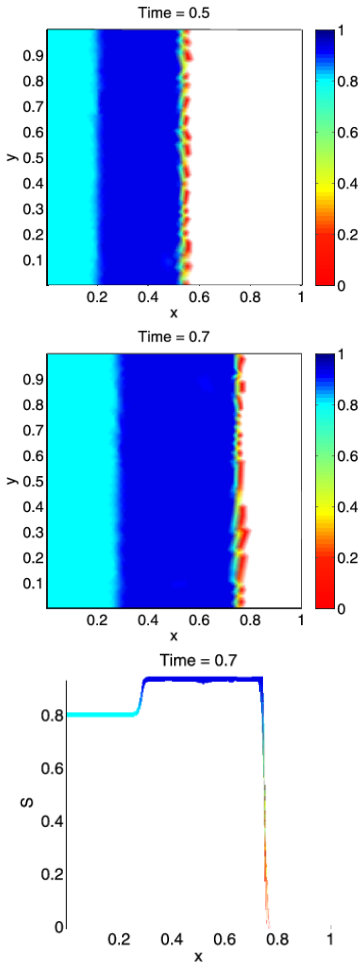
Parameters:
$\varepsilon = 10^{-5},\ \gamma = 1,$
$\delta t = \Delta t/10$

T	HMM		micro-scale model	
	N_T	cpu-time	n_t	cpu-time
$1,98 \cdot 10^{-4}$	1	57 s	4 594	$3,3 \cdot 10^5$ sec. $\approx$ 4 days
0,1	505	7 h	2 321 053	$1,7 \cdot 10^8$ sec. $\approx$ 5 years
0,5	2 526	34 h	11 605 263	$8,4 \cdot 10^8$ sec. $\approx$ 25 years

Limitation of DI-Micro-Scale Models

Test: Two-Phase Flow with Overshoot-Front:

		CPU-time
$2D$	Standard Finite-Volume Scheme	$38s$
	HMM with SI-micro solver	$66s$
	HMM with DI-micro solver	$24.7h$
	DI-micro solver over one edge	$2.6s$



Need for fast micro-scale solvers!

A Lower-Order Approximation

Micro-Scale Viscosity-Capillarity System:

$$\begin{aligned} w_t^\varepsilon - v_x^\varepsilon &= 0 \\ v_t^\varepsilon - \sigma(w^\varepsilon)_x &= \varepsilon v_{xx}^\varepsilon - \gamma\varepsilon^2 w_{xxx}^\varepsilon \end{aligned} \qquad (P_\varepsilon)$$

Lower-Order Approximation for (P_ε):

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Lower-Order Approximation for (P_ε):

$$\begin{aligned} w_t^{\varepsilon,\alpha} - v_x^{\varepsilon,\alpha} &= 0 \\ v_t^{\varepsilon,\alpha} - \sigma(w^{\varepsilon,\alpha})_x &= \varepsilon v_{xx}^{\varepsilon,\alpha} - \gamma\alpha(\lambda^{\varepsilon,\alpha} - w^{\varepsilon,\alpha})_x \quad (P_{\varepsilon,\alpha}) \\ -\varepsilon^2\lambda_{xx}^{\varepsilon,\alpha} &= \alpha(w^{\varepsilon,\alpha} - \lambda^{\varepsilon,\alpha}) \end{aligned}$$

Recover (P_ε) in the limit $\alpha \to \infty$.

Theorem: (Corli&R.&Viorel '10)
For $\varepsilon > 0$ let $\{(w^{\varepsilon,\alpha}, v^{\varepsilon,\alpha}, \lambda^{\varepsilon,\alpha})\}_{\alpha>0}$ be a family of solutions for $(P_{\varepsilon,\alpha})$. It satisfies

$$\frac{d}{dt}\int_{\mathbb{R}}\left(\Sigma(w^{\varepsilon,\alpha}) + \frac{\alpha}{2}(w^{\varepsilon,\alpha} - \lambda^{\varepsilon,\alpha})^2 + \gamma\varepsilon^2\frac{(\lambda_x^{\varepsilon,\alpha})^2}{2} + \frac{(v^{\varepsilon,\alpha})^2}{2}\right)\,dx \leq 0.$$

