Journée

Mathematical Modelling and Numerical Simulation

October 9, 2012

Multiscale Modelling for Interfaces in Fluids

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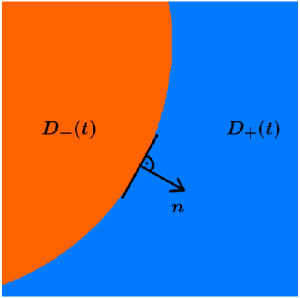
Sharp Interface Model



Sharp Interface $\Gamma(t)$
separating the domain
$D = D_-(t) \cup \Gamma(t) \cup D_+(t)$.

Find $U : D \times [0, T] \to \mathbb{R}^m$ and $\Gamma = \Gamma(t)$ with

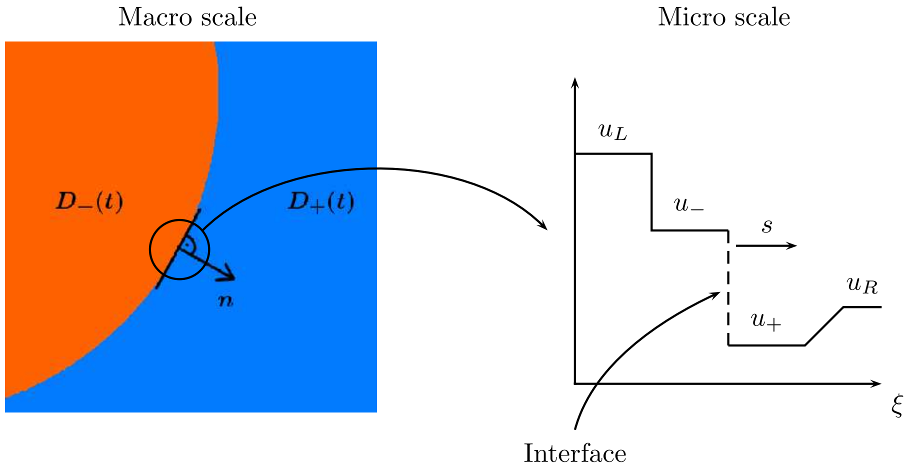
$$U(\mathbf{x}, t) = \begin{cases} U_-(\mathbf{x}, t) : \mathbf{x} \in D_-(t) \\ U_+(\mathbf{x}, t) : \mathbf{x} \in D_+(t) \end{cases}$$

and

$$\begin{aligned} U_{\pm,t} + \sum_{i=1}^{d} f_i(U_\pm)_{x_i} &= 0 \quad \text{in } D_\pm(t) \\ \mathcal{K}[U_-, U_+] &= 0 \quad \text{at } \Gamma(t) \end{aligned}$$

$$+IC/BC$$

Multiscale Approach I



Multiscale Approach I

Macroscale Model

Find $U : D \times [0,T] \to \mathbb{R}^m$ and $\Gamma = \Gamma(t)$ with

$$U(\mathbf{x},t) = \begin{cases} U_-(\mathbf{x},t) : \mathbf{x} \in D_-(t) \\ U_+(\mathbf{x},t) : \mathbf{x} \in D_+(t) \end{cases}$$

and

$$U_{\pm,t} + \sum_{i=1}^{d} f_i(U_\pm)_{x_i} \quad = \quad 0.$$

Microscale Model

For each $t \in [0,T]$ and $\mathbf{x} \in \Gamma(t)$ find $u : \mathbb{R} \times [0,\infty) \to \mathbb{R}^m$ with

