The Trace Finite Element Method for PDEs on Surfaces

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1 The Physical Problem

Consider a moving bubble of one liquid in a fluid milieu of a different liquid, with a certain concentration of some species, which adheres to the surface. Such a species is called a surfactant. An example for such a constellation would be molecules with a hydrophobic and a hydrophilic end on some bubble in water (e.g. tensides, lipids, ...).

1.1 Mathematical model

Let $\Omega \subseteq \mathbb{R}^n$ be an open domain and let Ω_1, $\Omega_2 \subseteq \mathbb{R}^d$ describe the interior and exterior part of our bubble such that $\overline{\Omega_1} \cup \overline{\Omega_2} = \Omega$, $\partial\Omega_1 := \Gamma$, $\Gamma \cap \partial\Omega = \emptyset$ and let n and κ denote the outward normal and mean curvature on Γ respectively.
Further we denote the densities and viscosities of our fluids by ρ_i and μ_i respectively. Then the classical two-phase fluid dynamics model reads (cf. **??**):

Problem 1.1. Find a velocity field $u(x,t)$ and a pressure $p(x,t)$, such that

$$\rho_i \left(\frac{\partial}{\partial t} u + (u \cdot \nabla)\, u \right) - \operatorname{div}(\mu_i D(u)) + \nabla p = \rho_i g, \qquad \text{in } \Omega_i(t)\,. \tag{1a}$$

$$\operatorname{div}(u) = 0, \qquad \text{in } \Omega_i(t)\,. \tag{1b}$$

$$[[\sigma \cdot n]] = -\tau\kappa n, \qquad \text{on } \Gamma(t)\,. \tag{1c}$$

$$[[u]] = 0, \qquad \text{on } \Gamma(t)\,, \tag{1d}$$

where $D(u) := \nabla u + \nabla u^T$, $[[\cdot]]$ denotes the jump in normal direction, τ is the surface tension force, σ the stress tensor, and g the gravitational force.

1.1.1 Some remarks on differential geometry

Let $\Gamma \subseteq \mathbb{R}^d$ be an oriented C^2-hypersurface and let $n(x)$ denote its outward normal. For a C^1-function f on Γ we define its tangential derivative by

$$\nabla_\Gamma f := P \nabla f, \tag{2}$$

where $P(x) := I - n(x)\, n(x)^T$ is the orthogonal projection on the tangential space. Further we define the tangential gradient $\operatorname{div}_\Gamma$ of some vector field $\vec{v}$ by

$$\operatorname{div}_\Gamma(\vec{v}) := \nabla_\Gamma \cdot \vec{v} = \sum_{n=1}^{d} (P\nabla)_n\, v_n = \operatorname{div}(\vec{v}) - n^T \vec{v} n. \tag{3}$$

Remark 1.2. For a differentiable scalar function f and a vector field $\vec{g}$ on Γ, there holds the product rule

$$\mathrm{div}_\Gamma(f\vec{g}) = f\mathrm{div}_\Gamma(\vec{g}) + \nabla_\Gamma f \cdot \vec{g}. \tag{4}$$

Remark 1.3. Let $W \subseteq \Gamma$ be an open subset and n_W denote its outward normal in the tangential plane of Γ. Then there holds integration of parts in Γ

$$\int_W f\,\mathrm{div}_\Gamma(\vec{v})\,ds = -\int_W \nabla_\Gamma f \cdot \vec{v} + \int_{\partial W} f\vec{v} \cdot n_W d\tilde{s}. \tag{5}$$