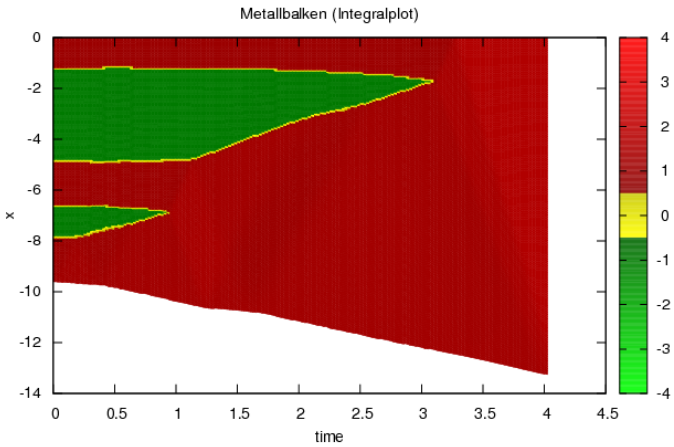
If σ is globally Lipschitz there are functions $w^{\varepsilon}, v^{\varepsilon} \in L^2_{loc}(\mathbb{R}\times(0,\infty))$ such that for a subsequence

$$w^{\varepsilon,\alpha}\to w^{\varepsilon},\ v^{\varepsilon,\alpha}\to v^{\varepsilon},\ \lambda^{\varepsilon,\alpha}\to w^{\varepsilon} \text{ in } L^p_{loc}(\mathbb{R}\times(0,\infty)), p\in[1,2)\ .$$

holds. The function $(w^{\varepsilon}, v^{\varepsilon})$ is a weak solution of (P_{ε}).

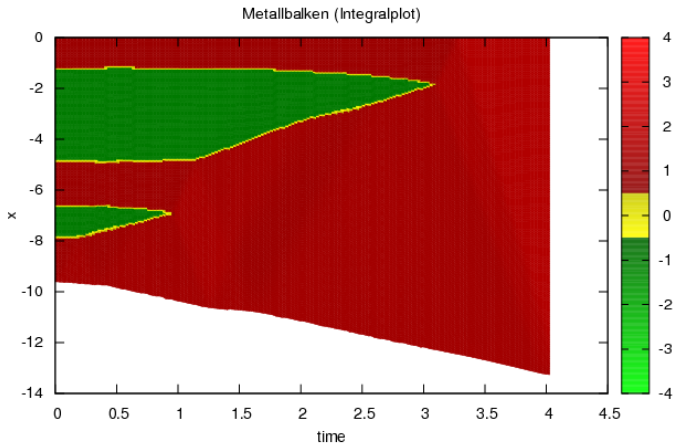
Note: For the static case refer to Brandon&Li&Rogers '95, Solci '03.

Back to Pull-Motion:



Viscosity-capillarity system

$\alpha = \infty$, $\varepsilon = 5 \cdot 10^{-4}$.

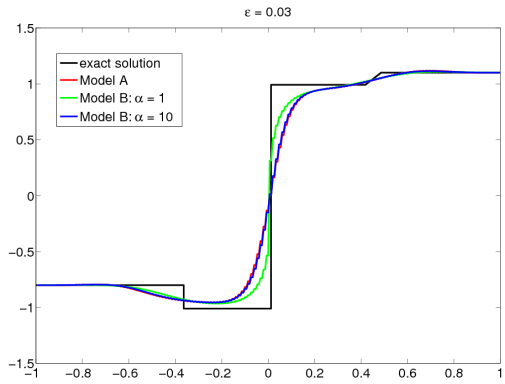


Lower-order approximation

$\alpha = 1$, $\varepsilon = 5 \cdot 10^{-4}$

Computing time:

α	∞	1	10	10^2	10^3
time	10.4	2.9	3.5	4.9	14.0



Numerical advantages of lower-order approximation:

$$
\begin{aligned}
w_t^{\varepsilon,\alpha} - v_x^{\varepsilon,\alpha} &= 0 \\
v_t^{\varepsilon,\alpha} - \underbrace{\left(\sigma(w^{\varepsilon,\alpha}) + \alpha\gamma w^{\varepsilon,\alpha}\right)_x}_{=:\tilde{\sigma}(w^{\varepsilon,\alpha})_x} &= \varepsilon v_{xx}^{\varepsilon,\alpha} - \gamma\alpha c_x^{\varepsilon,\alpha} \qquad (P_{\varepsilon,\alpha}) \\
-\varepsilon^2 c_{xx}^{\varepsilon,\alpha} &= \alpha\left(w^{\varepsilon,\alpha} - c^{\varepsilon,\alpha}\right)
\end{aligned}
$$

1) Eigenvalues (of first-order operator):

$$\lambda_{\mp}(w, v) = \mp\sqrt{\tilde{\sigma}'(w)} \text{ real for } \alpha >> 1.$$

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1) Eigenvalues (of first-order operator):

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2) Time-step control: An explicit scheme for $(P_{\varepsilon,\alpha})$ requires

$$\delta t \approx C\delta x^2,$$

but **not as for the third-order problem** (P_ε) like

$$\delta t \approx C\delta x^3.$$

5) Summary and Outlook:

- Two-scale approach seems to be mandatory for computation of dynamics phase boundaries.
- Increase of efficiency for micro-model solver is the key issue.
- Modelling **and** numerical ideas are needed for increasing efficiency.
- Modelling perspectives: A2C-bridging, Dafermos regularization,...
- Numerical perspectives: *hp*-adaptivity, local time stepping, kernel-based learning and and reduced-basis methods,...
- (Almost) no convergence analysis due to lack of theory.

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