Simulation of compressible two-phase flow using the Navier-Stokes-Allen-Cahn model

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Outline

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- Goal: Simulation of two phase flow (liquid and vapor)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
- The small size of the interfacial layer is one main difficulty for the numerical treatment.
- We want to use a phase field type model, where the thickness of the interface can be easily controlled, without changing the surface tension.

Governing Equations

The NS-AC-model (see [1, Witterstein1]) consists of the compressible Navier-Stokes equations and an Allen-Cahn like equation for the phase field parameter φ.

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

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

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

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

with a helmholtz free energy $\mathbf{F} = \mathbf{F}(\rho, \varphi, \nabla\varphi) = \frac{A}{\delta} W(\varphi) + \Psi(\rho, \varphi) + A\delta \frac{|\nabla\varphi|^2}{2}$ and mobility $\eta > 0$.

Governing Equations

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

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

and

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

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:

$$\frac{\delta F}{\delta \varphi} = \frac{A}{\delta} W_\varphi(\varphi) + \frac{\partial \Psi}{\partial \varphi}(\rho, \varphi) - \nabla \cdot (A\delta \nabla\varphi).$$

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*

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

Helmholtz free energy

The helmholtz free energy has the form

$$\mathbf{F}(\rho, \varphi, \nabla\varphi) := \frac{A}{\delta} W(\varphi) + \Psi(\rho, \varphi) + A\delta \frac{|\nabla\varphi|^2}{2}.$$

- Ψ is a nonlinear interpolation of the free energies f_1 and f_2 of the pure phases.

$$\Psi(\rho, \varphi) = \nu(\varphi) f_1(\rho) + (1 - \nu(\varphi)) f_2(\rho) \quad \text{with} \quad \nu'(1) = \nu'(0) = 0. \qquad (5)$$

- W is a double-well function in φ.
- The factors $\frac{A}{\delta}$ and $A\delta$ in front of W and $\frac{|\nabla\varphi|^2}{2}$ are chosen according the scaling in [1], which leads to nonvanishing surface tension in the sharp interface limit.

Helmholtz free energy

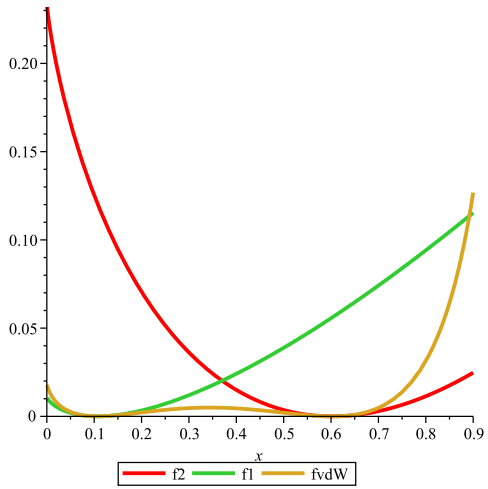
The helmholtz free energy has the form

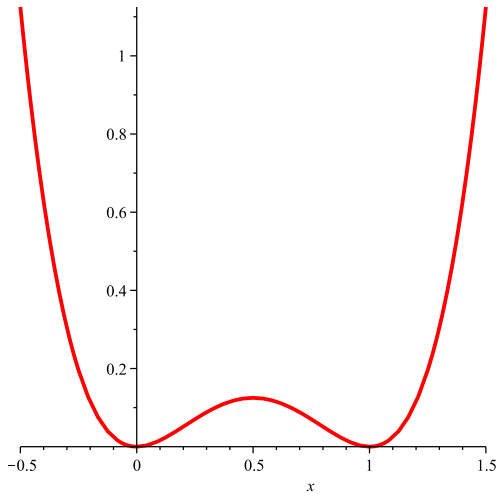
$$F(\rho, \varphi, \nabla\varphi) := \frac{A}{\delta} W(\varphi) + \psi(\rho, \varphi) + A\delta \frac{|\nabla\varphi|^2}{2}.$$

Bulk-Energy

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

$W(\varphi)$ is double-well function with respect to φ.





