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On a Diffuse Interface Approach to PDEs on Surfaces

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   surface conserved quantity, transport and diffusion, reparameterisation
2. Diffuse Interface Approach
   ideas and notions, strong and weak formulation
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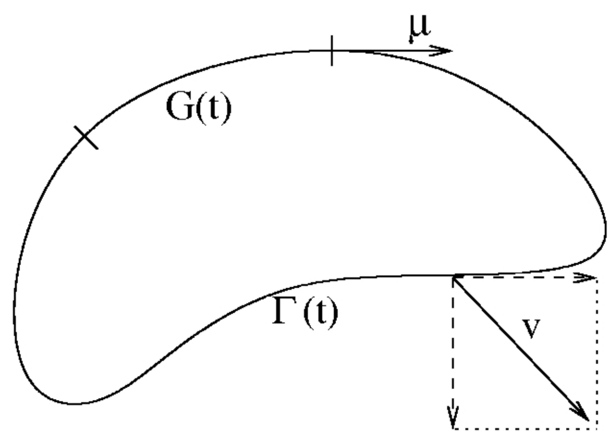
   narrow band, solvability, mass conservation, experimental convergence

Implementation: ALBERTA, http://www.alberta-fem.de

Surface Conserved Quantity

Given: evolving curve $\{\Gamma(t)\}_t$
and material velocity field $\boldsymbol{v}(t) : \Gamma(t) \longrightarrow \mathbb{R}^2$.



Consider a surface conserved quantity $c(t) : \Gamma(t) \longrightarrow \mathbb{R}$:

$$\frac{d}{dt}\Big(\int_G c\Big) = -\int_{\partial G} \boldsymbol{q}_c \cdot \boldsymbol{\mu} \, \Big[+\ldots\Big] \quad \forall G \subset \Gamma.$$

Strong equation with flux $\boldsymbol{q}_c = -D_c \nabla_\Gamma c$:

$$\underbrace{\partial_t c + \boldsymbol{v} \cdot \nabla c}_{\partial_t^\bullet c} + c \, \nabla_\Gamma \cdot \boldsymbol{v} - D_c \Delta_\Gamma c = 0.$$

Weak Problem

Assume that there is a smooth parametrisation

$$\boldsymbol{\gamma} : [0, T) \times (0, 2\pi) \to \{\Gamma(t)\}_{t \in [0,T)}, \quad (t, s) \to \boldsymbol{\gamma}(t, s)$$

with

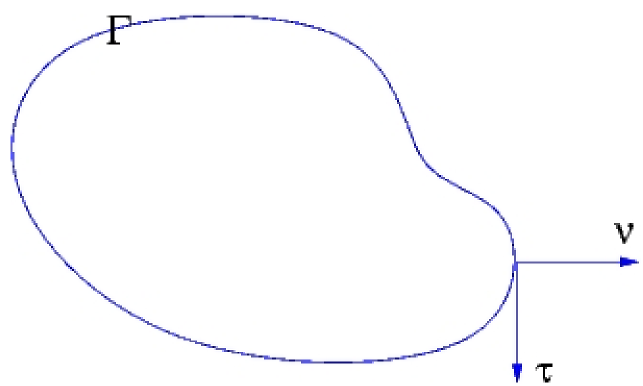
$$g(t, s) := |\partial_s \boldsymbol{\gamma}(t, s)| \geq C_g > 0$$

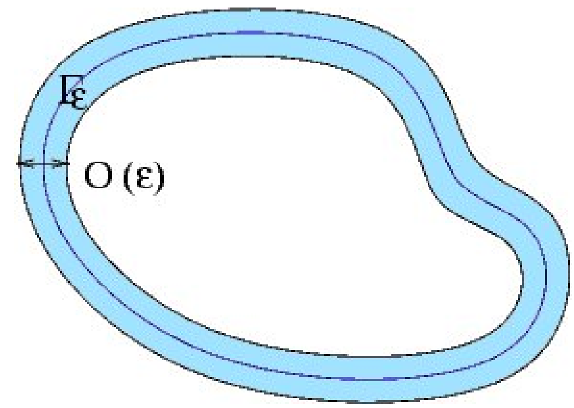
Weak formulation (in parameter space):

$$0 = \int_0^T \int_0^{2\pi} \Big(\partial_t c\, \chi g - c \partial_s \chi\, \boldsymbol{\tau} \cdot (\boldsymbol{v} - \partial_t \boldsymbol{\gamma}) + c\chi\, \boldsymbol{\tau} \cdot \partial_{st} \boldsymbol{\gamma} + \partial_s c\, \partial_s \chi\, \frac{1}{g} \Big) ds dt.$$

Here, $\boldsymbol{\tau} := \partial_s \boldsymbol{\gamma} / g$. and $g ds$ length element.

Diffuse Interface Extension, Notion





Γ_ε layer with thickness of order $O(\varepsilon)$.

$\boldsymbol{v}$ suitably extended to $\boldsymbol{v}_\varepsilon$.

