Energy Consistent DG Scheme for the Navier-Stokes-Allen-Cahn System

Albert-Ludwigs-Universität Freiburg

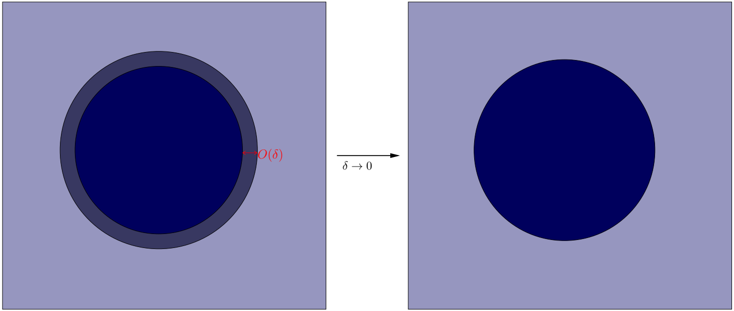
Mirko Kränkel

AAM Freiburg

9th DFG-CNRS WORKSHOP
Micro-Macro Modeling and Simulation of Liquid-Vapor Flows
25.2.-27.2.2014

Outline

- Goal: Simulation of two phase flow using a phase field approach.
- Diffuse interface model: Small positive width of the phase boundary. No explicit interface conditions needed.
- Additional variable φ which indicates the phases. $\varphi \approx 0$: phase 1, $\varphi \approx 1$: phase 2



- We want to use a phase field type model, where the thickness of the interface can be easily controlled.
- This should allow to artificially increase the transition layer between the two phases in numerical calculations.
- The small size of the interfacial layer is one main difficulty for the numerical treatment.
- In [1, Witterstein] and [2, Alt Witterstein] a compressible phase field model was derived where the Young-Laplace-Law was recovered in the sharp interface limit.

Governing Equations

The model from [1, Witterstein1] consists of the compressible Navier-Stokes and an Allen-Cahn like equation for the phase field parameter φ.

$$\partial_t \rho + \nabla \cdot \rho \mathbf{v} = 0, \tag{1}$$

$$\partial_t(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla \mathbb{P}(\rho, \varphi, \nabla \varphi) + \nabla \cdot (\mathbb{D}(\nabla v)) = 0, \tag{2}$$

$$\rho(\partial_t \varphi + \mathbf{v} \cdot \nabla \varphi) = -\eta \frac{\delta F}{\delta \varphi}. \tag{3}$$

for $x \in \Omega \subset \mathbb{R}^d, t > 0$.
with a free energy $F = F(\rho, \varphi, \nabla \varphi) = \frac{1}{\delta} h_1(\rho) W(\varphi) + \psi(\rho, \varphi) + \delta h_2(\rho) \frac{|\nabla \varphi|^2}{2}$
and $\eta > 0$.

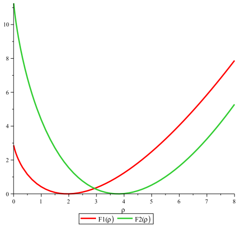
Governing Equations

The free Energy has the form

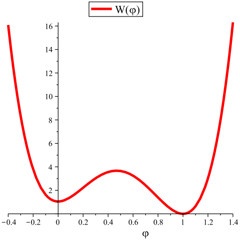
$$F(\rho,\varphi,\nabla\varphi) := \frac{1}{\delta}h_1(\rho)W(\varphi) + \psi(\rho,\varphi) + \delta h_2(\rho)\frac{|\nabla\varphi|^2}{2}.$$

The function ψ models the physics in the pure phases.

$$\psi(\rho,\varphi) := \nu(\varphi)f_2(\rho) + (1-\nu(\varphi))f_1(\rho).$$



$W(\varphi)$ is double-well function with respect to φ and possibly different heights of the minima.



