Micro-Macro Modelling and
Simulation of Liquid-Vapour Flow

DFG – CNRS

Curvature Driven Liquid-Vapour Flow in Compressible Fluids

Christoph Zeiler

Institut für Angewandte Analysis und Numerische Simulation

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Free Boundary Value Problem in $\mathbb{R}^d$

Bulk Phases

$$\begin{aligned} \varrho_t + \operatorname{div}(\varrho\, \boldsymbol{v}) &= 0, \\ (\varrho\, \boldsymbol{v})_t + \operatorname{div}\left(\varrho\, \boldsymbol{v} \otimes \boldsymbol{v} + p(\varrho)\, \boldsymbol{I}\right) &= \boldsymbol{0}. \end{aligned}$$

Phase Boundary

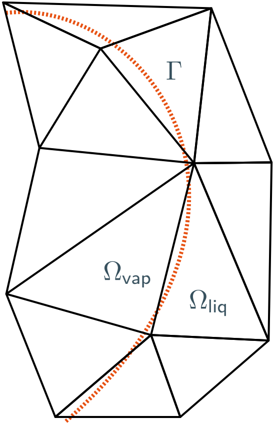
$$\begin{aligned} [\![\varrho(\boldsymbol{v}\cdot\boldsymbol{n} - \sigma)]\!] &= 0, \\ [\![\varrho(\boldsymbol{v}\cdot\boldsymbol{n} - \sigma)\, \boldsymbol{v} + p(\varrho)\, \boldsymbol{n}]\!] &= (d-1)\gamma\kappa\, \boldsymbol{n}. \end{aligned}$$

$+$ kinetic relation

[Stöhr, Binninger, Zeng]

Outline

Heterogeneous Multiscale Method



[Engquist et al. 2007]

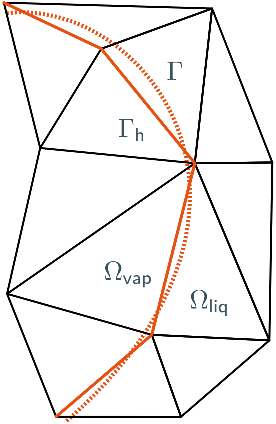
Domain $\Omega \in \mathbb{R}^d$ with fluid in two phases at time $t > 0$

- liquid $\Omega_{\text{liq}}(t)$,
- vapour $\Omega_{\text{vap}}(t)$,
- curved phase boundary $\Gamma(t) = \partial\Omega_{\text{liq}}(t) \cap \partial\Omega_{\text{vap}}(t)$.

We consider physical quantities in Euler coordinates $(\boldsymbol{x}, t)$

- density $\varrho(\boldsymbol{x}, t) > 0$,
- velocity $\boldsymbol{v}(\boldsymbol{x}, t) \in \mathbb{R}^d$.

Heterogeneous Multiscale Method



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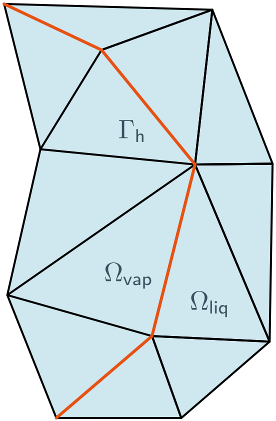
Phase Boundary

Approximate $\Gamma(t)$ with $\Gamma_\mathsf{h}(t)$ consisting of element edges.

[Engquist et al. 2007]

Heterogeneous Multiscale Method



[Engquist et al. 2007]

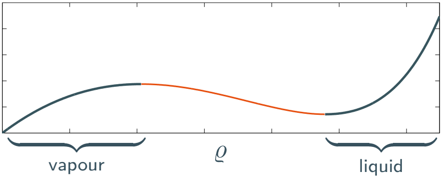
Macroscale

Dynamics of the bulk phases Ω_{liq} and Ω_{vap}.
Model: Isothermal Euler equation

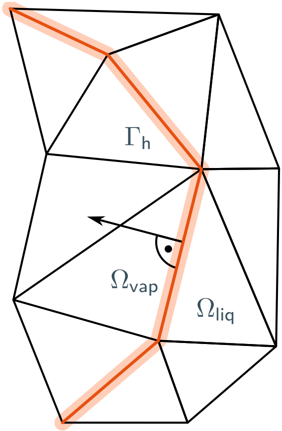
$$\begin{aligned} \varrho_t + \operatorname{div}(\varrho\, \boldsymbol{v}) &= 0, \\ (\varrho\, \boldsymbol{v})_t + \operatorname{div}\left(\varrho\, \boldsymbol{v} \otimes \boldsymbol{v} + p(\varrho)\, \boldsymbol{I}\right) &= \boldsymbol{0}, \end{aligned}$$

with a pressure function p that covers liquid and vapour phase.