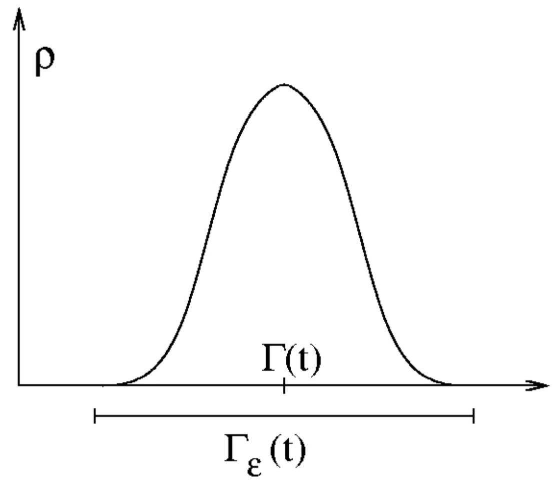
Goal: Formulate an appropriate problem for a bulk quantity $c_\varepsilon : \Gamma_\varepsilon \longrightarrow \mathbb{R}$
such that the problem on $\{\Gamma(t)\}_t$ is obtained as $\varepsilon \longrightarrow 0$.

Profile Function

Idea: approximate surface delta 'function' δ_Γ
by a smooth cross profile $\rho_\varepsilon : [0,T) \times \mathbb{R}^2 \longrightarrow \mathbb{R}$:

$$\tfrac{1}{\varepsilon}\rho_\varepsilon \longrightarrow \delta_\Gamma \text{ as measure,}$$

$$\Gamma_\varepsilon = \{\rho_\varepsilon(t) > 0\}.$$



To derive the equation for c_ε: $G = \Gamma \cap \mathcal{R}$, $G_\varepsilon = \Gamma_\varepsilon \cap \mathcal{R}$ with test volume $\mathcal{R} \subset \mathbb{R}^2$

$$\begin{array}{ccc} \frac{d}{dt}\Big(\int_G c\Big) & = & -\int_{\partial G} \boldsymbol{q}_c \cdot \boldsymbol{\mu} \\ \uparrow & \text{as } \varepsilon \longrightarrow 0 & \uparrow \\ \frac{d}{dt}\Big(\int_{G_\varepsilon} \rho_\varepsilon c_\varepsilon\Big) & = & -\int_{\partial G_\varepsilon} \rho_\varepsilon \boldsymbol{q}_{c,\varepsilon} \cdot \boldsymbol{\nu}_{G_\varepsilon} \end{array}$$

Equation on the Diffuse Interface

With the flux $\boldsymbol{q}_{c,\varepsilon} = -D_c \nabla c_\varepsilon$

$$0 = \frac{d}{dt}\Big(\int_{G_\varepsilon} \rho_\varepsilon c_\varepsilon \Big) + \int_{\partial G_\varepsilon} \rho_\varepsilon \boldsymbol{q}_{c,\varepsilon} \cdot \boldsymbol{\nu}_{G_\varepsilon} =$$

$$\int_{G_\varepsilon} \Big(\partial_t(\rho_\varepsilon c_\varepsilon) + \nabla \cdot (\boldsymbol{v}_\varepsilon \rho_\varepsilon c_\varepsilon) - D_c \nabla \cdot (\rho_\varepsilon \nabla c_\varepsilon) \Big) + \int_{\partial G_\varepsilon} \rho_\varepsilon c_\varepsilon (\boldsymbol{v}_{\partial G_\varepsilon} - \boldsymbol{v}_\varepsilon) \cdot \boldsymbol{\nu}_{G_\varepsilon}.$$

Proposal:

$$\partial_t^\bullet(\rho_\varepsilon c_\varepsilon) + \rho_\varepsilon c_\varepsilon \nabla \cdot \boldsymbol{v}_\varepsilon - D_c \nabla \cdot (\rho_\varepsilon \nabla c_\varepsilon) = 0.$$

In applications we expect that $\boldsymbol{v}_{\partial G_\varepsilon} - \boldsymbol{v}_\varepsilon$ is small but $\neq 0$ in general.
Since ρ_ε vanishes on $\partial \Gamma_\varepsilon$:

$$\frac{d}{dt}\Big(\int_{\Gamma_\varepsilon} \rho_\varepsilon c_\varepsilon \Big) = 0$$

Degeneration of ρ_ε keeps the mass on the interfacial layer.

Assumptions

Assumptions:

- Extension of the parametrisation is possible, with $z \in (-1, 1)$

$$\boldsymbol{\gamma}_\varepsilon(t, s, z) = \boldsymbol{\gamma}(t, s) + \varepsilon z \underbrace{q(t, s, z, \varepsilon)}_{\sim 1} \boldsymbol{\nu}(t, s).$$

- There is a function $\rho_0 : (-1, 1) \longrightarrow \mathbb{R}$ such that

$$||\rho_\varepsilon(t, s, z) - \rho_0(z)||_\infty \to 0, \quad C_1\rho_0 \leq \rho_\varepsilon \leq C_2\rho_0, \quad |\partial_t\rho_\varepsilon|, |\partial_{tt}\rho_\varepsilon| \leq C\rho_0$$

- The extension of the velocity field fulfils

$$|\boldsymbol{v}_\varepsilon(t, s, z) - \boldsymbol{v}(t, s)|, |\partial_t\boldsymbol{v}_\varepsilon(t, s, z) - \partial_t\boldsymbol{v}(t, s)| \leq C\varepsilon.$$

Weak Formulation

Weak formulation in parameter space:

$$0 = \int_0^T \int_0^{2\pi} \int_{-1}^1 \rho_0 \Big(a_0^\varepsilon \partial_t c_\varepsilon \chi + (a_1^\varepsilon \partial_s c_\varepsilon - b_3^\varepsilon \partial_z c_\varepsilon)(a_1^\varepsilon \partial_s \chi - b_3^\varepsilon \partial_z \chi) + b_0^\varepsilon c_\varepsilon \chi + b_1^\varepsilon c_\varepsilon \partial_s \chi + b_2^\varepsilon c_\varepsilon \partial_z \chi + \frac{1}{\varepsilon^2} a_2^\varepsilon \partial_z c_\varepsilon \partial_z \chi \Big) dz\, ds\, dt$$

The coefficients are bounded provided ε is small enough.

