

# Fitted ALE scheme for Two-Phase Navier–Stokes Flow

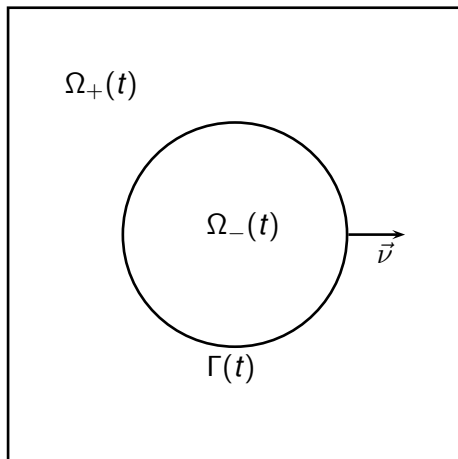
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# Problem setting

Domain  $\Omega$  in the 2-dimensional case.



# Governing equations

- Bulk equations

$$\begin{aligned}\rho(\vec{u}_t + (\vec{u} \cdot \nabla) \vec{u}) - \nabla \cdot \underline{\underline{\sigma}} &= \vec{f} = \rho \vec{f}_1 + \vec{f}_2 && \text{in } \Omega_{\pm}(t), \\ \nabla \cdot \vec{u} &= 0 && \text{in } \Omega_{\pm}(t),\end{aligned}$$

where

$$\underline{\underline{\sigma}} = \mu(\nabla \vec{u} + (\nabla \vec{u})^T) - p \underline{\underline{\text{id}}} = 2\mu \underline{\underline{D}}(\vec{u}) - p \underline{\underline{\text{id}}}.$$

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## ► Interface equations

$$\begin{aligned}[\vec{u}]_{-}^{+} &= \vec{0} && \text{on } \Gamma(t), \\ [\underline{\underline{\sigma}} \vec{\nu}]_{-}^{+} &= -\gamma \kappa \vec{\nu} && \text{on } \Gamma(t), \\ \vec{\nu} \cdot \vec{\nu} &= \vec{u} \cdot \vec{\nu} && \text{on } \Gamma(t).\end{aligned}$$

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- ▶ To close the system, we prescribe the initial data  $\Gamma(0) = \Gamma_0$  and some boundary condition for  $\vec{u}$  on  $\partial\Omega$ .

# Interface treatment

- ▶  $\Gamma(t)$  is a sufficiently smooth evolving hypersurface without boundary that is parameterized by  $\vec{x}(\cdot, t) : \Upsilon \rightarrow \mathbb{R}^d$ , therefore

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- ▶ It holds that

$$\Delta_s \vec{\text{id}} = \varkappa \vec{\nu} \quad \text{on } \Gamma(t),$$

where  $\Delta_s = \nabla_s \cdot \nabla_s$  is the Laplace-Beltrami operator on  $\Gamma(t)$  with  $\nabla_s \cdot$  and  $\nabla_s$  denoting surface divergence and surface gradient on  $\Gamma(t)$ .

# Stokes weak formulation

Using the function spaces

$$\mathbb{U} := [H_0^1(\Omega)]^d, \quad \mathbb{P} := L^2(\Omega) \quad \text{and}$$

$$\widehat{\mathbb{P}} := \{\eta \in \mathbb{P} : \int_{\Omega} \eta \, d\mathcal{L}^d = 0\},$$

the Stokes weak formulation is

$$2 \left( \mu \underline{\underline{D}}(\vec{u}), \underline{\underline{D}}(\vec{\xi}) \right) - \left( \vec{p}, \nabla \cdot \vec{\xi} \right) - \gamma \left\langle \varkappa \vec{\nu}, \vec{\xi} \right\rangle_{\Gamma(t)} = \left( \vec{f}, \vec{\xi} \right) \quad \forall \vec{\xi} \in \mathbb{U},$$

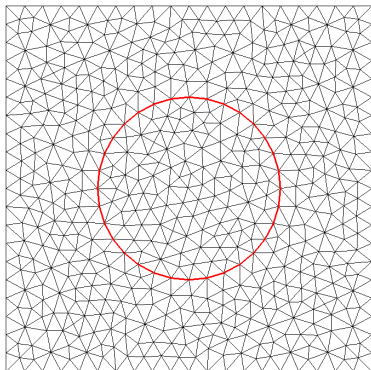
$$(\nabla \cdot \vec{u}, \varphi) = 0 \quad \forall \varphi \in \widehat{\mathbb{P}},$$

$$\left\langle \vec{\nu} - \vec{u}, \chi \vec{\nu} \right\rangle_{\Gamma(t)} = 0 \quad \forall \chi \in H^1(\Gamma(t)),$$