Van-der-Waals like Pressure p



Heterogeneous Multiscale Method



Microscale

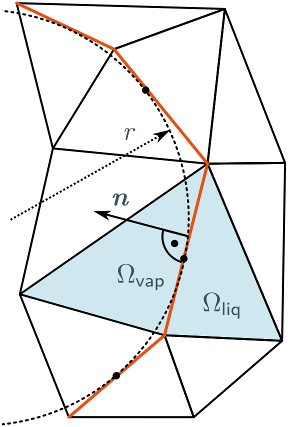
Dynamics at the phase boundary.

We assume that it is sufficient to consider a 1D Riemann type problem on the microscale.

- sharp interface
    - isothermal Euler equation and jump conditions across the phase boundary
- diffuse interface
    - Navier-Stokes-Korteweg model

[Engquist et al. 2007]

Heterogeneous Multiscale Method



Transfer Operator

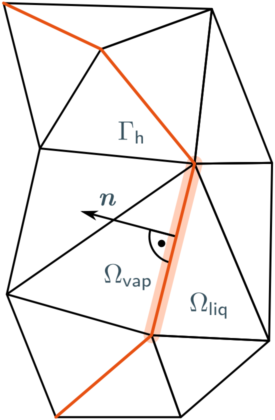
Macro- to microscale

- data reconstruction
    - initial states for microscale problems
- curvature reconstruction
    - applying Γ_{h} (figure: $\kappa = \frac{1}{r}$)
    - level set function

$$\kappa = \operatorname{div}\left(\frac{\operatorname{grad}\varphi}{|\operatorname{grad}\varphi|}\right)$$

[Engquist et al. 2007]

Heterogeneous Multiscale Method



Transfer Operator

Micro- to macroscale

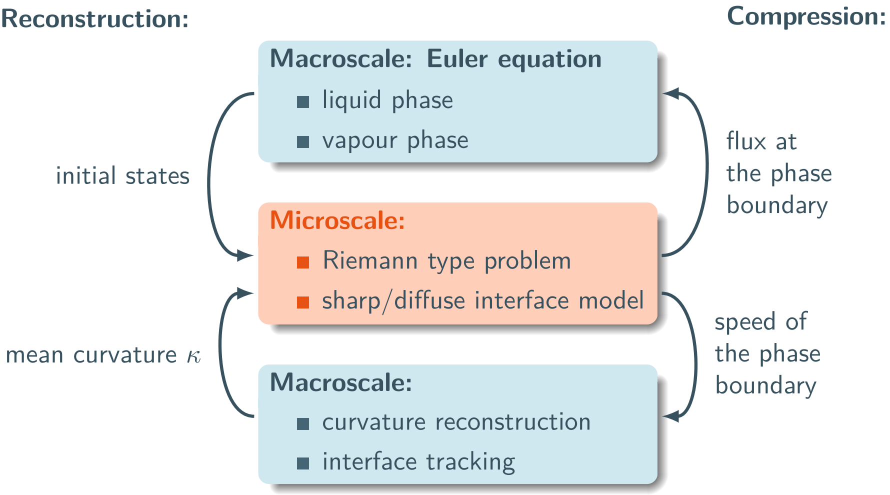
- data compression
    - fluxes for phase boundary edges
- interface tracking
    - level set function

$$\frac{\partial \varphi}{\partial t} + (\sigma\, \boldsymbol{n}) \cdot \operatorname{grad} \varphi = \mathbf{0}$$

[Engquist et al. 2007]

Heterogeneous Multiscale Method

Algorithm



Reconstruction:

Compression:

Macroscale: Euler equation

- liquid phase
- vapour phase

initial states

flux at the phase boundary

Microscale:

- Riemann type problem
- sharp/diffuse interface model

mean curvature κ

speed of the phase boundary

Macroscale:

- curvature reconstruction
- interface tracking

Microscale

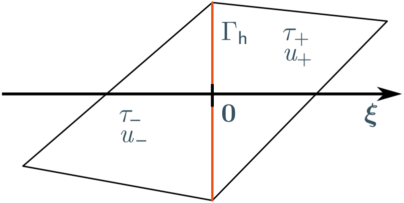
Sharp Interface Model

Within a macro time step, there are essentially Riemann problems to solve:

$$(\tau, u)(\xi, 0) :=\begin{cases}(\tau_-, u_-) & \text{for } \xi \leq 0,\\ (\tau_+, u_+) & \text{for } \xi > 0.\end{cases} \tag{RP}$$

In Lagrange coordinates (ξ, t):

- specific volume $\tau := \varrho^{-1} > 0$
- velocity $u \in \mathbb{R}$



Microscale

Sharp Interface Model

$$\begin{pmatrix} \tau \\ u \end{pmatrix}_t + \begin{pmatrix} -u \\ \tilde{p}(\tau) \end{pmatrix}_\xi = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{in} \quad \mathbb{R} \times (0, \infty). \tag{Euler}$$

We solve the Riemann problem (RP) for the isothermal Euler equation (Euler) such that

1. the solution in bulk phases is entropy solution,
2. there exists one phase boundary that satisfies

$$\begin{aligned} \sigma \llbracket \tau \rrbracket + \llbracket u \rrbracket &= 0, \\ \sigma \llbracket u \rrbracket + \llbracket \tilde{p}(\tau) \rrbracket &= (d-1)\gamma\kappa, \end{aligned} \tag{RH$^\kappa$}$$

3. Liu's entropy criterion holds ([Liu 1974]).

σ	speed of the phase boundary	d	spatial dimension
$\gamma > 0$	surface tension coefficient	κ	mean curvature
$\tilde{p}(\tau)$	$:= p(\tau^{-1})$ Van-der-Waals Pressure	$\llbracket \tau \rrbracket$	$:= \tau_- - \tau_+$

Microscale

A Curvature Dependent Pressure Function

We introduce a curvature dependent pressure function $\tilde{p}^{\kappa}$:

$$\tilde{p}^{\kappa}(\tau) := \begin{cases} \tilde{p}(\tau) + (d-1)\gamma\kappa & \text{in the liquid phase,} \\ \tilde{p}(\tau) & \text{in the vapour phase.} \end{cases}$$

$$\begin{pmatrix} \tau \\ u \end{pmatrix}_t + \begin{pmatrix} -u \\ \tilde{p}^{\kappa}(\tau) \end{pmatrix}_{\xi} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{in} \quad \mathbb{R} \times (0,\infty) \qquad (\text{Euler}^{\kappa})$$

The Rankine Hugoniot conditions for (Euler$^{\kappa}$) coincides with (RH$^{\kappa}$).

Appropriate free energy

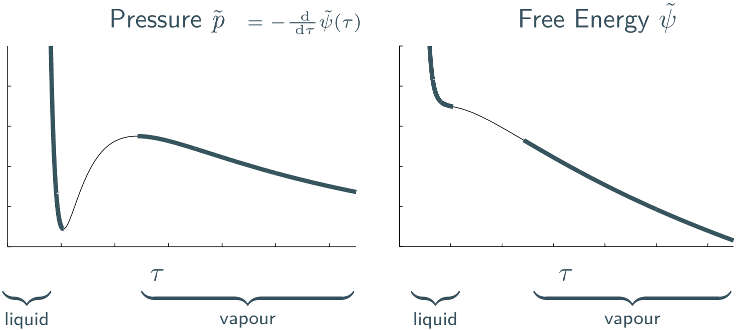
$$\tilde{\psi}^{\kappa}(\tau) := \begin{cases} \tilde{\psi}(\tau) - (d-1)\tau\gamma\kappa & \text{in the liquid phase,} \\ \tilde{\psi}(\tau) & \text{in the vapour phase.} \end{cases}$$

such that $\frac{\mathrm{d}}{\mathrm{d}\tau}\tilde{\psi}^{\kappa}(\tau) = -\tilde{p}^{\kappa}(\tau)$ and $\tilde{\psi}^{\kappa} + \tau\,\tilde{p}^{\kappa} = \tilde{\psi} + \tau\,\tilde{p}$.