Surface tension

In an equilibrium situation, one can show that the gibbs free energy defined as $\frac{\partial \mathbf{F}}{\partial \rho}$ has to be constant:

$$\frac{\partial \mathbf{F}}{\partial \rho}(\rho, \varphi) = \mu_{eq}. \tag{6}$$

As $\mathbf{F}$ is convex in ρ, there is by the implicit function theorem, a function $\rho^*(\varphi)$ so that,

$$\frac{\partial \mathbf{F}}{\partial \rho}(\rho^*(\varphi), \varphi) = \mu_{eq}. \tag{7}$$

For a planar interface in equilibrium the surface tension can be expressed as:

$$\begin{aligned} \sigma &= \int_{-\infty}^{\infty} A\delta \frac{\partial \varphi}{\partial z}^2 \, \mathrm{d}z = \int_0^1 \sqrt{\delta 2(\frac{A}{\delta} W(\varphi) + \mathbf{\Psi}(\rho^*(\varphi), \varphi))} \, \mathrm{d}\varphi \\ &= A \int_0^1 \sqrt{2(W(\varphi) + \frac{\delta}{A} \mathbf{\Psi}(\rho^*(\varphi), \varphi))} \, \mathrm{d}\varphi. \end{aligned} \tag{8}$$

Modified double-well

For numerical reasons, we modify the helmholtz free energy so that,

$$\mathbf{F} = \frac{A}{\delta} W(\varphi) - \Psi(\rho^*(\varphi), \varphi) + \Psi(\rho, \varphi) + A\delta \frac{|\nabla|^2}{2}$$

Then

$$\sigma = A \int_0^1 \sqrt{2W(\varphi)}\, \mathrm{d}\varphi = A \cdot Const. \tag{9}$$

- σ is independent of δ.
- In a similar way one can show, that the width of the interface does not depend on A.
- The interface can be enlarged in numerical simulation.
- The limit $\delta \to 0$ is not changed, as the correction term is $\mathcal{O}(\delta)$.
- If ρ is too far from equilibrium, or δ is too large, unphysical states may occur, as the corrected W might have additional extrema.

The Energy consistent DG-Method

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- 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 environment: 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 auxiliary variables τ, μ, σ

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

and noting that

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

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

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

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

Definition

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

$$V_h := \{u \in L^2(\Omega) : u_{|E} \in \mathbb{P}_k \text{for all } E \in \mathcal{T}\} \tag{10}$$

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:

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

The jump operators on e are given by:

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

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 $\mathbf{U}_h^n := (\rho^n, \mathbf{v}^n, \varphi^n, \tau^n, \mu^n, \sigma^n) \in \mathcal{V}_h$

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:

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

$$\begin{aligned} 0 = \sum_{E\in\mathcal{T}} \int_E \Big(& \rho^{n+\frac{1}{2}} d_t(v^n) + \nabla \cdot (\rho^{n+\frac{1}{2}} v^{n+\frac{1}{2}} \otimes v^{n+\frac{1}{2}}) - \nabla \cdot (\rho^{n+\frac{1}{2}} v^{n+\frac{1}{2}}) v^{n+\frac{1}{2}} \\ & - \frac{1}{2} \rho^{n+\frac{1}{2}} \nabla |v^{n+\frac{1}{2}}|^2 \rho^{n+\frac{1}{2}} \left[DS(\nabla v^{n+\frac{1}{2}}) \right] v^{n+\frac{1}{2}} + \rho^{n+\frac{1}{2}} \nabla \mu^{n+\frac{1}{2}} - \tau^{n+\frac{1}{2}} \nabla \varphi^n \Big) \chi dx \\ & - \int_\Gamma [\![\mu^{n+\frac{1}{2}}]\!] \{\!\{ \rho^{n+\frac{1}{2}} \chi \}\!\} - [\![\varphi^{n+\frac{1}{2}}]\!] \{\!\{ \tau^{n+\frac{1}{2}} \chi \}\!\} ds + \mathbb{B}(v^{n+\frac{1}{2}}, \chi) \end{aligned}$$

