

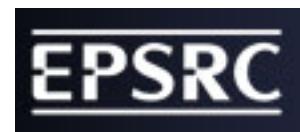
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On a Diffuse Interface Method
for an Advection Diffusion Equation
on a Moving Surface

In collaboration with
Charles M. Elliott (Warwick)

Supported by



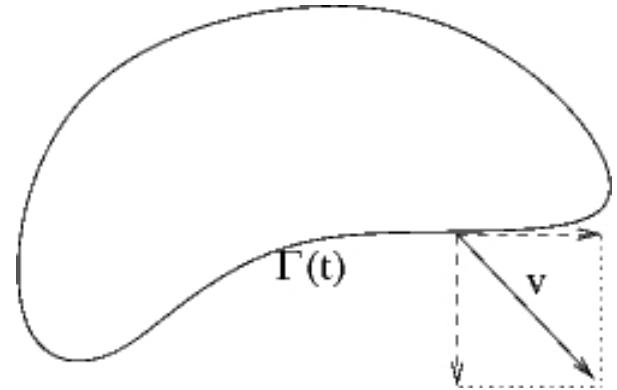
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Surface Conserved Quantity

Given:

Evolving closed curve $\{\Gamma(t)\}_{t \in I}$ in a domain $\Omega \subset \mathbb{R}^2$,
 a material velocity field $\mathbf{v}(t) : \Gamma(t) \rightarrow \mathbb{R}^2$,
 and a source term $f(t) : \Gamma(t) \rightarrow \mathbb{R}$.



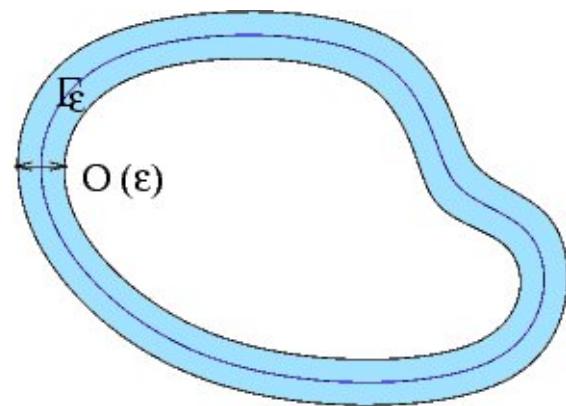
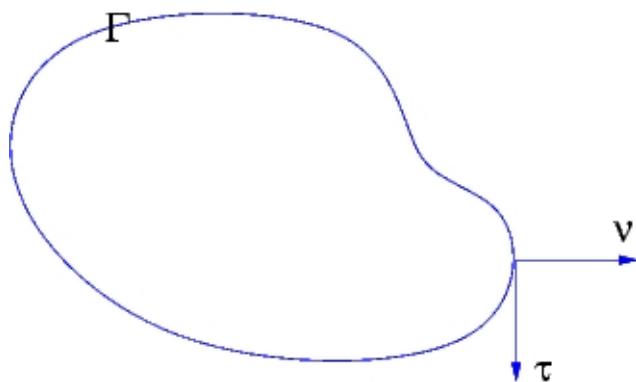
Problem:

Find a field $c(t) : \Gamma(t) \rightarrow \mathbb{R}$ such that

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

Diffuse Interface Extension, Notion

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

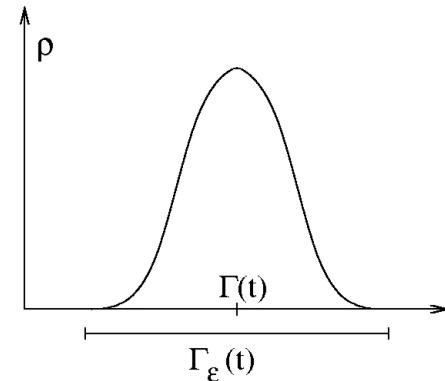


Motivation: (a) no need for surface triangulations but (fixed) bulk meshes sufficient,
(b) surface described implicitly, for example by a distance function,
(c) surface may be unknown and solution to a level-set or phase-field equation.

Equation on the Diffuse Interface

Idea: approximate surface delta 'function' δ_Γ by cross profile functions $\rho_\varepsilon : I \times \Omega \rightarrow \mathbb{R}$:

$$\frac{1}{\varepsilon} \rho_\varepsilon \rightarrow \delta_\Gamma \text{ as measure, } \Gamma_\varepsilon(t) = \{\rho_\varepsilon(t) > 0\}.$$



Extend \mathbf{v} and f in a suitable way to functions \mathbf{v}_ε and f_ε on Γ_ε .