The b_j^ε belong to lower order terms, e.g.

$$b_1 = -\frac{(q + z\partial_z q)\rho_\varepsilon}{\rho_0} \boldsymbol{\tau} \cdot (\boldsymbol{v}_\varepsilon - \partial_t \boldsymbol{\gamma}) \longrightarrow -\boldsymbol{\tau} \cdot (\boldsymbol{v} - \partial_t \boldsymbol{\gamma}) \text{ as } \varepsilon \to 0.$$

The a_i^ε bounded from below by positive constants, e.g.

$$a_2^\varepsilon = \frac{\rho_\varepsilon g_\varepsilon}{\rho_0 (q + z\partial_z q)} \longrightarrow g \text{ as } \varepsilon \to 0.$$

Existence and Uniqueness

$$0 = \int_0^T \int_0^{2\pi} \int_{-1}^1 \rho_0 \Big(a_0^\varepsilon \partial_t c_\varepsilon \chi + (a_1^\varepsilon \partial_s c_\varepsilon - b_3^\varepsilon \partial_z c_\varepsilon)(a_1^\varepsilon \partial_s \chi - b_3^\varepsilon \partial_z \chi) + b_0^\varepsilon c_\varepsilon \chi + b_1^\varepsilon c_\varepsilon \partial_s \chi + b_2^\varepsilon c_\varepsilon \partial_z \chi + \frac{1}{\varepsilon^2} a_2^\varepsilon \partial_z c_\varepsilon \partial_z \chi \Big) dz ds dt$$

Th.: *There is a unique weak solution* c_ε *in* $L^2(0,T;X) \cap H^1(0,T;B)$ *where*

$$B = \Big\{ f : (0,2\pi)_{per} \times (-1,1) \to \mathbb{R} \,\Big|\, \int_0^{2\pi} \int_{-1}^1 \rho_0 |f|^2 dz ds < \infty \Big\},$$

$$X = \Big\{ f \in B \,\Big|\, \int_0^{2\pi} \int_{-1}^1 \rho_0 \big(|\partial_s f|^2 + |\partial_z f|^2 \big) dz ds < \infty \Big\}.$$

Essential ingredient for the proof is that $X \hookrightarrow B$ is compact [Antoci, 2003].

Estimates

Test with c_ε:

$$\sup_{t\in[0,T)} \int_0^{2\pi}\int_{-1}^{1} \rho_0 |c_\varepsilon(t)|^2 + \|\partial_s c_\varepsilon\|^2_{L^2(0,T;B)} + \frac{1}{\varepsilon^2}\|\partial_z c_\varepsilon\|^2_{L^2(0,T;B)} \le C \int_0^{2\pi}\int_{-1}^{1} \rho_0 |c_\varepsilon(0)|^2,$$

Test with $\partial_t c_\varepsilon$:

$$\sup_{t\in[0,T)} \int_0^{2\pi}\int_{-1}^{1} \left(|\partial_s c_\varepsilon(t)|^2 + \frac{1}{\varepsilon^2}|\partial_z c_\varepsilon(t)|^2 \right) + \|\partial_t c_\varepsilon\|^2_{L^2(0,T;B)} \le C.$$

For going to the limit follow the lines of
[Hale, Raugel, 1992], [Rodriguez, Viaño, 1998], [Prizzi, Rinaldi, Rybakowski, 2002]

Convergence

Sharp interface:

$$0 = \int_0^T \int_0^{2\pi} \big(\partial_t c\, \chi g - c\partial_s \chi\, \boldsymbol{\tau} \cdot (\boldsymbol{v} - \partial_t \boldsymbol{\gamma}) + c\chi\, \boldsymbol{\tau} \cdot \partial_{st}\boldsymbol{\gamma} + \partial_s c\, \partial_s \chi \frac{1}{g}\big) ds dt.$$

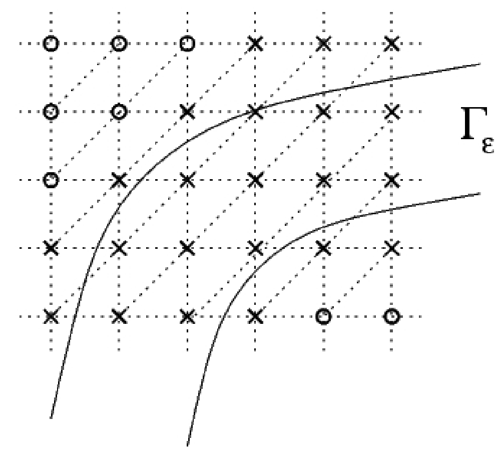
Diffuse interface:

$$0 = \int_0^T \int_0^{2\pi} \int_{-1}^1 \rho_0(z) \Big(\partial_t c_\varepsilon \chi a_0^\varepsilon + c_\varepsilon \partial_s \chi\, b_1^\varepsilon + c_\varepsilon \chi\, b_0^\varepsilon + c_\varepsilon \partial_z \chi\, b_2^\varepsilon$$
$$+ (\tilde{a}_1^\varepsilon \partial_s c_\varepsilon - b_3^\varepsilon \partial_z c_\varepsilon)(\tilde{a}_1^\varepsilon \partial_s \chi - b_3^\varepsilon \partial_z \chi) + \frac{1}{\varepsilon^2} a_2^\varepsilon \partial_z c_\varepsilon \partial_z \chi \Big) dz ds dt.$$

Th.: *As* $\varepsilon \longrightarrow 0$, *the solutions* c_ε *converge to a function* c *in* $C^0(0,T;B)$ *with*

- $\partial_z c = 0$, *hence* $c = c(t,s)$,
- $c \in L^2(0,T;H^1_{per}(0,2\pi)) \cap H^1(0,T;L^2_{per}(0,2\pi))$,
- c *solves the weak sharp interface problem.*

Numerical Setup



Approximation in **physical space** Ω.
Timestep τ, triangulation $\mathcal{T}_h$, vertices $\{\boldsymbol{x}_i\}_i$.
Linear FE:

$$S_h := \left\{ \eta \in C^0(\Omega) \,\middle|\, \eta\big|_e \text{ linear on each } e \in \mathcal{T}_h \right\}.$$

Projection:

$$\pi^h : C^0(\Omega) \to S_h, \quad \pi^h(\eta)(\boldsymbol{x}_i) = \eta(\boldsymbol{x}_i)\, \forall i.$$

Discrete interfacial layer:

$$\mathcal{N}_h^n := \left\{ \text{vertex } i \,\middle|\, \text{there is a connected vertex } j \text{ with } \rho_\varepsilon(t^n, \boldsymbol{x}_j) \neq 0 \right\},$$
$$\Gamma_h^n := \left\{ e \in \mathcal{T}_h \,\middle|\, \text{vertices of } e \text{ belong to } \mathcal{N}_h^n \right\}.$$

Proposed Method

Weak formulation: find c such that for all χ

$$0 = \int_\Omega \partial_t(\rho c)\chi - \rho c \boldsymbol{v} \cdot \nabla\chi + D_c \rho \nabla c \cdot \nabla \chi.$$

Scheme: given $c_h^{n-1} = \sum_{i \in \mathcal{N}_h^{n-1}} c_i^{n-1}\chi_i$ compute $c_h^n = \sum_{i\in\mathcal{N}_h^n} c_i^n \chi_i$ such that for all $j \in \mathcal{N}_h^n$

$$0 = \int_{\Gamma_h^n} \frac{1}{\tau}\Big(\pi^h(\rho^n c_h^n \chi_j) - \pi^h(\rho^{n-1} c_h^{n-1}\chi_j)\Big) - \pi^h(\rho^n c_h^n)\pi^h(\boldsymbol{v}^n)\cdot\nabla\chi_j + D_c \pi^h(\rho^n)\nabla c_h^n \cdot \nabla \chi_j$$

Q: solvable? mass conserved?

Other methods:
[Schwartz, Adalsteinsson et. al., 2005], [Rätz, Voigt, 2006, 2007]

Solvability

Scheme:

$$0 = \int_{\Gamma_h^n} \frac{1}{\tau}\Big(\pi^h(\rho^n c_h^n \chi_j) - \pi^h(\rho^{n-1} c_h^{n-1} \chi_j)\Big) - \pi^h(\rho^n c_h^n)\pi^h(\boldsymbol{v}^n)\cdot\nabla\chi_j + D_c \pi^h(\rho^n)\nabla c_h^n \cdot \nabla \chi_j$$

Th.: *If $\tau \leq 4D_c/\|\boldsymbol{v}\|_\infty^2$ the scheme has a unique solution c_h^n.*

Proof:
Linear system, number of equations = number of unknown
$\Rightarrow$ uniqueness sufficient $\rightsquigarrow$ set $c_h^{n-1} = 0$.
Test with c_h^n aiming to use nonnegativity of mass and stiffness matrix.
Control of advective term $\rightsquigarrow$ restriction on timestep.
Mass matrix degenerate, have only that $c_h^n = 0$ in interior vertices.
Stiffness matrix always with contribution $\Rightarrow \nabla c_h^n = 0$. $\square$

Mass Conservation

Scheme: for all $j \in \mathcal{N}_h^n$

$$0 = \int_{\Gamma_h^n} \frac{1}{\tau}\Big(\pi^h(\rho^n c_h^n \chi_j) - \pi^h(\rho^{n-1} c_h^{n-1} \chi_j)\Big) - \pi^h(\rho^n c_h^n)\pi^h(\boldsymbol{v}^n)\cdot\nabla\chi_j + D_c \pi^h(\rho^n)\nabla c_h^n \cdot \nabla\chi_j$$

Assumption: If $i \in N_h^{n-1}$ does not belong to N_h^n then $\rho^{n-1}(\boldsymbol{x}_i) = 0$.

