

Theory and Applications of Local Discontinuous-Galerkin Schemes in Phase Transition Theory

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A1: Numerical Solution of the NSK-System

Model problems in phase transition theory

$$\begin{aligned}\rho_t + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ (\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}^T) + \nabla p(\rho) &= \varepsilon \nabla \cdot \boldsymbol{\tau} + \lambda \rho \nabla (D^\varepsilon[\rho])\end{aligned}$$

in $\mathbb{R}^d \times (0, T)$

with either the **local version** $D_{local}^\varepsilon[\rho] = \varepsilon^2 \Delta \rho$

or the **non-local version** $D_{global}^\varepsilon[\rho] = \gamma(\Phi_\varepsilon * \rho - \rho)$

Convolution $[\Phi_\varepsilon * \rho](x) = \int_{\mathbb{R}^d} \Phi_\varepsilon(x - y) \rho(y) dy$

with a symmetric, non-negative kernel function satisfying

$\Phi_\varepsilon(x) = \frac{1}{\varepsilon^d} \Phi\left(\frac{x}{\varepsilon}\right)$ and $\int_{\mathbb{R}^d} \Phi(x) dx = 1$.

$$\begin{aligned}D_{global}^\varepsilon[\rho](x) &= \gamma \int_{\mathbb{R}} \Phi_\varepsilon(x - y) [\rho(y) - \rho(x)] dy \\ &\approx \gamma \int_{\mathbb{R}} \frac{1}{\varepsilon} \Phi\left(\frac{x-y}{\varepsilon}\right) \left[\rho_x(x)(y-x) + \rho_{xx}(x) \frac{1}{2}(y-x)^2 \right] dy \\ &= \varepsilon^2 \rho_{xx}(x) \frac{\gamma}{2} \int_{\mathbb{R}} \Phi(z) z^2 dz \quad \left(\text{set } \gamma := \frac{2}{\int_{\mathbb{R}} \Phi(z) z^2 dz} \right) \\ &= D_{local}^\varepsilon[\rho](x)\end{aligned}$$

Outline

1. Scalar model problem
2. Elasticity system
3. Navier-Stokes-Korteweg system

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2. Elasticity system
3. Navier-Stokes-Korteweg system

2. Scalar model problem

$$u_t + f(u)_x = \varepsilon u_{xx} + \lambda D_{local/global}^\varepsilon [u]_x \quad \text{in } \mathbb{R} \times (0, T)$$

Unknown: $u = u(x, t) \in \mathbb{R}$

Given parameters: $\lambda > 0$, parameter $\varepsilon > 0$ scales between diffusion and dispersion

Local version: $D_{local}^\varepsilon [u] = \varepsilon^2 u_{xx}$

(Jacobs&McKinney&Shearer '95, Hayes&LeFloch '97, ...)

Non-local version: $D_{global}^\varepsilon [u] = \gamma(\Phi_\varepsilon * u - u)$

(Rohde '05)

2. Scalar model problem

$$u_t + f(u)_x = \varepsilon u_{xx} + \lambda D_{local/global}^\varepsilon [u]_x \quad \text{in } \mathbb{R} \times (0, T)$$

Unknown: $u = u(x, t) \in \mathbb{R}$

Given parameters: $\lambda > 0$, parameter $\varepsilon > 0$ scales between diffusion and dispersion

Local version: $D_{local}^\varepsilon [u] = \varepsilon^2 u_{xx}$

$$u_t + (f(u) - \varepsilon q - \lambda \varepsilon^2 p)_x = 0$$

$$q - u_x = 0$$

$$p - q_x = 0$$

2. Scalar model problem

$$u_t + f(u)_x = \varepsilon u_{xx} + \lambda D_{local/global}^\varepsilon [u]_x \quad \text{in } \mathbb{R} \times (0, T)$$

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Local version: $D_{local}^\varepsilon [u] = \varepsilon^2 u_{xx}$

$$\begin{aligned} 0 &= \int_{I_j} u_{h,t} \phi \, dx - \int_{I_j} (f(u_h) - \varepsilon q_h - \lambda \varepsilon^2 p_h) \phi_x \, dx \\ &\quad + (\tilde{f}_{j+1/2} - \varepsilon \tilde{q}_{j+1/2} - \lambda \varepsilon^2 \tilde{p}_{j+1/2}) \phi(x_{j+1/2}) \\ &\quad - (\tilde{f}_{j-1/2} - \varepsilon \tilde{q}_{j-1/2} - \lambda \varepsilon^2 \tilde{p}_{j-1/2}) \phi(x_{j-1/2}) \end{aligned}$$

$$0 = \int_{I_j} q_h \phi \, dx + \int_{I_j} u_h \phi_x \, dx - \tilde{u}_{j+1/2} \phi(x_{j+1/2}) + \tilde{u}_{j-1/2} \phi(x_{j-1/2})$$

$$0 = \int_{I_j} p_h \phi \, dx + \int_{I_j} q_h \phi_x \, dx - \tilde{q}_{j+1/2} \phi(x_{j+1/2}) + \tilde{q}_{j-1/2} \phi(x_{j-1/2})$$

2. Scalar model problem

$$u_t + f(u)_x = \varepsilon u_{xx} + \lambda D_{local/global}^\varepsilon [u]_x \quad \text{in } \mathbb{R} \times (0, T)$$

Unknown: $u = u(x, t) \in \mathbb{R}$

Given parameters: $\lambda > 0$, parameter $\varepsilon > 0$ scales between diffusion and dispersion

Non-local version: $D_{global}^\varepsilon [u] = \gamma(\Phi_\varepsilon * u - u)$

- ▶ Derivation of LDG-schemes, especially for the non-local version two different schemes
- ▶ Several numerical experiments