Bulk pde: Find a function $c_\varepsilon : I \times \Omega \rightarrow \mathbb{R}$ such that

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

Degeneration of ρ_ε keeps the mass on the interfacial layer:

$$\frac{d}{dt} \left(\int_{\Gamma_\varepsilon} \rho_\varepsilon c_\varepsilon \right) = \int_{\Gamma_\varepsilon} \rho_\varepsilon f_\varepsilon + \underbrace{\int_{\partial\Gamma_\varepsilon} \rho_\varepsilon (c_\varepsilon \mathbf{v}_{\partial\Gamma_\varepsilon} - c_\varepsilon \mathbf{v}_\varepsilon + D_c \nabla c_\varepsilon) \cdot \boldsymbol{\nu}_{ext}}_{=0}$$

Weak Solutions

Transfer to fixed space with a parametrisation

$$\boldsymbol{\gamma}_\varepsilon : [0, T) \times (0, 2\pi) \times (-1, 1) \rightarrow \{\Gamma_\varepsilon(t)\}_{t \in I}, \quad \boldsymbol{\gamma}_\varepsilon(t, s, z) = \boldsymbol{\gamma}_0(t, s) + \varepsilon z q \boldsymbol{\nu}(t, s).$$

Weak formulation in parameter space:

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

Th.: (Unique weak solvability) [Elliott, S. 2008]

There is a unique weak solution c_ε in $L^2(H_{\rho_0}^1) \cap H^1(L_{\rho_0}^2)$.

Convergence

For going to the limit (energy method) follow the lines of
 [Hale, Raugel, 1992], [Rodriguez, Viaño, 1998],
 [Prizzi, Rinaldi, Rybakowski, 2002], [Prizzi, Rybakowski, 2003]

Estimates:

$$\begin{aligned} \|c_\varepsilon\|_{L^\infty(L^2_{\rho_0})}^2 + \|\partial_s c_\varepsilon\|_{L^2(L^2_{\rho_0})}^2 + \frac{1}{\varepsilon^2} \|\partial_z c_\varepsilon\|_{L^2(L^2_{\rho_0})}^2 &\leq C \|c_\varepsilon(0)\|_{L^2_{\rho_0}}^2, \\ \|\partial_s c_\varepsilon\|_{L^\infty(L^2_{\rho_0})}^2 + \frac{1}{\varepsilon^2} \|\partial_z c_\varepsilon(t)\|_{L^\infty(L^2_{\rho_0})}^2 + \|\partial_t c_\varepsilon\|_{L^2(L^2_{\rho_0})}^2 &\leq C. \end{aligned}$$

Th.: (Convergence) [Elliott, S. 2008]

As $\varepsilon \rightarrow 0$, the weak solutions c_ε converge to a function $c \in C^0(I; L^2_{\rho_0})$ with

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

Numerical Setup

[Elliott, S., submitted]

Approximation in **physical space** Ω .

Timestep τ , triangulation \mathcal{T}_h , vertices $\{\mathbf{x}_i\}_i$.

Linear FE:

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

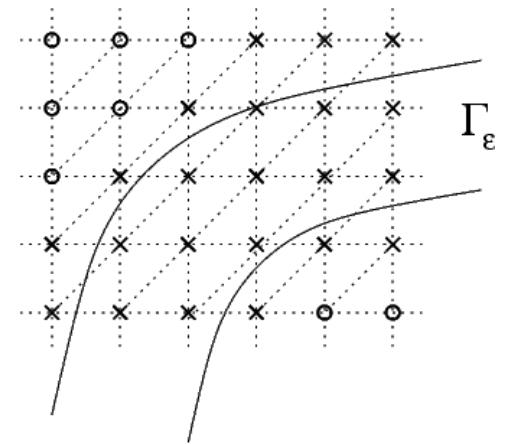
Projection:

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

Discrete interfacial layer:

$$\mathcal{N}_h^n := \left\{ \text{vertex } i \mid \text{there is a connected vertex } j \text{ with } \rho_\varepsilon(t^n, \mathbf{x}_j) \neq 0 \right\},$$

$$\Gamma_h^n := \left\{ e \in \mathcal{T}_h \mid \text{vertices of } e \text{ belong to } \mathcal{N}_h^n \right\}.$$



