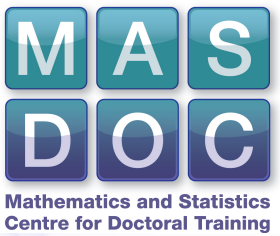
Soap to Simulation: A phase field story

Oliver Dunbar
MASDOC, Warwick Mathematics Institute

Postgraduate Seminar, Wednesday 30/11/16



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2. Introduce and incorporate surfactants into this model. **The soap!**

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2. Introduce and incorporate surfactants into this model. **The soap!**
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2. Introduce and incorporate surfactants into this model. **The soap!**
3. Introduce phase field modelling, a technique to study an approximation of the above. **The "diffuse" approximation.**
4. Discuss discretisation and present some simulations solutions to the phase field problem.**The simulation!**

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Multi Fluid Bubble Cluster

Free boundary problem

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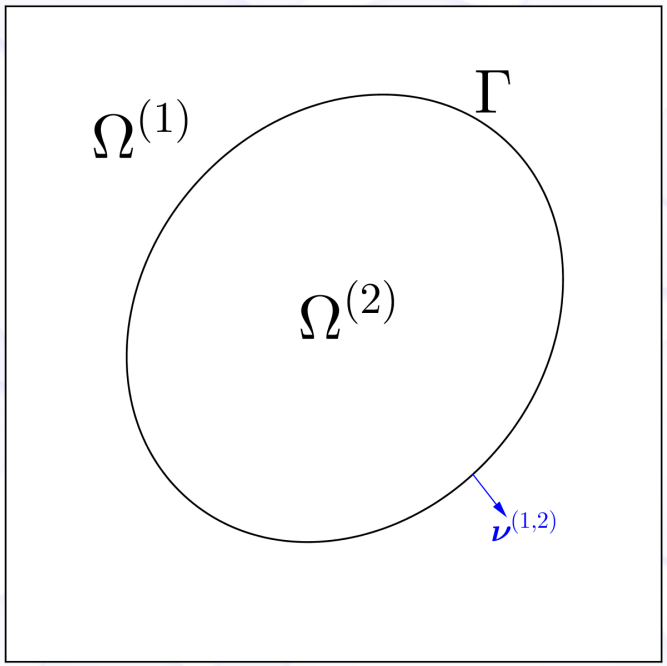

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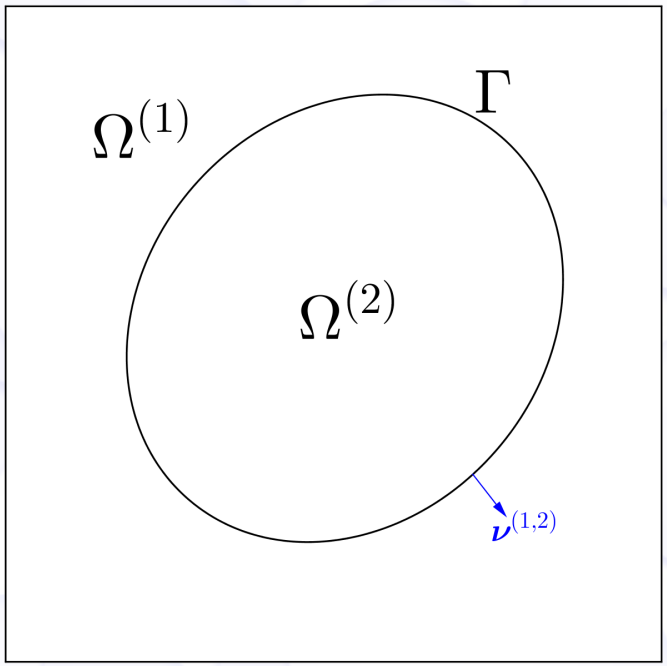

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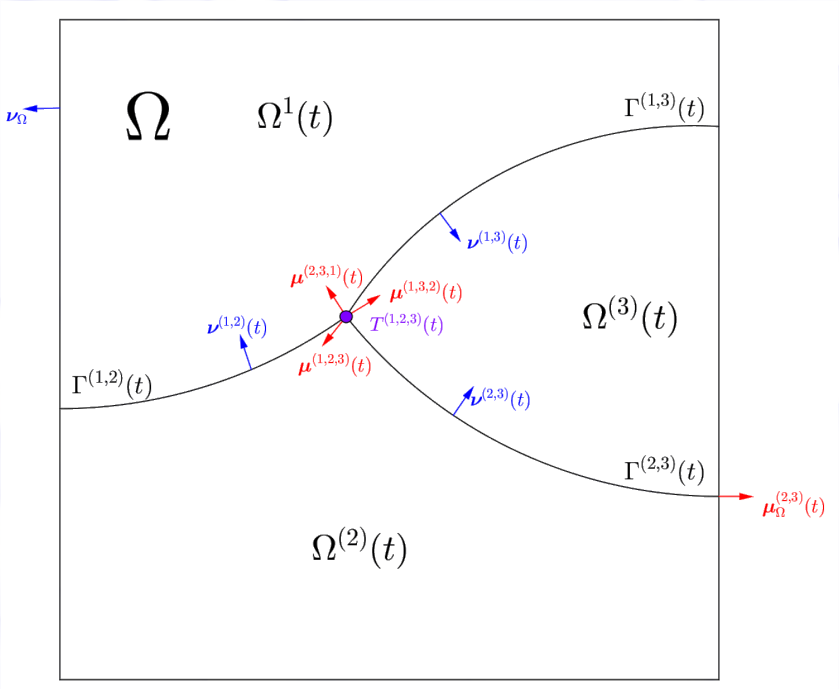

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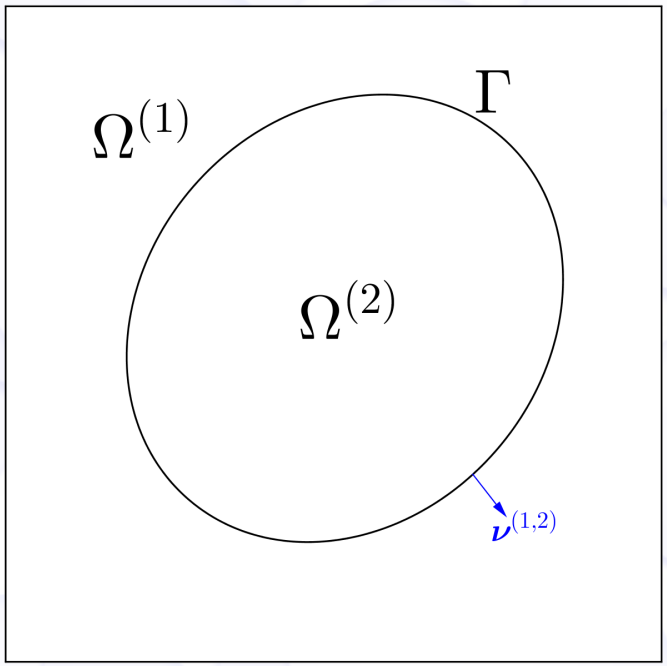