2. Scalar model problem

$$u_t + f(u)_x = \varepsilon u_{xx} + \lambda D_{local/global}^\varepsilon [u]_x \quad \text{in } \mathbb{R} \times (0, T) \quad (*)$$

For any smooth solution u of $(*)$ that decays sufficiently fast together with its spatial derivatives as $x \rightarrow \pm\infty$ we have

$$\frac{d}{dt} \int_{\mathbb{R}} \frac{u^2}{2} dx + \varepsilon \int_{\mathbb{R}} u_x^2 dx = 0.$$

Theorem: (L^2 -stability)

The LDG-solution u_h of $(*)$ is L^2 -stable

$$\frac{d}{dt} \int_{\mathbb{R}} \frac{u_h^2}{2} dx \leq 0.$$

2. Scalar model problem

$$u_t + f(u)_x = \varepsilon u_{xx} + \lambda D_{local}^\varepsilon[u]_x \quad \text{in } (0, 1) \times (0, T) \quad (*)$$

Theorem: (L^2 -error estimate)

Take $f(u) = au$, $a \in \mathbb{R}$. Let $u \in C^{\mathbf{p}+3}([0, 1] \times [0, T])$ be a solution of $(*)$ and $u_h(., t) \in \mathcal{V}_h^{\mathbf{p}}$ be the LDG-solution of $(*)$, where we consider special numerical fluxes. Then there exists a constant $C = C(\mathbf{p}, a, \varepsilon, \lambda, T) > 0$

$$\|u - u_h\|_{L^2(0,1)} \leq Ch^{\mathbf{p}+1/2}$$

holds true for all $t \in [0, T]$.

(Proof similar as in Yan&Shu '02 for $u_t + u_x + u_{xxx} = 0$)

2. Scalar model problem

$$u_t + f(u)_x = \varepsilon u_{xx} + \lambda D_{global}^\varepsilon[u]_x \quad \text{in } (0, 1) \times (0, T) \quad (*)$$

Theorem: (L^2 -error estimate)

Take $f(u) = au$, $a \in \mathbb{R}$. Let $u \in C^{\mathbf{p}+2}([0, 1] \times [0, T])$ be a solution of $(*)$ and $u_h(., t) \in \mathcal{V}_h^{\mathbf{p}}$ be the LDG-solution of $(*)$, where we consider special numerical fluxes. Furthermore let Φ be an even function from $W^{1,\infty}(\mathbb{R})$ with compact support. Then there exists a constant $C = C(\mathbf{p}, a, \varepsilon, \lambda, \gamma, T) > 0$

$$\|u - u_h\|_{L^2(0,1)} \leq Ch^{\mathbf{p}+1/2}$$

holds true for all $t \in [0, T]$.

2. Scalar model problem

Convergence order due to L^∞ -estimates for the projection operators \mathcal{P} and \mathcal{S} defined by

$$\int_{I_j} \mathcal{P}w(x)\phi_h(x) dx = \int_{I_j} w(x)\phi_h(x) dx \quad \forall \phi_h \in \mathbb{P}^{\mathbf{p}} \quad (\text{L^2-projection}),$$

$$\int_{I_j} \mathcal{S}w(x)\phi_h(x) dx = \int_{I_j} w(x)\phi_h(x) dx \quad \forall \phi_h \in \mathbb{P}^{\mathbf{p}-1}, \quad \mathcal{S}w(x_{j-1/2}^+) = w(x_{j-1/2}^+).$$

To prove the non-local error estimate we need:

- ▶ $[\Phi_\varepsilon * (\mathcal{S}w - w)](x_{j-1/2}) \leq C(\mathbf{p}) \|w^{(\mathbf{p}+1)}\|_{L^\infty(0,1)} \|\Phi_\varepsilon\|_{L^1(\mathbb{R})} h^{\mathbf{p}+1}$
- ▶
$$\sum_{j=1}^N \int_{I_j} [\Phi_\varepsilon * (\mathcal{S}w - w)](x) (\mathcal{S}w - w_h)_x(x) dx$$
$$\leq \frac{1}{2} \int_0^1 (\mathcal{S}w - w_h)^2(x) dx + C(\mathbf{p}) \|w^{(\mathbf{p}+1)}\|_{L^\infty(0,1)}^2 \|\Phi'_\varepsilon\|_{L^\infty(\mathbb{R})}^2 h^{2\mathbf{p}+2}$$

(work submitted to Proceedings of Hyp2008)

Outline

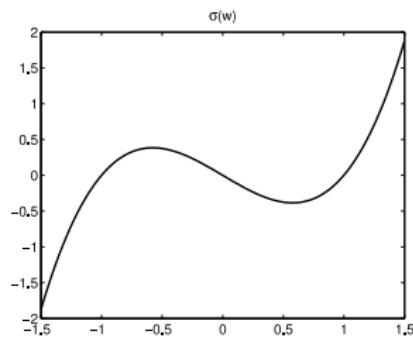
1. Scalar model problem
2. Elasticity system
3. Navier-Stokes-Korteweg system

3. Elasticity system

$$\begin{aligned} w_t - v_x &= 0 \\ v_t - \sigma(w)_x &= \varepsilon v_{xx} - \lambda D_{local/global}^\varepsilon[w]_x \end{aligned} \quad \text{in } \mathbb{R} \times (0, T)$$

Unknowns: stress $w = w(x, t) \in \mathbb{R}$, velocity $v = v(x, t) \in \mathbb{R}$