Proposed Method

Weak formulation: find c such that for all χ

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

Scheme: given $c_h^{n-1} = \sum_{i \in \mathcal{N}_h^{n-1}} c_i^{n-1} \chi_i$ and $c_h^{n-1}(\mathbf{x}_i) = c_i^{n-1} = 0$ if $i \notin \mathcal{N}_h^{n-1}$
compute $c_h^n = \sum_{i \in \mathcal{N}_h^n} c_i^n \chi_i$ such that for all $j \in \mathcal{N}_h^n$

$$\begin{aligned} 0 &= \int_{\Gamma_h^n} \frac{1}{\tau} \left(\pi^h(\rho^n c_h^n \chi_j) - \pi^h(\rho^{n-1} c_h^{n-1} \chi_j) \right) \\ &\quad - \int_{\Gamma_h^n} \pi^h(\rho^n c_h^n) \pi^h(\mathbf{v}^n) \cdot \nabla \chi_j + D_c \int_{\Gamma_h^n} \pi^h(\rho^n) \nabla c_h^n \cdot \nabla \chi_j - \int_{\Gamma_h^n} \pi^h(\rho^n f^n \chi_j) \end{aligned}$$

and set $c_h^n(\mathbf{x}_i) = c_i^n = 0$ if $i \notin \mathcal{N}_h^n$.

Other methods:

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

Questions: solvable? (total) mass conserved?

Solvability

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

$$\begin{aligned} 0 = & \int_{\Gamma_h^n} \frac{1}{\tau} \left(\pi^h(\rho^n c_h^n \chi_j) - \pi^h(\rho^{n-1} c_h^{n-1} \chi_j) \right) \\ & - \int_{\Gamma_h^n} \pi^h(\rho^n c_h^n) \pi^h(\mathbf{v}^n) \cdot \nabla \chi_j + D_c \int_{\Gamma_h^n} \pi^h(\rho^n) \nabla c_h^n \cdot \nabla \chi_j - \int_{\Gamma_h^n} \pi^h(\rho^n f^n \chi_j) \end{aligned}$$

Th.: (Unique Solvability) [Elliott, S., submitted]

If $\tau \leq 4D_c/\|\mathbf{v}\|_{L^\infty(L^\infty)}$ the scheme has a unique solution c_h^n .

Proof:

Uniqueness sufficient \rightsquigarrow set $c_h^{n-1} = 0, f^n = 0$.

Test with c_h^n .

Mass matrix degenerate, have only that $c_h^n = 0$ in interior vertices.

Stiffness matrix always with contribution $\Rightarrow \nabla c_h^n = 0$. □

Mass Conservation

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

Ensured, for example, if $\tau \leq Ch/\|\mathbf{v}\|_{L^\infty(L^\infty)}$.

Th.: (Total Mass Conservation) [Elliott, S., submitted] ($f = 0$)

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

Proof: In the scheme, summing up over $j \in \mathcal{N}_h^n$ yields

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

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

Narrow Band

Full fine triangulation \mathcal{T}_h not stored but dynamically adapted,
coarsened away from the diffusive interfacial layer Γ_ε .

(Loading Movie)

Numerical Convergence

From [Dziuk, Elliott 2007].

Surface: $\Gamma(t) = \{\mathbf{x} \in \mathbb{R}^3 \mid \frac{x_1^2}{a(t)} + x_2^2 + x_3^2 = 1\}$, $a(t) = 1 + \sin(t)/4$.

Solution: $c(t, \mathbf{x}) = e^{-6t}x_1x_2$ for appropriate f .

Profile function: $\rho(t, \mathbf{x}) = \cos^2(\text{dist}(\mathbf{x}, \Gamma(t))/\varepsilon)$.

For ε fixed: Convergence quadratic in $L^\infty(L^2)$ and $L^2(H_{norm}^1)$, linear in $L^2(H_{tang}^1)$ as $h \rightarrow 0$.