Microscale

A Curvature Dependent Pressure Function

Generalised Maxwell construction for $\tilde{p}^{\kappa}$



Microscale

A Curvature Dependent Pressure Function

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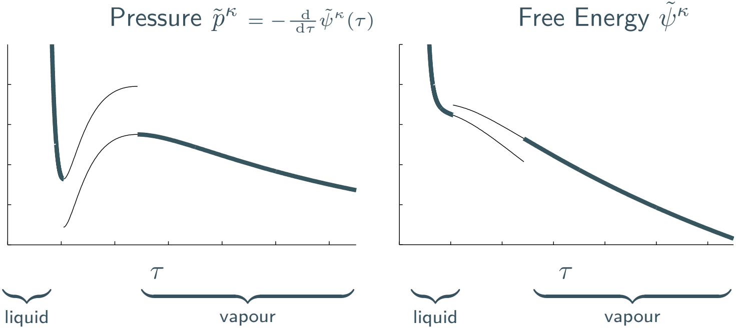


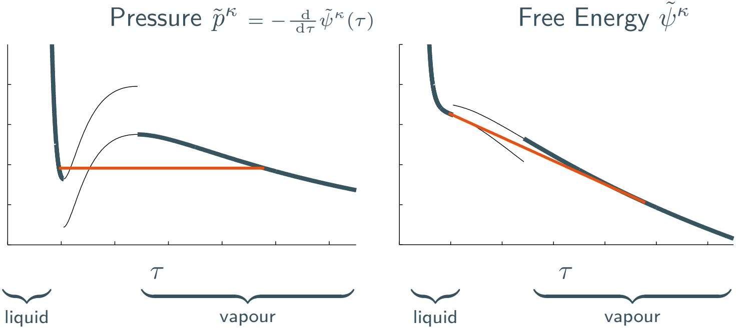
Pressure $\tilde{p}^{\kappa} = -\frac{\mathrm{d}}{\mathrm{d}\tau}\tilde{\psi}^{\kappa}(\tau)$

Free Energy $\tilde{\psi}^{\kappa}$

Microscale

A Curvature Dependent Pressure Function

Generalised Maxwell construction for $\tilde{p}^{\kappa}$



Microscale

A Curvature Dependent Pressure Function

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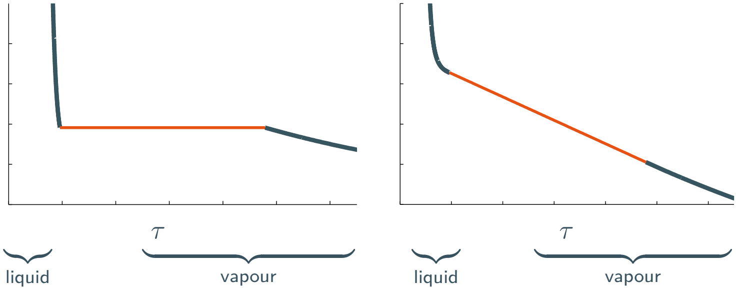


Pressure $\tilde{p}^{\kappa} = -\frac{\mathrm{d}}{\mathrm{d}\tau}\tilde{\psi}^{\kappa}(\tau)$

Free Energy $\tilde{\psi}^{\kappa}$

Microscale

Solution

$$\begin{pmatrix}\tau\\ u\end{pmatrix}_t+\begin{pmatrix}-u\\ \tilde{p}^\kappa(\tau)\end{pmatrix}_\xi=\begin{pmatrix}0\\ 0\end{pmatrix}\quad \text{in}\quad \mathbb{R}\times(0,\infty). \qquad (\text{Euler}^\kappa)$$

Theorem [Z 2012]

The Riemann problem for (Euler$^\kappa$) with moderate surface tension, has a unique (Liu) entropy solution. The solution consist of elementary waves and exactly one phase boundary satisfying (RH$^\kappa$).