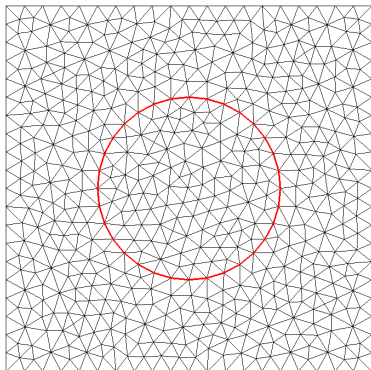
$$\left\langle \varkappa \vec{\nu}, \vec{\eta} \right\rangle_{\Gamma(t)} + \left\langle \nabla_s \text{id}, \nabla_s \vec{\eta} \right\rangle_{\Gamma(t)} = 0 \quad \forall \vec{\eta} \in [H^1(\Gamma(t))]^d.$$



# Fitted approach

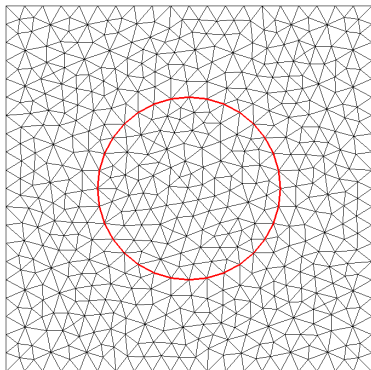


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- ▶ Pros: naturally captured discontinuity jumps in  $\rho, \mu, p$  and no need to interpolate bulk quantities over interface.
- ▶ Cons: possible bulk mesh distortion and difficult bulk mesh adaptation.

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- ▶ Let  $(\mathbf{U}^m, \mathbb{P}^m)$  be an LBB-stable pair of velocity/pressure finite element spaces in the bulk, e.g. P2-P0 (only in 2d) or P2-P1, with  $\mathbb{P}^m$  possibly extended by an additional basis function.

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- ▶ Then our finite element approximation is based directly on the discretization of the weak formulation.

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- ▶ Pressure jumps at the interface are captured accurately for standard pressure finite element spaces without the need for XFEM extensions.
- ▶ The surface mesh quality is maintained and for the semidiscrete scheme an equidistribution property can be shown in 2d.

# Solution method

Find  $(\vec{U}^{m+1}, \mathbf{P}^{m+1}, \kappa^{m+1}, \delta \vec{X}^{m+1})$  such that

$$\begin{pmatrix} \vec{B}_\Omega & \vec{C}_\Omega & -\gamma \vec{N}_{\Gamma,\Omega} & 0 \\ \vec{C}_\Omega^T & 0 & 0 & 0 \\ \vec{N}_{\Gamma,\Omega}^T & 0 & 0 & -\frac{1}{\tau_m} \vec{N}_\Gamma^T \\ 0 & 0 & \vec{N}_\Gamma & \vec{A}_\Gamma \end{pmatrix} \begin{pmatrix} \vec{U}^{m+1} \\ \mathbf{P}^{m+1} \\ \kappa^{m+1} \\ \delta \vec{X}^{m+1} \end{pmatrix} = \begin{pmatrix} \vec{c} \\ 0 \\ 0 \\ -\vec{A}_\Gamma \vec{X}^m \end{pmatrix},$$

where  $\vec{X}^{m+1} = \vec{X}^m + \delta \vec{X}^{m+1}$ .

# Schur complement approach

Let

$$\Xi_{\Gamma} := \begin{pmatrix} 0 & -\frac{1}{\tau_m} \vec{N}_{\Gamma}^T \\ \vec{N}_{\Gamma} & \vec{A}_{\Gamma} \end{pmatrix}.$$

Therefore

$$\begin{pmatrix} \vec{B}_{\Omega} + \gamma (\vec{N}_{\Gamma, \Omega} \ 0) \Xi_{\Gamma}^{-1} \begin{pmatrix} \vec{N}_{\Gamma, \Omega}^T \\ 0 \end{pmatrix} & \vec{C}_{\Omega} \\ \vec{C}_{\Omega}^T & 0 \end{pmatrix} \begin{pmatrix} \vec{U}^{m+1} \\ \vec{P}^{m+1} \end{pmatrix} = \\ \begin{pmatrix} \vec{c} - \gamma (\vec{N}_{\Gamma, \Omega} \ 0) \Xi_{\Gamma}^{-1} \begin{pmatrix} 0 \\ \vec{A}_{\Gamma} \vec{X}^m \end{pmatrix} \\ 0 \end{pmatrix}$$

and

$$\begin{pmatrix} \kappa^{m+1} \\ \delta \vec{X}^{m+1} \end{pmatrix} = \Xi_{\Gamma}^{-1} \begin{pmatrix} -\vec{N}_{\Gamma, \Omega}^T \vec{U}^{m+1} \\ -\vec{A}_{\Gamma} \vec{X}^m \end{pmatrix}.$$

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As preconditioner we use the matrix

$$\mathcal{P} = \begin{pmatrix} \vec{B}_{\Omega} & \vec{C}_{\Omega} \\ 0 & -M_{\Omega} \end{pmatrix}.$$