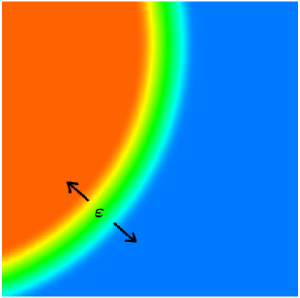
$$u_t + \left(\sum_{i=1}^{d} f_i(u) n_i(\mathbf{x}) \right)_\xi = 0$$

$$u(\xi,0) = \begin{cases} U_L & : \quad \xi < 0, \\ U_R & : \quad \xi > 0, \end{cases}$$

such that the solution contains a shock wave connecting states $u_- \xrightarrow{s} u_+$ with

$$\mathcal{K}[u_-,u_+] = 0, \; \dot{\Gamma}(t) = s.$$

Diffuse Interface Model



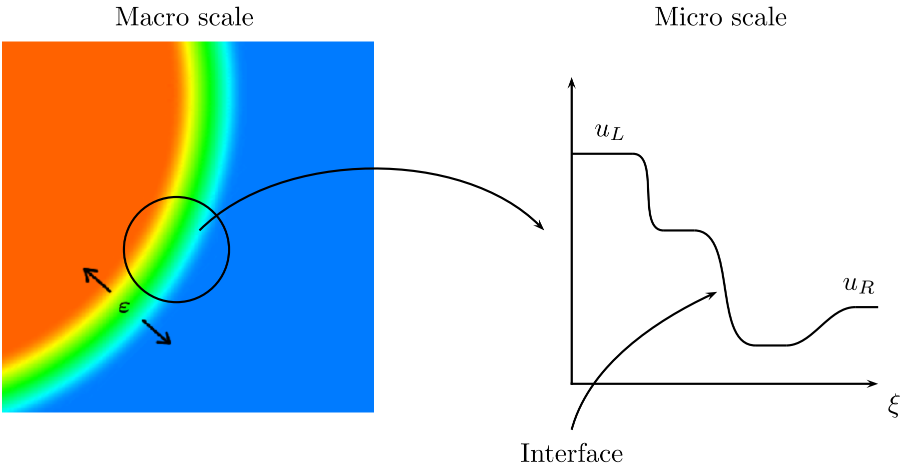
Diffuse interface in D.

Find $U^\epsilon : D \times [0, T] \to \mathbb{R}^m$ with

$$U_t^\epsilon + \sum_{i=1}^{d} f_i(U^\epsilon)_{x_i} = R^\epsilon[U^\epsilon] \quad \text{in } D \times (0, T)$$
$$+IC/BC$$

e.g. $R^\epsilon[U] = \epsilon \Delta U$.

Multiscale Approach II



Multiscale Approach II

Macroscale Model

Find $U : D \times [0, T] \to \mathbb{R}^m$ and $\Gamma = \Gamma(t)$ with

$$U(\mathbf{x}, t) = \begin{cases} U_-(\mathbf{x}, t) : \mathbf{x} \in D_-(t) \\ U_+(\mathbf{x}, t) : \mathbf{x} \in D_+(t) \end{cases}$$

and

$$U_{\pm,t} + \sum_{i=1}^{d} f_i(U_\pm)_{x_i} \quad = \quad 0.$$

Microscale Model

For some $\varepsilon > 0$ and each $t \in [0, T]$ and $\mathbf{x} \in \Gamma(t)$ find $u^\varepsilon : \mathbb{R} \times [0, \infty) \to \mathbb{R}^m$ with

$$u^\varepsilon_t + \left(\sum_{i=1}^{d} f_i(u^\varepsilon) n_i(\mathbf{x}) \right)_\xi = R^\varepsilon[u^\varepsilon]$$

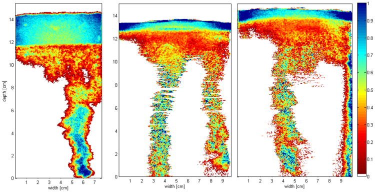
$$u^\varepsilon(\xi, 0) = \begin{cases} U_L & : \quad \xi < 0, \\ U_R & : \quad \xi > 0. \end{cases}$$

Plan of the Talk

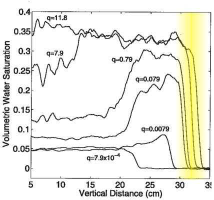
1) Interfaces in Porous Media
2) Interfaces in Compressible Liquid-Vapour Flow
3) Summary and Outlook

1) Interfaces in Porous Media

Overshoot Waves in Porous Media



Viscous fingering (Neuweiler&Schütz '10)



Saturation front with overshoot (DiCarlo '04)