- entropy dissipativity condition:

$$\sigma\,[\![E^\kappa(\tau,u)]\!]-[\![F^\kappa(\tau,u)]\!]\le 0,$$

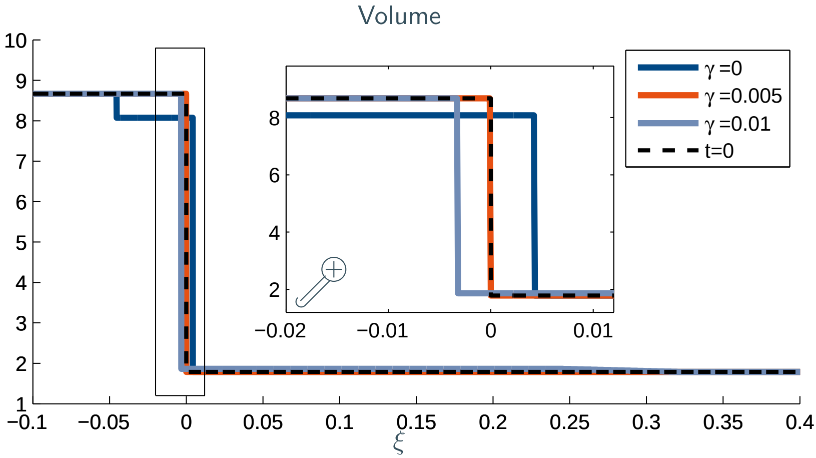
$E^\kappa(\tau,u)=\frac{1}{2}u^2+\tilde{\psi}^\kappa(\tau),\ F^\kappa(\tau,u)=u\,\tilde{p}^\kappa(\tau).$

For a construction, we follow [Müller, Voß 2006].

Microscale

Solution

Solution for a bubble of radius 1
with different surface tension coefficients γ.



Microscale

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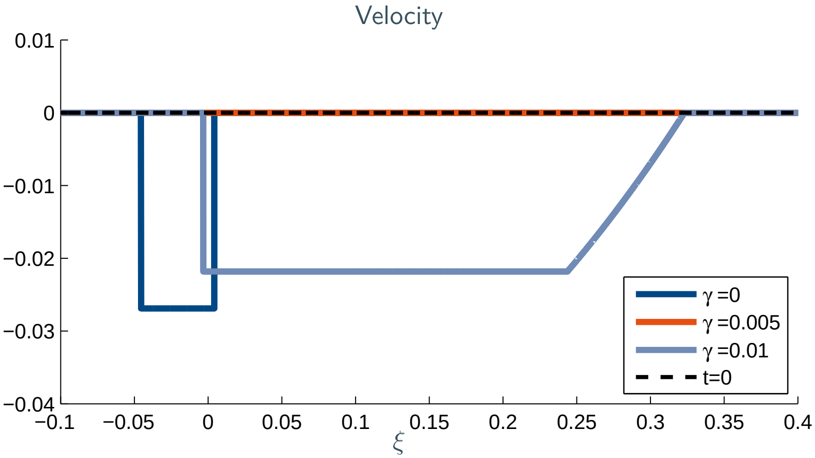


Application of the HMM in 2d (with P. Engel)

Macroscale Solver

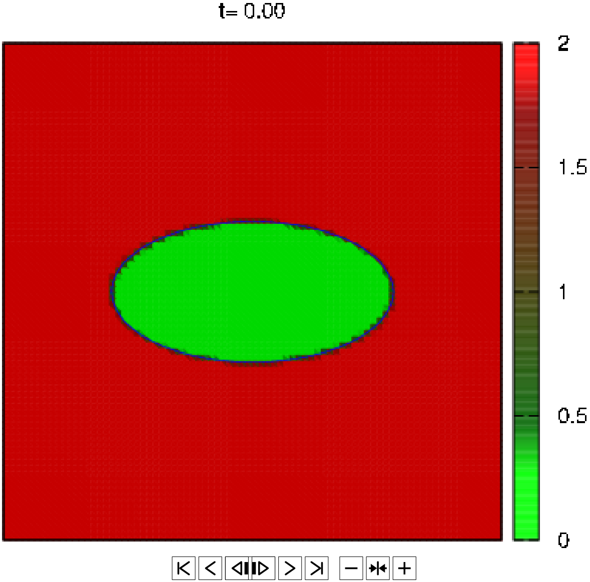
- Finite Volume method for the 2d Euler system
- unstructured grid
- cut cells along the level set zero
- level set driving

$$\frac{\partial \varphi}{\partial t} + (\sigma\, \boldsymbol{n}) \cdot \operatorname{grad} \varphi = \mathbf{0}$$

- curvature

$$\kappa = \operatorname{div}\left(\frac{\operatorname{grad} \varphi}{|\operatorname{grad} \varphi|}\right)$$