Given: stress-strain-relation $\sigma(w) = w^3 - w$



Local version:

$$D_{local}^\varepsilon[w] = \varepsilon^2 w_{xx}$$

Non-local version:

$$D_{global}^\varepsilon[w] = \gamma(\Phi_\varepsilon * w - w)$$

3. Elasticity system

$$w_t - v_x = 0$$

$$v_t - \sigma(w)_x = \varepsilon v_{xx} - \lambda D_{local/global}^\varepsilon [w]_x$$

in $\mathbb{R} \times (0, T)$

Classical solutions satisfy the following energy inequality

$$\frac{d}{dt} \left(\int_{\mathbb{R}} \left(\frac{1}{2} |v(x)|^2 + W(w(x)) + E^\varepsilon[w](x) \right) dx \right) \leq 0$$

with

$$E^\varepsilon[w](x) = \begin{cases} \frac{1}{2} \lambda \varepsilon^2 |w_x(x)|^2 & (\text{local case}) \\ \frac{1}{4} \lambda \gamma \int_{\mathbb{R}} \Phi_\varepsilon(x-y) [w(y) - w(x)]^2 dy & (\text{non-local case}) \end{cases}$$

Theorem: (Discrete energy estimate for the non-local elasticity system)

The LDG-solution for the non-local elasticity system satisfies

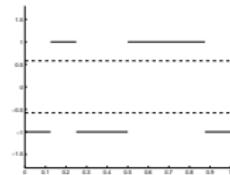
$$\frac{d}{dt} \left(\int_{\mathbb{R}} \left(\frac{1}{2} |v_h(x)|^2 + W(w_h(x)) + \frac{1}{4} \lambda \gamma \sum_{k \in \mathbb{Z}} h \Phi_\varepsilon^h(x-x_k) [w(x_k) - w(x)]^2 \right) dx \right) \leq 0.$$

(see also Dressel&Rohde '07)

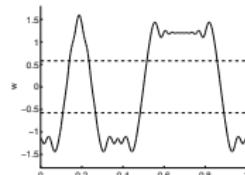
3. Elasticity system

Test: Phase separation

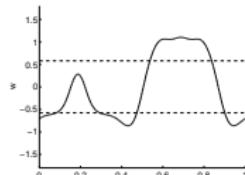
Local case



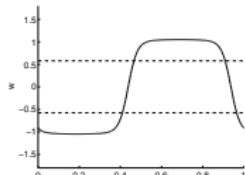
$t = 0$



$t = 0.01$

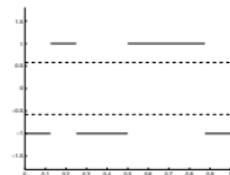


$t = 0.1$

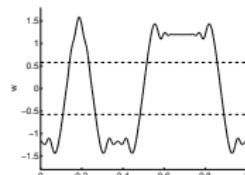


$t = 5$

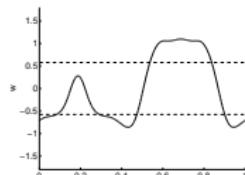
Non-local case



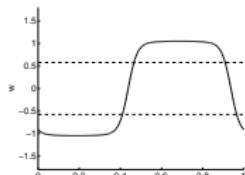
$t = 0$



$t = 0.01$



$t = 0.1$



$t = 5$

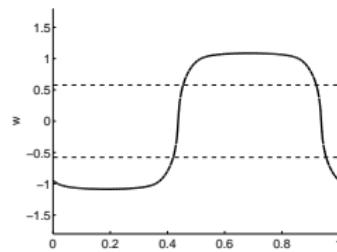
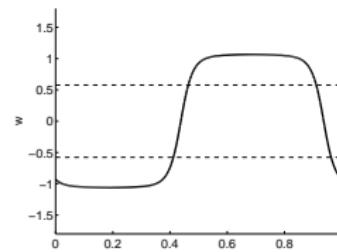
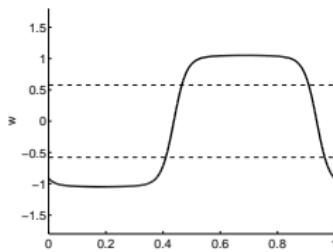
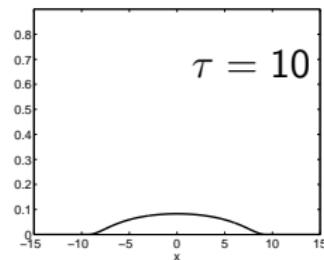
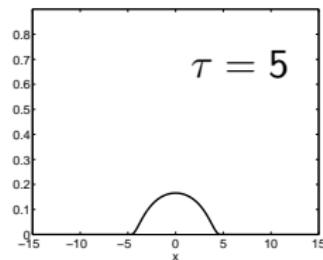
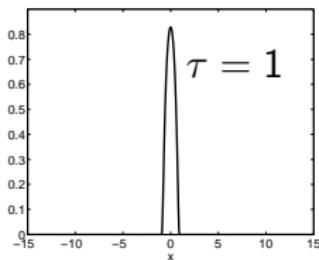
3. Elasticity system

Test: Phase separation, $\gamma(\Phi_\varepsilon * w - w) \approx \varepsilon^2 w_{xx}$

3. Elasticity system

Test: Phase separation, $\gamma(\tau)(\Phi_\varepsilon^\tau * w - w) \approx \varepsilon^2 w_{xx}$, $\gamma(\tau) = \frac{2}{\int_{\mathbb{R}} \Phi_\varepsilon^\tau(x) x^2 dx}$

$$\begin{aligned} w_t - v_x &= 0 \\ v_t - \sigma(w)_x &= \varepsilon v_{xx} - \lambda \gamma(\tau)(\Phi_\varepsilon^\tau * w - w)_x \end{aligned}$$



$t = 5$

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Outline

1. Scalar model problem
2. Elasticity system
- 3. Navier-Stokes-Korteweg system**

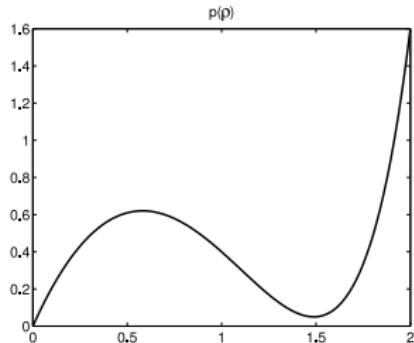
4. Navier-Stokes-Korteweg system

$$\begin{aligned}\rho_t + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ (\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}^T) + \nabla p(\rho) &= \varepsilon \nabla \cdot \boldsymbol{\tau} + \lambda \rho \nabla (D_{local/global}^\varepsilon[\rho])\end{aligned}$$