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

Fully Discrete System

$$
\begin{aligned}
0 &= \sum_{E\in\mathcal{T}} \int_E \left(\tau^{n+\frac{1}{2}} - \frac{\Psi(\rho^{n-1},\varphi^n) - \mathbf{F}(\rho^{n-1},\varphi^{n-1})}{\varphi^n - \varphi^{n-1}} + \delta \nabla\cdot\sigma^{n+\frac{1}{2}} \right) \zeta dx \\
&\quad - \int_\Gamma \delta [\![\sigma^{n+\frac{1}{2}}]\!] \{\!\{\zeta\}\!\} ds, \\
0 &= \sum_{E\in\mathcal{T}} \int_E \left(\mu^{n+\frac{1}{2}} - \frac{\mathbf{F}(\rho^n,\varphi^n) - \mathbf{F}(\rho^{n-1},\varphi^n)}{\rho^n - \rho^{n-1}} - \frac{1}{4}(|v^n|^2 + |v^{n-1}|^2) \right) \eta ds \\
0 &= \sum_{E\in\mathcal{T}} \int_E \left(\sigma^n - \nabla\varphi^n\right) \xi dx + \int_\Gamma [\![\varphi^n]\!] \{\!\{\xi\}\!\} ds.
\end{aligned}
\tag{11}
$$

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

The interior penalty bilinear form

The diffusion part of the momentum balance equation is discretized the symmetric interior penalty bilinear form:

$$\mathbb{B}(\mathbf{v},\mathbf{w}) := \sum_{E\in\mathcal{T}}\int_E \mathbb{D}(\nabla\mathbf{v})\nabla\mathbf{w}dx - \sum_{e\in\Gamma}\int_e \{\{\mathbb{D}(\nabla\mathbf{v})\}\}[\![\mathbf{w}]\!] + \{\{\mathbb{D}(\nabla\mathbf{w})\}\}[\![\mathbf{v}]\!] + \sum_{e\in\Gamma}\int_e \frac{\alpha}{|e|}[\![\mathbf{v}]\!][\![\mathbf{w}]\!]ds. \tag{12}$$

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 (11) *conserves mass*

$$\int_\Omega \rho_h^n dx = \int_\Omega \rho_h^0 \quad 0 \leq n \leq N \tag{13}$$

and dissipates energy.

$$\begin{aligned} &\int_\Omega F(\rho_h^n, \varphi_h^n) + \frac{|\sigma_h^n|^2}{2} + \rho_h^n \frac{|\mathbf{v}_h^n|^2}{2} dx \\ &- \int_\Omega F(\rho_h^{n-1}, \varphi_h^{n-1}) + \frac{|\sigma_h^{n-1}|^2}{2} + \rho_h^{n-1} \frac{|\mathbf{v}_h^{n-1}|^2}{2} dx \\ &= -\frac{(\tau_h^{n-\frac{1}{2}})^2}{\rho_h} - \mathbb{B}(\nabla \mathbf{v}_h^{n+\frac{1}{2}}, \nabla \mathbf{v}_h^{n+\frac{1}{2}}) \end{aligned} \tag{14}$$

