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NITSCHE-XFEM FOR A TRANSPORT PROBLEM IN TWO-PHASE INCOMPRESSIBLE FLOWS

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Summary. We present a finite element discretization method for a mass transport problem with a solution that is discontinuous across an interface. The grids are regular and unfitted. The method is based on a combination of Nitsche's method and an XFEM approach.

1 INTRODUCTION

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, be a convex polygonal domain that contains two different immiscible incompressible phases Ω_1 and Ω_2. We assume that the interface $\Gamma = \Gamma(t) = \bar{\Omega}_1 \cap \bar{\Omega}_2$ is sufficiently smooth. We consider a model which describes the transport of a dissolved species in a divergence-free velocity field $\mathbf{w}$, i.e. $\operatorname{div} \mathbf{w} = 0$, as follows:

$$\frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u - \operatorname{div}(\alpha \nabla u) = f \quad \text{in } \Omega_i,\ i = 1, 2,\ t \in [0, T], \tag{1}$$

$$[\alpha \nabla u \cdot \mathbf{n}]_\Gamma = 0, \quad [\beta u]_\Gamma = 0, \tag{2}$$

where $\mathbf{n}$ is the unit normal at Γ pointing from Ω_1 into Ω_2. For a sufficiently smooth function v, $[v]$ denotes the jump of v across Γ. The first interface condition in (2) results from the conservation of mass principle while the second one is the so-called *Henry condition*.[1] The diffusion coefficient α and the Henry coefficient β are positive and piecewise constant in the two subdomains, so the solution u is in general *discontinuous across the interface*. For the special case $\beta_1 = \beta_2$ and with a triangulation which is *fitted* to the interface, standard finite element spaces have (close to) optimal approximation properties.[2] Here we allow $\beta_1 \neq \beta_2$ and use triangulations that are *un*fitted (as in level set of VOF approaches), i.e. the interface crosses the elements. We will use a variant of Nitsche's method combined with a special finite element method for the spatial discretization of this problem. From this semi-discrete problem a full discretization is obtained by using a standard θ-scheme for time discretization. We use the same Nitsche method as presented and analyzed for a *stationary* diffusion problem by Hansbo.[3] We apply this method to the *nonstationary* problem described above, with discontinuous solution, and furthermore allow a convection term in (1).

2 Weak formulation

In this section we give a weak formulation. For simplicity we only consider homogeneous Dirichlet boundary conditions. Due to the fact that the underlying two-phase fluid dynamics concerns two incompressible immiscible phases it is reasonable to make the following assumption about the velocity field $\mathbf{w}$: $\operatorname{div} \mathbf{w} = 0$ in $\Omega_i,\ i = 1,2$, $\mathbf{w} \cdot \mathbf{n} = 0$ at Γ, and $\|\mathbf{w}\|_{L^\infty(\Omega)} \leq c < \infty$. We define $H_0^1(\Omega_1 \cup \Omega_2) := \{\, v \in L^2(\Omega) \,|\, v_i \in H^1(\Omega_i),\ i = 1,2,\ v_{|\partial\Omega} = 0 \,\}$, where $v_i := v_{|\Omega_i}$, and

$$
\begin{aligned}
H &:= L^2(\Omega), \quad V := \{\, v \in H_0^1(\Omega_1 \cup \Omega_2) \,|\, [\beta v]_\Gamma = 0 \,\}, \\
(u,v)_0 &: = \int_\Omega \beta u v \, dx, \quad u,v \in H, \\
(u,v)_{1,\Omega_1\cup\Omega_2} &:= (u,v)_{1,\Omega_1} + (u,v)_{1,\Omega_2} = \sum_{j=1}^{2} \Big(\frac{\partial u}{\partial x_j}, \frac{\partial v}{\partial x_j} \Big)_0, \quad u,v \in V.
\end{aligned}
$$

We now introduce the bilinear form

$$
a(u,v) := (\alpha u, v)_{1,\Omega_1\cup\Omega_2} + (\mathbf{w}\cdot\nabla u, v)_0, \quad u,v \in V.
$$