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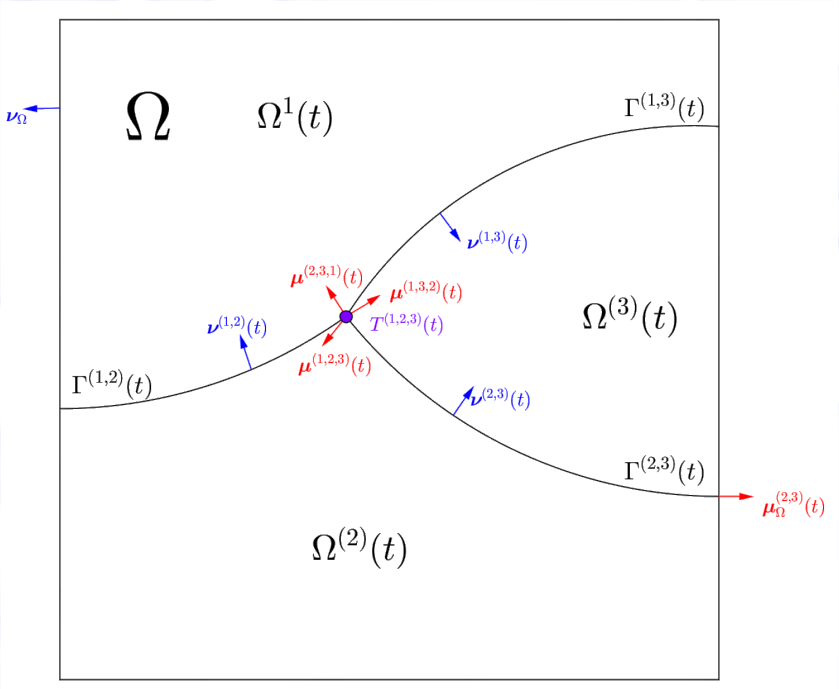
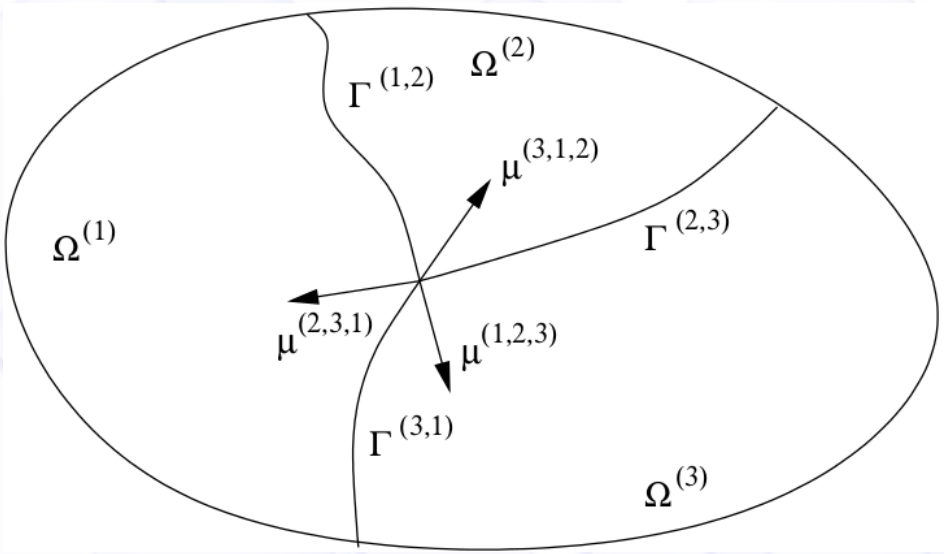


Applications: Phase change in materials (Stefan problem), fluid dynamics (two/multi-phase flow, wetting phenomena), obstacle problems, tumour growth

Multi Fluid Bubble Cluster

Multi phase flow



Quantities of interest

- velocity $\mathbf{v}^{(i)}$
- (constant) density,viscosity $\overline{\rho}^{(i)}$ $\eta^{(i)}$
- surface tension $\sigma_{i,j}$ of $\Gamma^{(i,j)}$
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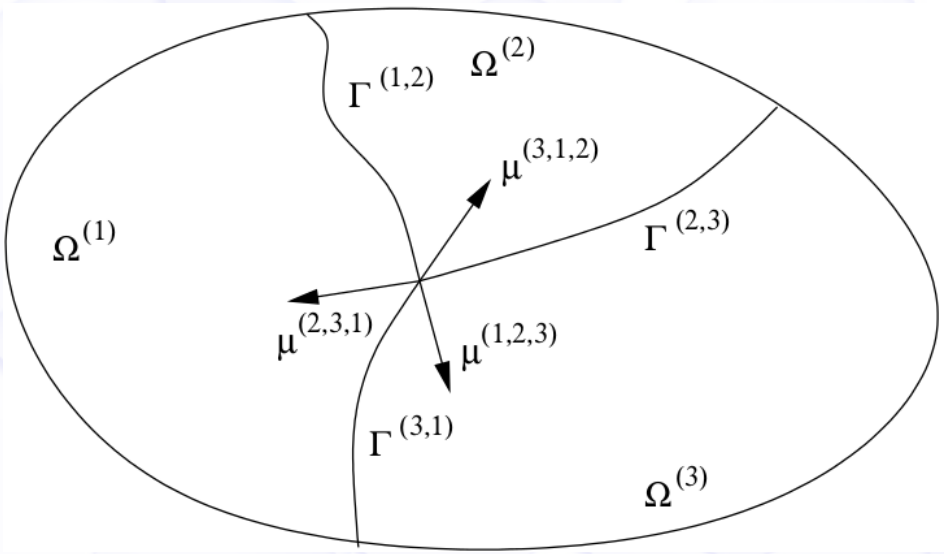