Unknowns: density $\rho = \rho(x, t) > 0$, velocity $\mathbf{v} = \mathbf{v}(x, t) \in \mathbb{R}^d$

Given: van-der-Waals pressure $p = p(\rho) = \frac{RT^* \rho}{b - \rho} - a\rho^2$

Navier-Stokes tensor $\boldsymbol{\tau} = \mu(\nabla \mathbf{v} + \nabla \mathbf{v}^T) + \lambda(\nabla \cdot \mathbf{v})\mathbf{I}$



Local version:

$$D_{local}^\varepsilon[\rho] = \varepsilon^2 \Delta \rho$$

Non-local version:

$$D_{global}^\varepsilon[\rho] = \gamma(\Phi_\varepsilon * \rho - \rho)$$

4. Navier-Stokes-Korteweg system

Dennis Diehl: LDG-code for the local NSK-system

Convolution $\Phi_\varepsilon * \rho$ in the LDG-scheme:

$$\int_{\Delta_j} [\Phi_\varepsilon * \rho_h(., t)](\mathbf{x}) \phi_h(\mathbf{x}) \, d\mathbf{x} = \int_{\Delta_j} \left(\int_{\mathbb{R}^d} \Phi_\varepsilon(\mathbf{x} - \mathbf{y}) \rho_h(\mathbf{y}, t) \, d\mathbf{y} \right) \phi_h(\mathbf{x}) \, d\mathbf{x}$$

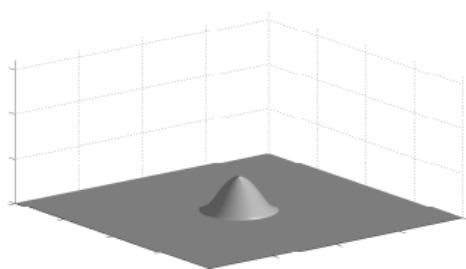
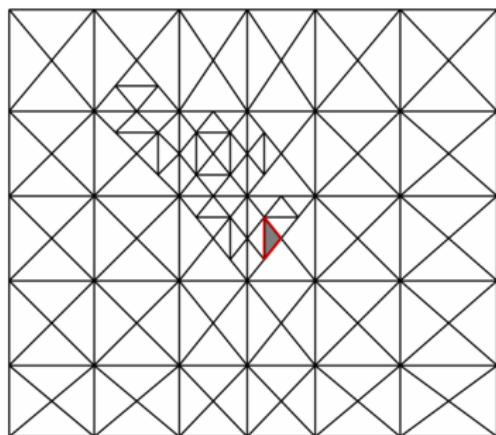
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- Identify the essential triangles



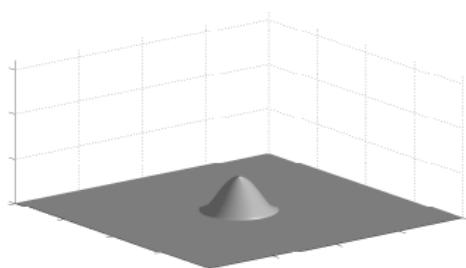
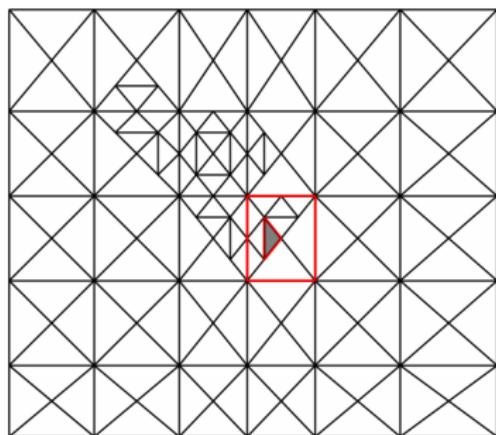
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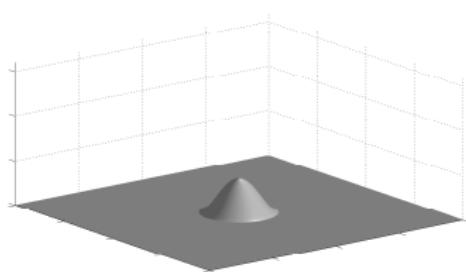
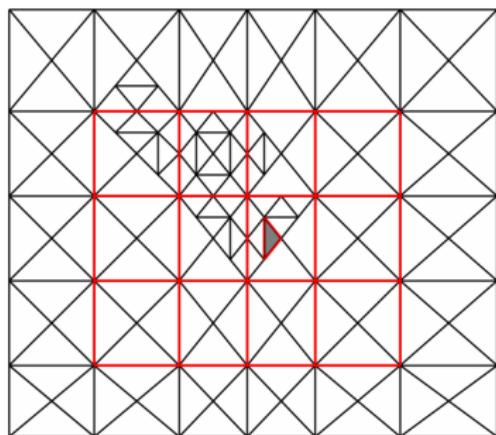
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- Identify the essential triangles