In the momentum equation

$$\partial_t(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla \mathbb{P}(\rho, \varphi, \nabla \varphi) + \nabla \cdot (\mathbb{D}(\nabla v)) = 0,$$

the pressure and stress tensor $\mathbb{P}$,$\mathbb{D}$ are given

$$\mathbb{P} := \mathbb{P}(\rho, \varphi, \nabla \varphi) = (-F + \rho F_\rho)\mathbb{I} + \delta(h_2(\rho)\nabla \varphi \otimes \nabla \varphi)$$

and

$$\mathbb{D}(\nabla \mathbf{v}) := \mu_1 \nabla \cdot \mathbf{v}\mathbb{I} + \mu_2(\frac{1}{2}(\nabla \mathbf{v} + (\nabla \mathbf{v}))^T - \frac{1}{d}\nabla \cdot \mathbf{v}\mathbb{I})$$

with $\mu_1, \mu_2 > 0$ so that $\mathbb{D}(\nabla \mathbf{v}) \cdot \nabla v > 0$.
The source term in the phase field equation reads:

$$\frac{\delta F}{\delta \varphi} = \frac{1}{\delta} h_1(\rho) W_\varphi(\varphi) + \psi_\varphi(\rho, \varphi) - \delta \nabla \cdot (h_2(\rho)\nabla \varphi).$$

Energy Inequality

Proposition (G.Witterstein [1])

If the boundary values are chosen so that $\mathbf{v} = 0$ *and* $\nabla\varphi \cdot \boldsymbol{n} = 0$ *on* $\partial\Omega$ *than*

$$\frac{d}{dt}E(\rho,\varphi,v,\nabla\varphi) = \frac{d}{dt}\int_\Omega F(\rho,\varphi) + h_2(\rho)\frac{|\nabla\varphi|^2}{2} + \rho\frac{|v|^2}{2}dx \leq 0. \quad (4)$$

The Energy consistent DG-Method

UNI FREIBURG

- The scheme presented in this talk is a direct extension for the Navier-Stokes-Allen-Cahn System of the scheme developed by J. Giesselmann et. al. for the Navier-Stokes-Korteweg system.
- It can be shown that the scheme fulfills a discrete Version of the energy inequality (4).
- Implemented using the DUNE and DUNE-FEM software enviroment: http://dune.mathematik.uni-freiburg.de/

J. GIESSELMANN, C. MAKRIDAKIS, T. PRYER
Energy consistent DG methods for the Navier-Stokes-Korteweg system
Mathematics of Computation, 2014

Nonconservative Mixed Form

To derive an energy consistent numerical method we introduce the auxilliary variables τ, μ, σ

$$\tau = F_\varphi + \delta \nabla \cdot (h_2(\rho)\sigma),$$
$$\mu = F_\rho - \frac{1}{2}|v|^2$$
$$\sigma = \nabla\varphi.$$

and noting that

$$\nabla \cdot \mathbb{P}(\rho, \varphi, \nabla\varphi) = \nabla \cdot \left[(-F + \rho F|_\rho)\mathbf{I} + h_2(\rho)\nabla\varphi \otimes \nabla\varphi\right]$$
$$= \rho\nabla\mu + \frac{1}{2}\rho\nabla|v|^2 - \nabla\varphi(F_\varphi - \delta\nabla \cdot (h_2(\rho)\sigma)$$

we can rewrite the Navier-Stokes-Allen-Cahn-System in the following mixed form:

Find $\rho, \mathbf{v}, \varphi, \tau, \mu, \sigma$ so that

$$
\begin{aligned}
\partial_t \rho + \nabla \cdot \rho \mathbf{v} &= 0, \\
\rho \partial_t(\mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) - \nabla \cdot (\rho \mathbf{v}) v + \rho \nabla \mu - \tau \nabla \varphi - \frac{1}{2} \rho \nabla |\mathbf{v}|^2 - \nabla \cdot (\mathbb{D}(\nabla \mathbf{v})) &= 0, \\
\partial_t \varphi + \nabla \varphi \cdot \mathbf{v} + \eta \frac{\tau}{\rho} &= 0, \\
\tau - F_\varphi + \delta \nabla \cdot \sigma &= 0, \\
\mu - F_\rho - \frac{1}{2} |v|^2 &= 0, \\
\sigma - \nabla \varphi &= 0.
\end{aligned}
$$