Th.: *With this assumption*

$$\int_{\Gamma_h^n} \pi^h(\rho^n c_h^n) = \int_{\Gamma_h^{n-1}} \pi^h(\rho^{n-1} c_h^{n-1}).$$

Proof: Summing up over $j \in \mathcal{N}_h^n$ yields

$$\sum_{i \in \mathcal{N}_h^n} \Big(\int \chi_i\Big)\rho^n(\boldsymbol{x}_i) c_i^n = \sum_{i \in \mathcal{N}_h^n} \Big(\int \chi_i\Big)\rho^{n-1}(\boldsymbol{x}_i) c_i^{n-1}.$$

Thanks to both assumptions we can replace $\mathcal{N}_h^n$ by $\mathcal{N}_h^{n-1}$ on the right hand side. $\square$

Stationary Surface

The function $c = e^{-4t}x_1x_2$ is a solution to $\partial_t c - \Delta_\Gamma c = 0$ on $\Gamma = S^1$.

ρ stretched $\cos^2$ profile, argument is $\mathrm{dist}(\boldsymbol{x}, \Gamma)/\varepsilon$.

For ε fixed: quadratic in $L^\infty(0, T, L^2(\Gamma))$, and linear in $L^2(0, T, H^1(\Gamma))$ as $h \to 0$.

Ratio ε/h fixed (≥ 3 grid points across the interface sufficient, here ≥ 8):

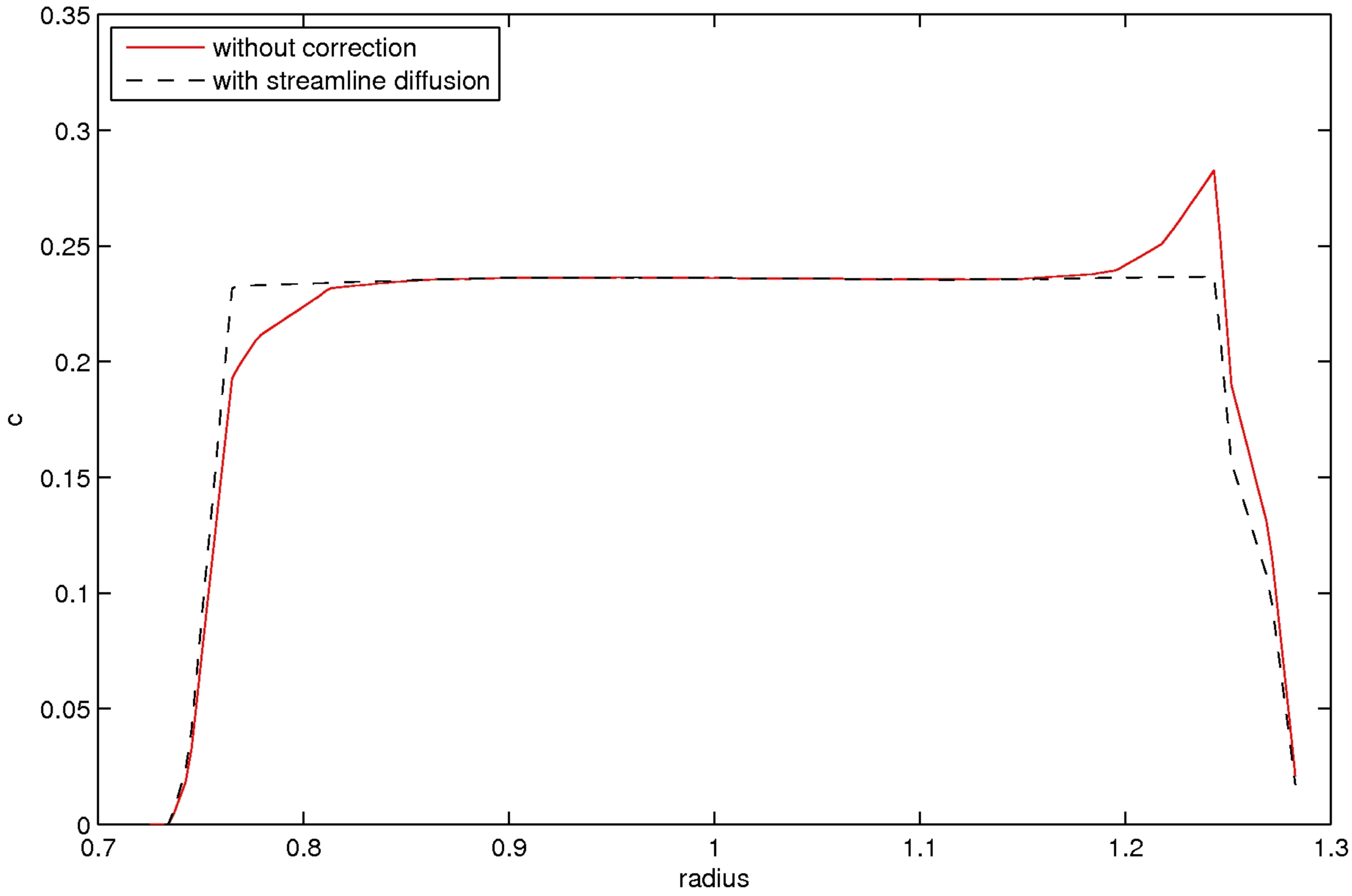
ε	h	$e[L^\infty, L^2]$	$\mathrm{eoc}_{e[L^\infty, L^2]}$	$e[L^2, H^1]$	$\mathrm{eoc}_{e[L^2, H^1]}$
$\sqrt{2}/10$	$2^{-4.5}$	0.00141612	—	0.01664609	—
$1/10$	$2^{-5.0}$	0.00073612	1.887884	0.01054201	1.318067
$\sqrt{2}/20$	$2^{-5.5}$	0.00036690	2.009086	0.00692233	1.213642
$1/20$	$2^{-6.0}$	0.00017812	2.085131	0.00436128	1.333009
$\sqrt{2}/40$	$2^{-6.5}$	0.00008500	2.134493	0.00291098	1.166492