Setting

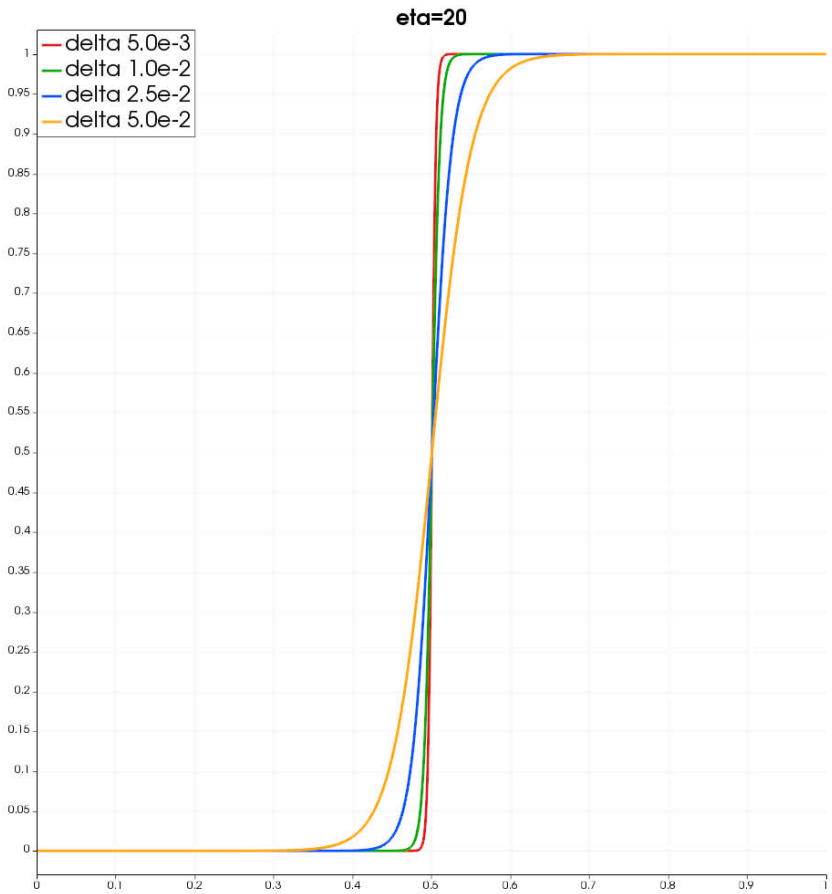
- The free energies of the bulk phases are convex functions of Stiffened-Gas Type:

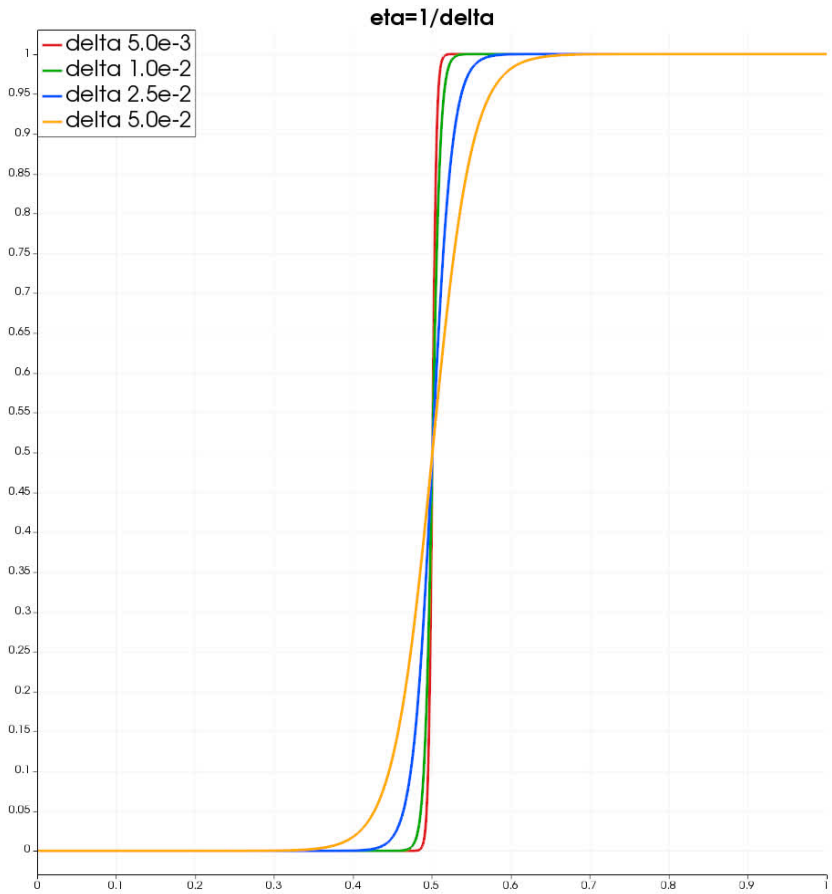
$$f_i := a_i \rho \log(\rho) + (b_i - a_i)\rho + c_i. \tag{15}$$

- Pressure, chemical and sound speed are matched to the values at saturation given by the vanderWaals-EOS at $0.85 T_{crit}$.
- $\mu_1 = 1e-3$ and $\mu_2 = -\frac{2}{3}\mu_1$
- $A = 1e-4$
- In 2d an adaptive method is used, which guarantees ≈ 10 elements in the interfacial layer.
- In each time step a nonlinear system is solved by an inexact newton method.
- The linear subproblem is solved using the preconditioned GMRES method.