Let $\mathcal{T}$ be a triangulation of Ω. Then we define the **Discontinuous Galerkin Space** by

$$V_h := \{u \in L^2(\Omega) : u_{|E} \in \mathbb{P}_k \text{for all } E \in \mathcal{T}\} \tag{5}$$

where $\mathbb{P}_k$ is the space of polynomials of degree $\leq K$.
The mean value of φ on the edge e is defined by:

$$\{\{\varphi\}\} = \frac{1}{2}(\varphi^+ + \varphi^-).$$

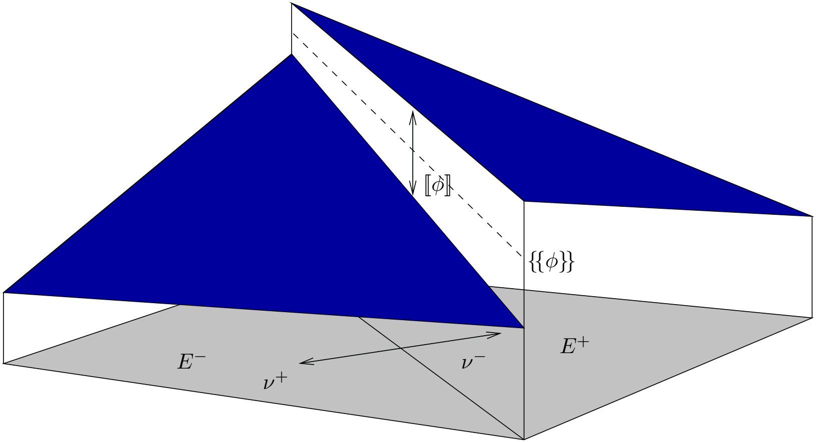
The jump operators on e are given by:

$$[\![\mathbf{v}]\!] = \mathbf{v}^+ \otimes \boldsymbol{n}^+ + \mathbf{v}^- \otimes \boldsymbol{n}^-,$$
$$[\![\varphi]\!] = \varphi^+ \boldsymbol{n}^+ + \varphi^- \boldsymbol{n}^-.$$

Where $\varphi, \mathbf{v}$ take values in $\mathbb{R}, \mathbb{R}^d$.
The set of all edges in the triangulation $\mathcal{T}$ is denoted by

$$\Gamma := \bigcup_{E, E' \in \mathcal{T}} E \cap E'.$$

Mean values and Jumps



Notation

- Let $t_0 = 0 < t_1 < t_2 < \cdots < t_N = T$ a subdivision of the time interval $[0, T]$ and $\Delta t^n := t_n - t_{n-1}$ the n-th time step.
- The backward difference quotient for a time dependent function Φ is denoted by $d_t \Phi^n := \frac{\Phi(\cdot,t_n) - \Phi(\cdot,t_{n-1})}{\Delta t^n}$
- $\Phi^{n-\frac{1}{2}} := \frac{\Phi(\cdot,t_n) + \Phi(\cdot,t_{n-1})}{2}$
- Define $\mathcal{V}_h := V_h \times V_h^d \times V_h \times V_h \times V_h \times V_h^d$
- and $\mathbf{U}_h^n := (\rho^n, \mathbf{v}^n, \varphi^n, \tau^n, \mu^n, \sigma^n) \in \mathcal{V}_h$

We test the continuity equation with a testfunction $\psi \in V_h$

$$\begin{aligned}\sum_{E\in\mathcal{T}}\int_E(\partial_t\rho+\nabla\cdot\rho\mathbf{v})\psi dx \approx & \sum_{E\in\mathcal{T}}\int_E \partial_t\rho\,\psi-\rho\mathbf{v}\cdot\nabla\psi dx \\ & +\int_{\partial_E} G(\rho^+\mathbf{v}^+,\rho^-\mathbf{v}^-)\cdot\boldsymbol{n}^+\psi^+ ds \\ & =\sum_{E\in\mathcal{T}}\int_E(\partial_t\rho+\nabla\cdot\rho\mathbf{v})\psi \\ & -\int_{\partial_E}\rho^+\mathbf{v}^+\cdot\boldsymbol{n}^+\psi^+ ds \\ & +\int_{\partial_E} G(\rho^+\mathbf{v}^+,\rho^-\mathbf{v}^-)\cdot\boldsymbol{n}^+\psi^+ ds\end{aligned} \tag{6}$$