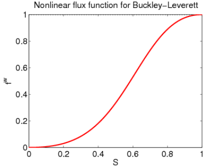
Interfaces in Porous Media

Macroscale Mathematical Model:

$$\left.\begin{array}{c} S_t + \operatorname{div}\left(\mathbf{V} f(S)\right) = 0 \\ \operatorname{div}\mathbf{V} = 0,\ \ \mathbf{V} = \mathbf{K}\lambda\nabla P \end{array}\right. \qquad (P_0)$$

Unknowns:

$$\begin{array}{ll} S = S(\mathbf{x}, t) \in [0,1] & : \text{saturation} \\ P = P(\mathbf{x}, t) & : \text{pressure} \\ \mathbf{V} = \mathbf{V}(\mathbf{x}, t) \in \mathbb{R}^d & : \text{velocity} \end{array}$$



Fractional flow function f

Microscale Mathematical Model:

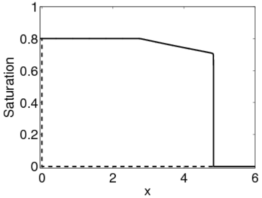
$$\left.\begin{array}{c} s_t^{\epsilon} + \operatorname{div}\left(\mathbf{v}^{\varepsilon} f(s^{\epsilon})\right) = \epsilon \operatorname{div}\left(\mathbf{K}\overline{\lambda}\nabla s^{\epsilon}\right), \\ \operatorname{div}\mathbf{v}^{\varepsilon} = 0,\ \ \mathbf{v}^{\varepsilon} = \mathbf{K}\lambda\nabla p^{\varepsilon} \end{array}\right. \qquad (P_{\varepsilon})$$

Theorem

Let $\{s^\varepsilon\}_{\varepsilon>0}$ be a family of regular solutions to an initial value problem for (P_ε) with $S_0 \in (L^1 \cap L^\infty)(\mathbb{R}^d)$ and $\mathbf{v}^\varepsilon = \mathbf{v}$ given.
Then, there exist a function $S = S(t) \in (L^\infty \cap L^1)(\mathbb{R}^d)$ and a subsequence of $\{s^\varepsilon\}_{\varepsilon>0}$ such that

(i) $\lim_{\varepsilon\to 0} \|S - s^\varepsilon\|_{L^1} = 0$.

(ii) S is a weak solution of (P_0) with $\mathrm{essinf}\{S_0\} \leq S \leq \mathrm{esssup}\{S_0\}$ a.e.



Monotone rarefaction-shock solution.

Interfaces in Porous Media

Macroscale Mathematical Model:

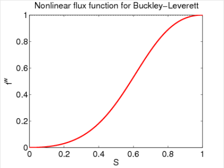
$$\begin{aligned} S_t + \operatorname{div}(\mathbf{V} f(S)) &= 0 \\ \operatorname{div} \mathbf{V} = 0, \ \mathbf{V} &= \mathbf{K}\lambda \nabla P \end{aligned} \qquad (P_0)$$

Unknowns:

$S = S(\mathbf{x}, t) \in [0,1]$: saturation

$P = P(\mathbf{x}, t)$: pressure

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



Fractional flow function f

Microscale Mathematical Model:

(Stauffer '78, Hassanizadeh&Gray '93, Van Duijn&Peletier&Pop '07,...)

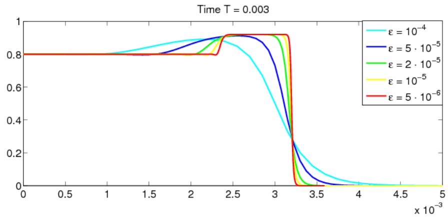
$$\begin{aligned} s^\epsilon_t + \operatorname{div}(\mathbf{v}^\varepsilon f(s^\epsilon)) &= \epsilon \operatorname{div}\left(\mathbf{K}\bar{\lambda}\nabla\left(s^\epsilon + \epsilon\gamma s^\epsilon_t\right)\right) \\ \operatorname{div} \mathbf{v}^\varepsilon = 0, \ \mathbf{v}^\varepsilon &= \mathbf{K}\lambda\nabla p^\varepsilon, \end{aligned} \qquad (P_\varepsilon)$$