Application of the HMM in 2d

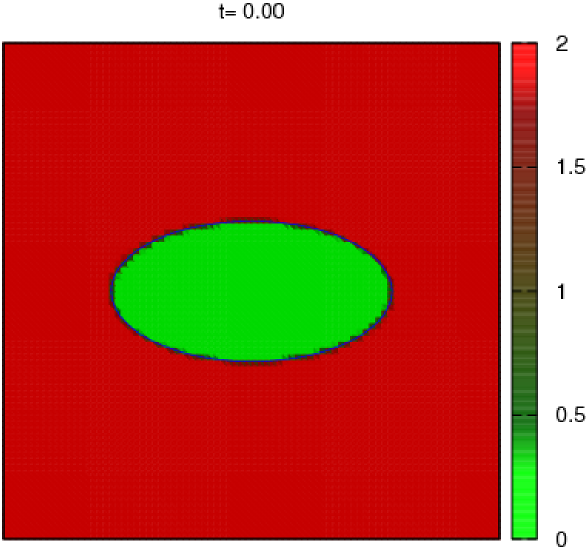


$$\varrho(\boldsymbol{x},0) = \begin{cases} 0.3191 & : \text{inside} \\ 1.8063 & : \text{outside}, \end{cases}$$

$$\boldsymbol{v}(\boldsymbol{x},0) = \mathbf{0},$$

$$\gamma = 0.001$$

Application of the HMM in 2d



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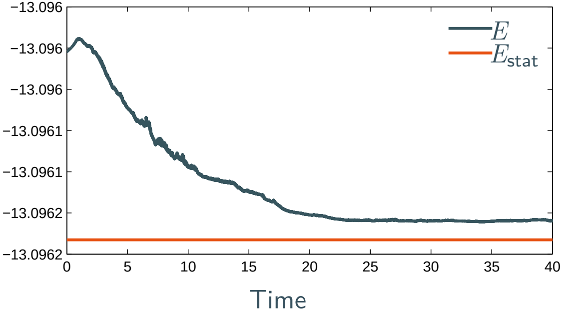
Application of the HMM in 2d

Energy (cf. [Gurtin 1985])

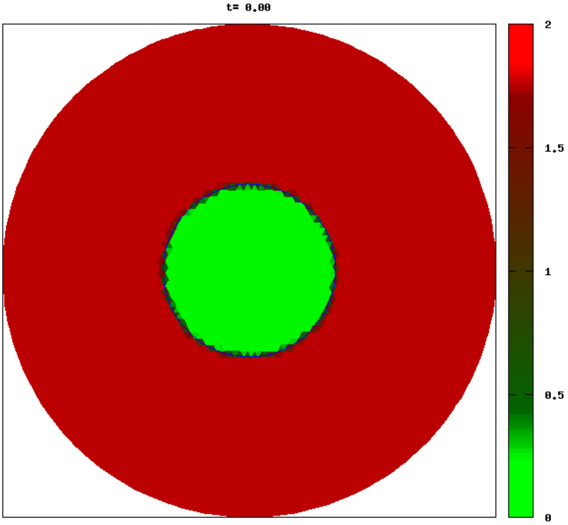
$$E(\varrho, \boldsymbol{v}) = \int_\Omega \frac{1}{2}\varrho\,|\boldsymbol{v}|^2 + W(\varrho)\,\mathrm{d}x + \gamma\,|\Gamma|\,, \qquad W(\varrho) = \varrho\,\tilde{\psi}(1/\varrho),$$

$$E_{\mathsf{stat}} = \min\left\{ E(\varrho, \mathbf{0}) \;\middle|\; \int_\Omega \varrho\,\mathrm{d}x = \text{const.} \right\}$$



Application of the HMM in 2d

Solution



$$\varrho(\boldsymbol{x},0) = \begin{cases} 0.3 & : |\boldsymbol{x}| \leq 0.42 \\ 1.8 & : |\boldsymbol{x}| > 0.42, \end{cases}$$

$$\boldsymbol{v}(\boldsymbol{x},0) = \mathbf{0},$$

$$\gamma = 0.001$$

Application of the HMM in 3d (with F. Jägle)

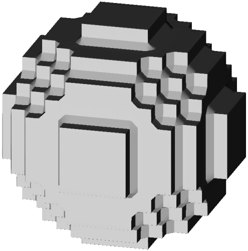
Macroscale Solver [Jägle, Rohde, Z 2012]