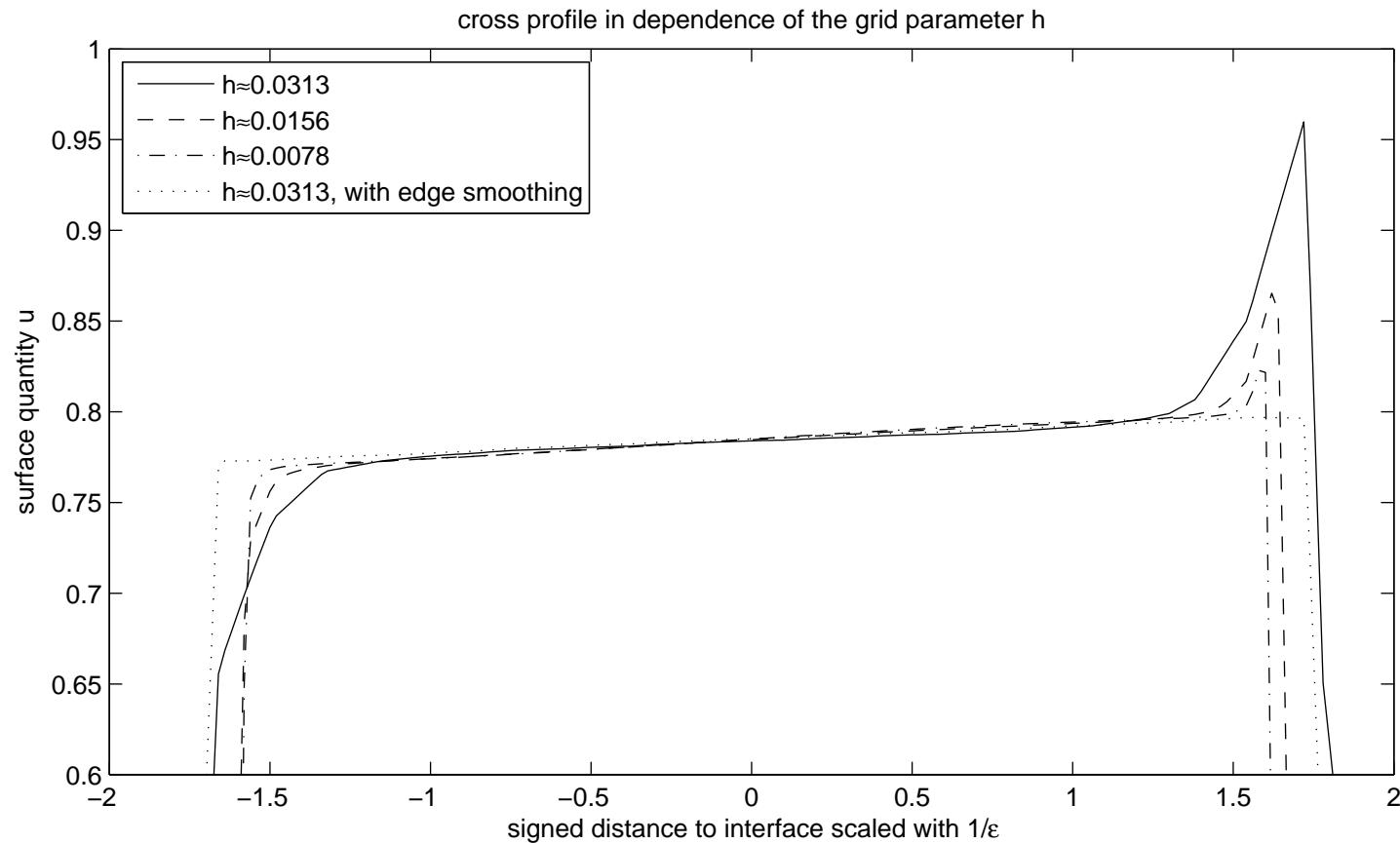
Ratio ε/h fixed:

ε	h	$\frac{e[L^\infty, L^2]}{10^{-3}}$	eoc	$\frac{e[L^2, H_{norm}^1]}{10^{-2}}$	eoc	$\frac{e[L^2, H_{tang}^1]}{10^{-2}}$	eoc
2/10	0.0628	9.0617	—	4.7355	—	3.4891	—
$\sqrt{2}/10$	0.0544	5.1481	1.6259	2.7484	1.5698	2.5583	0.8953
1/10	0.0314	2.2238	2.4220	1.5070	1.7338	1.7187	1.1477
$\sqrt{2}/20$	0.0272	1.2871	1.5778	0.9499	1.3317	1.2695	0.8741

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

Interfacial Profile, Edge Smoothing

Influence of motion in normal direction:



Streamline diffusion $\int_{\Gamma_h^n} g_h^n \mathbf{v}_{\nu,h}^n \cdot \nabla c_h^n \mathbf{v}_{\nu,h}^n \cdot \nabla \chi$ for flat profile, **not necessary for convergence!**

Insoluble Surfactants in Two-Phase Flow

Fluid flow in phases Ω_+ and Ω_- :

$$\begin{aligned}\nabla \cdot \mathbf{v} &= 0, \\ \rho \partial_t^\bullet \mathbf{v} &= \nabla \cdot (-p\mathbf{I} + 2\eta D(\mathbf{v})).\end{aligned}$$

On two-phase interface $\Gamma = \partial\Omega_+ \cap \partial\Omega_-$:

$$\begin{aligned}[\mathbf{v}]_+^+ &= 0, \\ [-p\mathbf{I} + 2\eta D(\mathbf{v})]_-^+ &= -(\sigma(c)\boldsymbol{\kappa} + \nabla_\Gamma \sigma(c)), \\ \partial_t^\bullet c + c \nabla_\Gamma \cdot \mathbf{v} &= -\nabla_\Gamma \mathbf{j}_\Gamma, \quad \mathbf{j}_\Gamma = -D_\Gamma \nabla_\Gamma \gamma'(c).\end{aligned}$$

Energy dissipation ($\mathcal{R}(t)$ material test volume):

$$\begin{aligned}\frac{d}{dt} \left(\int_{\mathcal{R}(t) \cap \Omega} \frac{1}{2} \rho |\mathbf{v}|^2 + \int_{\mathcal{R}(t) \cap \Gamma} \gamma(c) \right) &= - \int_{\mathcal{R}(t) \cap \Omega} \eta |D(\mathbf{v})|^2 - \int_{\mathcal{R}(t) \cap \Gamma} D_\Gamma |\nabla_\Gamma \gamma'(c)|^2 \\ &\quad + \int_{\partial(\mathcal{R}(t) \cap \Omega)} \mathbf{v} \cdot \mathbf{S} \boldsymbol{\nu}_{ext} - \int_{\partial(\mathcal{R}(t) \cap \Gamma)} \gamma'(c) \mathbf{j}_\Gamma \cdot \boldsymbol{\mu}_{ext}.\end{aligned}$$

Diffuse Interface Description

[Elliott, S., in preparation]

Model:

$$\begin{aligned}\partial_t^\bullet \phi &= \nabla \cdot (M(\phi) \nabla \mu), \quad \mu = -\nabla \cdot (\varepsilon \sigma(c) \nabla \phi) + \frac{\sigma(c)}{\varepsilon} W'(\phi). \\ \nabla \cdot \mathbf{v} &= 0, \quad \rho \partial_t^\bullet \mathbf{v} = \nabla \cdot (-p \mathbf{I} + 2\eta D(\mathbf{v}) - \varepsilon \sigma(c) \nabla \phi \otimes \nabla \phi). \\ \partial_t^\bullet (\rho c) + \rho c \nabla \cdot \mathbf{v} &= D_\Gamma \nabla \cdot (\rho \nabla \gamma'(c)).\end{aligned}$$

Asymptotics: Obtain sharp interface model as $\varepsilon \rightarrow 0$ by matching asymptotic expansions.

Energy dissipation: ($\delta = \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} W(\phi)$)