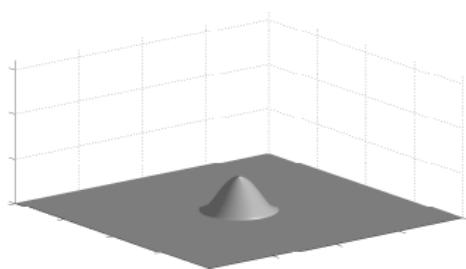
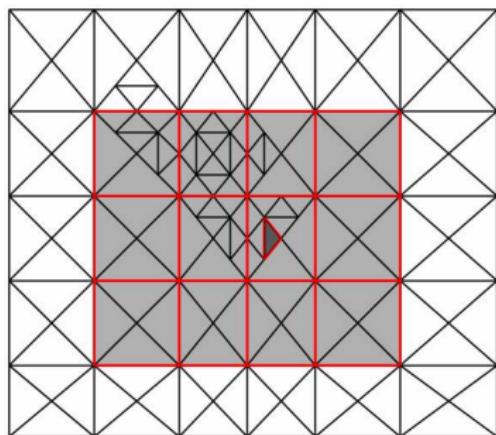
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- Identify the essential triangles



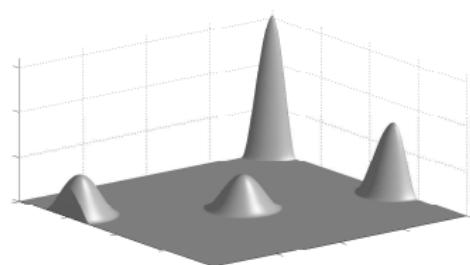
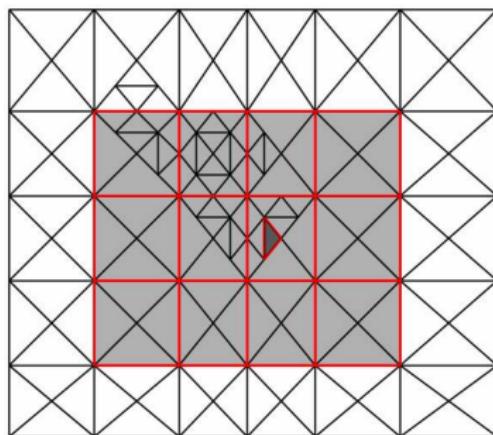
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Convolution $\Phi_\varepsilon * \rho$ in the LDG-scheme:

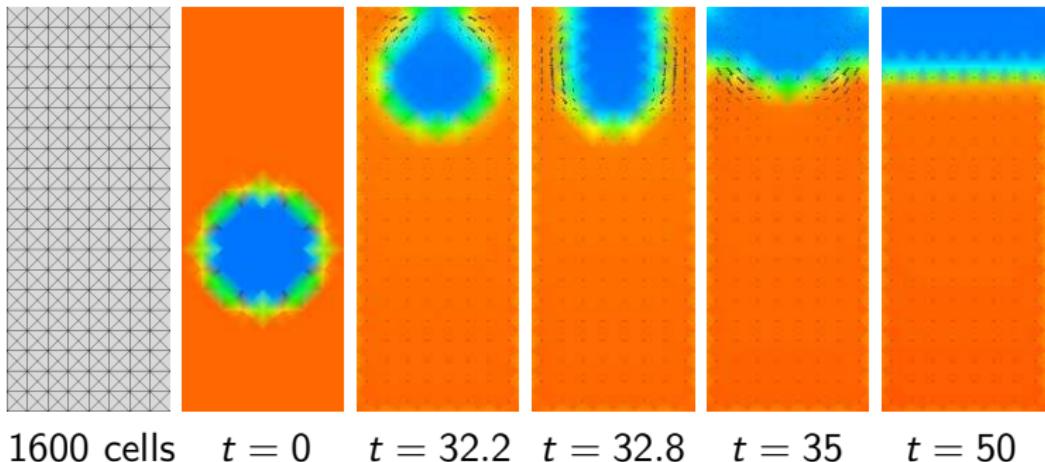
$$\int_{\Delta_j} [\Phi_\varepsilon * \rho_h(., t)](\mathbf{x}) \phi_h(\mathbf{x}) \, d\mathbf{x} = \int_{\Delta_j} \left(\int_{\mathbb{R}^d} \Phi_\varepsilon(\mathbf{x} - \mathbf{y}) \rho_h(\mathbf{y}, t) \, d\mathbf{y} \right) \phi_h(\mathbf{x}) \, d\mathbf{x}$$

- Identify the essential triangles
- Steepen kernel next to boundaries



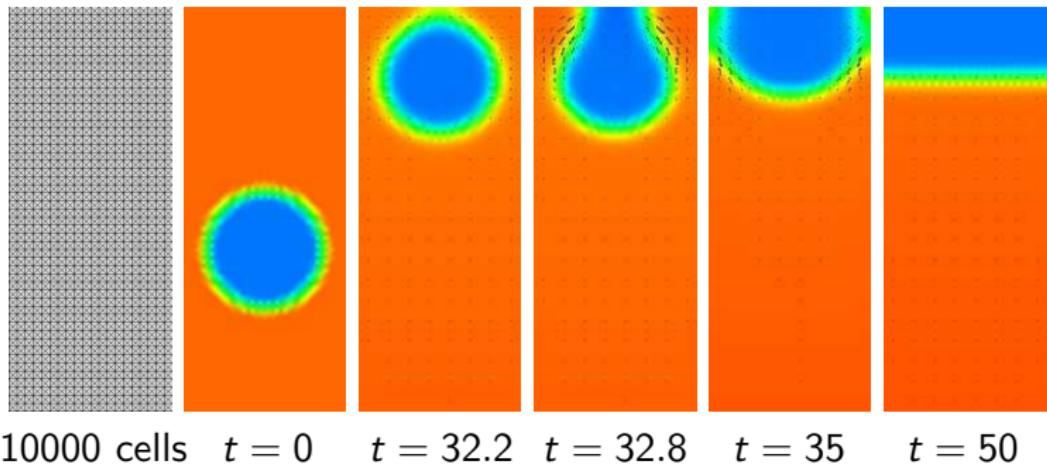
4. Navier-Stokes-Korteweg system

Test 1: Rising bubble in liquid (grid convergence)