Theorem

Let $\{s^\varepsilon\}_{\varepsilon>0}$ be a family of regular solutions to an initial value problem for (P_ε) with $S_0 \in (L^1 \cap L^\infty)(\mathbb{R}^d)$ and $\mathbf{v}^\varepsilon = \mathbf{v}$ given.
Then, there is a function $S = S(t) \in L^p(\mathbb{R}^d)$, $p \in [1,2]$, and a subsequence of $\{s^\varepsilon\}_{\varepsilon>0}$ such that

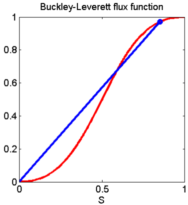
(i) $\lim_{\varepsilon\to 0} \|S - s^\varepsilon\|_{L^2} = 0$,

(ii) S is a weak solution of (P_0).

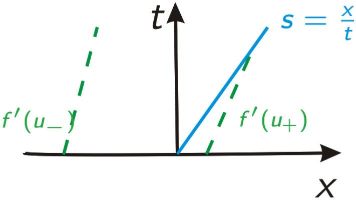


Numerical convergence to sharp overshoot front.

Overshoots as Shock Waves for (P_0):



Buckley-Leverett flux.



Characteristics for overshoot.

The limit $S := \lim_{\varepsilon \to 0} s^\varepsilon$ is **not** a (standard) Kruzkov solution of (P_0).

Numerics

Failure of Standard Approach for Planar Front:

$$S_t + \operatorname{div}\left(\mathbf{v} f(S)\right) = 0,\ \mathbf{v} = (1,0)^T, \qquad S(\mathbf{x},0) = \begin{cases} 0.8 : x_1 < 0 \\ 0 : x_1 > 0 \end{cases}$$

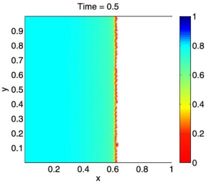
$$\text{Overshoot Solution:} \quad S(\mathbf{x},t) = \begin{cases} 0.8 : x_1 < st \\ S^* > 0.8 : st < x_1 < st \\ 0.0 : x_1 > st \end{cases}$$

Monotone Finite-Volume Scheme:

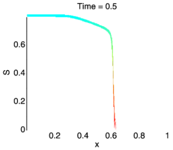
$$\begin{aligned} S_r^0 &= \frac{1}{|T_r|}\int_{T_r} S(\mathbf{x},0)\,d\mathbf{x}, \\ S_r^{n+1} &= S_r^n - \frac{\Delta t^n}{|T_r|}\sum_{l\in N(r)} g_{rl}\left(S_r^n, S_l^n\right) \end{aligned} \qquad (r \in \mathcal{I})$$

Failure of Standard Approach for Planar Front:

$$S_t + \operatorname{div}(\mathbf{v} f(S)) = 0,\ \mathbf{v} = (1,0)^T, \qquad S(\mathbf{x},0) = \begin{cases} 0.8 : x_1 < 0 \\ 0 : x_1 > 0 \end{cases}$$



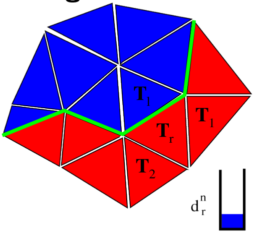
Saturation



Vertical Sampling.

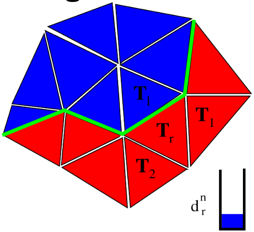
Note: Convergence towards Kruzkov solution is proven.

A Heterogeneous Multiscale Method (Engel&Kissling&R. 10/11)



Front position at $t = t^n$.

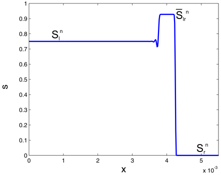
A Heterogeneous Multiscale Method (Engel&Kissling&R. 10/11)



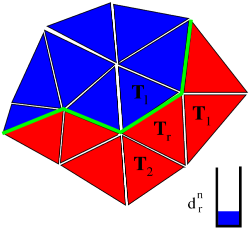
Front position at $t = t^n$.

