Local Discontinuous-Galerkin Schemes for Model Problems in Phase Transition Theory

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A1: Numerical Solution of the NSK-System

Overview

1. Compressible models for phase transition problems
   - Sharp interface model
   - Diffuse interface model
2. Model problems in phase transition theory
   - LDG-schemes
   - Analytical results
3. Various numerical examples
   - Scalar model problem (1D)
   - Equations of elasticity (1D)
   - NSK-system (2D)

1. Compressible models for phase transition problems

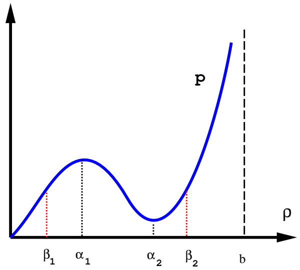
1.1. Sharp interface model

Isothermal equations of hydrodynamics:

$$\boxed{\begin{array}{cccc} \rho_t & + & \nabla \cdot (\rho v) & = & 0 \\ (\rho v)_t & + & \nabla \cdot (\rho v v^T + p(\rho) Id) & = & 0 \end{array}} \quad \text{in } \Omega \times (0, T)$$

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

Given: pressure $p = p(\rho)$



van-der-Waals-function

$$p(\rho) = \frac{RT^*\rho}{b - \rho} - a\rho^2$$

Remark:

The system is hyperbolic for $\rho \leq \alpha_1$ resp. $\rho \geq \alpha_2$.

Definition:

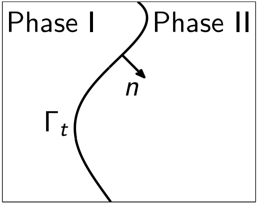
A state $(\rho, v)^T$ is called **vapour** resp. **liquid** if $\rho \leq \alpha_1$ resp. $\rho \geq \alpha_2$.

1.1. Sharp interface model

Interface conditions in 2D:

$$
\begin{aligned}
[\![\rho(v\cdot n - s)]\!] &= 0 && \text{(Mass conservation)}\\
[\![\rho v(v\cdot n - s) + p(\rho)n]\!] &= \sigma\kappa n && \text{(Young-Laplace)}\\
-[\![W'(\rho) + \tfrac{1}{2}(v\cdot n - s)^2]\!] &= \psi(j) && \text{(Kinetic relation)}\\
& & & j := \rho^-(v^- \cdot n - s)
\end{aligned}
$$

Theorem: (Benzoni-Gavage & Freistühler (2004), $\psi = 0$)
Local existence of an interface solution (and more important stability results).



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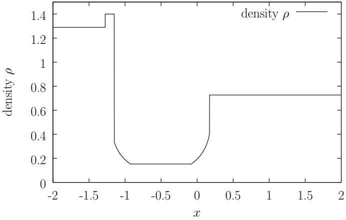
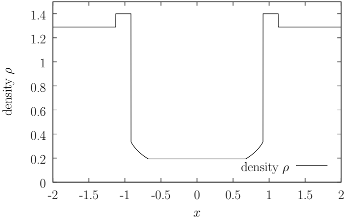
& && j := \rho^-(v^- \cdot n - s)
\end{aligned}
$$

Theorem: (Merkle & Rohde (2006, M^{2}AN), isothermal 1D Riemann problem)
Existence theory for $\kappa = 0$.





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& && j := \rho^-(v^- \cdot n - s)
\end{aligned}
$$

Theorem: (Dressel & Rohde (2008), nonisothermal Riemann problem)
Existence theory for $\kappa > 0$ (as a perturbation of monotone balance).