- Discontinuous Galerkin spectral element method for the 3d Euler system
- polynomials of degree 2
- $20 \times 20 \times 20$ hexahedral cells
- cells are either liquid or vapour
- level set driving

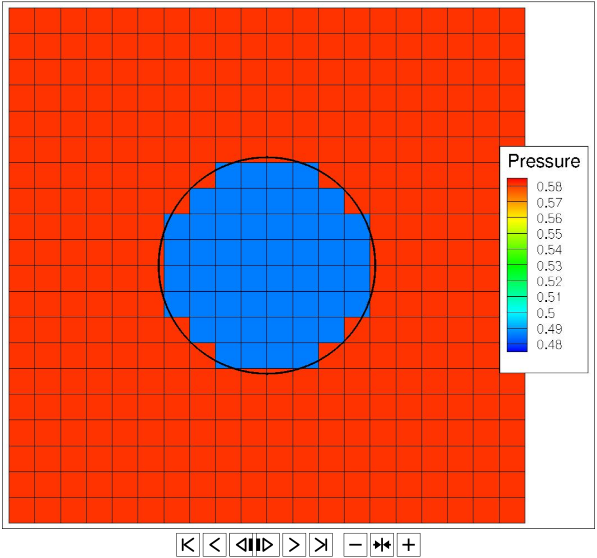
$$\frac{\partial \varphi}{\partial t} + (\sigma\, \boldsymbol{n}) \cdot \operatorname{grad} \varphi = \mathbf{0}$$

- curvature

$$\kappa = \operatorname{div}\left(\frac{\operatorname{grad} \varphi}{|\operatorname{grad} \varphi|}\right)$$



Application of the HMM in 3d



$$\varrho(\boldsymbol{x},0) =$$

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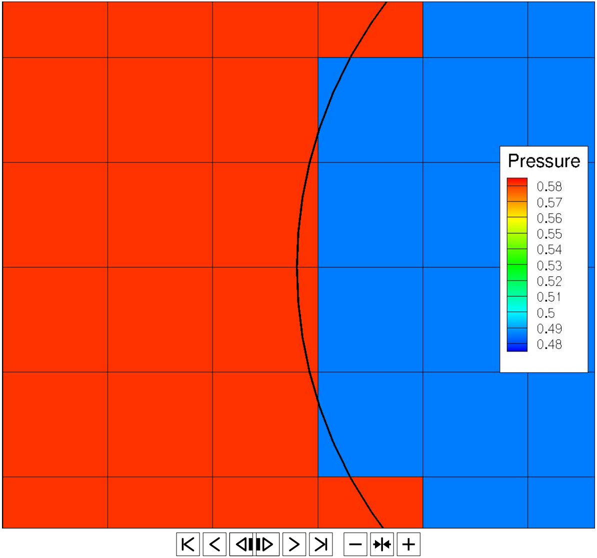
$$\boldsymbol{v}(\boldsymbol{x},0) = \mathbf{0},$$

$$\gamma = 0.0025$$

Application of the HMM in 3d



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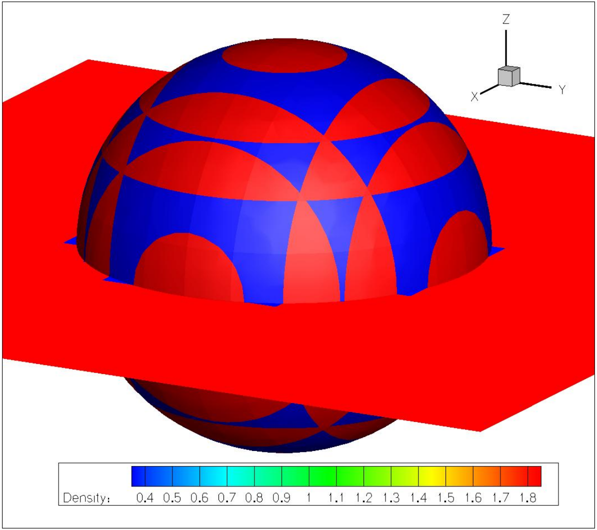

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$$\boldsymbol{v}(\boldsymbol{x},0) = \boldsymbol{0},$$

$$\gamma = 0.0025$$

Outlook

Macroscale

- level set reinitialization for the 3d HMM
- implementation for the 2d HMM in Dune / C++
- interface tracking
- curvature reconstruction

Microscale

- Navier-Stokes-Korteweg model

Literature

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