Mobility Scaling

Effect of the mobility η in the situation of compressed vapor, for different delta.
The vapor density is $2\rho_{sat}^{va}$, the fluid density is ρ_{sat}^{liq}.

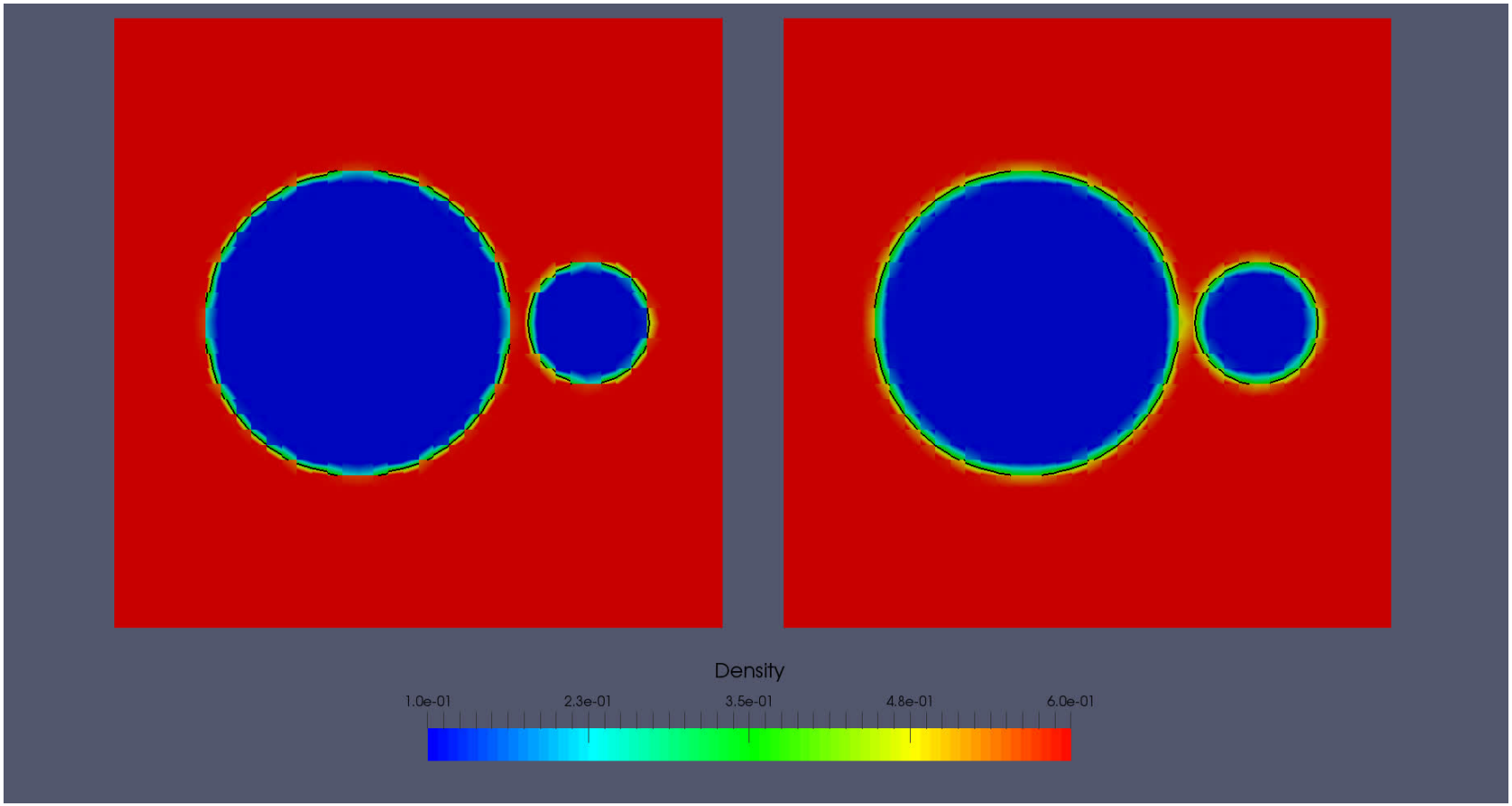




Two Bubbles

Vapor and Liquid density are at the saturation values.