If we set $G(\rho^+v^+\rho^-,\rho^-\mathbf{v}^-)=\{\{\rho\mathbf{v}\}\}$ one can check:

$$\begin{aligned}&-\int_{\partial_E}\rho^+\mathbf{v}^+\cdot\boldsymbol{n}^+\psi^+ ds+\int_{\partial_E} G(\rho^+\mathbf{v}^+,\rho^-\mathbf{v}^-)\cdot\boldsymbol{n}^+\psi^+ ds \\ &=-\int_\Gamma [\![\rho\mathbf{v}]\!]\{\{\psi\}\} ds\end{aligned} \tag{7}$$

Fully Discrete System

Given $\mathbf{U}_h^0 \in \mathcal{V}_h$ find a sequence $(\mathbf{U}_h^n)_{i=1\cdots N}$ so that:

$$0 = \sum_{E\in\mathcal{T}} \int_E \left(d_t\rho^n + \nabla\cdot(\rho^{n-\frac{1}{2}} v^{n-\frac{1}{2}}) \right) \psi dx - \int_\Gamma [\![\rho^{n-\frac{1}{2}} \mathbf{v}^{n-\frac{1}{2}}]\!] \{\{\psi\}\} ds =: \langle F_1(\mathbf{U}_h^n), \psi\rangle,$$

$$0 = \sum_{E\in\mathcal{T}} \int_E \Big(\rho^{n-\frac{1}{2}} d_t(v^n) + \nabla\cdot(\rho^{n-\frac{1}{2}} v^{n-\frac{1}{2}} \otimes v^{n-\frac{1}{2}}) - \nabla\cdot(\rho^{n-\frac{1}{2}} v^{n-\frac{1}{2}}) v^{n-\frac{1}{2}}$$

$$-\frac{1}{2}\rho^{n-\frac{1}{2}} \nabla |v^{n-\frac{1}{2}}|^2 + \rho^{n-\frac{1}{2}} \nabla\mu^{n-\frac{1}{2}} - \tau^{n-\frac{1}{2}} \nabla\varphi^n \Big) \chi dx$$

$$- \int_\Gamma [\![\mu^{n-\frac{1}{2}}]\!] \{\{\rho^{n-\frac{1}{2}} \chi\}\} - [\![\varphi^{n-\frac{1}{2}}]\!] \{\{\tau^{n-\frac{1}{2}} \chi\}\} ds + \mathbb{B}(v^{n-\frac{1}{2}}, \chi) =: \langle F_2(\mathbf{U}_h^n), \chi\rangle,$$

$$0 = \sum_{E\in\mathcal{T}} \int_E \left(d_t\varphi^n + \nabla\varphi^n \cdot v^{n-\frac{1}{2}} + \frac{\tau^{n-\frac{1}{2}}}{\rho^{n-\frac{1}{2}}} \right) \theta dx - \int_\Gamma [\![\varphi^{n-\frac{1}{2}}]\!] \{\{\theta \mathbf{v}^{n-\frac{1}{2}}\}\} ds$$

$$=: \langle F_3(\mathbf{U}_h^n), \theta\rangle,$$

Fully Discrete System

$$
\begin{aligned}
0 = \sum_{E\in\mathcal{T}} \int_E \left(\tau^{\boldsymbol{n}-\frac{1}{2}} - \frac{\Psi(\rho^{n-1},\varphi^n) - \Psi(\rho^{n-1},\varphi^{n-1})}{\varphi^n - \varphi^{n-1}} + \delta\nabla\cdot\sigma^{n-\frac{1}{2}} \right) \zeta dx \\
- \int_\Gamma \delta[\![\sigma^{n-\frac{1}{2}}]\!]\{\{\zeta\}\} ds =: \langle F_4(\mathbf{U}_h^n), \zeta\rangle, \\
0 = \sum_{E\in\mathcal{T}} \int_E \left(\mu^{n-\frac{1}{2}} - \frac{\Psi(\rho^m,\varphi^m) - \Psi(\rho^{m-1},\varphi^m)}{\rho^m - \rho^{m-1}} - \frac{1}{4}(|v^n|^2 + |v^{n-1}|^2) \right) \eta ds \\
=: \langle F_5(\mathbf{U}_h^n), \eta\rangle, \\
0 = \sum_{E\in\mathcal{T}} \int_E (\sigma^n - \nabla\varphi^n)\,\xi dx + \int_\Gamma [\![\varphi^n]\!]\{\{\xi\}\} ds =: \langle F_6(\mathbf{U}_h^n), \xi\rangle.
\end{aligned} \tag{8}
$$

for all $\psi, \chi, \theta, \zeta, \eta, \xi$.

