A Local Discontinuous Galerkin method for a compressible phase field model

Mirko Kränkel, Dietmar Kröner

14. Februar 2012

Albert-Ludwigs-Universität Freiburg

Introduction

Phase field Model

The LDG-Method

Numerical Results

Summary

Introduction

Phase field Model

The LDG-Method

Numerical Results

Summary

- Goal: Simulation of phase transitions between liquid and vapor
- 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.
- In [3, Diehl] the smallness of the interface was the 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.

Introduction

Phase field Model

The LDG-Method

Numerical Results

Summary

Governing Equations

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

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

$$\partial_t(\rho v) + \nabla \cdot (\rho v \otimes v + \Pi) = 0, \tag{2}$$

$$\rho(\partial_t \phi + v \cdot \nabla \phi) = -\frac{1}{\delta} \frac{\delta f}{\delta \phi}. \tag{3}$$

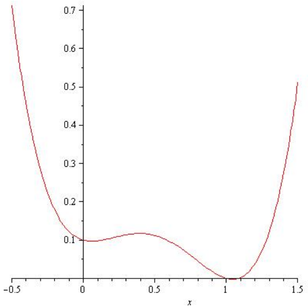
for $x \in \Omega \subset \mathbb{R}^d$, $t > 0$.
With a tension tensor $\Pi := D(\nabla v) + P(\rho, \phi, \nabla \phi)$, a free energy $f = f(\rho, \phi, \nabla \phi)$ and $\frac{\delta f}{\delta \phi}$ denoting the first Variation $f_{|\phi} - \nabla \cdot (f_{|\nabla \phi})$

Governing Equations

The free Energy has the form

$$f(\rho, \phi, \nabla\phi) := \frac{1}{\delta}\rho W(\phi) + \delta\rho\frac{|\nabla\phi|^2}{2} + \psi(\rho, \phi) \qquad (4)$$

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



Governing Equations

The free Energy has the form

$$f(\rho, \phi, \nabla\phi) := \frac{1}{\delta}\rho W(\phi) + \delta\rho\frac{|\nabla\phi|^2}{2} + \psi(\rho, \phi) \tag{5}$$

The function ψ models the physics in the pure phases.

$$\psi(\rho, \phi,) := \nu(\phi) f_2(\rho) + (1 - \nu(\phi)) f_1(\rho) \tag{6}$$

here f_1, f_2 are free energy densities for the two phases and ν is interpolation function with

$$\nu'(1) = \nu'(0) = 0 \tag{7}$$

The pressure and stress tensor P, D are given

$$P := P(\rho, \phi, \nabla\phi) = (-\psi + \rho\psi_{|\rho})\mathbb{I} + \delta(\rho\nabla\phi \otimes \nabla\phi) \tag{8}$$

and the stress tensor D

$$D := \mu_1 \nabla \cdot v\mathbb{I} + \mu_2(\frac{1}{2}(\nabla v + (\nabla v))^T - \frac{1}{d}\nabla \cdot v\mathbb{I}) \tag{9}$$

with $\mu_1, \mu_2 > 0$ so that $D \cdot \nabla v > 0$ and the source term

$$\frac{\delta f}{\delta\phi} = \frac{1}{\delta}\rho W_{|\phi}(\phi) + \psi_{|\phi}(\rho, \phi) - \delta\nabla \cdot (\rho\nabla\phi) \tag{10}$$

Using the conservation of total mass we can write

$$\partial_t \rho + \nabla \cdot \rho v = 0 \tag{11}$$

$$\partial_t(\rho v) + \nabla \cdot (\rho v \otimes v + \Pi) = 0 \tag{12}$$

$$\rho(\partial_t \phi + v \cdot \nabla \phi) = -\frac{1}{\delta}\frac{\delta f}{\delta \phi} \tag{13}$$

as second-order balance law of the form

$$\partial_t U + \nabla \cdot F(U) + \nabla \cdot T(U, \nabla U) + \nabla \cdot D(U, \nabla U) = S(U) \tag{14}$$

with

$$U := \begin{pmatrix} \rho \\ \rho v \\ \rho\phi \end{pmatrix} \qquad F(U) := \begin{pmatrix} \rho v \\ \rho v \otimes v + p \\ \rho\phi v \end{pmatrix}$$

$$T(U, \nabla U) := \begin{pmatrix} 0 \\ \rho\nabla\phi \otimes \nabla\phi \\ 0 \end{pmatrix} \quad S(U) := \begin{pmatrix} 0 \\ 0 \\ -\frac{1}{\delta}\frac{\delta f}{\delta\phi} \end{pmatrix}$$