Step 1: For $\varepsilon > 0$ solve (P_ε) **in 1D** and **in micro-scale interval** $(t^n, t^n + \delta t)$ for

$$s^\varepsilon(\xi, 0) = \begin{cases} S_l^n & : \xi < 0 \\ S_r^n & : \xi > 0 \end{cases}$$



Determine (only) $\bar{S}_{lr}^n$ from solution.

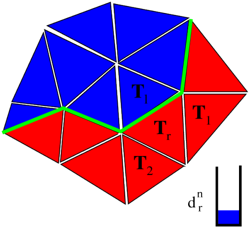


Front position at $t = t^n$.

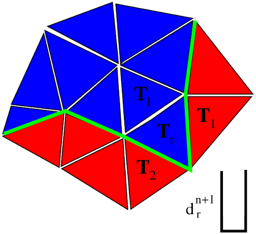
Step 2: Flux balance for T_r (using a numerical flux $g = g_{rl}$)

$$|T_r|\tilde{S}_r := |T_r|S_r^n - \Delta t(g(S_r^n, S_1^n) + g(S_r^n, S_2^n) + g(\bar{S}_{lr}^n, S_l^n)) + d_r^n$$

Numerics



Front position at $t = t^n$.



Front position at $t = t^{n+1}$ for case (A).

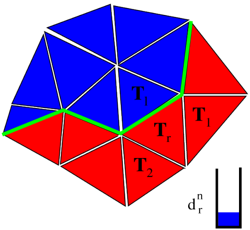
Step 2: Flux balance for T_r (using a numerical flux $g = g_{rl}$)

$$|T_r|\tilde{S}_r := |T_r|S_r^n - \Delta t(g(S_r^n, S_1^n) + g(S_r^n, S_2^n) + g(\bar{S}_{lr}^n, S_l^n)) + d_r^n$$

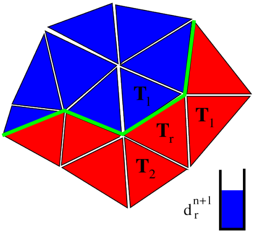
Step 3: Update and front propagation for case (A): $\tilde{S}_r \geq \bar{S}_{lr}^n$

$$S_r^{n+1} = \tilde{S}_r, \quad d_r^{n+1} = 0$$

Numerics



Front position at $t = t^n$.



Front position at $t = t^{n+1}$ for case (B).

Step 2: Flux balance for T_r (using a numerical flux $g = g_{rl}$)

$$|T_r|\tilde{S}_r := |T_r|S_r^n - \Delta t(g(S_r^n, S_1^n) + g(S_r^n, S_2^n) + g(\bar{S}_{lr}^n, S_l^n)) + d_r^n$$

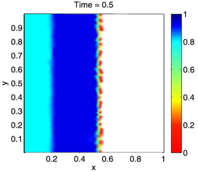
Step 3: Update and front propagation for case (B): $\tilde{S}_r < \bar{S}_{lr}^n$

$$|T_r|S_r^{n+1} = |T_r|S_r^n - \Delta t(g(S_r^n, S_1^n) + g(S_r^n, S_2^n) + g(S_r^n, S_r^n))$$
$$d_r^{n+1} = d_r^n + \Delta t(g(\bar{S}_{lr}^n, S_l^n) - g(S_r^n, S_r^n))$$

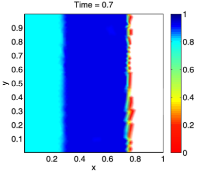
Planar Front with HMM:

$$S_t + \operatorname{div}\left(\mathbf{V} f(S)\right) = 0,\ \mathbf{V} = (1,0)^T, \quad S(\mathbf{x},0) = \begin{cases} 0.8 : x_1 < 0 \\ 0 : x_1 > 0 \end{cases}$$