The interior penalty bilinear form

The diffusion part of the momentum balance equation is discretized the bilinear form

$$\mathbb{B}(\mathbf{v},\mathbf{w}) := \sum_{E\in\mathcal{T}} \int_E \mathbb{D}(\nabla\mathbf{v})\nabla\mathbf{w}dx - \sum_{e\in\Gamma}\int_e \{\{\mathbb{D}(\nabla\mathbf{v})\}\}[\![\mathbf{w}]\!] + \{\{\mathbb{D}(\nabla\mathbf{w})\}\}[\![\mathbf{v}]\!] + \sum_{e\in\Gamma}\int_e \frac{\alpha}{|e|}[\![\mathbf{v}]\!][\![\mathbf{w}]\!]ds. \tag{9}$$

Which is coercive if the penalty parameter $\alpha > 0$ is large enough.

D. Arnold, F. Brezzi, B. Cockburn, D. Marini *Unified analysis of discontinuous Galerkin methods for elliptic problems.* SIAM J. Numer. Anal. ,2002

Proposition

The scheme (8) *conserves mass*

$$\int_\Omega \rho_h^n dx = \int_\Omega \rho_h^0 \quad 0 \le n \le N \tag{10}$$

and dissipates energy.

$$\begin{aligned} &\int_\Omega F(\rho_h^n, \varphi_h^n) + \frac{|\sigma_h^n|^2}{2} + \rho_h^n \frac{|\mathbf{v}_h^n|^2}{2} dx \\ &- \int_\Omega F(\rho_h^{n-1}, \varphi_h^{n-1}) + \frac{|\sigma_h^{n-1}|^2}{2} + \rho_h^{n-1} \frac{|\mathbf{v}_h^{n-1}|^2}{2} dx \\ &= -\frac{(\tau_h^{n-\frac{1}{2}})^2}{\rho_h} - \mathbb{B}(\nabla \mathbf{v}_h^{n-\frac{1}{2}}, \nabla \mathbf{v}_h^{n-\frac{1}{2}}) \end{aligned} \tag{11}$$

Approximate Jacobian

UNI FREIBURG

With

$$\langle F_1(\mathbf{U}_h^n), \psi\rangle = \sum_{E\in\mathcal{T}} \int_E \left(d_t\rho^n + \nabla\cdot(\rho^{n-\frac{1}{2}} v^{n-\frac{1}{2}})\right)\psi dx - \int_\Gamma [\![\rho^{n-\frac{1}{2}}\mathbf{v}^{n-\frac{1}{2}}]\!]\{\{\psi\}\} ds,$$
$$\langle F_2(\mathbf{U}_h^n), \chi\rangle = \cdots$$
$$\cdots \tag{12}$$

the scheme defines a mapping

$$F : \mathcal{V}_h \to \mathcal{V}_h^*$$

Let $\mathbf{V} = (\psi, \chi, \theta, \zeta, \eta, \xi) \in \mathcal{V}_h$

$$\langle F(\mathbf{U}_h), \mathbf{V}\rangle = \langle F_1(\mathbf{U}_h^n), \psi\rangle + \langle F_2(\mathbf{U}_h^n), \chi\rangle + \langle F_1(\mathbf{U}_h^n), \theta\rangle + \langle F_4(\mathbf{U}_h^n), \zeta\rangle + \langle F_5(\mathbf{U}_h^n), \eta\rangle + \langle F_5(\mathbf{U}_h^n), \xi\rangle$$

Approximate Jacobian

Writing $\mathbf{U}_h^n$ as

$$\mathbf{U}_h^n = \sum_{i=1}^{dim\mathcal{V}_h} u_i^n \varphi_i$$

the discrete Operator

$$\bar{F} : \mathbb{R}^{dim\mathcal{V}_h} \to \mathbb{R}^{dim\mathcal{V}_h}$$

is defined by

$$\bar{F}(u_1 \cdots u_{dim\mathcal{V}_h})_j = \langle F(\mathbf{U}_h^n), \varphi_j \rangle.$$