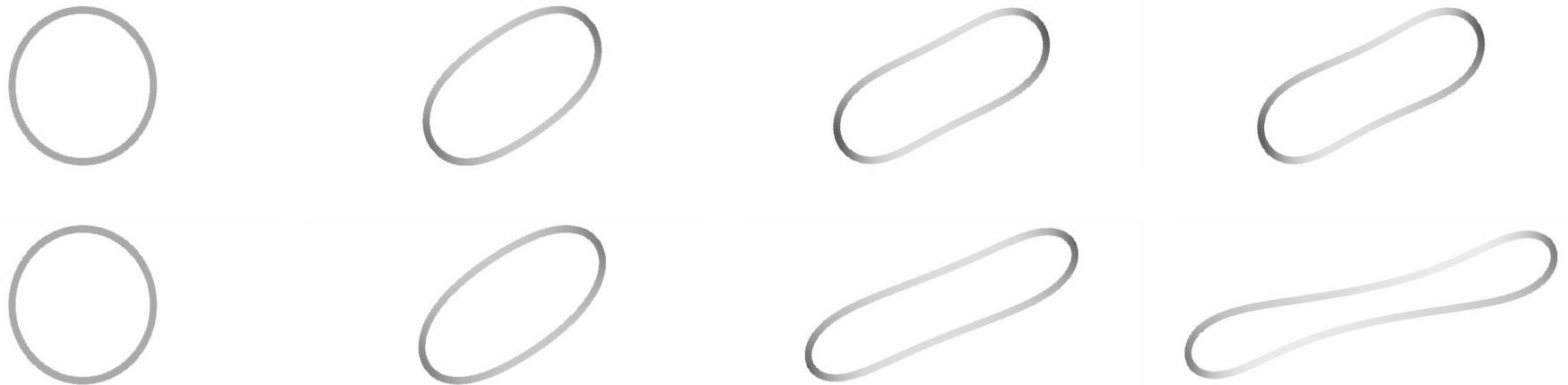
$$\begin{aligned}\frac{d}{dt} \left(\int_{\mathcal{R}(t)} \frac{1}{2} \rho |\mathbf{v}|^2 + \gamma(c) \delta(\varphi, \nabla \varphi) \right) \\ = \int_{\mathcal{R}(t)} -2\eta |D(\mathbf{v})|^2 - M(\varphi) |\nabla \mu|^2 - D_c \delta(\varphi, \nabla \varphi) |\nabla \gamma'(c)|^2 \\ + \int_{\partial \mathcal{R}(t)} (\mathbf{S} \mathbf{v} + K \varepsilon \sigma(c) \partial_t \varphi \nabla \varphi - \mu \mathbf{q}_\varphi - \gamma'(c) \mathbf{q}_c) \cdot \boldsymbol{\nu}_{ext}.\end{aligned}$$

Discretisation

- [Kay, Styles, Welford, 2007] for σ constant.
- Double-obstacle potential, interfacial regions of finite thickness.
- Navier-Stokes with Taylor-Hood \rightsquigarrow saddle point problem,
employed GMRES with preconditioner of [Kay, Loghin, Wathen, 2002].
- Linear FE for Cahn-Hilliard variational inequality,
solved with Gauss-Seidel type iterative method
[Elliott Gardiner, 1994], [Barrett, Nürnberg, Styles, 2004].
- $\gamma(c) = \beta c \log(c) + \alpha$, $\sigma(c) = \alpha - \beta c$ with $\alpha, \beta > 0$.

Numerical Example

Diffuse interface with surfactant:



Upper row: no surfactant dependence.

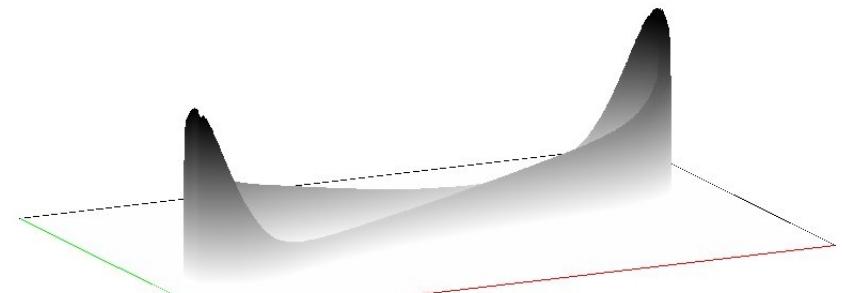
Lower row: $\sigma(c) = 1 - c/4$.

Displayed at times $t = 0, 2, 6, 12$,

$\Omega = [-5, 5] \times [-2, 2]$, $\text{Re} = 10$, $\text{Ca} = 0.7$,

$\mathbf{v}(x, y) = (0.5y, 0)$ on $\partial\Omega$,

$\text{Pe}_c = 10$.



Conclusion

- Diffuse interface approach to pdes on moving surfaces involving degenerate coefficients.
- Sharp interface analysis, convergence of weak solutions as $\varepsilon \rightarrow 0$.
- Numerical method based on unfitted FE, mass conservation.
- Discussion of the discretisation error (h convergence) and modelling error (ε convergence).
- Diffuse interface model for insoluble surfactants in two-phase flow.
- Related to sharp interface model by formal asymptotic analysis.
- Simulation of a droplet in shear flow.