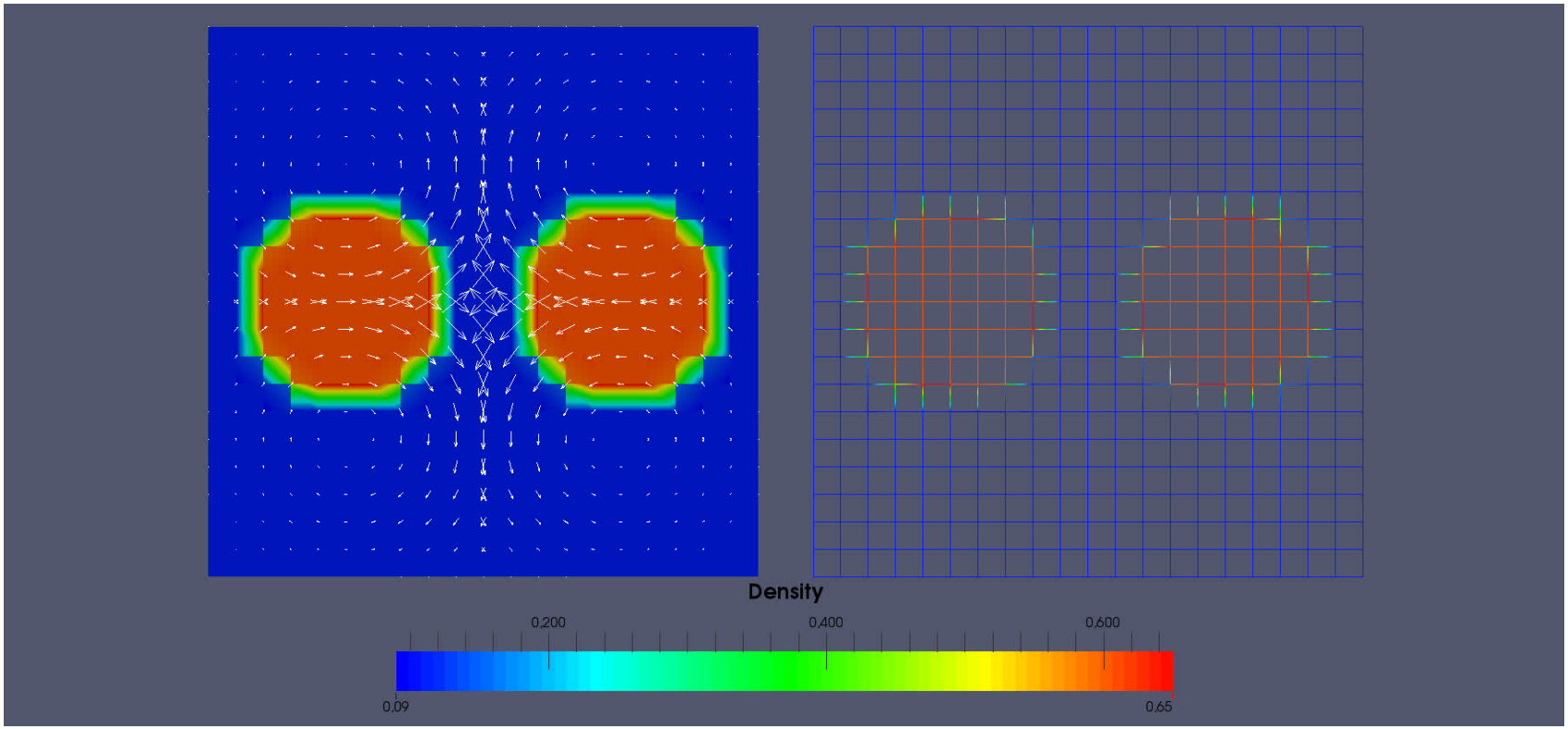
$\delta = 0.01$ *vs.* $\delta = 0.02$



Droplet Collision

Two droplets are pushed against each other by an initial velocity field.