Comparable to [Schwartz, Adalsteinsson et. al., 2005].

Rk.: Can also take tangential motion into account.

Interfacial Profile on Moving Surface

Influence of motion in normal direction:



Boundary condition

Continuous problem: no boundary condition since $\rho = 0$ on $\partial\Gamma(\varepsilon, t)$.

Discrete in 1D, i boundary vertex, $\rho_i^n = \rho_{i+1}^n = 0$, $\rho_{i-1}^n > 0$:

$$0 = -\frac{h\rho_i^{n-1}}{\Delta t} c_i^{n-1} - \frac{\boldsymbol{v}_{i-1,i}^n \rho_{i-1}^n}{2} c_{i-1}^n + \frac{\rho_{i-1,i}^n}{h}(c_i^n - c_{i-1}^n)$$

$\rightsquigarrow$ no homogeneous Neumann boundary condition.

Streamline Diffusion

Overcome by adding a streamline diffusion to scheme:

$$\int_{\Gamma_h^n} g_h^n \, \boldsymbol{\omega}_h^n \cdot \nabla c_h^n \, \boldsymbol{\omega}_h^n \cdot \nabla \chi$$

- $\boldsymbol{\omega} := (\boldsymbol{v} \cdot \boldsymbol{\nu})\boldsymbol{\nu}$ with unit normal $\boldsymbol{\nu}$ on Γ,
- g_h nonnegative function of order h present close to the interface boundary.

Leads to an additional term of the form

$$\frac{g_h (\boldsymbol{\omega}_{i,i-1}^n)^2}{h} (c_i^n - c_{i-1}^n)$$

Solvability and mass conservation are not affected.

Moving Surface

Transport of unit circle with constant velocity field $\boldsymbol{v}(\boldsymbol{x}, t) = (2, 0)^T$.

Same profile for c as in stationary case solves $\partial_t c + \boldsymbol{v} \cdot \nabla c - \Delta_\Gamma c = 0$.

Errors quantitatively comparable (with/without motion or with/without streamline diffusion).

Exemplary $e[H^1_{tang}]$: converging linearly for $h \to 0$, for fixed ε as well as when keeping ε/h fixed.

$h \setminus \varepsilon$	$\sqrt{2}/10$	$1/10$	$\sqrt{2}/20$	$1/20$
$2^{-4.0}$	0.032217			
$2^{-4.5}$	0.022567	0.022738		
$2^{-5.0}$	0.016381	0.016446	0.016531	
$2^{-5.5}$	0.011504	0.011408	0.011426	0.011428
$2^{-6.0}$	0.008672	0.008432	0.008398	0.008395
$2^{-6.5}$	0.006424	0.006003	0.005910	0.005895

Application Example

Two-phase flow modelled by

1. Navier-Stokes system with interfacial contribution to stress tensor for two fluids of same mass density and viscosity,
2. advective degenerate Cahn-Hilliard equation with double-obstacle potential for fluid-fluid interface.

[Kay, Styles, Welford, 2007]

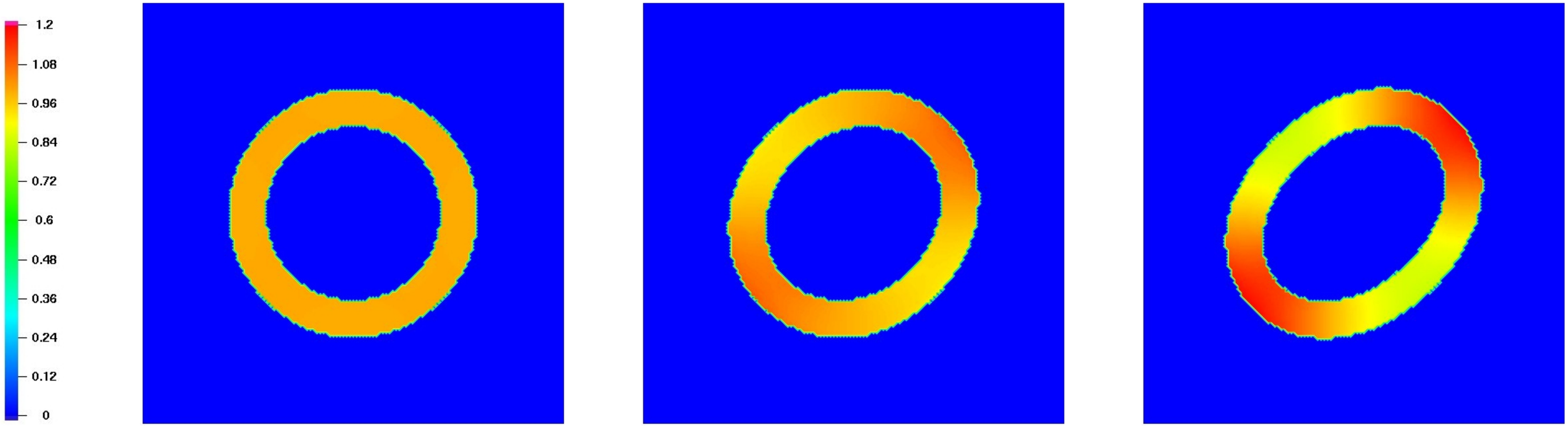
Initially: drop of fluid 1 in fluid 2, then external fluid exposed to shear flow.