The diffusion tensor

$$D(U,\nabla U) \quad := \quad \begin{pmatrix} 0 \\ -D_v(U,\nabla U) \\ \delta\rho\nabla\phi \end{pmatrix}$$

with

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

Note that D_v can be written as

$$D_v(U,\nabla U) = A(U)\nabla U$$

We want to solve the system

$$\partial_t U + \nabla \cdot F(U) + \nabla \cdot T(U, \nabla U) + \nabla \cdot [A(U)\nabla U] = S(U) \quad (15)$$

with boundary conditions:

$$\nabla \rho \cdot \boldsymbol{\nu} = 0, v = 0, \nabla \phi \cdot \boldsymbol{\nu} = 0 \quad \text{on } \partial\Omega \quad (16)$$

and initial conditions

$$\rho(0, x) = \rho_0(x), v(0, x) = v_0(x), \phi(0, x) = \phi_0(x) \quad (17)$$

Introduction

Phase field Model

The LDG-Method

Numerical Results

Summary

The LDG-Method

To discretize the system of equations we used a Local-Discontinuous-Galerkin Method, similar to the LDG-method developed in [3, Diehl]

- Write the system as a first order system.
- On a given grid elementwise polynomial ansatzfunctions are used , which are allowed to be discontinuous over element boundaries.
- The values on the edges are approximated using numerical fluxes.
- Suitable for adaptive and parallel computations.
- For the numerical results presented the **DUNE** and **DUNE-FEM** software environment was used.

The first order system

We introduce the auxiliary variables σ and θ to write the equation

$$\partial_t U + \nabla \cdot F(U) + \nabla \cdot T(U, \nabla U) + \nabla \cdot [A(U)\nabla U] = S(U). \quad (18)$$

as a system of first order equations

$$\begin{aligned} \sigma - \nabla U &= 0, && (19) \\ \theta - T(U, \sigma) &= 0, && (20) \\ \partial_t U + \nabla \cdot F(U) + \nabla \cdot \theta + \nabla \cdot [A(U)\sigma] &= S(U). && (21) \end{aligned}$$

Definition

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

$$V_h := \{u \in L^2(\Omega) : u_{|E} \in \mathbb{P}_k \text{for all } E \in \mathcal{T}\} \qquad (22)$$

where $\mathbb{P}_k$ is the space of polynomials of degree $\leq K$.

Mean values and Jumps

Definition

The mean value of ϕ on the edge e is defined by:

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

The jump operators on e are given by:

$$[\![u]\!] = u^+ \otimes \boldsymbol{\nu}^+ + u^- \otimes \nu^-,$$
$$[\![\sigma]\!] = \sigma^+ n^+ + \sigma^- n^-,$$

Where u, σ take values in $\mathbb{R}^{d+2}, \mathbb{R}^{(d+2)\times d}$.

multiplying

$$\sigma - \nabla U = 0, \quad (23)$$

$$\theta - T(U,\sigma) = 0, \quad (24)$$

$$\partial_t U + \nabla \cdot F(U) + \nabla \cdot \theta + \nabla \cdot A(U)\sigma = S(U). \quad (25)$$

with test functions and integrating by parts on each element $E \in \mathcal{T}$

$$\int_E \sigma : \tau \,\mathrm{dx} = -\int_e u \cdot \nabla \cdot \tau \,\mathrm{dx} + \int_{\partial E} u\tau \cdot \boldsymbol{\nu} \,\mathrm{ds}, \quad (26)$$

$$\int_E \theta : \xi \,\mathrm{dx} = \int_E T(u,\sigma) : \xi \,\mathrm{dx}, \quad (27)$$

$$\int_E \partial_t u \cdot \phi = -\int_E [F(u) + \theta + A(u)\sigma] \cdot \nabla\phi - S(u)\phi \,\mathrm{dx} \quad (28)$$

$$+ \int_{\partial E} [F(u) + \theta + A(u)\sigma] \cdot \boldsymbol{\nu}\phi \,\mathrm{ds}. \quad (29)$$

where $\tau \in [V_h]^{(d+2)\times d}, \xi \in [V_h]^{(d+2)\times d}, \phi \in [V_h]^{d+2}$.

The numerical fluxes

The numerical fluxes on the edge e are given by:

$$\begin{aligned}\widehat{\sigma} &:= \{\!\{A(U)\sigma\}\!\} - [\![A(U)\sigma]\!] \otimes \boldsymbol{\beta} - \frac{\alpha}{h}\{\!\{A(U)\}\!\}[\![U]\!],\\ \widehat{\theta} &:= \{\!\{\theta\}\!\} - [\![\theta]\!] \otimes \boldsymbol{\beta} - \frac{\alpha}{h}[\![U]\!],\\ \widehat{U} &:= \{\!\{U\}\!\} + [\![U]\!] \cdot \boldsymbol{\beta}.\end{aligned}$$

where h denotes the mesh size, $\alpha > 0$ and $\boldsymbol{\beta}$ a *switch function*. For an edge e with neighboring elements E_e^+, E_e^- it holds $\boldsymbol{\beta} = \frac{1}{2}\boldsymbol{\nu}_{E_e^-} = -\frac{1}{2}\boldsymbol{\nu}_{E_e^+}$.