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In each $\Omega^{(i)}(t)$:

- Incompressible Navier Stokes equations:

$$\nabla \cdot \mathbf{v}^{(i)} = 0$$

$$\partial_t(\overline{\rho}^{(i)}\mathbf{v}^{(i)}) + \nabla \cdot (\overline{\rho}^{(i)}\mathbf{v}^{(i)} \otimes \mathbf{v}^{(i)}) = \nabla \cdot (p\mathcal{I} + 2\eta^{(i)} D(\mathbf{v}^{(i)}))$$

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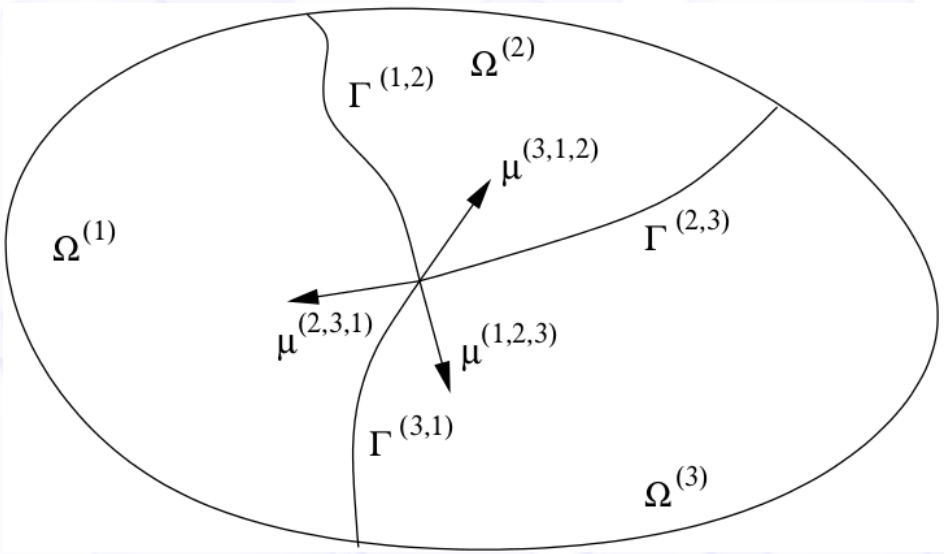

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On each $\Gamma^{(i,j)}(t)$:

- Young-Laplace law, $[p\mathcal{I} + 2\eta^{(\cdot)} D(\mathbf{v}^{(\cdot)})]^i_j \cdot \nu^{(i,j)} = \sigma_{i,j}\kappa^{(i,j)}\nu^{(i,j)}$,

All $\Gamma^{(i,j)}(t)$, $\mathbf{T}^{(i,j,k)}(t)$:

Transported with the flow.

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Incorporating Surfactants

Surfactant introduction

What are surfactants?

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Industries: Detergents, cosmetics, oil/petroleum industry, pharmaceuticals,. . .

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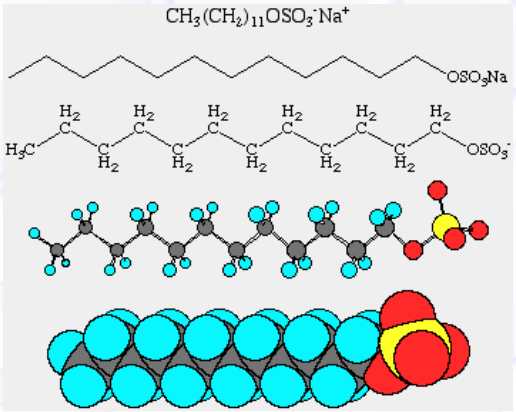
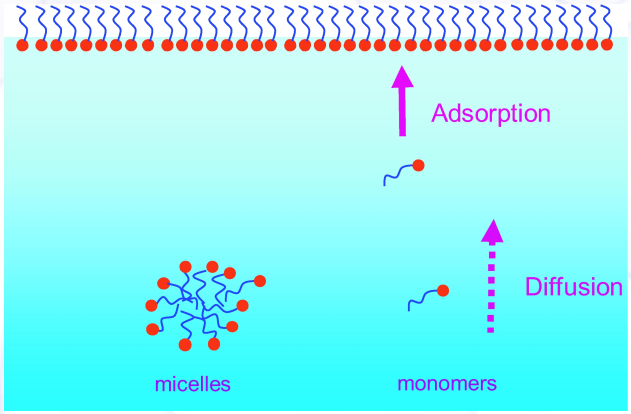




The -philic/-phobic structure causes **adsorbtion** to interfaces between fluids

$\Longrightarrow$ gives a **loss of surface tension.**

[http://www.ilpi.com/genchem/demo/tension/, https://people.maths.ox.ac.uk/griffit4/surfactant.html]

Incorporating Surfactants

Effects

Demonstration of an effect of surfactants

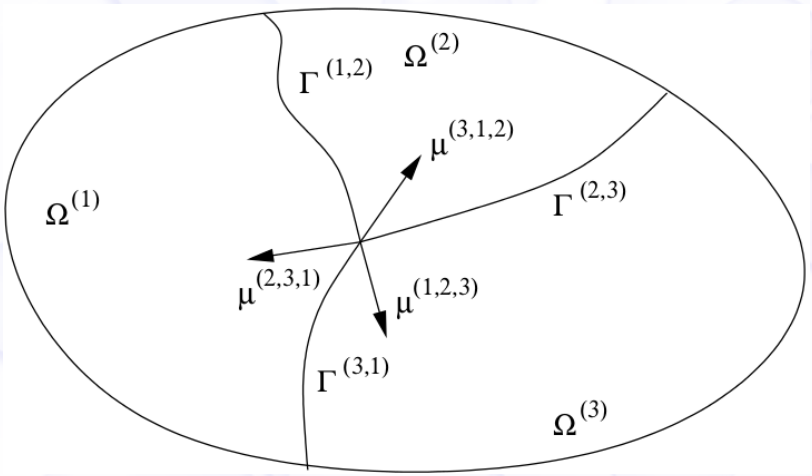
This is the **Marangoni effect**, caused by tangential surface forces. Captured by a new interfacial condition:

$$[p\mathcal{I} + 2\eta^{(\cdot)} D(\mathbf{v}^{(\cdot)})]^i_j \nu^{(i,j)} = \sigma_{i,j}(c^{(i,j)})\kappa^{(i,j)}\nu^{(i,j)} + \nabla_{\Gamma^{(i,j)}} \sigma_{i,j}(c^{(i,j)})$$