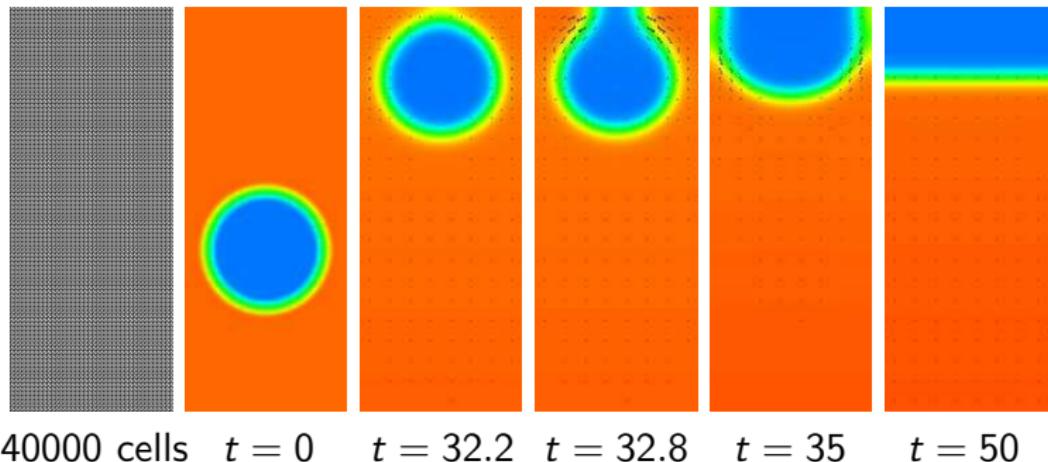
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4. Navier-Stokes-Korteweg system

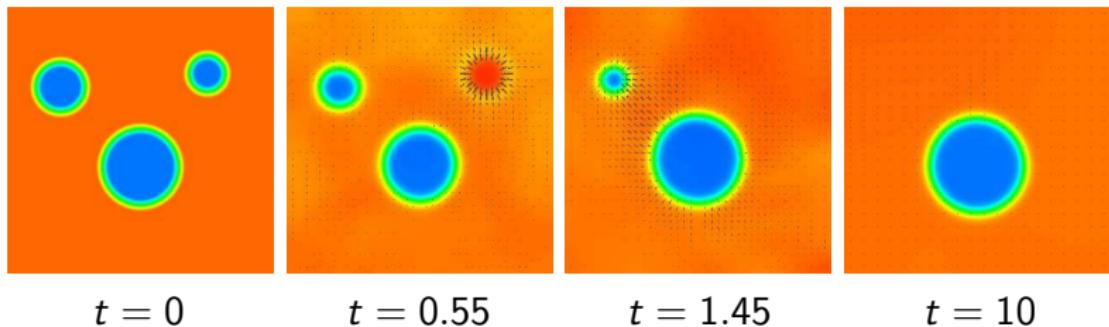
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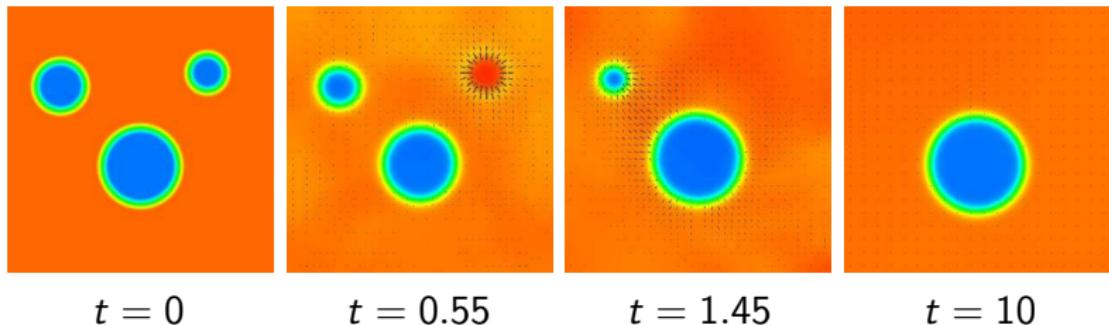
4. Navier-Stokes-Korteweg system

Test 2: Three bubbles in liquid

Local NSK



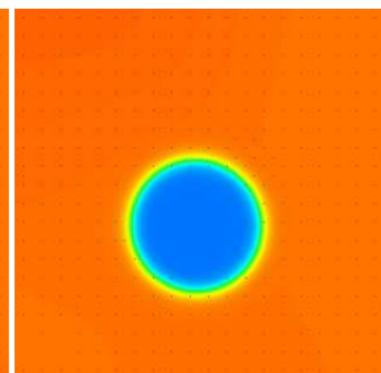
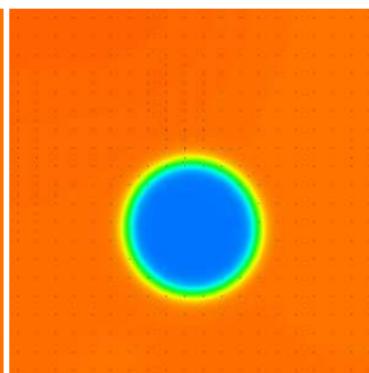
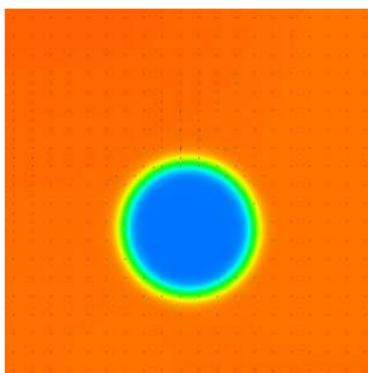
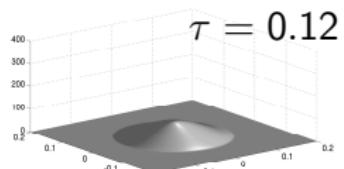
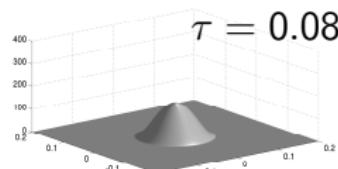
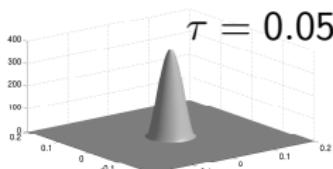
Non-local NSK