In each time step we have to solve an equation of the form

$$\bar{F}(u_1^n \cdots u_k^n) = 0. \tag{13}$$

Approximate Jacobian

- To use Newton's method we need the Jacobian $J\bar{F}(u) := D\bar{F}(u)$
- Matrix free method:Only the application

$$J\bar{F}(u)v$$

  is calculated.
- standard preconditioning methods are not applicable.
- Therefore the we compute the components of the Jacobian matrix by finite differences:

$$(JF(u))_{i,j} = (\partial_{u_i} F(u)_j) \approx \frac{1}{\varepsilon} \left[\langle F(u_h + \varepsilon \varphi_j), \varphi_i \rangle - \langle F(u_h), \varphi_i \rangle \right] \quad (14)$$

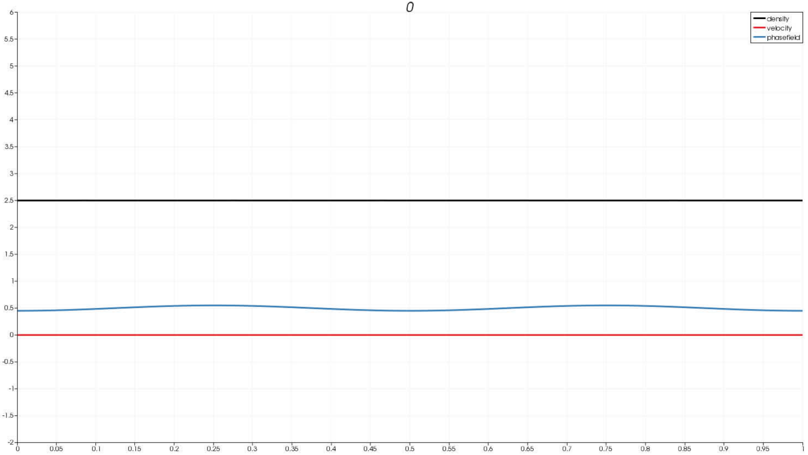
- The DG basisfunctions vanish outside of one mesh element.
- The matrix can be computed traversing each element and it's neighbors for the flux part.

Numerical Experiments

- μ_1 and μ_2 are chosen so that $\nabla \cdot \mathbb{D}(\nabla \mathbf{v}) = \varepsilon \Delta \mathbf{v}$ with $\varepsilon = 0.01$.
- $h_1 = h_2 = 1$ are constant.
- GMRES with *ILU* preconditioning for the linear subproblem of the Newton solver.
- $\Delta t = 1e - 3$.
- 320 cells in $1d$.
- 200×200 cells in 2d.