[https://www.youtube.com/watch?v=IeVA0ZcW5Ik]

Incorporating Surfactants

Multi phase flow with Surfactant



(More!) quantities of interest

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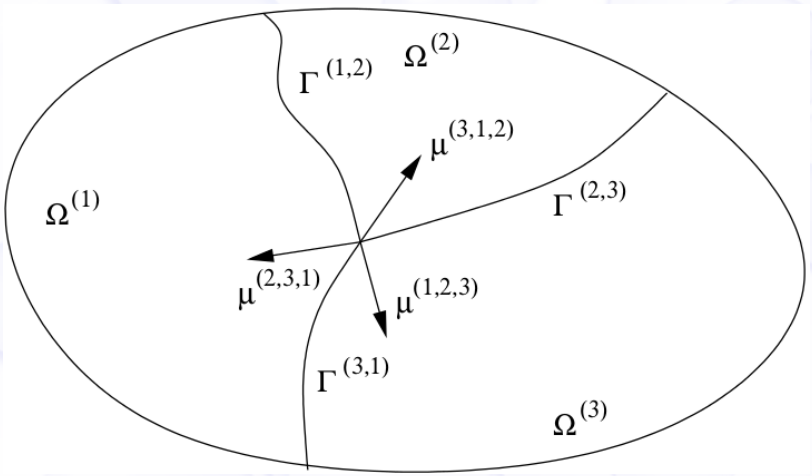

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Balance of mass of the surfactant:

In each $\Omega^{(i)}(t)$:

$$\partial_t^\bullet c^{(i)} = \nabla \cdot \mathbf{J}_c^{(i)}$$

On each $\Gamma^{(i,j)}(t)$:

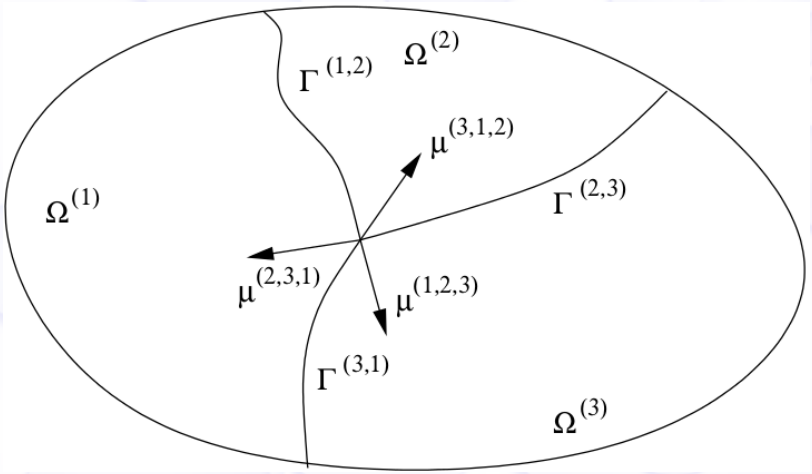
$$\partial_t^\bullet c^{(i,j)} + c^{(i,j)} \nabla_{\Gamma^{(i,j)}} \cdot \mathbf{v}^{(i)} = \nabla_{\Gamma^{(i,j)}} \cdot \mathbf{J}_c^{(i,j)} + \text{Adsorption}$$

On $\mathbf{T}^{(i,j,k)}(t)$:

No mass is deposited.

Incorporating Surfactants

Energetic framework



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- Surfactant concentration $c^{(i)}$ in $\Omega^{(i)}$
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Total system energy:

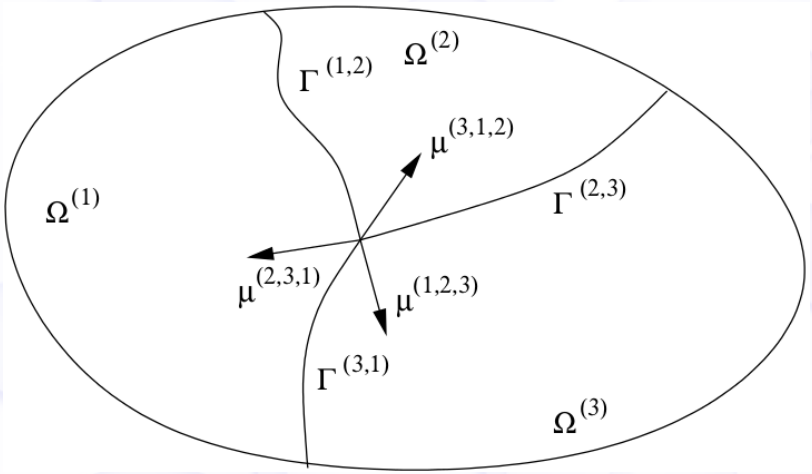
$$E := \sum_i \int_{\Omega^{(i)}} \Big(\underbrace{\frac{\overline{\rho}^{(i)} |\mathbf{v}^{(i)}|^2}{2}}_{\text{Fluid}} + \underbrace{G_i(c^{(i)}) \Big) + \sum_{i<j} \int_{\Gamma^{(i,j)}} \gamma_{i,j}(c^{(i,j)})}_{\text{surfactant}}$$

How to choose G_i,$\gamma_{i,j}$?

$\sigma_{i,j}(c^{(i,j)}) = \gamma_{i,j}(c^{(i,j)}) - c^{(i,j)}\gamma'_{i,j}(c^{(i,j)})$ well defined

Incorporating Surfactants

Energetic framework



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Simplifying assumption:

- **Instantaneous adsorption:** continuous chemical potential q.
- $\tilde{\sigma}_{i,j}(q) = \gamma_{i,j}(c^{(i,j)}(q)) - c^{(i,j)}(q)q$ well defined
- Equilibrium relation (Isotherm): **e.g Langmuir** $c^{(i)}(q) = \frac{K c^{(i,j)}(q)}{c^{(i,j)}_{\max} - c^{(i,j)}(q)}$

