

A Local Discontinuous Galerkin method for a compressible phase field model

MIRKO KRÄNKEL, DIETMAR KRÖNER

14. Februar 2012

Albert-Ludwigs-Universität Freiburg

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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.

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

$$\partial_t \rho + \nabla \cdot \rho \mathbf{v} = 0, \quad (1)$$

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

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

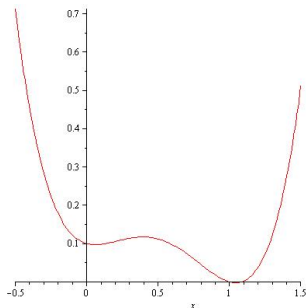
for $x \in \Omega \subset \mathbb{R}^d$, $t > 0$.

With a tension tensor $\Pi := D(\nabla \mathbf{v}) + P(\rho, \phi, \nabla \phi)$, a free energy $f = f(\rho, \phi, \nabla \phi)$ and $\frac{\delta f}{\delta \phi}$ denoting the first Variation $f|_{\phi} - \nabla \cdot (f|_{\nabla \phi})$

The free Energy has the form

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

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



The free Energy has the form

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

The function ψ models the physics in the pure phases.

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

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

$$\nu'(1) = \nu'(0) = 0 \quad (7)$$

The pressure and stress tensor P, D are given

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

and the stress tensor D

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

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

$$\frac{\delta f}{\delta \phi} = \frac{1}{\delta} \rho W|_{\phi}(\phi) + \psi|_{\phi}(\rho, \phi) - \delta \nabla \cdot (\rho \nabla \phi) \quad (10)$$

Using the conservation of total mass we can write

$$\partial_t \rho + \nabla \cdot \rho \mathbf{v} = 0 \quad (11)$$

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

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

as second-order balance law of the form

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

with

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

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

The diffusion tensor

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

with

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

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:

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

and initial conditions

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

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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.

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

$$\sigma - \nabla U = 0, \quad (19)$$

$$\theta - T(U, \sigma) = 0, \quad (20)$$

$$\partial_t U + \nabla \cdot F(U) + \nabla \cdot \theta + \nabla \cdot [A(U) \sigma] = S(U). \quad (21)$$

Definition

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

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

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

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:

$$\begin{aligned} \llbracket u \rrbracket &= u^+ \otimes \nu^+ + u^- \otimes \nu^-, \\ \llbracket \sigma \rrbracket &= \sigma^+ n^+ + \sigma^- n^-, \end{aligned}$$

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
 $E \in \mathcal{T}$

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

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

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

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

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 on the edge e are given by:

$$\hat{\sigma} := \{A(U)\sigma\} - \llbracket A(U)\sigma \rrbracket \otimes \beta - \frac{\alpha}{h} \{A(U)\} \llbracket U \rrbracket,$$

$$\hat{\theta} := \{\theta\} - \llbracket \theta \rrbracket \otimes \beta - \frac{\alpha}{h} \llbracket U \rrbracket,$$

$$\hat{U} := \{U\} + \llbracket U \rrbracket \cdot \beta.$$

where h denotes the mesh size, $\alpha > 0$ and β a *switch function*.

For an edge e with neighboring elements E_e^+ , E_e^- it holds

$$\beta = \frac{1}{2} \nu_{E_e^-} = -\frac{1}{2} \nu_{E_e^+}.$$

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

for the advective part a Lax-Friedrich flux is chosen

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

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

$$\int_E \sigma_h : \tau \, dx = \int_E U_h \cdot \nabla \cdot \tau \, dx - \int_{\partial E} \hat{U} \cdot \tau \cdot \nu \, ds, \quad (31)$$

$$\int_E \theta_h : \xi \, dx = \int_E T(U_h, \sigma_h) \cdot \xi \, dx, \quad (32)$$

$$\begin{aligned} \int_E \partial_t U_h \cdot \psi &= \int_E (F(U_h) + \theta + A(U)\sigma_h) \cdot \nabla \psi - S(U_h)\psi \, dx, \quad (33) \\ &\quad - \int_{\partial E} (\hat{F} + \hat{\theta} + \hat{\sigma})\psi \cdot \nu \, ds. \end{aligned}$$

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

$$\sigma_h = L_1[U_h], \quad (34)$$

$$\theta_h = L_2[\sigma_h, U_h], \quad (35)$$

$$\partial_t U_h = L_3[\theta_h, \sigma_h, U_h]. \quad (36)$$

We know have to solve the nonlinear system of ODEs

$$\partial_t U_h = L[U_h] := L_3[L_2[L_1[U_h], U_h], L_1[U_h], U_h]. \quad (37)$$

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 and refine the elements where

$$|\phi - \frac{1}{2}| \leq \frac{\eta}{2}. \quad (38)$$

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

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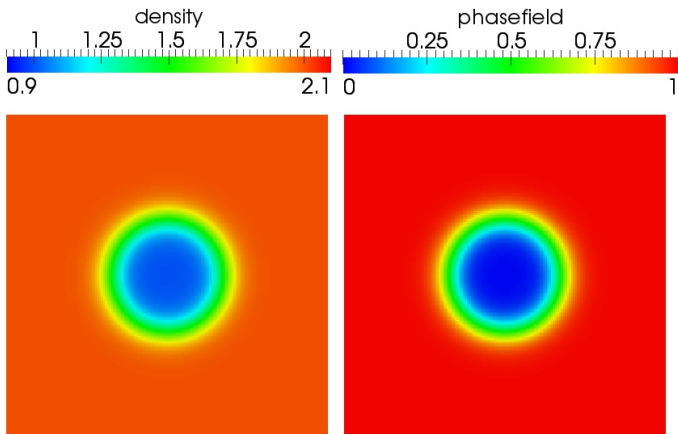
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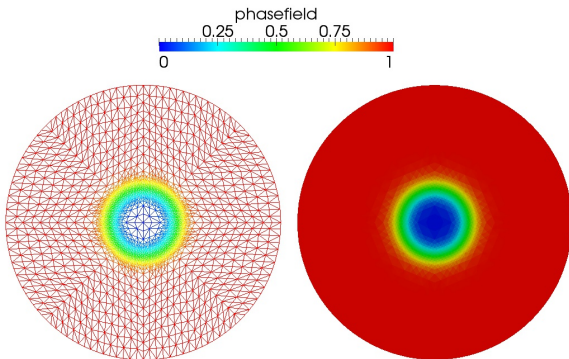
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Ideal gas EOS in both phases, $\delta = 0.01$



Locally refined mesh, $\delta = 0.01$



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- ▶ 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.



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