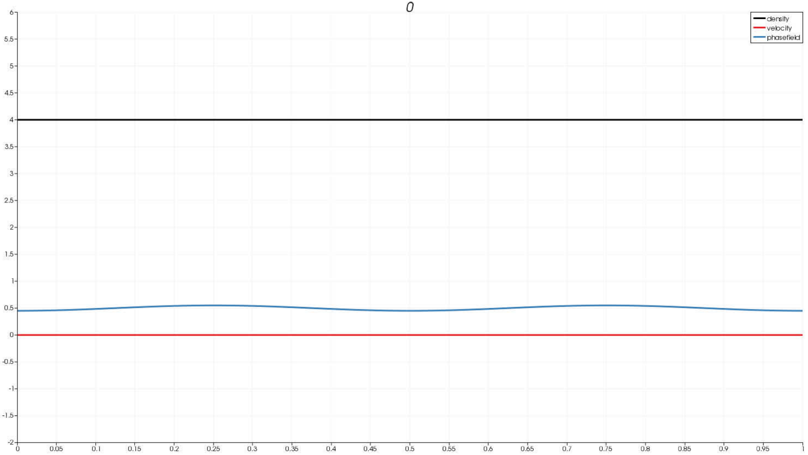
Numerical Experiments

$\delta = 0.025, \rho_0 = 2.5$

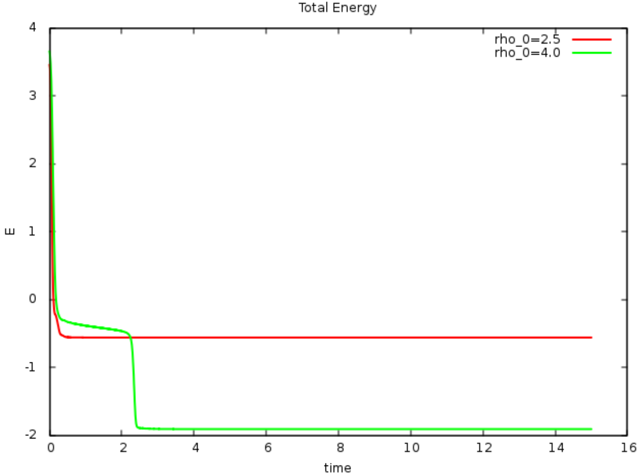


Numerical Experiments

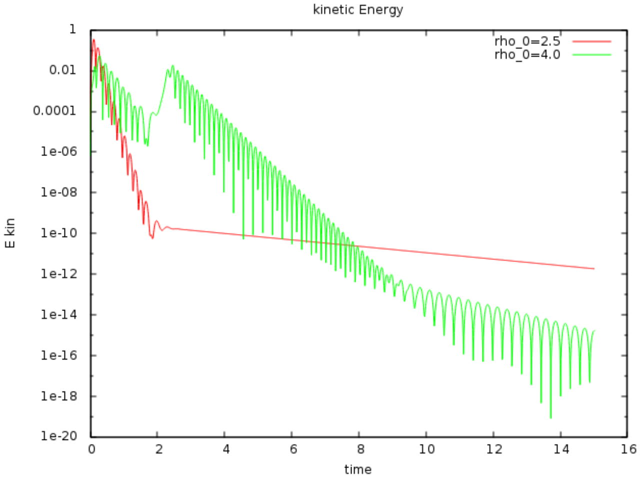
$\delta = 0.025, \rho_0 = 4$



Total and Kinetic Energy

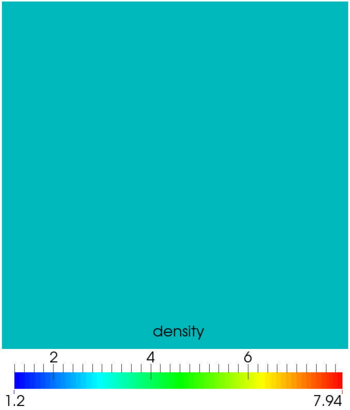


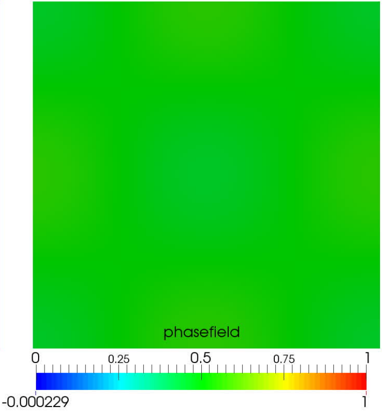
Total and Kinetic Energy



Numerical Experiments

$$\delta = 0.025, \rho_0 = 2.2$$





- A energy consistent numerical method was presented.
- Using an approximated Jacobian Matrix in the Newton-Method allows for general preconditioning methods.
- Because of the preconditioning the use of the approximated matrix is more efficient than the matrix free version.

G. WITTERSTEIN
Sharp Interface Limit of Phase Change Flows,
Adv. Math. Sci. Appl.,2010

H.W. ALT, G. WITTERSTEIN
Distributional equation in in the limit of phase transition for fluids,
Interfaces and Boundaries.,2011

J. GIESSELMANN, C. MAKRIDAKIS, T. PRYER
Energy consistent DG methods for the Navier-Stokes-Korteweg system
Mathematics of Computation, 2014

Y. SAAD
Iterative Methods for Sparse Linear Systems
PWS Publishing Company, Boston,1996

D. ARNOLD, F. BREZZI, B. COCKBURN, D. MARINI *Unified analysis of discontinuous Galerkin methods for elliptic problems.*
SIAM J. Numer. Anal. ,2002