Take an additional conserved surface quantity into account, initially homogeneously distributed.

Application Example

Fluid drop in another fluid exposed to shear flow
with conserved surface quantity (later on surfactant),
solved with a double obstacle Cahn-Hilliard-Navier-Stokes system.

[Lowengrub, Truskinowsky, 1998], [Boyer, 2002], [Kay, Welford, 2007]



$t = 0.01$ $t = 0.20$ $t = 0.50.$

Application Example

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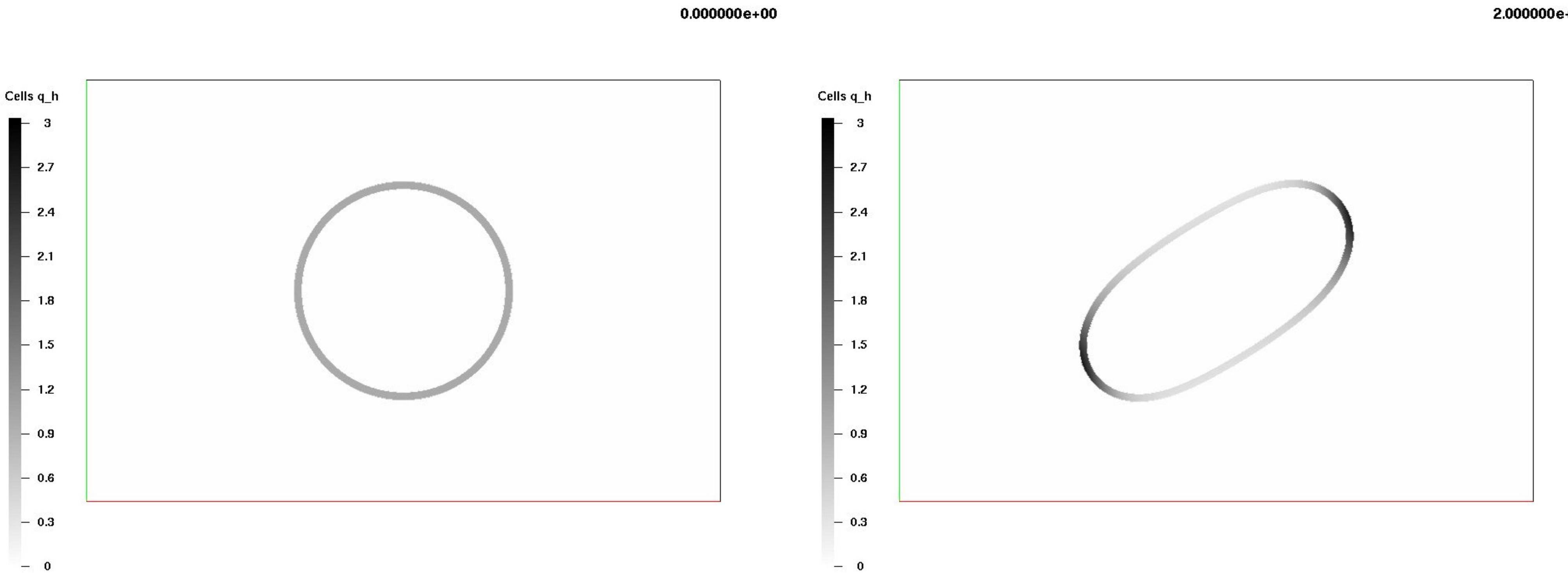
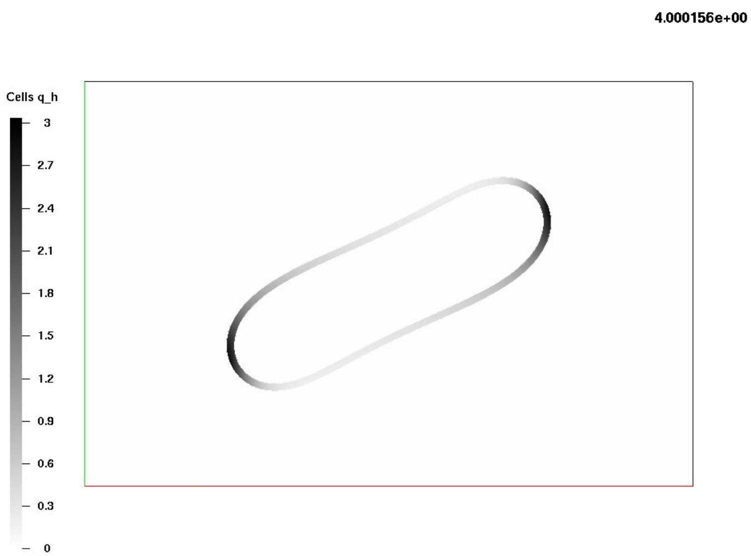
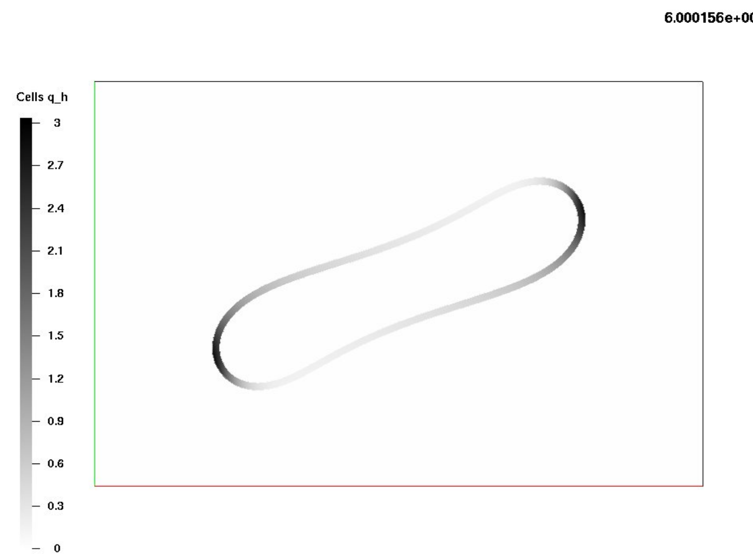
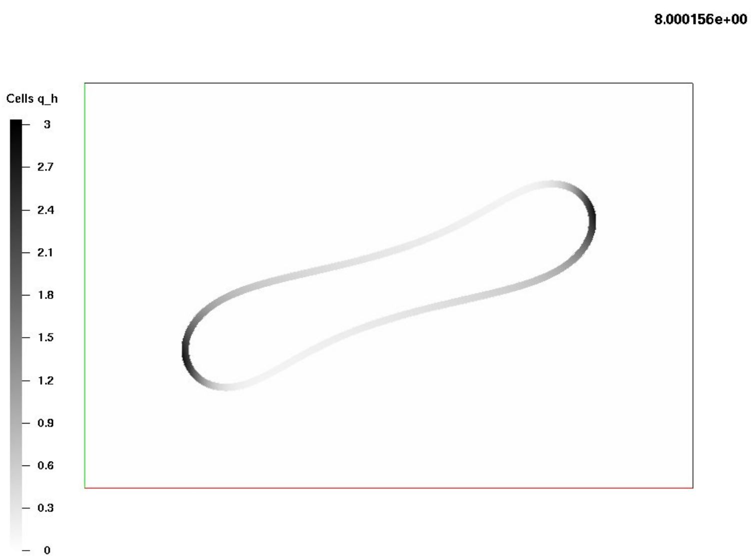
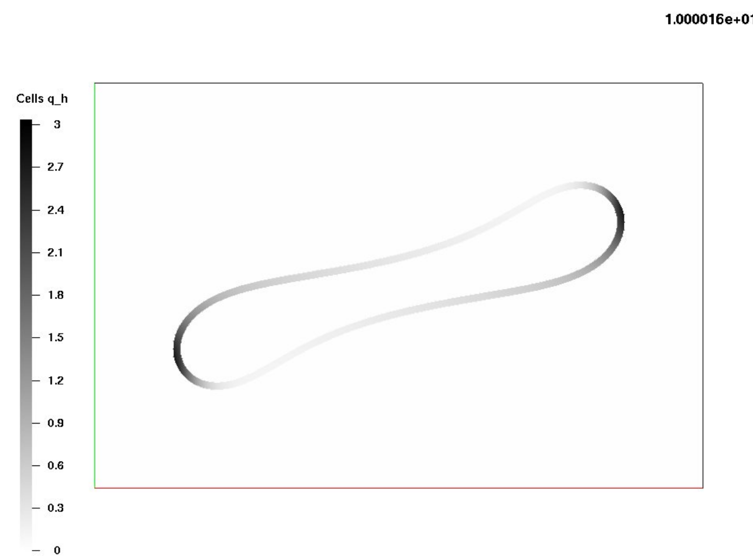


Application Example









Application Example

ALBERTA-FEM

An Adaptive Hierarchical Finite Element Toolbox
by ALfred Schmidt and KuniBERT Siebert.

Core parts of FE programs:
assembly and solution of the discretised problems.

Goals: provide data structures which allow an easy and efficient implementation of the problem-dependent parts, in particular with respect to

- mesh modification (adaptive methods),
- solving linear and nonlinear systems of equations.

www.alberta-fem.de

Conclusion

We considered three different approaches to solve pdes on moving surfaces:

1. ESFEM on moving polyhedral surfaces,
2. implicit surfaces as level sets $\rightsquigarrow$ degenerate equations to be solved in a narrow band
3. diffuse interface approach $\rightsquigarrow$ bulk equations to be solved in a narrow band.

Applications:

- biomechanics, dynamics of lipid bilayer vesicles,
- fluid dynamics, rheology properties of emulsions in dependence of surfactant presence,
- materials science, enhanced species diffusion along (moving) grain boundaries.