An accurate finite element solution of interface flows with surfactants

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... present collaborator

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Outline

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1. Aim and objective
   - flows with surfactants
2. Modelling of two-phase flows with surfactants
   - mathematical model
   - numerical scheme
   - spurious velocities
   - FE discretisation
3. Results
   - computational results
   - summary and outlook

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Aim

to develop an accurate and robust numerical scheme for two-phase flows with insoluble/soluble surfactants

Properties

- surfactant (surface active agent) is a substance that lowers the surface/interfacial tension on liquid-gas/liquid-liquid interface
- nonuniform distribution of surfactants on surface/interface induce Marangoni convection

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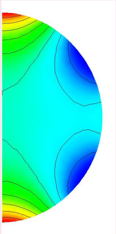
Application

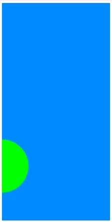
- surfactant transport on the mucus film in nasal cavity
- mucus film is responsible for filtration and air-conditioning in nasal cavity

Assumptions and model problems

- the fluid is Newtonian and incompressible
- insoluble surfactant in free surface flows (e.g., freely oscillating droplet)
- insoluble/soluble surfactant in two-phase flows (e.g., rising bubble in a cylinder)

Axisymmetric representation of the computational domains





Definitions

- Γ_F be a hypersurface in $\mathbb{R}^{n+1}$ $n = 1, 2$
- for any function ϕ defined on a open set $\mathcal{N}$ of $\mathbb{R}^{n+1}$ containing Γ we define tangential gradient

$$\underline{\nabla}\phi = \nabla\phi - (\nu \cdot \nabla\phi)\nu, \qquad \underline{\nabla}\phi = (\underline{D}_1\phi, ..., \underline{D}_{n+1}\phi)$$

- the Laplace-Beltrami operator

$$\underline{\Delta} = \underline{\nabla} \cdot \underline{\nabla}\phi = \sum_{i=1}^{n+1} \underline{D}_i \underline{D}_i \phi$$

Navier-Stokes equations

$$\rho_k \left(\frac{\partial u}{\partial t} + (u \cdot \nabla) u \right) - \nabla \cdot \mathbb{S}_k(u,p) = \rho_k \mathbf{e} \qquad \text{in } \Omega_k(t) \subset \mathbb{R}^3$$

$$\nabla \cdot u = 0 \qquad \text{in } \Omega_k(t) \subset \mathbb{R}^3$$

$$[|u|] = 0, \quad \nu \cdot [|\mathbb{S}(u,p)|] \cdot \nu + \sigma(\Gamma)\mathcal{K} = 0 \qquad \text{on } \Gamma_F(t)$$

$$u = w, \quad \tau_i \cdot [|\mathbb{S}(u,p)|] \cdot \nu - \tau_i \cdot \nabla \sigma(\Gamma) = 0 \qquad \text{on } \Gamma_F(t)$$

$$+ \text{ appropriate BCs} \qquad \text{on } \partial\Omega_k(t) \setminus \Gamma_F(t)$$

for $k = 1, 2.$

$$\mathbb{S}_k(u,p) = \mu_k \mathbb{D}(u) - p\mathbb{I}, \qquad \mathbf{e} = (0, 0, \text{-g})$$

u - velocity, p - pressure, t - time, ρ_k - density, μ_k - dynamic viscosity, σ - surface tension, Γ - surfactant concentration, g - gravity

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Surfactant concentration in outer phase

$$\begin{aligned} \frac{\partial C}{\partial t} + (u \cdot \nabla) C &= D_c \Delta C && \text{in } \Omega_1(t) \subset \mathbb{R}^3 \\ -D_c(\nu \cdot \nabla C) &= S(\Gamma, C) && \text{on } \Gamma_F(t) \\ + \text{ appropriate BCs} & && \text{on } \partial\Omega_1(t) \setminus \Gamma_F(t) \end{aligned}$$

Surfactant concentration on the interface

$$\frac{\partial \Gamma}{\partial t} + U \cdot \underline{\nabla} \Gamma + \Gamma \underline{\nabla} \cdot u = D_s \underline{\Delta} \Gamma + S(\Gamma, C) \quad \text{on } \Gamma_F(t)$$

where

$$S(\Gamma, C) = k_a C \left(1 - \frac{\Gamma}{\Gamma_\infty}\right) - k_d \Gamma$$

C - surfactant in outer phase, D_c - diffusion coefficient of C, Γ - surfactant on interface, D_s - diffusion coefficient of Γ

k_a - adsorption coefficient, k_d - desorption coefficient, Γ_∞ - maximum surface packing surfactant concentration

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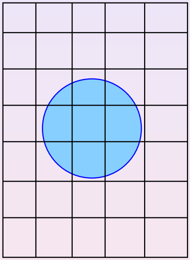
Eulerian Approach

- mesh is fixed, interface moves through it
- interface non-resolving mesh



Pros and cons

- easy to implement
- merging and breaking of interface can be handled easily
- require special techniques to incorporate the surface force and material properties
- spurious velocities