# Mesh smoothing and remeshing

- Smoothing: find a displacement  $\vec{\psi} \in [H^1(\Omega)]^d$  such that

$$\begin{aligned}\nabla \cdot \underline{\underline{S}} &= \vec{0} && \text{in } \Omega_{\pm}^m, \\ \vec{\psi} &= \delta \vec{X} && \text{on } \Gamma^m, \\ \vec{\psi} \cdot \vec{n} &= 0 && \text{on } \partial\Omega,\end{aligned}$$

where  $\underline{\underline{S}} = 2 \underline{\underline{D}}(\vec{\psi}) + (\nabla \cdot \vec{\psi}) \underline{\underline{Id}}$  is the stress tensor and where  $\vec{n}$  is the outer unit normal to  $\Omega$  on  $\partial\Omega$ .



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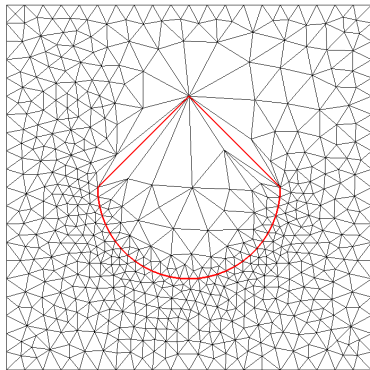
- Remeshing: perform remeshing when

$$\frac{\max_{o \in \mathcal{T}^{m+1}} (\mathcal{H}^d(o))}{\min_{o \in \mathcal{T}^{m+1}} (\mathcal{H}^d(o))} \geq C_r,$$

where  $C_r \geq 1$  is a fixed constant.

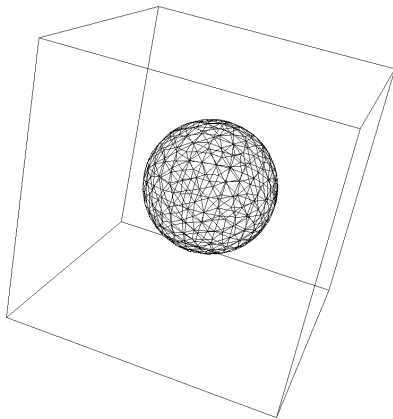
# Equidistribution property experiment

$$\rho_{\pm} = 0, \quad \mu_{\pm} = 1, \quad \gamma = 1$$



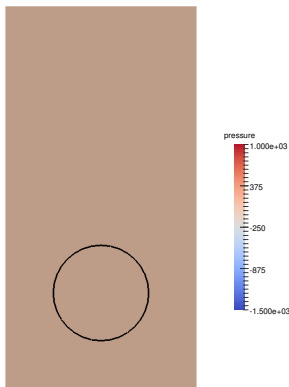
# Shear flow experiment

$$\rho_{\pm} = 0, \quad \mu_{\pm} = 1, \quad \gamma = 3, \quad \vec{g}(\vec{x}) = x_3 \vec{e}_1 \quad \text{on } \partial\Omega$$



# Rising bubble experiment

$$\rho_+ = 10^3, \rho_- = 10^2, \mu_+ = 10, \mu_- = 1, \gamma = 24.5, \vec{f} = -0.98\vec{e}_2$$



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- ▶ In order to reduce the computational cost of the interpolation, bulk elements are sorted and traversed following a continuous path; barycentric coordinates are used to locate the interpolation points in the previous bulk mesh.
- ▶ On the other hand, to improve the accuracy, the interpolation should be performed only after a remeshing.



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- ▶ This prescribed flow needs to be accounted for in the approximation of the momentum equation; in practice, it adds a convective-type term to the momentum balance.
- ▶ The movement of the bulk mesh is incorporated in the finite element approximation therefore it avoids the repeated interpolation onto the bulk mesh.

# Outlook

- ▶ Test other solvers/preconditioners to solve the algebraic linear system more efficiently.
- ▶ Include surface active agents (surfactants) to the model.
- ▶ Use adaptive meshes to increase the accuracy of the scheme.
- ▶ Test higher order spaces to approximate the displacement of the interface.

# References

1. J. W. BARRETT, H. GARCKE, AND R. NÜRNBERG, *A parametric finite element method for fourth order geometric evolution equations*, [J. Comput. Phys.](#), (2007).
2. ———, *On the parametric finite element approximation of evolving hypersurfaces in  $\mathbb{R}^3$* , [J. Comput. Phys.](#), (2008).
3. ———, *Eliminating spurious velocities with a stable approximation of viscous incompressible two-phase Stokes flow*, [Comput. Methods Appl. Mech. Engrg.](#), (2013).
4. ———, *A stable parametric finite element discretization of two-phase Navier–Stokes flow*, [J. Sci. Comput.](#), (2013).
5. M. AGNESE AND R. NÜRNBERG, *Fitted Finite Element Discretization of Two-Phase Stokes Flow*, [Int. J. Numer. Meth. Fluids](#), (2016).