**DROPS Package**

for Simulation of Two Phase Incompressible Flows

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### Model

**Fluid Dynamics**

\[
\begin{aligned}
\rho(\phi) &= \rho_1 + (\rho_2 - \rho_1)H(\phi), \\
\rho(\phi)\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) &= \nabla p + \text{div}(\rho(\phi)\mathbf{D}(\mathbf{u})) + \rho(\phi)\mathbf{g} \\
\text{div}\mathbf{u} &= 0
\end{aligned}
\]

\(\text{in } \Omega_1, \quad i = 1, 2, \quad \mathbf{u}|_{\Gamma} = 0 \quad \text{on } \Gamma_1, \quad \mathbf{u}|_{\Gamma} = \mathbf{n}_1 \quad \text{on } \Gamma_2, \quad \frac{\partial \phi}{\partial n} + \mathbf{n} \cdot \nabla \phi = 0 \quad \text{on } \Omega_2 \)

with proper boundary and initial conditions

**Mass Transport**

\[
\frac{D}{Dt} + \mathbf{u} \cdot \nabla \mathbf{v} = \text{div}(D(\phi)\nabla \mathbf{v}) \quad \text{in } \Omega_1, \quad \mathbf{v}|_{\Gamma} = 0 \quad \text{on } \Gamma_1, \quad \mathbf{v}|_{\Gamma} = \mathbf{n}_1 \quad \text{on } \Gamma_2
\]

**Transport of Surfactants**

\[
\frac{\partial S}{\partial t} + \mathbf{u} \cdot \nabla S + S \text{div}\mathbf{u} = D_I \nabla^2 S \quad \text{on } \Gamma_1
\]

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### Aims

- Parallel simulation of coupled fluid dynamics, mass- and surfactant transport with variable surface property.
- Simulation of real physical systems; validation of numerics.
- Development and analysis of numerical methods.

### Key Components

- Adaptive multilevel hierarchy of tetrahedral triangulations. Local refinement / coarsening.
- Level set method for interface representation.
- Finite Element methods. Extended-FEM(XFEM) for discretization of discontinuous quantities.
- Special Laplace-Beltrami method for surface tension force discretization.
- New FE method for discretization of surfactant transport equation.
- Implicit time discretization method with strong coupling of fluid dynamics and interface dynamics.
- Fast iterative solvers.
- Parallelization with MPI.

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### Fluid Dynamics

**XFEM (Extended FEM)**

- By extending the standard finite element space with additional basis functions, the jump at the interface can be formulated as

\[
\mathbf{q}_j \mathbf{P}_j = q_j (H_1(x) - H_2(x))
\]

**Approximation quality**

\[
\inf_{\mathbf{q} \in Q_0} \| \mathbf{q} - \mathbf{p} \|_{L^2(\Omega)} \leq \begin{cases} \mathcal{O}(\sqrt{h}), & \text{Standard PI-FE} \\
\mathcal{O}(h^2), & \text{XFEM} \end{cases}
\]

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### Parallelization

- Implementation based on MPI.
- Distributed multilevel hierarchy of tetrahedral triangulations.
- Dynamic load-balancing.
- Treatment of distributed unknowns.

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### Improved Laplace-Beltrami discretization

\[
\int_{\Gamma_1} (\mathbf{v}_1 \cdot \mathbf{t}_1) = -\tau \int_{\Gamma_1} P_1 \nabla \mathbf{u}_1 \cdot \mathbf{t}_1 ds, \quad P_1(x) = 1 - n_1(x) n_2(x)^T
\]

\[
\mathcal{O}(\sqrt{h}) \sim \mathcal{O}(h^2)
\]

**Variable surface tension coefficients**

\[
\begin{aligned}
\mathbf{f}_1(\mathbf{v}) &= \int_{\Gamma_1} \mathbf{P}_1 \nabla \mathbf{u}_1 \cdot \mathbf{t}_1 \mathbf{v} ds \\
&= \int_{\Gamma_1} \mathbf{P}_1 \nabla \mathbf{u}_1 \cdot \mathbf{t}_1 \mathbf{v} - \mathbf{P}_1 \mathbf{u}_1 \cdot \mathbf{t}_1 \mathbf{v} \mathbf{t}_1 \cdot \mathbf{n}_1 \mathbf{v} \mathbf{n}_1 ds
\end{aligned}
\]

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### Publications


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**Figures**

- Simulation evolution with refinement and load-balancing
- From left to right: interfacial tension $$\tau = 1.63 \times 10^{-3} \text{N/m}, 8.15 \times 10^{-3} \text{N/m}, 32.6 \times 10^{-3} \text{N/m}$$