$$
\begin{aligned}
\{\!\{A(U)\sigma\}\!\} - [\![A(U)\sigma]\!] \otimes \boldsymbol{\beta} &:= \begin{cases} A(U)^+\sigma^+ \\ A(U)^-\sigma^- \end{cases} \\
\{\!\{\theta\}\!\} - [\![\theta]\!] \otimes \boldsymbol{\beta} &:= \begin{cases} \theta^+ \\ \theta^- \end{cases} \\
\{\!\{U\}\!\} + [\![U]\!] \cdot \boldsymbol{\beta} &:= \begin{cases} U^- \\ U^+ \end{cases}
\end{aligned}
$$

for the advective part a Lax-Friedrich flux is chosen

$$
\widehat{F}(u^+, u^-) := \frac{1}{2}(F(u^+) + F(u^-)) \cdot \boldsymbol{\nu} - \lambda(u^+ - u^-). \qquad (30)
$$

The numerical solution U_h can then be computed by solving the discrete system

$$\int_E \sigma_h : \tau \,\mathrm{d}x = \int_E U_h \cdot \nabla \cdot \tau \,\mathrm{d}x - \int_{\partial E} \widehat{U} \cdot \tau \cdot \boldsymbol{\nu} \,\mathrm{d}s, \tag{31}$$

$$\int_E \theta_h : \xi \,\mathrm{d}x = \int_E T(U_h, \sigma_h) \cdot \xi \,\mathrm{d}x, \tag{32}$$

$$\int_E \partial_t U_h \cdot \psi = \int_E (F(U_h) + \theta + A(U)\sigma_h) \cdot \nabla\psi - S(U_h)\psi \,\mathrm{d}x, \tag{33}$$
$$- \int_{\partial E} (\widehat{F} + \widehat{\theta} + \widehat{\sigma})\psi \cdot \boldsymbol{\nu} \,\mathrm{d}s.$$

for all $\tau \in [V_h]^{(d+2)\times d}, \xi \in [V_h]^{(d+2)\times d}, \psi \in [V_h]^{d+2}$.

Solving locally for σ_h, θ_h and $\partial_t U_h$ we can write (31) – (33) in operator form

$$\sigma_h = L_1[U_h], \tag{34}$$

$$\theta_h = L_2[\sigma_h, U_h], \tag{35}$$

$$\partial_t U_h = L_3[\theta_h, \sigma_h, U_h]. \tag{36}$$

We know have to solve the nonlinear system of ODEs

$$\partial_t U_h = L[U_h] := L_3[L_2[L_1[U_h], U_h], L_1[U_h], U_h]. \tag{37}$$

For solving

$$\partial_t U_h = L[U_h]$$

we use explicit and implicit Runge-Kutta schemes. In the implicit case the nonlinear system is solved by an inexact Newton-method, for the inner solver restarted GMRES is used.

We want to resolve the interfacial region, therefore a simple indicator for refining the mesh is to use the phase field variable ϕ an refine the elements where

$$|\phi - \frac{1}{2}| \leq \frac{\eta}{2}. \tag{38}$$

If η is chosen close to 1 the mesh is refined around the interface as desired.

Introduction

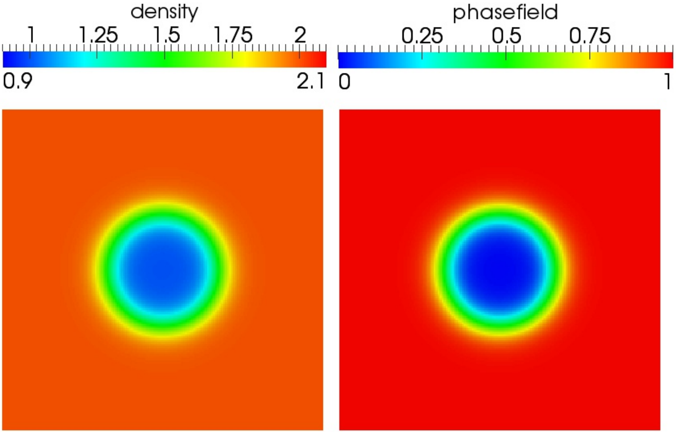
Phase field Model

The LDG-Method

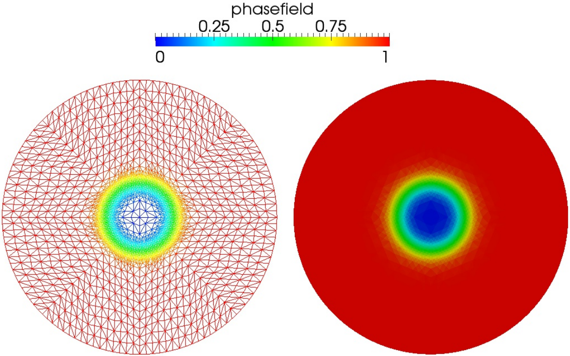
Numerical Results

Summary

Ideal gas EOS in both phases, $\delta = 0.01$



Locally refined mesh, $\delta = 0.01$



Introduction

Phase field Model

The LDG-Method

Numerical Results

Summary

- The explicit numerical scheme needs very small time steps to be stable
- In the implicit case the solver converge slowly, therefore preconditioning for the matrix free operator is needed.
- This difficulties might arise due to the different timescales in the Allen-Cahn equation and the Navier-Stokes system.
- A nonconservative scheme should lead to better results.

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

D.DIEHL
Higher Order Schemes for Simulation of Compressible Liquid-Vapour Flows with phase change,
doctoral thesis,2007