1.2. Diffuse interface model

Isothermal equations of hydrodynamics:

$$\begin{array}{rcccl} \rho_t & + & \nabla \cdot (\rho v) & = & 0 \\ (\rho v)_t & + & \nabla \cdot (\rho v v^T + p(\rho) Id) & = & 0 \end{array}$$

Unknowns: density $\rho = \rho(x,t) > 0$, velocity $v = v(x,t) \in \mathbb{R}^d$
Given: pressure $p = p(\rho)$ (van-der-Waals-function)

1.2. Diffuse interface model

Isothermal equations of hydrodynamics:

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\rho_t & + & \nabla \cdot (\rho v) & = & 0 \\
(\rho v)_t & + & \nabla \cdot (\rho v v^T + p(\rho) Id) & = & \mu\varepsilon\Delta v + \lambda\rho\nabla(D^\varepsilon[\rho])
\end{array}
$$

Unknowns: density $\rho = \rho(x, t) > 0$, velocity $v = v(x, t) \in \mathbb{R}^d$
Given: pressure $p = p(\rho)$ (van-der-Waals-function)
Given parameters: $\mu, \lambda > 0$
Parameter $\varepsilon > 0$ scales between viscosity and capillarity

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Unknowns: density $\rho = \rho(x,t) > 0$, velocity $v = v(x,t) \in \mathbb{R}^d$
Given: pressure $p = p(\rho)$ (van-der-Waals-function)
Given parameters: $\mu, \lambda > 0$
Parameter $\varepsilon > 0$ scales between viscosity and capillarity

Local version: (Diehl)

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

Non-local version:

$$D^\varepsilon_{global}[\rho] = \Phi_\varepsilon * \rho - \rho$$

Kernel function $\Phi_\varepsilon(x) = \frac{1}{\varepsilon^d}\Phi(\frac{x}{\varepsilon})$ with
Φ symmetric, nonnegative and $\int_{\mathbb{R}^d}\Phi(x)\,dx = 1$

2. Model problems in phase transition theory

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Diffusive-dispersive scalar model problem (1D):
(LeFloch, Shearer, ...)

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

Unknown: $u = u(x, t) \in \mathbb{R}$
Given parameters: $\lambda > 0$, parameter $\varepsilon > 0$ scales between diffusion and dispersion

Local version:

$$\boxed{D^{\varepsilon}_{local}[u] = \varepsilon^2 u_{xx}}$$

Non-local version:

$$\boxed{D^{\varepsilon}_{global}[u] = \gamma(\Phi_{\varepsilon} * u - u)}$$

$\Phi_{\varepsilon}(x) = \frac{1}{\varepsilon}\Phi(\frac{x}{\varepsilon})$ with Φ symmetric, nonnegative, $\int_{\mathbb{R}} \Phi(x)\, dx = 1$

2. Model problems in phase transition theory

Local version:

$$\boxed{D^{\varepsilon}_{local}[u] = \varepsilon^2 u_{xx}}$$

Non-local version:

$$\boxed{D^{\varepsilon}_{global}[u] = \gamma(\Phi_\varepsilon * u - u)}$$

$\Phi_\varepsilon(x) = \frac{1}{\varepsilon}\Phi(\frac{x}{\varepsilon})$ with Φ symmetric, nonnegative, $\int_{\mathbb{R}} \Phi(x)\,dx = 1$

$$\begin{aligned} D^{\varepsilon}_{global}[u](x) &= \gamma \int_{\mathbb{R}} \Phi_\varepsilon(x-y)[u(y)-u(x)]\,dy \\ &\approx \gamma \int_{\mathbb{R}} \frac{1}{\varepsilon}\Phi\left(\frac{x-y}{\varepsilon}\right)\left[u_x(x)(y-x) + u_{xx}(x)\frac{1}{2}(y-x)^2\right]dy \\ &= \varepsilon^2 u_{xx}(x)\ \frac{\gamma}{2}\int_{\mathbb{R}} \Phi(z)z^2\,dz \\ &= D^{\varepsilon}_{local}[u](x) \end{aligned}$$

if $\gamma := \frac{2}{\int_{\mathbb{R}} \Phi(z)z^2\,dz}$

2. Model problems in phase transition theory

Theorem:
Consider

$$u_t + f(u)_x = \varepsilon u_{xx} + \lambda D^{\varepsilon}_{local/global}[u]_x. \qquad (*)$$

Let u be any smooth solution of $(*)$ that decays sufficiently fast together with its spatial derivatives as $x \to \pm\infty$. Then for both, the local and non-local model problem, we have