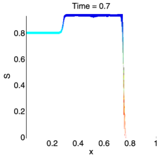
Nonclassical Overshoot Solution: $S(\mathbf{x},t) = \begin{cases} 0.8 : x_1 < st \\ S^* > 0.8 : st < x_1 < st \\ 0.0 : x_1 > st \end{cases}$



Saturation at $t = 0.5$



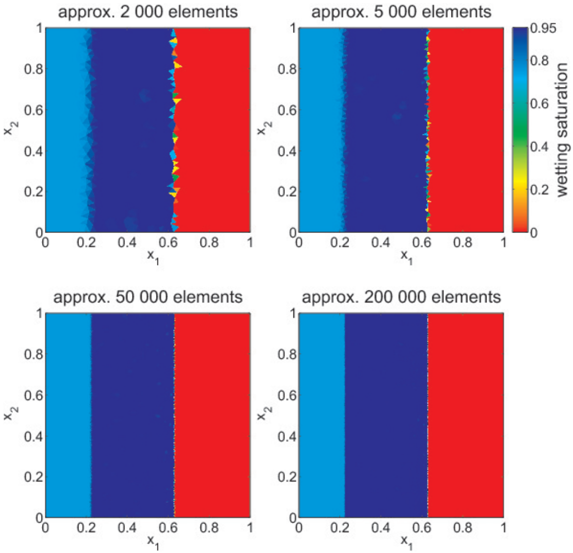
Saturation at $t = 0.7$



Vertical Sampling.

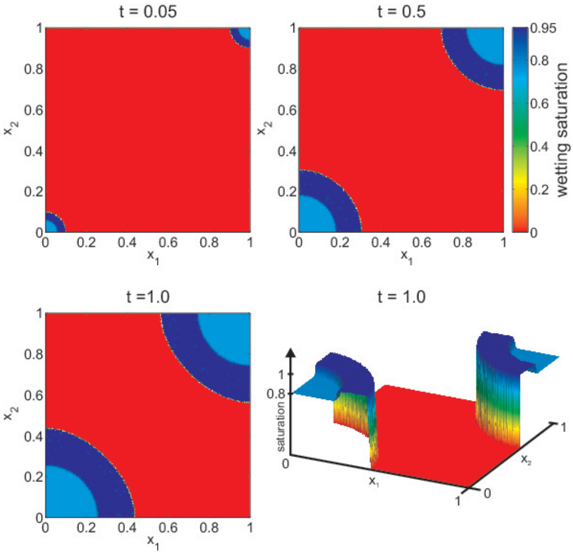
Numerics

Planar Front
Grid Convergence:
$(\mathbf{V} = (1, 0)^T)$



Numerics

Five-Spot Waterflood:
(with Darcy)

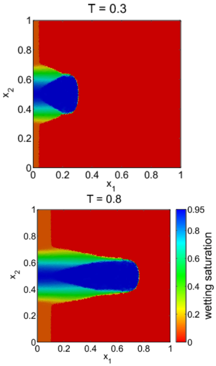


Numerics

Performance-Comparison:

Two-Phase Flow in 2D (Viscous Fingering with Darcy)

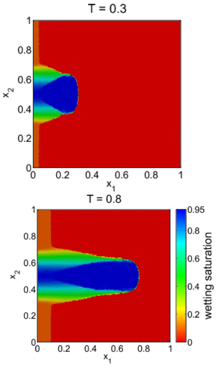
		CPU-time
$2D$	monotone FV- IMPES	165 min
	HMM (solving microscale problem on the fly)	1300 min
$1D$	microscale problem over one edge	$0.1s$
$1D$		



$\rightsquigarrow$ 3D implementation within open source solver DuMuX

Performance-Comparison:
Two-Phase Flow in 2D (Viscous Fingering with Darcy)

		CPU-time
$2D$	monotone FV- IMPES	165 min
	HMM (solving microscale problem on the fly)	1300 min
	HMM (solving microscale problem by kernel method)	215 min
$1D$	microscale problem over one edge	$0.1s$
$1D$	microscale problem one edge (kernel method)	$1.2 \cdot 10^{-4}s$