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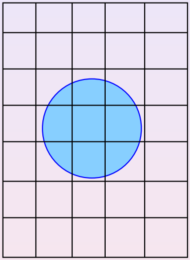

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Lagrangian Approach

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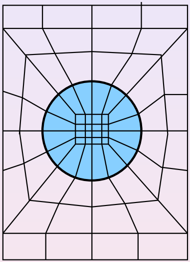

Pros and cons

- surface force can be incorporated accurately
- no convection term
- handling of merging and breaking of interface is more challenging

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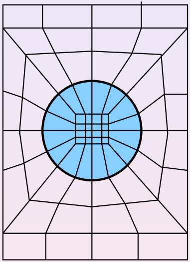

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Arbitrary Lagrangian Eulerian approach

- interface resolving mesh
- interface moves with the fluid (Lagrangian manner)
- inner points can be displaced arbitrarily
- spurious velocities can be avoided
- needs remeshing occasionally

ALE form of the NSE

$$\frac{\partial u}{\partial t}\Big|_{\hat{\Omega}} + (u\cdot\nabla)u - (w\cdot\nabla)u - \nabla\cdot\mathbb{T}(u,p) = f, \qquad \nabla\cdot u = 0$$

w - grid velocity

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Spurious velocities

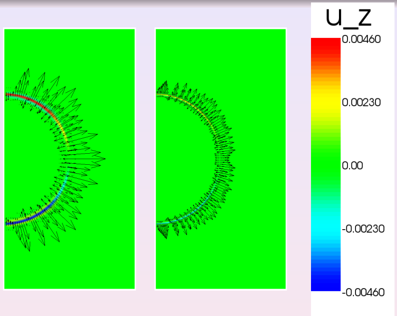
Static bubble problem

$$
\begin{aligned}
-\nabla \cdot \mathbb{T}(u,p) &= 0 && \text{in } \Omega_1 \cup \Omega_2 \\
\nabla \cdot u &= 0 && \text{in } \Omega_1 \cup \Omega_2 \\
u &= 0 && \text{on } \Gamma_D \\
[|u|] &= 0 && \text{on } \Gamma_F \\
n \cdot [|\mathbb{T}(u,p)|] &= n \cdot \sigma \mathcal{K} && \text{on } \Gamma_F
\end{aligned}
$$

Error estimate

$$
|u_h|_1 \le C \left(\inf_{q_h \in Q_h} \|p - q_h\|_0 + \sup_{v_h \in V_{h,0}} \frac{|\langle \mathcal{K}_h, v_h \cdot n \rangle - \langle \mathcal{K}, v_h \cdot n \rangle|}{|v_h|_1} \right)
$$

Spurious velocities



continuous pressure approximations, analytically u=0 !

Suppresing spurious velocities

- discontinuous pressure approximation in interface resolved mesh
- cubic spline or Laplace-Beltrami operator with iso-parametric elements has to be used for curvature approximation

Weak Formulation

Implementing the boundary conditions

- Dirichlet type boundary conditions in both ansatz and test space
- all other boundary conditions in the weak form

Material properties in two-phase flows

$$\rho(x) = \begin{cases} 1 & \text{for } x \text{ in } \Omega_1(t) \\ \frac{\rho_2}{\rho_1} & \text{for } x \text{ in } \Omega_2(t) \end{cases} \qquad Re(x) = \begin{cases} \frac{\rho_1 UL}{\mu_1} & \text{for } x \text{ in } \Omega_1(t) \\ \frac{\rho_1 UL}{\mu_2} & \text{for } x \text{ in } \Omega_2(t) \end{cases}$$

Weak form of NSE

$$\left(\rho(x)\frac{\partial u}{\partial t}, v\right) + a(u - w, u, v) - b(p, v) + b(q, u) \quad = \quad f(\mathcal{K}, v)$$

$$a(\hat{u}, u, v) = 2\int_{\Omega_t} \frac{1}{Re(x)}\mathbb{D}(u) : \mathbb{D}(v)\; dx + \int_{\Omega_t} \rho(x)(\hat{u}\cdot\nabla)u\cdot v\; dx,$$

$$b(q, v) = \int_{\Omega_t} q\; \nabla\cdot v\; dx,$$

$$f(\mathcal{K}, v) = \int_{\Omega_t} \rho(x)\,\mathbf{e}\cdot v\; dx - \frac{1}{Eo}\int_{\Gamma_{F_t}} \left(1 + E\left(\frac{\Gamma_0}{\Gamma_\infty} - \Gamma\right)\right)\;(v\cdot\nu)\,\mathcal{K}\, dS$$
$$- \frac{E}{Eo}\int_{\Gamma_{F_t}} (v\cdot\tau_i)\nabla\,\Gamma\cdot\tau_i\, dS$$

with $\sigma(\Gamma) = \sigma_1 + RT_a(\Gamma_1 - \Gamma)$, and $E = RT_a\Gamma_\infty/\sigma_0$