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

2.1. LDG-schemes

(work submitted to: Communications in Computational Physics)

Local diffusive-dispersive model:

$$\boxed{u_t + f(u)_x = \varepsilon u_{xx} + \lambda \varepsilon^2 u_{xxx}}$$

LDG-discretization: (Cockburn, Shu)

$$\begin{aligned} u_t + \left(f(u) - \varepsilon q - \lambda \varepsilon^2 p\right)_x &= 0 \\ q - u_x &= 0 \\ p - q_x &= 0 \end{aligned}$$

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$$\boxed{u_t + f(u)_x = \varepsilon u_{xx} + \lambda\varepsilon^2 u_{xxx}}$$

LDG-discretization: (Cockburn, Shu)

$$\begin{aligned}
0 &= \int_{I_j} u_t\phi \, dx - \int_{I_j} (f(u) - \varepsilon q - \lambda\varepsilon^2 p)\phi_x \, dx \\
&\qquad + (\tilde{f}_{j+1/2} - \varepsilon\tilde{q}_{j+1/2} - \lambda\varepsilon^2\tilde{p}_{j+1/2})\phi(x_{j+1/2}) \\
&\qquad - (\tilde{f}_{j-1/2} - \varepsilon\tilde{q}_{j-1/2} - \lambda\varepsilon^2\tilde{p}_{j-1/2})\phi(x_{j-1/2}) \\
0 &= \int_{I_j} q\phi \, dx + \int_{I_j} u\phi_x \, dx - \tilde{u}_{j+1/2}\phi(x_{j+1/2}) + \tilde{u}_{j-1/2}\phi(x_{j-1/2}) \\
0 &= \int_{I_j} p\phi \, dx + \int_{I_j} q\phi_x \, dx - \tilde{q}_{j+1/2}\phi(x_{j+1/2}) + \tilde{q}_{j-1/2}\phi(x_{j-1/2})
\end{aligned}$$

2.1. LDG-schemes

- Find $u_h \in \mathcal{V}_h^k = \{\phi \colon \phi|_{I_j} \text{ is a polyomial of degree} \leq k, \forall j \in \mathbb{Z}\}$
- Ansatz: $u_h(.,t)\big|_{I_j} = \sum_{l=0}^{k} \alpha_l^j(t)\phi_l^j(.)$ (analogue for q_h, p_h)
- Choose test functions $\phi \in \mathcal{V}_h^k$, i.e., $\phi = \phi_l^j$
- Choose numerical flux functions $\tilde{f}, \tilde{q}, \tilde{p}, \tilde{u}$, e.g. central flux

$$\tilde{f} = \tilde{f}(a,b) = \frac{1}{2}(f(a) + f(b))$$

$\Rightarrow$ Ordinary differential equations and explicit formulas for the unknown coefficients

- Quadrature formulas
- Runge-Kutta time discretization

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- Choose numerical flux functions $\tilde{f}, \tilde{q}, \tilde{p}, \tilde{u}$, e.g. E-flux

$$\operatorname{sign}(b-a)\left(\tilde{f}(a,b) - f(u)\right) \leq 0 \quad \forall u \in [\min\{a,b\}, \max\{a,b\}]$$

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- Choose numerical flux functions $\tilde{f}, \tilde{q}, \tilde{p}, \tilde{u}$, e.g. Tadmor's flux

$$\tilde{g} = \tilde{g}(a,b) = \int_0^1 g(a + s(b-a))\,ds \quad \big(g(v) = f(u), v = \eta'(u)\big)$$

$\Rightarrow$ Ordinary differential equations and explicit formulas for the unknown coefficients

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2.1. LDG-schemes

Non-local diffusive-dispersive model:

$$\boxed{u_t + f(u)_x = \varepsilon u_{xx} + \lambda\gamma(\Phi_\varepsilon * u - u)_x}$$

LDG-discretization:

(Flux-like variant)

$$\begin{aligned} u_t + (f(u) - \varepsilon q - \lambda\gamma(\Phi_\varepsilon * u - u))_x &= 0 \\ q - u_x &= 0 \end{aligned}$$

(Source-like variant)

$$\begin{aligned} u_t + (f(u) - \varepsilon q)_x &= \lambda\gamma(\Phi_\varepsilon * q - q) \\ q - u_x &= 0 \end{aligned}$$

2.2. Analytical results

Local diffusive-dispersive model:

$$\boxed{u_t + f(u)_x = \varepsilon u_{xx} + \lambda \varepsilon^2 u_{xxx}} \qquad (*)$$

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

Theorem: (cell entropy inequality)
Let $u_h \in \mathcal{V}_h^k$ be the solution of the LDG-scheme of $(*)$, $\tilde{u}, \tilde{q}, \tilde{p}$ central fluxes and $\tilde{f}$ arbitrary. Then

$$\frac{d}{dt} \int_{I_j} \frac{u_h^2}{2}\, dx + g_{j+1/2} - g_{j-1/2} + \varepsilon \int_{I_j} q_h^2\, dx + \theta_{j-1/2} = 0.$$

If $\tilde{f}$ is an E-flux or Tadmor's flux then $\theta_{j-1/2} \geq 0$ holds true.

2.2. Analytical results

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$$\frac{d}{dt} \int_{I_j} \frac{u_h^2}{2}\, dx + g_{j+1/2} - g_{j-1/2} + \varepsilon \int_{I_j} q_h^2\, dx + \theta_{j-1/2} = 0.$$

If $\tilde{f}$ is an E-flux or Tadmor's flux then $\theta_{j-1/2} \geq 0$ holds true.

Corollary: (L^2-stability)
Let $u_0 \in L^2(\mathbb{R})$ and $|u_h|, |q_h|, |p_h| \to 0$ as $x \to \pm\infty$. Then

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

2.2. Analytical results

Local diffusive-dispersive model: (with linear flux)

$$\boxed{u_t + au_x = \varepsilon u_{xx} + \lambda\varepsilon^2 u_{xxx}} \qquad (**)$$

(similar to Yan, Shu: $u_t + u_x + u_{xxx} = 0$)

Theorem: (L^2-error estimate)
Let u be a smooth solution of $(**)$ and $u_h \in \mathcal{V}_h^k$ be the solution of the LDG-scheme of $(**)$. Then, under some assumptions, we have

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

2.3. Analytical results

Non-local diffusive-dispersive model:

$$\boxed{u_t + f(u)_x = \varepsilon u_{xx} + \lambda\gamma(\Phi * u - u)_x} \qquad (\#)$$

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

Theorem:

Let $u_h \in \mathcal{V}_h^k$ be the solution of the flux-like LDG-scheme of $(\#)$, $\tilde{u}, \tilde{q}$ central fluxes and $\tilde{f}$ arbitrary. Then

$$\frac{d}{dt}\int_{I_j} \frac{u_h^2}{2}\, dx + g_{j+1/2} - g_{j-1/2} + \varepsilon \int_{I_j} q_h^2\, dx + \theta_{j-1/2}$$

$$- \lambda\gamma\left(\int_{I_j} [\Phi_\varepsilon * u_h] u_{h,x}\, dx + [\Phi_\varepsilon * u_h](x_{j-1/2}) \left(u_h(x_{j-1/2}^+) - u_h(x_{j-1/2}^-)\right)\right)$$

$$+ \lambda\gamma\left(\int_{I_j} u_h u_{h,x}\, dx + \tilde{u}_{j-1/2} \left(u_h(x_{j-1/2}^+) - u_h(x_{j-1/2}^-)\right)\right) = 0.$$

If $\tilde{f}$ is an E-flux or Tadmor's flux then $\theta_{j-1/2} \geq 0$ holds true.