$\rightsquigarrow$ 3D implementation within open source solver DuMuX

3) Interfaces in Liquid-Vapour Flow

Liquid-Vapour Flow

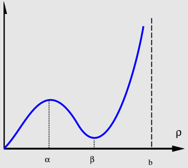
Macroscale Model: Euler Equations

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

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

Microscale Model: (in Lagrangian coordinates)

$$
\begin{aligned}
\tau_t &- v_\xi &= 0\\
v_t &+ \tilde{p}(\tau)_\xi &= 0
\end{aligned}
$$

Unknowns:

$\tau = \tau(\xi, t)$: specific volume

$v = v(\xi, t)$: longitudinal velocity

Jump conditions at phase boundary:

$$
\begin{aligned}
[\![\tilde{s}\tau + v]\!] &= 0,\\
[\![-\tilde{s}v + \tilde{p}]\!] &= (d-1)\gamma\kappa,
\end{aligned}
$$

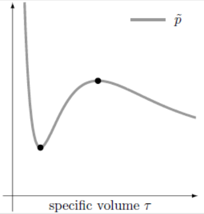
+ entropy criterion.

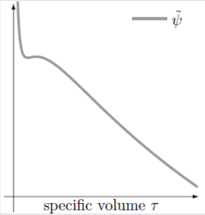
The Riemann Problem for a modified system: $(d = 2)$

$$\begin{array}{rcrcl} \tau_t & - & v_\xi & = & 0 \\ v_t & + & \tilde{p}(\tau)_\xi & = & 0 \end{array}$$

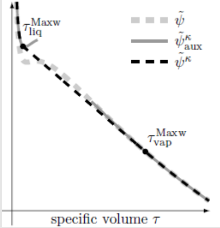
The pressure $\tilde{p}$ satisfies

$$\tilde{p}(\tau) = -\tilde{\psi}'(\tau).$$





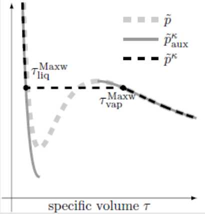
$$\tilde{\psi}^\kappa_{aux}(\tau) = \begin{cases} \tilde{\psi}(\tau) - \gamma\kappa\tau & : \tau \in (0, \tau_{liq}^{Maxw}) \\ \tilde{\psi}(\tau) & : \tau \in (\tau_{vap}^{Maxw}, \infty). \end{cases}$$



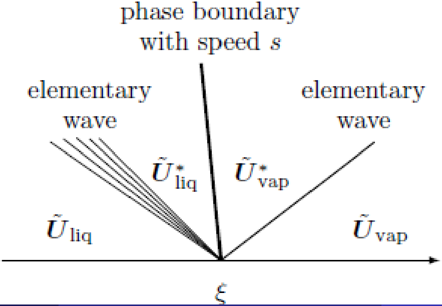
Define the pressure $\tilde{p}^\kappa$ as the derivative of the convex hull of $\tilde{\psi}^\kappa_{aux}$!

The Riemann Problem for the Final Microscale Model:

$$\begin{aligned} \tau_t \quad &- \quad v_x &= \quad 0 \\ v_t \quad &+ \quad \tilde{p}^\kappa(\tau)_x &= \quad 0 \end{aligned}$$

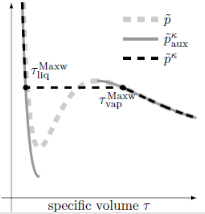


Riemann solutions: (Müller&Voss, Godlewski&Seguin '06)

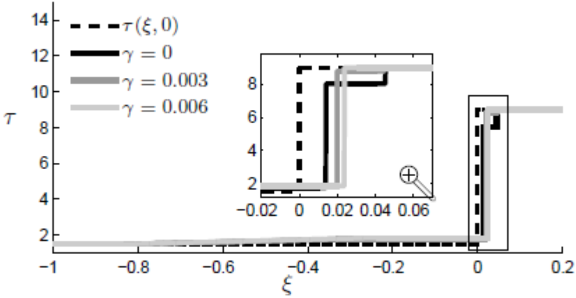


The Riemann Problem for the Final Microscale Model:

$$\begin{aligned} \tau_t &- v_x &= 0 \\ v_t &+ \tilde{p}^\kappa(\tau)_x &= 0 \end{aligned}$$