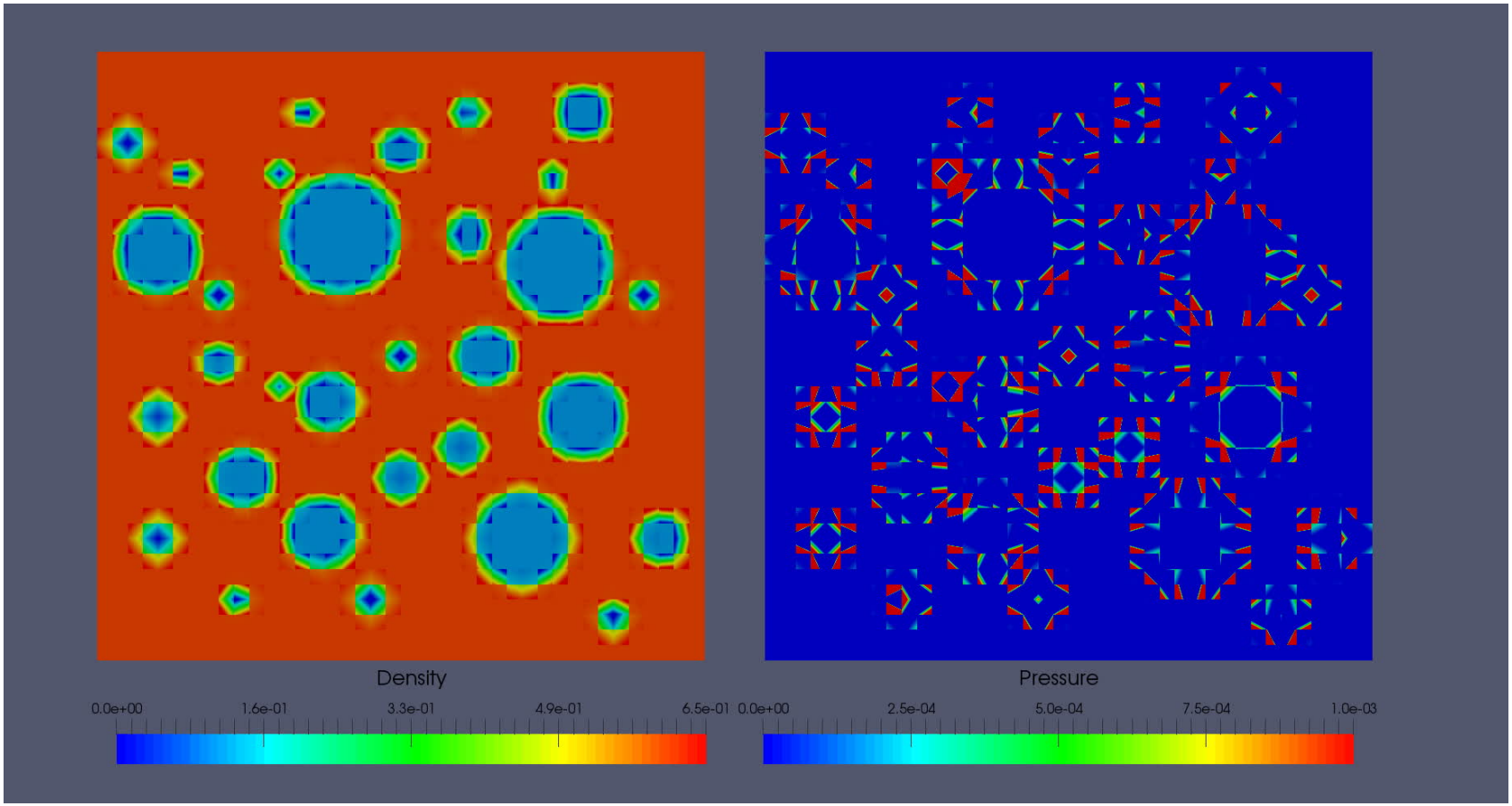
$\delta = 0.02$



Bubble Ensemble

Vapor and Liquid density are at the saturation values.

$\delta = 0.01$

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Thank you for your attention!