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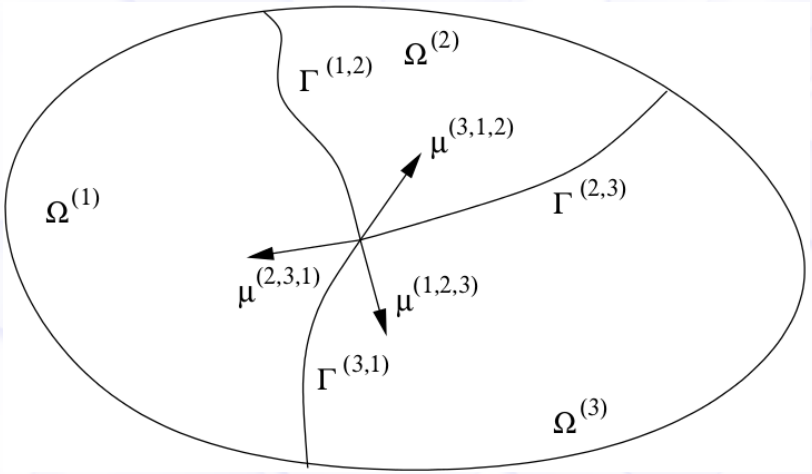
Incorporating Surfactants

Surfactant equations



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Choose fluxes $\mathbf{J}_c^{(i)}$, $\mathbf{J}_c^{(i,j)}$:

In each $\Omega^{(i)}(t)$:

$$\partial_t^\bullet c^{(i)}(q) = \nabla \cdot \left(M_c^{(i)} \nabla G_i'(c^{(i)}(q))\right)$$

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This choice $\implies$ Energy dissipation: $\frac{\mathrm{d}}{\mathrm{d}t} E \leq \int_{\partial\Omega} (\text{working terms})$

Incorporating Surfactants

Full system

The fluid mass and momentum equations

$$\nabla \cdot \mathbf{v}^{(i)} = 0 \qquad \text{in } \Omega^{(i)}(t)$$

$$\partial_t(\overline{\rho}^{(i)}\mathbf{v}^{(i)}) + \nabla \cdot (\overline{\rho}^{(i)}\mathbf{v}^{(i)} \otimes \mathbf{v}^{(i)}) = \nabla \cdot \left(p\mathcal{I} + 2\eta^{(i)} D(\mathbf{v}^{(i)})\right) \qquad \text{in } \Omega^{(i)}(t)$$

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The surfactant balances in bulk and interface

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$$- [M_c^{(\cdot)} \nabla G_\cdot'(c^{(\cdot)}(q))]_j^i \cdot \nu^{(i,j)}$$

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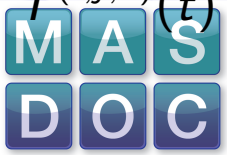
$$- [M_c^{(\cdot)} \nabla G_\cdot'(c^{(\cdot)}(q))]_j^i \cdot \nu^{(i,j)}$$

Force balance on interfaces and triple junctions

$$[p\mathcal{I} + 2\eta^{(\cdot)} D(\mathbf{v}^{(\cdot)})]_j^i \nu^{(i,j)} = \tilde{\sigma}_{i,j}(q)\kappa^{(i,j)}\nu^{(i,j)} + \nabla_{\Gamma^{(i,j)}}\tilde{\sigma}_{i,j}(q) \qquad \text{on } \Gamma^{(i,j)}(t)$$

$$0 = \tilde{\sigma}_{i,j}(q)\mu^{(i,j,k)} + \tilde{\sigma}_{j,k}(q)\mu^{(j,k,i)} + \tilde{\sigma}_{k,i}(q)\mu^{(k,i,j)} \qquad \text{on } T^{(i,j,k)}(t)$$



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Issues with interface tracking of free boundary problems

- For many regions, there are can be large systems of coupled equations,
- We must solve for the free boundaries as we must solve equations on them,
- Solving across two/three different dimensions, (bulk,boundary and boundary intersections)
- Only able to model a narrow range of effects, the geometry tracking is highly sensitive to topological change
- Discretisation errors associated with discretising the free boundaries
- Grid complexity (match grid to the free boundaries or not)
- ...

$\Longrightarrow$ **More difficult for analysis and simulation.**

Phase field modelling

Phase field model

The idea: **Interface capturing.**

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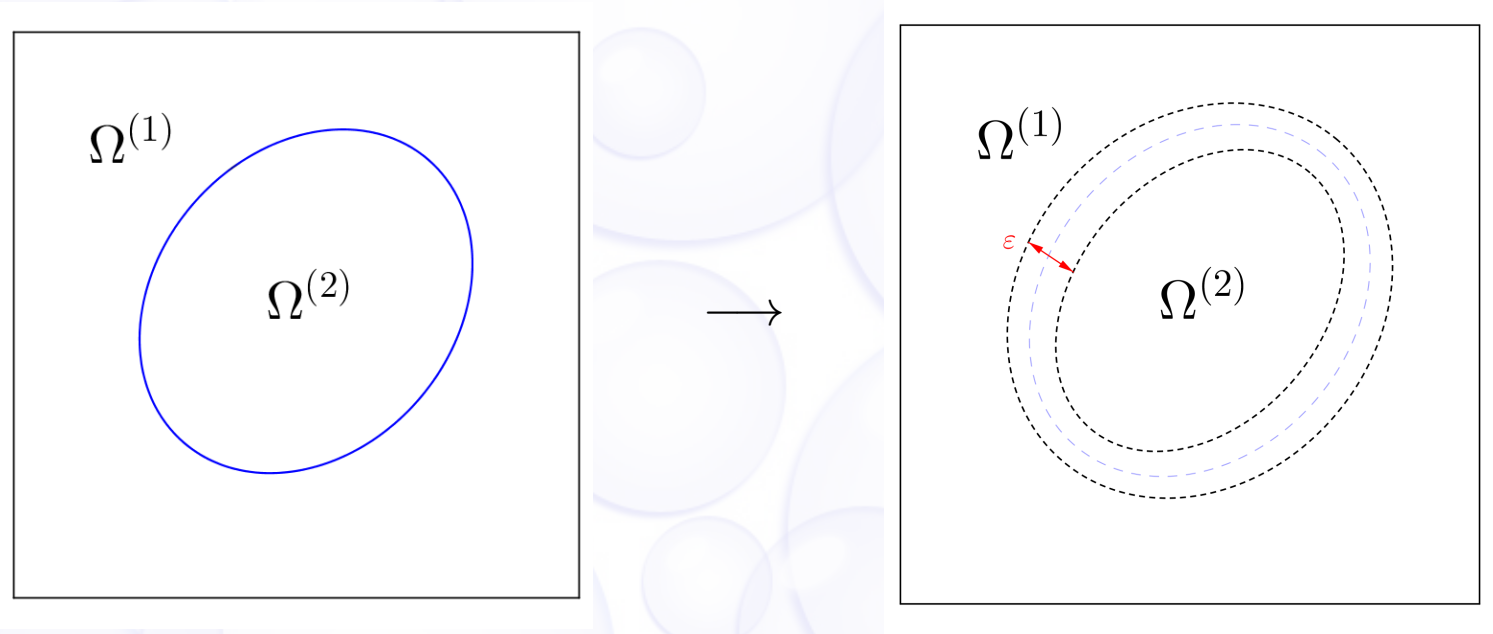
Regularise quantities we care about, by converting:

$$\text{infinitesimal interfaces} \rightarrow \text{ interfacial layer width } \epsilon > 0$$

then smoothly change quantities over these strips.