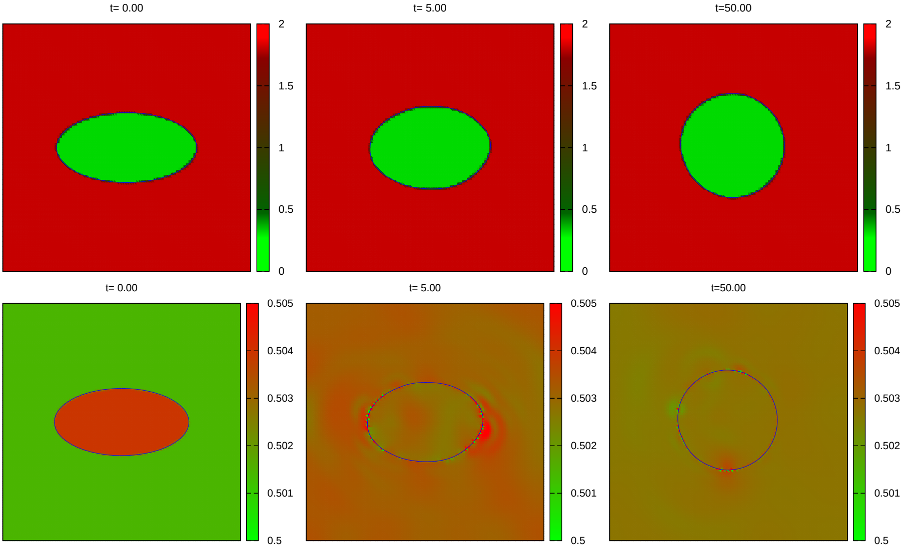


Riemann solutions: (Müller&Voss, Godlewski&Seguin '06)



Numerics (Engel, Jaegle, Zeiler)

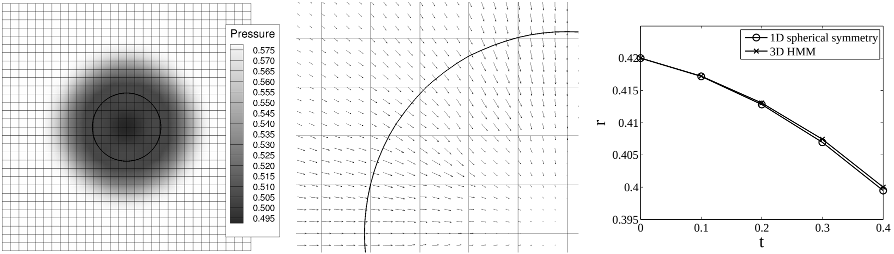
Relaxation to spherical equilibrium: (density (upper line) and pressure)



Numerics

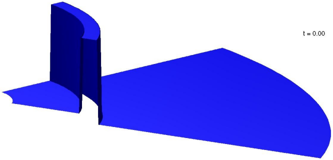
Unsteady bubble in 3D:
(Spectral DG-code with $\approx$ 100000 elements and polynomial degree 3)

Initial radius	Surface tension	Inner state	Outer state
$r_{\text{ini}} = 0.42$	$\gamma = 0.0025$	$\rho = 0.3$, $\lvert\mathbf{v}\rvert = 0.0$	$\rho = 1.83$, $\lvert\mathbf{v}\rvert = 0.0$

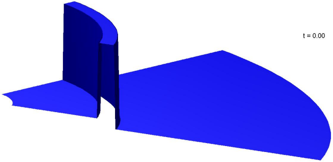


Pressure field and level set at $t = 0.2$, comparison with 1D reference solution

Droplets in Rotational-Symmetric Geometry:



Initial Density, Volume-Weighted Total Mass in Vapour Phase



Initial Density, Volume-Weighted Total mass in Elliptic Region.

3) Summary and Outlook:

- Construction of MultiD algorithms for flow problems with interfaces
- Increase of efficiency is a key issue for HMM...
- (Almost) no convergence analysis due to lack of theory

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