4. Navier-Stokes-Korteweg system

$$\gamma(\tau)(\Phi_\varepsilon^\tau * \rho - \rho) \approx \varepsilon^2 \Delta \rho$$

$$\Phi^\tau(\mathbf{x}) = \begin{cases} \frac{3}{\pi\tau^4} \left(\tau - \frac{|\mathbf{x}|^2}{\tau} \right)^2 & \text{for } |\mathbf{x}| < \tau, \\ 0 & \text{otherwise.} \end{cases} \Rightarrow \gamma(\tau) = \frac{16}{\tau^2}$$



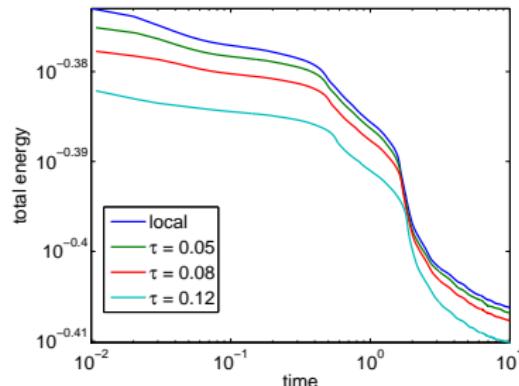
4. Navier-Stokes-Korteweg system

Energy inequality:

$$\frac{d}{dt} \left(\int_{\mathbb{R}^d} \left(\frac{1}{2} \rho(\mathbf{x}) |\mathbf{v}(\mathbf{x})|^2 + W(\rho(\mathbf{x})) + E^\varepsilon[\rho](\mathbf{x}) \right) d\mathbf{x} \right) \leq 0$$

with

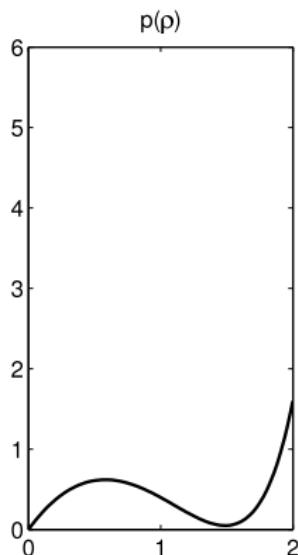
$$E^\varepsilon[\rho](\mathbf{x}) = \begin{cases} \frac{1}{2} \lambda \varepsilon^2 |\nabla \rho(\mathbf{x})|^2 & (\text{local NSK}) \\ \frac{1}{4} \lambda \gamma \int_{\mathbb{R}^d} \Phi_\varepsilon^\tau(\mathbf{x} - \mathbf{y}) [\rho(\mathbf{y}) - \rho(\mathbf{x})]^2 d\mathbf{y} & (\text{non-local NSK}) \end{cases}$$



4. Navier-Stokes-Korteweg system

Momentum balance equation:

$$(\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}^T) + \nabla p(\rho) = \varepsilon \nabla \cdot \boldsymbol{\tau} + \lambda \gamma \rho \nabla (\Phi_\varepsilon^\tau * \rho - \rho)$$

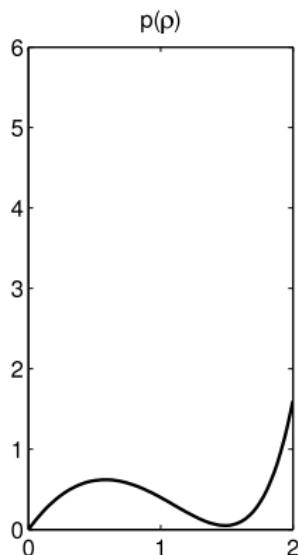


Remark: The Euler-part of the NSK-system is hyperbolic for increasing branches of p .

4. Navier-Stokes-Korteweg system

Momentum balance equation:

$$(\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}^T) + \nabla p(\rho) = \varepsilon \nabla \cdot \boldsymbol{\tau} + \lambda \gamma \rho \nabla (\Phi_\varepsilon^\tau * \rho - \rho)$$

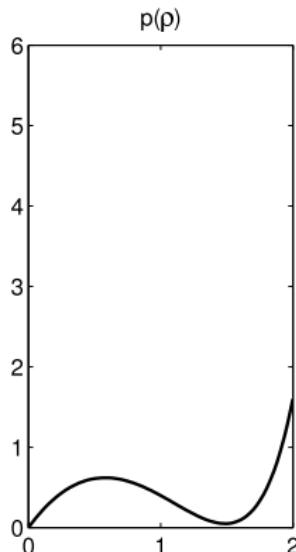


Remark: The Euler-part of the NSK-system is hyperbolic for increasing branches of p .

4. Navier-Stokes-Korteweg system

Momentum balance equation:

$$(\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}^T) + \nabla \left(p(\rho) + \frac{1}{2} \lambda \gamma \rho^2 \right) = \varepsilon \nabla \cdot \boldsymbol{\tau} + \lambda \gamma \rho \nabla (\Phi_\varepsilon^\tau * \rho)$$

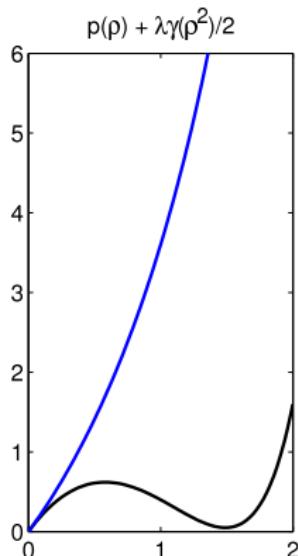


Remark: The Euler-part of the NSK-system is hyperbolic for increasing branches of p .