2.2. Analytical results

Non-local diffusive-dispersive model:

$$\boxed{u_t + f(u)_x = \varepsilon u_{xx} + \lambda\gamma(\Phi * u - u)_x}$$

- Corollary: L^2-stability for the numerical solution

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Non-local diffusive-dispersive model:

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- Corollary: L^2-stability for the numerical solution
- L^2-error estimate for the non-local model problem with linear flux

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Open problems:

- L^2-error estimates in the multidimensional case

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- L^2-error estimate for the non-local model problem with linear flux

Open problems:

- L^2-error estimates in the multidimensional case
- Generalization of the L^2-error estimates to nonlinear flux functions (Feistauer et al.)

3. Various numerical examples

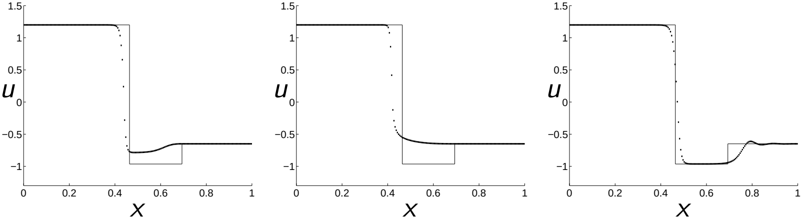
3.1. Scalar model problem (1D)

(cf. Shearer et al.)

$$\boxed{u_t + (u^3)_x = \varepsilon u_{xx} + \lambda D^{\varepsilon}_{local/global}[u]_x} \quad \text{with } \varepsilon = 0.004, \;\; \lambda = 4$$

Initial datum: $u_0(x) = \begin{cases} 1.2 & \text{for } x \leq 0.1 \\ -0.65 & \text{for } x > 0.1 \end{cases}$

Piecewise constant approximation



(Local) (Non-local, flux-like) (Non-local, source-like)

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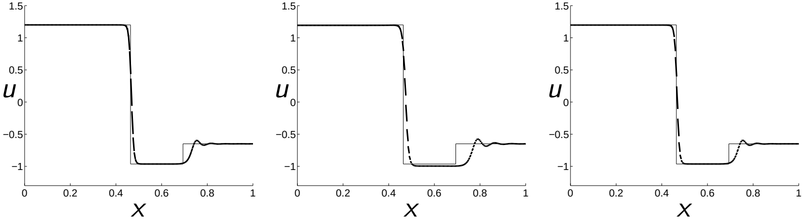
Piecewise linear approximation



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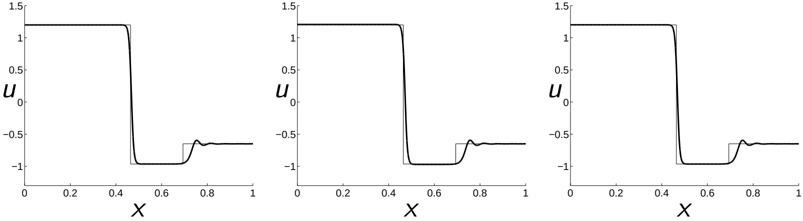
Piecewise quadratic approximation



(Local) (Non-local, flux-like) (Non-local, source-like)

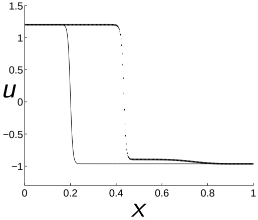
3.1. Scalar model problem (1D)

Traveling wave: (cf. Shearer et al.)

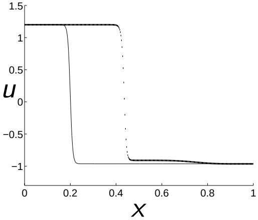
$$\boxed{u_t + (u^3)_x = \varepsilon u_{xx} + \lambda \varepsilon^2 u_{xxx}} \quad \text{with } \varepsilon = 0.004,\ \lambda = 4$$

Initial datum: $$u_0(x) = \frac{1}{2}\left(u_l + u_r - (u_l - u_r)\tanh\left(\frac{u_l - u_r}{2\varepsilon\sqrt{2\lambda}}(x - 0.2)\right)\right)$$