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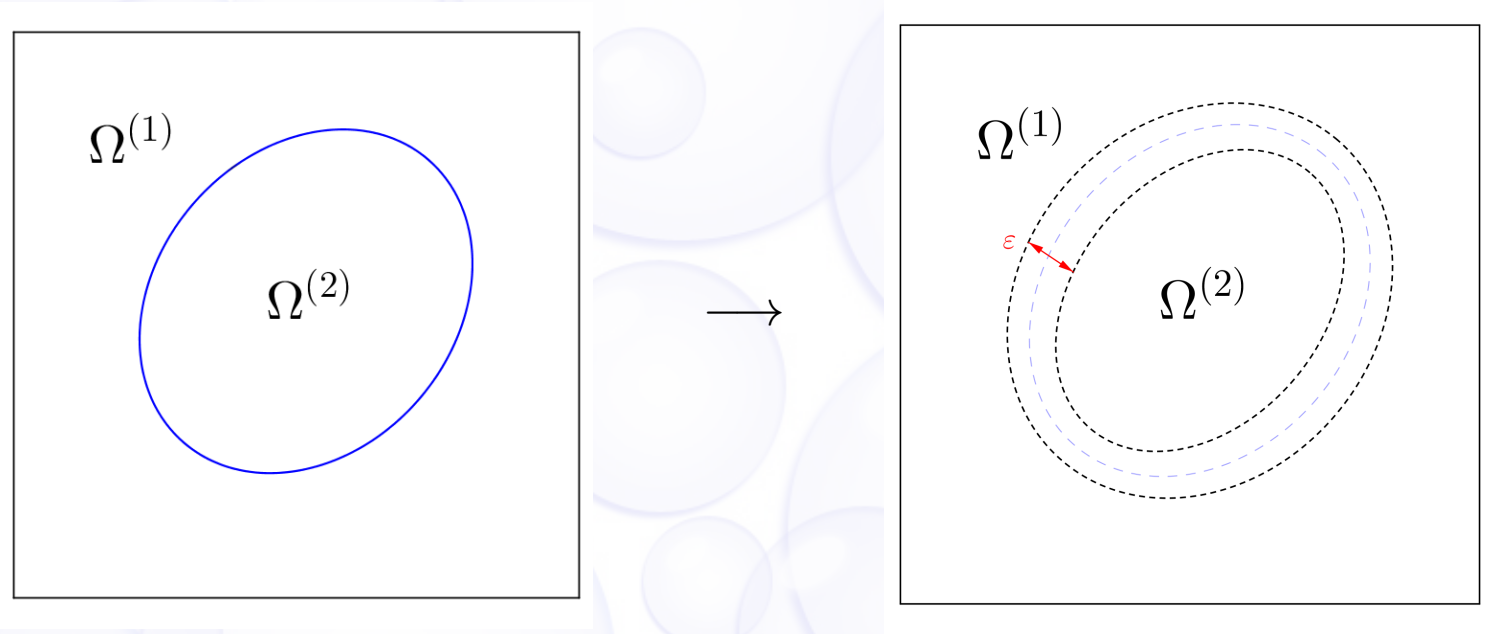

Some questions

How do we characterise the bulk domains and interfacial strips?
How do we preserve structures as $\varepsilon \rightarrow 0$?

Phase field modelling

More Precisely

Define

$$\Sigma^M := \left\{ u = (u^{(1)}, \ldots, u^{(M)}) \in \mathbb{R}^M \ : \ \sum_{i=1}^{M} u^{(i)} = 1, \text{ where } 0 \leq u^{(i)} \leq 1 \right\}$$

Then the **phase field variables** (or **order parameters**) are functions

$$\varphi = (\varphi^{(1)}, \ldots, \varphi^{(M)}) \colon \Omega \to \Sigma^M$$

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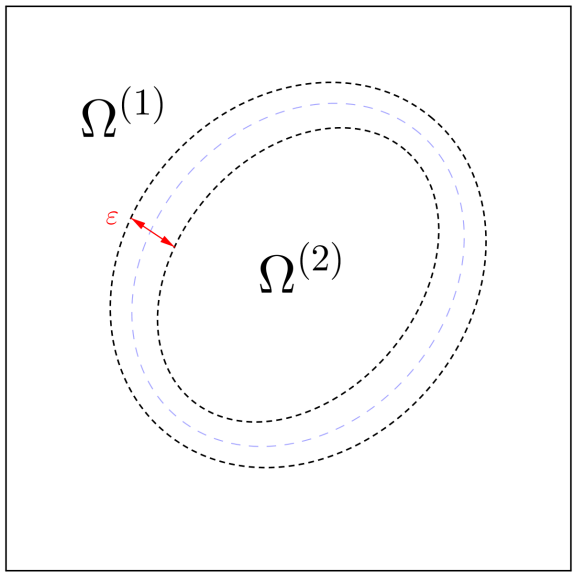
Essentially: The $\varphi^{(i)}$'s "represent the presence of fluid i" at the state (x, t), and

$$\varphi^{(i)}(x, t) = 1 \implies x \in \Omega^{(i)} \text{ at time } t$$

$$0 < \varphi^{(i)}(x, t) < 1 \implies x \in \Gamma^{(i,j)} \text{ at time } t$$



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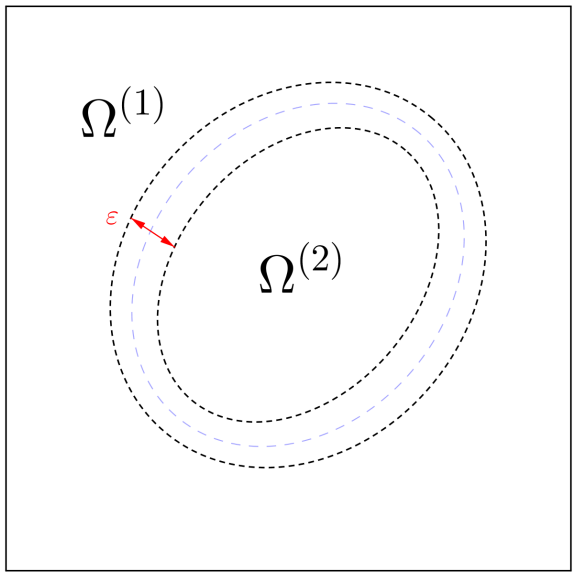