Laplace Beltrami operator technique for curvature

$$\frac{1}{Eo}\int_{\Gamma_{F_t}}\left(1+E\left(\frac{\Gamma_0}{\Gamma_\infty}-\Gamma\right)\right) v\,(\mathcal{K}\cdot\nu)\,dS$$

$$=\frac{1}{Eo}\int_{\Gamma_F}\left(1+E\left(\frac{\Gamma_0}{\Gamma_\infty}-\Gamma\right)\right) v\,\underline{\Delta} id_{\Gamma_F}\,dS$$

$$=-\frac{1}{Eo}\int_{\Gamma_{F_t}}\underline{\nabla} id : \left(\left[1+E\left(\frac{\Gamma_0}{\Gamma_\infty}-\Gamma\right)\right]\underline{\nabla} v - E\,\underline{\nabla}\Gamma\otimes v\right)\,dS$$

Note: Only first order derivatives needed!

Semi-implicit time discretisation of the curvature term

$$\int_{\Gamma_{F_t}}\underline{\nabla} id_{\Gamma_F} : \underline{\nabla} v\,dS \approx \int_{\Gamma_{F_t}}\underline{\nabla} id_{\Gamma_F(t_{n+1})} : \underline{\nabla} v\,dS$$

Weak form of surfactant equations

$$\left(\frac{\partial C}{\partial t}, \phi\right) + ((u - w)\cdot\nabla)C, \phi) + \frac{1}{Pe_C}(\nabla C, \nabla\phi) = -\langle S_C(\Gamma, C), \phi\rangle$$

Surfactant concentration on the interface

$$\left(\frac{\partial \Gamma}{\partial t}, \psi\right) + \frac{1}{Pe_\Gamma}(\underline{\nabla}\Gamma, \underline{\nabla}\psi) + (\Gamma\underline{\nabla}\cdot u, \psi) = (S_\Gamma(\Gamma, C), \psi)$$

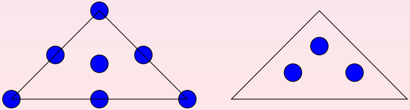
Discretization in time and space

Time discretisation

- Euler schemes are only first order, Crank-Nicolson scheme is second order but not strongly A-stable
- fractional step Θ-scheme is second order and strongly A-stable

Stable finite elements

- partition of the domain into simplices
- isoparametric P_2^{bubble}/P_1^{disc} element for velocity and pressure



$$P_2^{bubble} = P_2(K) \oplus \text{span}\{\lambda_1\lambda_2\lambda_3\}$$

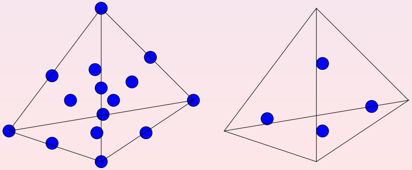
P_2^{bubble}/P_1^{disc} element

Advantages

- second order in energy norm
- satisfies Babuška-Brezzi stability condition
- allows extension to 3D

$$P_2^{bubble} = P_2(K) \oplus \text{span}\{\lambda_1\lambda_2\lambda_3\lambda_4\} \oplus \text{span}\{\lambda_i\lambda_j\lambda_k \ : \ i \neq j \neq k\}$$

3 × 15 dofs



4 dofs

Elastic mesh deformation

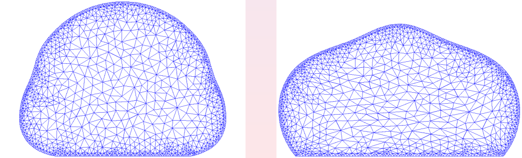
move the boundary points (X^n) and compute their displacement

$$X^{n+1} = X^n + (t_{n+1} - t_n)\, u^{n+1}, \quad d^n = X^{n+1} - X^n$$

compute the inner points displacement (Ψ^n)

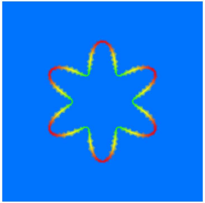
$$\nabla \cdot \mathbb{T}(\Psi^n) = 0 \quad \text{in } \Omega_k(t_n), \qquad \Psi^n(x^n) = d^n \quad \text{on } \partial\Omega_k(t_n)$$

where $\mathbb{T}(\phi) = \lambda_1(\nabla \cdot \phi)\mathbb{I} + 2\lambda_2\mathbb{D}(\phi)$.



Computational results

- surfactant diffusion over a solid sphere
- surfactant diffusion over a torus
- mass flux test (soluble surfactant)
- 2D oscillating bubble with insoluble surfactant
- 2D rising bubble with insoluble surfactant



Summary and outlook

- second order isoparametric finite element scheme for solving two-phase flows with soluble/insoluble surfactants
- optimal rate of convergence is obtained
- extend the numerical scheme for flows in nasal cavity

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