Theorem 1.4 (Reynold's transport theorem on an interface)**.** *The rate of change for a smooth function $f(x,t)$ on $W(t) \subseteq \Gamma$ can be described by*

$$\frac{d}{dt}\int_{W(t)} f(x,t)\,ds = \int_{W(t)} \dot{f}(x,t) + f(x,t)\,\mathrm{div}_\Gamma(\vec{v})\,ds \tag{6}$$

with the material derivative $\dot{f}$ for a given velocity field $\vec{v}$ defined as

$$\dot{f} := \frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f \tag{7}$$

1.1.2 Transport of a surfactant

Next let $c(x,t)$ describe the concentration of the surfactant on Γ. Then conservation of mass in an arbitrary control volume $W(t) \subseteq \Gamma$, with source f yields

$$\frac{d}{dt}\int_{W(t)} c\,ds = -\int_{\partial W(t)} \vec{q} \cdot n_W\,d\tilde{s} + \int_{W(t)} f\,ds \tag{8}$$

If we assume $\vec{q}$ to be a diffusive flux $\vec{q} := -\alpha\nabla_\Gamma c$ and use integration by parts, we obtain

$$\begin{aligned}\frac{d}{dt}\int_{W(t)} c\,ds &= \int_{\partial W(t)} \alpha\nabla_\Gamma c \cdot n_W\,d\tilde{s} + \int_{W(t)} f\,ds \\ &= \int_{W(t)} \mathrm{div}_\Gamma(\alpha\nabla_\Gamma c)\,ds + \int_{W(t)} f\,ds. \end{aligned} \tag{9}$$

Combined with Reynold's transport theorem we arrive at

$$\frac{d}{dt}\int_{W(t)} c\,ds = \int_{W(t)} \dot{c} + c\,\mathrm{div}_\Gamma(\vec{v})\,ds \tag{10}$$

$$= \int_{W(t)} \frac{\partial c}{\partial t} + \vec{v} \cdot \nabla c + c\,\mathrm{div}_\Gamma(\vec{v})\,ds \tag{11}$$

$$= \int_{W(t)} \mathrm{div}_\Gamma(\alpha\nabla_\Gamma c)\,ds + \int_{W(t)} f\,ds. \tag{12}$$

If we assume, that the velocity $\vec{v}$ is always tangential to the surface (i.e. $\vec{v} \cdot n = 0$) there holds

$$\vec{v} \cdot \nabla c = P\vec{v} \cdot \nabla c = \vec{v} \cdot P\nabla c = \vec{v} \cdot \nabla_\Gamma c \tag{13}$$

and

$$\vec{v} \cdot \nabla c + c \operatorname{div}_\Gamma(\vec{v}) = \operatorname{div}_\Gamma(c\vec{v}) \,. \tag{14}$$

Our final problem for the surfactant species transport in strong form reads:

Problem 1.5. Given suitable boundary and initial conditions for $\vec{v}$ and c and a source function f, find $\vec{v}$, p and c such that

$$\rho_i \left(\frac{\partial}{\partial t}\vec{v} + (u \cdot \nabla)\,\vec{v} \right) - \operatorname{div}(\mu_i D(\vec{v})) + \nabla p = \rho_i g, \qquad \text{in } \Omega_i(t)\,, \tag{15a}$$

$$\operatorname{div}(\vec{v}) = 0, \qquad \text{in } \Omega_i(t)\,, \tag{15b}$$

$$[[\sigma \cdot n]] = -\tau\kappa n, \qquad \text{on } \Gamma(t)\,, \tag{15c}$$

$$[[\vec{v}]] = 0, \qquad \text{on } \Gamma(t)\,, \tag{15d}$$

$$\frac{\partial}{\partial t}c + \operatorname{div}_\Gamma(c\vec{v}) - \operatorname{div}_\Gamma(\alpha\nabla_\Gamma c) = f, \qquad \text{on } \Gamma(t)\,. \tag{15e}$$

In the following, we will concentrate on equation (15e) for a given velocity field $\vec{v}$.