Essentially: The $\varphi^{(i)}$'s "represent the presence of fluid i" at the state (x, t), and

$$\varphi^{(i)}(x,t) = 1 \implies x \in \Omega^{(i)} \text{ at time } t$$

$$0 < \varphi^{(i)}(x,t) < 1 \implies x \in \Gamma^{(i,j)} \text{ at time } t$$

Key question: What equations should $\varphi^{(i)}$ satisfy?

For 2 phases: Define the **Ginzburg Landau** energy functional: For certain potentials F

$$E_\varepsilon(\varphi, \nabla\varphi) := \int_\Omega \frac{1}{\varepsilon} F(\varphi) + \frac{\varepsilon}{2} |\nabla\varphi|^2 dx$$

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$$E_\varepsilon(\varphi, \nabla\varphi) \overset{\varepsilon \to 0}{\to} \int_\Gamma 1 dx = \text{Area}_\Gamma(x, t)$$

$\to$ represents the notion of de Giorgi's Gamma-Convergence for functionals.

$\Longrightarrow$ **Minimizers of** $E_\varepsilon(\varphi, \nabla\varphi)$ **converge to minimizers of** Area_Γ **as** $\varepsilon \to 0$.

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Two gradient flows of this energy:

- L^2 flow: the Allen-Cahn
- H^{-1} flow: the Cahn-Hilliard

Phase field modelling

Two important PDEs

For 2 phases, $\varphi^{(1)} = \varphi$ and $\varphi^{(2)} = 1 - \varphi$, consider:

The Allen-Cahn Equation

$$\boxed{\varphi_t = \varepsilon \Delta \varphi + \frac{1}{\varepsilon} F'(\varphi)}$$

The Cahn-Hilliard Equation

$$\boxed{\varphi_t = \Delta \mu, \quad \mu = \varepsilon \Delta \varphi + \frac{1}{\varepsilon} F'(\varphi)}$$

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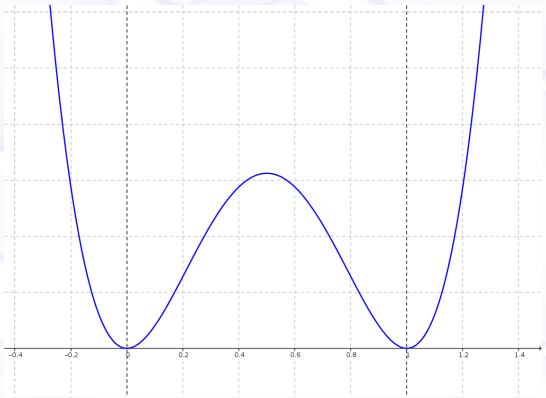
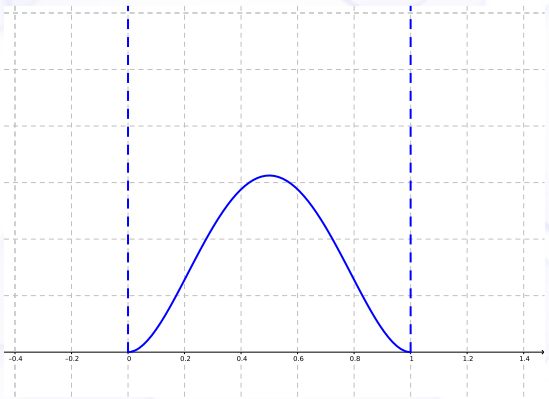
F is the **phase field potential**: Typically a double well, double obstacle or approximation of this:





Behaviour: "F" forces the φ's to sit in the wells of the potential, and $\Delta\varphi$ induces continuity of φ across the interface as it changes wells.

Approximating the multi fluid problem

Approximating the multi fluid problem

- We change variables so they depend on φ :

$$\left\{\mathbf{v}^{(i)}, \overline{\rho}^{(i)}, \eta^{(i)} \ \forall i\right\} \rightarrow \left\{ \underbrace{\sum_i \mathbf{v}^{(i)}\varphi^{(i)}}_{\mathbf{v}}, \underbrace{\sum_i \overline{\rho}^{(i)}\varphi^{(i)}}_{\rho(\varphi)}, \underbrace{\sum_i \eta^{(i)}\varphi^{(i)}}_{\eta(\varphi)} \right\}$$

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- Preserved energy framework $\Longrightarrow$ Forced Navier-Stokes:

$$\nabla \cdot \mathbf{v} = 0$$

$$\partial_t(\rho\mathbf{v}) + \nabla \cdot (\rho\mathbf{v} \otimes \mathbf{v}) = \nabla \cdot \left(\mathbf{v} \otimes (\sum_{k,l} \mathcal{L}^{(k,l)}\overline{\rho}^{(k)}\nabla\mu^{(l)}) - p\mathcal{I} + 2\eta D(\mathbf{v})\right)$$

and transported multiphase Cahn-Hilliard: For $k = 1, \ldots, M$

$$\partial_t(\varphi^{(k)}) + \nabla \cdot (\varphi^{(k)}\mathbf{v}) = \nabla \cdot \left(\sum_{l=1}^{M} \mathcal{L}^{(k,l)}(\varphi)\nabla\mu^{(l)}\right)$$

$$\mu^{(k)} = D_{\varphi^{(k)}, \nabla\varphi^{(k)}}\left[\varepsilon a(\varphi, \nabla\varphi) + \frac{1}{\varepsilon}F(\varphi)\right]$$

Approximating the surfactants

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- We approximate the **characteristic functions** of bulk ($\chi_{\Omega^{(i)}}$) and interfacial ($\chi_{\Gamma^{(i,j)}}$) regions by **smoothed** distributions ($\xi_i(\varphi)$ and $\delta_{ij}(\varphi, \nabla\varphi)$).