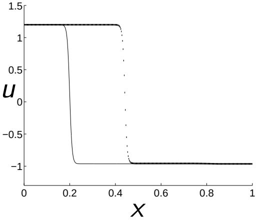
$$u_l = 1.2,\ u_r = -u_l + \tfrac{1}{3}\sqrt{\tfrac{2}{\lambda}} \approx -0.964$$



(LLF-flux)



(Upwind-flux)



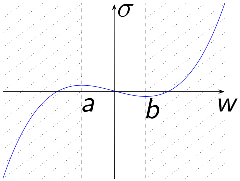
(Tadmor's flux)

3.2 Equations of elasticity (1D)

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

with $\varepsilon = 0.01, \;\; \lambda = 1$

Unknowns: stress $w = w(x,t) \in \mathbb{R}$, velocity $v = v(x,t) \in \mathbb{R}$
Given parameters: $\lambda > 0$, parameter $\varepsilon > 0$ scales between diffusion and dispersion



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

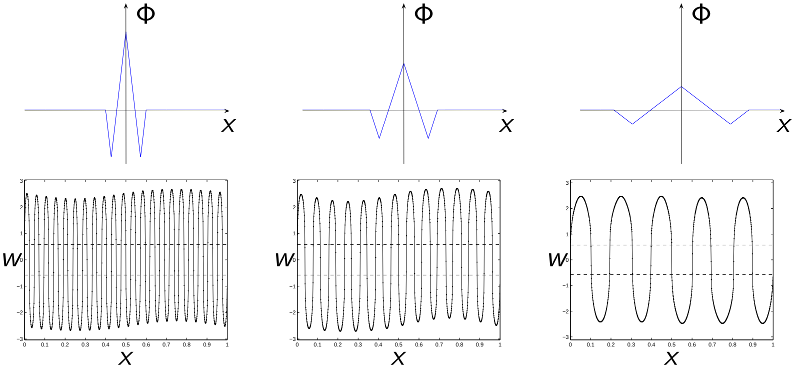
Dressel & Rohde (to appear 2008, IUMJ): Existence for kernel with indefinite sign.

3.2 Equations of elasticity (1D)

$$\begin{array}{|l|}\hline w_t - v_x = 0 \\ v_t - \sigma(w)_x = \varepsilon v_{xx} - \lambda(\Phi_\varepsilon * w - w)_x \\ \hline \end{array}$$

with $\varepsilon = 0.01, \ \lambda = 1$

Initial data: $w_0(x) = \begin{cases} 1.2 & \text{for } x < 0.5 \\ -1.2 & \text{for } x \geq 0.5 \end{cases}, \quad v_0(x) = 0 \ \text{ for all } x \in \mathbb{R}$



3.2 Equations of elasticity (1D)

Energy decay:

Classical solutions satisfy the following energy inequality

$$\frac{d}{dt}\Bigg(\int_{\mathbb{R}} \Big(\frac{1}{2}|v|^2 + W(w) + \frac{1}{4}\lambda\gamma \int_{\mathbb{R}} \Phi_\varepsilon(x-y)[w(y)-w(x)]^2 \, dy\Big) \, dx\Bigg) \le 0$$

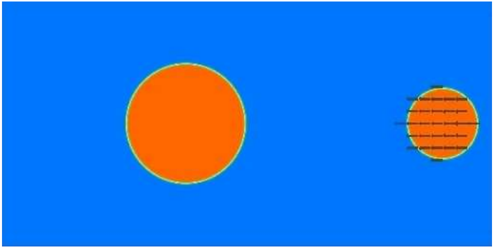
The numerical solution of the LDG-scheme satisfies

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

3.3. NSK-system (2D)

$$\begin{array}{ccccc} \rho_t & + & \nabla \cdot (\rho v) & = & 0 \\ (\rho v)_t & + & \nabla \cdot (\rho v v^T + p(\rho) Id) & = & \mu\varepsilon\Delta v + \lambda\varepsilon^2 \rho \nabla \Delta \rho \end{array}$$

Pressure p: van-der-Waals-function
Setting: drop-shoot
(parDG-Code by Dennis Diehl)



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