Example 1.6 (Stokes flow past a sphere). Let $\Omega_1 \subseteq \mathbb{R}^d$ $(d = 2, 3)$ be a sphere (circle) with radius r_0 rising with constant velocity v_0. We are interested in the resulting velocity field $\vec{v}$ relative to the sphere. To this end we study a stationary, linearized version of (15a) and (15b), namely

$$\operatorname{div}(\vec{v}) = 0 \tag{16a}$$

$$-\nabla p + \mu_i \Delta\vec{v} = 0, \tag{16b}$$

In general an axial symmetric solution of (16) can be written in the form

$$\vec{v} = v_r\vec{e}_r + v_\theta\vec{e}_\theta = \frac{1}{r^2 \sin\theta}\frac{\partial\psi}{\partial\theta}\vec{e}_r - \frac{1}{r\sin\theta}\frac{\partial\psi}{\partial r}\vec{e}_\theta \tag{17}$$

with a stream function

$$\psi(r,\theta) = r\sin^2\theta \left(A + Br^2 + Cr^3 + Dr^5\right). \tag{18}$$

and some coefficients A, B, C, D (r and θ are the usual spherical coordinates). To deduce the coefficients A_i, B_i, C_i, D_i for the inner and outer stream function, we need the following boundary conditions

$$\lim_{r\to\infty} v_r(r,\theta) = -v_0 \tag{19a}$$

$$\lim_{r\to 0} |v_r(r,\theta)| < \infty \tag{19b}$$

$$\lim_{r\to r_{0-}} v_\theta(r,\theta) = \lim_{r\to r_{0+}} v_\theta(r,\theta) \tag{19c}$$

$$\lim_{r\to r_{0-}} \sigma(r,\theta) = \lim_{r\to r_{0+}} \sigma(r,\theta) \tag{19d}$$

$$\lim_{r\to r_{0-}} v_r(r,\theta) = \lim_{r\to r_{0+}} v_r(r,\theta) = 0, \tag{19e}$$

which lead to a system of linear equations

$$2C_2 = v_0 \tag{20a}$$

$$A_1 = B_1 = 0 \tag{20b}$$

$$-A_2 + B_2 r_0^2 + v_0 r_0^3 = 2C_1 r_0^3 + 4D_1 r_0^5 \tag{20c}$$

$$\mu_2 A_2 = \mu_1 D_1 r_0^5 \tag{20d}$$

$$A_2 + B_2 r_0^2 + \frac{1}{2} v_0 r_0^3 = 0 \tag{20e}$$

$$C_2 + D_2 r_0^2 = 0. \tag{20f}$$

Solving (20) gives a stream function

$$\psi(r,\theta) = \begin{cases} \frac{v_0}{4}\sin^2\theta \frac{1}{\mu_1+\mu_2}\left(\frac{r_0^3}{r}\mu_2 - r_0\left(2\mu_2+3\mu_1\right)r + 2\left(\mu_1+\mu_2\right)r^2\right), & r \geq r_0 \\ \frac{v_0}{4}\sin^2\theta \frac{\mu_2}{\mu_1+\mu_2} r^2\left(\frac{r^2}{r_0^2} - 1\right) & r \leq r_0. \end{cases} \tag{21}$$

Calculating the radial and tangential component and substituting $r = r_0$ yields the sought-after velocity field on the sphere, namely

$$\vec{v} = \vec{e}_\theta \frac{v_0}{2}\frac{\mu_2}{\mu_1+\mu_2}\sin\theta. \tag{22}$$

In cartesian coordinates and two dimensions, this reads

$$\vec{v} = \frac{v_0}{2}\frac{\mu_2}{\mu_1+\mu_2}\frac{1}{r_0^2}\begin{pmatrix} yx \\ -x^2 \end{pmatrix}. \tag{23}$$

In three dimensions we obtain

$$\vec{v} = \frac{v_0}{2}\frac{\mu_2}{\mu_1+\mu_2}\frac{1}{r_0^2}\begin{pmatrix} zx \\ zy \\ -x^2-y^2 \end{pmatrix}. \tag{24}$$

2 Discretization

3 Implementation

4 Numerical Experiments