4. Navier-Stokes-Korteweg system

Momentum balance equation:

$$(\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}^T) + \nabla \left(p(\rho) + \frac{1}{2} \lambda \gamma \rho^2 \right) = \varepsilon \nabla \cdot \boldsymbol{\tau} + \lambda \gamma \rho \nabla (\Phi_\varepsilon^\tau * \rho)$$



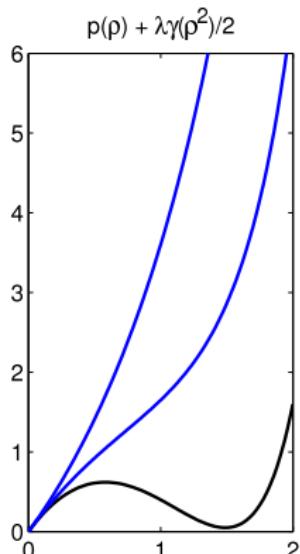
τ	$\gamma(\tau) = \frac{16}{\tau^2}$
0.05	6400

Remark: The Euler-part of the NSK-system is hyperbolic for increasing branches of p .

4. Navier-Stokes-Korteweg system

Momentum balance equation:

$$(\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}^T) + \nabla \left(p(\rho) + \frac{1}{2} \lambda \gamma \rho^2 \right) = \varepsilon \nabla \cdot \boldsymbol{\tau} + \lambda \gamma \rho \nabla (\Phi_\varepsilon^\tau * \rho)$$



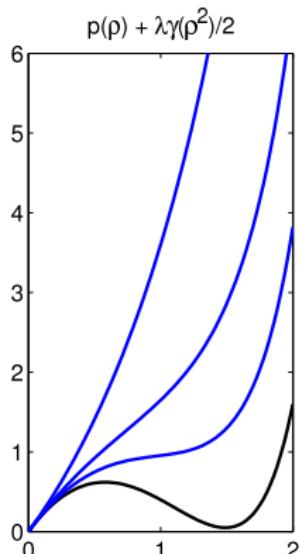
τ	$\gamma(\tau) = \frac{16}{\tau^2}$
0.05	6400
0.08	2500

Remark: The Euler-part of the NSK-system is hyperbolic for increasing branches of p .

4. Navier-Stokes-Korteweg system

Momentum balance equation:

$$(\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}^T) + \nabla \left(p(\rho) + \frac{1}{2} \lambda \gamma \rho^2 \right) = \varepsilon \nabla \cdot \boldsymbol{\tau} + \lambda \gamma \rho \nabla (\Phi_\varepsilon^\tau * \rho)$$



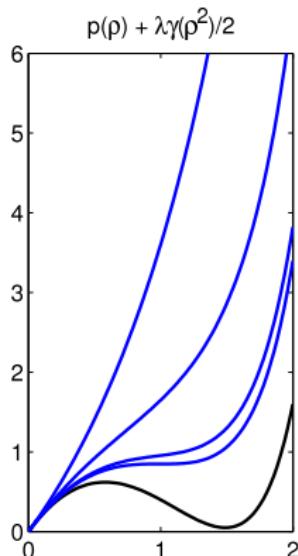
τ	$\gamma(\tau) = \frac{16}{\tau^2}$
0.05	6400
0.08	2500
0.12	1111

Remark: The Euler-part of the NSK-system is hyperbolic for increasing branches of p .

4. Navier-Stokes-Korteweg system

Momentum balance equation:

$$(\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}^T) + \nabla \left(p(\rho) + \frac{1}{2} \lambda \gamma \rho^2 \right) = \varepsilon \nabla \cdot \boldsymbol{\tau} + \lambda \gamma \rho \nabla (\Phi_\varepsilon^\tau * \rho)$$



τ	$\gamma(\tau) = \frac{16}{\tau^2}$
0.05	6400
0.08	2500
0.12	1111
0.13	900

Remark: The Euler-part of the NSK-system is hyperbolic for increasing branches of p .

4. Navier-Stokes-Korteweg system

Energy inequality:

$$\frac{d}{dt} \left(\int_{\mathbb{R}^d} \left(W(\rho(\mathbf{x})) + \frac{1}{2} \lambda \gamma (\rho(\mathbf{x}))^2 - \frac{1}{2} \lambda \gamma [\Phi_\varepsilon * \rho](\mathbf{x}) \rho(\mathbf{x}) \right) d\mathbf{x} \right) \leq 0$$

$$\frac{d}{dt} \left(\int_{\mathbb{R}^d} \left(W(\rho(\mathbf{x})) + \frac{1}{4} \lambda \gamma \int_{\mathbb{R}^d} \Phi_\varepsilon(\mathbf{x}-\mathbf{y}) [\rho(\mathbf{y}) - \rho(\mathbf{x})]^2 d\mathbf{y} \right) d\mathbf{x} \right) \leq 0$$

⇒ Energy density function W “convexified” to $W^* := W + \frac{1}{2} \lambda \gamma \rho^2$
(see also Brandon&Lin&Rogers '95)

Remark: This does not work for the local NSK-system

Remarks about future work

- ▶ Numerical tests for interfaces as thin as possible (increase τ)
- ▶ Comparison of numerical results and experimental data
- ▶ Investigate the contact angle in the non-local model
- ▶ Existence of weak solutions for the boundary value problem of the NSK-system (with Boris Haspot)