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- New system energy

$$E_\varepsilon := \int_\Omega \left(\frac{\rho(\varphi)|\mathbf{v}|^2}{2} + e_G(q,\varphi)\right) + e_\gamma(\varepsilon, q, \varphi, \nabla\varphi)$$

Where

- $e_G = \sum_i \xi_i G_i, \quad e_\gamma(\varphi) = \sum_{i<j}\delta_{ij}\gamma_{i,j}$
- $\delta_{ij} := \varepsilon$(gradient part) $+\frac{1}{\varepsilon}$(multi well potential)

Phase Field Modelling

The full system

The Diffuse interface approximation.

$$\nabla \cdot \mathbf{v} = 0$$

$$\partial_t(\rho\mathbf{v}) + \nabla\cdot(\rho\mathbf{v}\otimes\mathbf{v}) = \nabla\cdot\Big(\sum_{i<j}\sigma_{ij}\Big(\delta_{ij}\mathcal{I} - \sum_k \nabla\varphi^{(k)}\otimes a_{ij,\nabla\varphi^{(k)}}\Big) - \mathbf{v}\otimes\bar{\mathbf{J}} - p\mathcal{I} + 2\eta D(\mathbf{v})\Big)$$

For $k = 1,\dots,M$

$$\partial_t(\varphi^{(k)}) + \nabla\cdot(\varphi^{(k)}\mathbf{v}) = \nabla\cdot\Big(\sum_{l=1}^{M}\mathcal{L}^{(k,l)}(\varphi,q)\nabla\mu^{(l)}\Big)$$

$$\mu^{(k)} = \sum_{i<j} -\varepsilon\nabla\cdot(\tilde{\sigma}_{ij}a_{ij,\nabla\varphi^{(k)}}) + \varepsilon\tilde{\sigma}_{ij}a_{ij,\varphi^{(k)}} + \frac{1}{\varepsilon}\tilde{\sigma}_{ij}w_{ij,\varphi^{(k)}} + \xi_k'(G_k - c^{(k)}q)$$

$$\partial_t\Big(\sum_i \xi_i c^{(i)}(q) + \sum_{i<j}\delta_{ij}c^{(i,j)}(q)\Big) + \nabla\cdot\Big(\Big(\sum_i \xi_i c^{(i)}(q) + \sum_{i<j}\delta_{ij}c^{(i,j)}(q)\Big)\mathbf{v}\Big) = \nabla\cdot\Big(\sum_i \xi_i M_c^{(i)}\nabla q + \sum_{i<j}\delta_{ij}M_c^{(i,j)}\nabla q\Big)$$

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Table of Contents

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Use a **fractional−θ scheme**:

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Example: (2 phase) Cahn-Hilliard Navier-Stokes:

$$w = (\mathbf{v}, p, \varphi, \mu)^T, \quad F_i = (G_i, H_i)^T \text{ for } i = 1, 2$$

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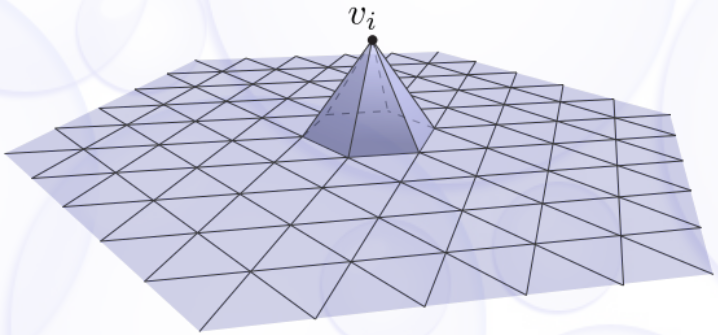
Benefits of this θ scheme

- Optimal θ can be found. This yields a second order in time scheme, A-stable for $\alpha > 0.5$.
- Separates nonlinear terms (advection and incompressibility) - Fast solvers.
- I have shown conditional stability using energy methods for this system.

Finite element framework:

- Triangulate the domain.
- Choose an FE space of functions to approximate your solution
- Approximating problem using basis functions ψ_i and representation $u = \sum_i u_i \psi_i$
- Solve the sparse linear system for u_i.



[http://mooseframework.org/wiki/MooseTraining/FEM/ShapeFunctions/]

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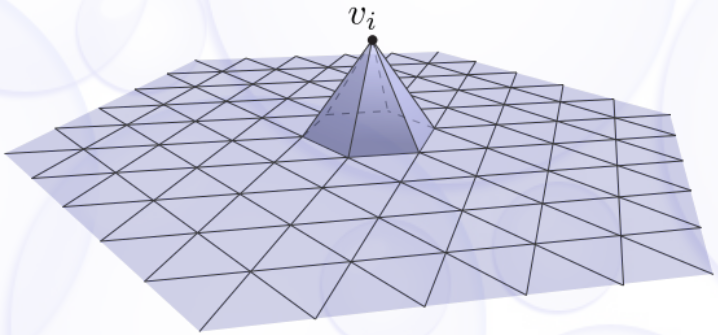

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We use:

- P^1 elements for φ, μ, q
- Taylor-Hood $P^2 - P^1$ or MINI for the fluid $(\mathbf{v}, p)$

Created in the DUNE-FEM C++ package and uses UMFPACK,PETSC, solvers and Alugrid grid manager.

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Discretisation and Simulation

Surfactants supplied on left. Highly viscous fluid

Demonstrates recovery of
$0 = \sigma_{i,j}(q)\mu^{(i,j,k)} + \sigma_{j,k}(q)\mu^{(j,k,i)} + \sigma_{k,i}(q)\mu^{(k,i,j)}$ on $T^{(i,j,k)}(t)$

Discretisation and Simulation

Marangoni force with surfactants(low fluid viscosity)

Demonstrates recovery of $[\mathbf{T}^{(\cdot)}]^i_j \nu^{(i,j)} = \tilde{\sigma}_{i,j}(q)\kappa^{(i,j)}\nu^{(i,j)} + \underbrace{\nabla_{\Gamma^{(i,j)}}\tilde{\sigma}_{i,j}(q)}_{\text{Marangoni force}}$ on $\Gamma^{(i,j)}$

Example of an effect **not** satisfied in the sharp interface model.

Thank you for listening!