We have[4] well-posedness of a weak formulation for the case with a stationary interface:

Lemma 1 *Assume that Γ does not depend on t. Take $f \in H$, $u_0 \in V_{\mathrm{reg}} := \{\, v \in V \,|\, v_i \in H^2(\Omega_i),\ i = 1,2 \,\}$. There exists a unique $u \in C([0,T]; V_{\mathrm{reg}})$ such that $u(0) = u_0$ and*

$$
(\frac{\partial u}{\partial t}, v)_0 + a(u,v) = (f,v)_0 \quad \textit{for all } \ v \in V. \tag{3}
$$

The distributional time derivative satisfies $\frac{\partial u}{\partial t} \in L^2(0,T;V) \cap C([0,T];H)$.

3 XFEM space and Nitsche's method

Let $\{\mathcal{T}_h\}_{h>0}$ be a family of shape regular triangulations of Ω. A triangulation $\mathcal{T}_h$ consists of triangles T, with $h_T := \operatorname{diam}(T)$ and $h := \max\{\, h_T \mid T \in \mathcal{T}_h \}$. Let $T_i := T \cap \Omega_i$ be the part of T in Ω_i. We now introduce the finite element space

$$
V_h^\Gamma := \{\, v \in H_0^1(\Omega_1 \cup \Omega_2) \,|\, v_{|T_i} \ \text{ is linear for all } \ T \in \mathcal{T}_h,\ i = 1,2 \,\}. \tag{4}
$$

Note that $V_h^\Gamma \subset H_0^1(\Omega_1\cup\Omega_2)$, but $V_h^\Gamma \not\subset V$, since the Henry interface condition $[\beta v_h] = 0$ does not necessarily hold for $v_h \in V_h^\Gamma$. We define $(\kappa_i)_{|T} = \frac{|T_i|}{|T|}$ for all $T \in \mathcal{T}_h,\ i = 1,2$, and the weighted average $\{v\} := \kappa_1 (v_1)_{|\Gamma} + \kappa_2 (v_2)_{|\Gamma}$. Let $(f,g)_\Gamma := \int_\Gamma f g \, ds$ be the $L^2(\Gamma)$ scalar product. We introduce the bilinear form

$$
\begin{aligned}
a_h(u,v) := {} & (\alpha u, v)_{1,\Omega_1\cup\Omega_2} + (\mathbf{w}\cdot\nabla u, v)_0 - ([\beta u], \{\alpha \nabla v \cdot \mathbf{n}\})_\Gamma \\
& - (\{\alpha\nabla u\cdot\mathbf{n}\}, [\beta v])_\Gamma + \lambda h^{-1} ([\beta u],[\beta v])_\Gamma,
\end{aligned} \tag{5}
$$

with a positive parameter λ. The following consistency result holds[4] : Let $u = u(t) \in V_{\mathrm{reg}}$ be the solution defined in lemma 1. Then $u(t)$ satisfies

$$
(\frac{\partial u}{\partial t}, v_h)_0 + a_h(u, v_h) = (f, v_h) \quad \text{for al } \ v_h \in V_h^\Gamma, \ \ t \in [0,T]. \tag{6}
$$

For the spatial discretization error we have the following result[4] .

Theorem 1 *Assume that Γ does not depend on t. Let $u = u(t) \in V_{\mathrm{reg}}$ be the solution defined in lemma 1 and $u_h = u_h(t) \in V_h^\Gamma$ the solution of* (6) *with $u_h(0) = \hat{u}_0$. The following holds, with R_h the elliptic projection on V_h^Γ,*

$$\|u_h(t) - u(t)\|_0 \leq \|\hat{u}_0 - R_h u_0\|_0 + c\,h^2 \big\{ \|u_0\|_{2,\Omega_1\cup\Omega_2} + \int_0^t \left\| \frac{\partial u}{\partial t} \right\|_{2,\Omega_1\cup\Omega_2} d\tau \big\}, \quad 0 \leq t \leq T.$$

From this result we conclude that for the semi-discretization of our transport problem we have an optimal error bound for the spatial discretization.

4 Numerical experiments

4.1 Experiment with a stationary interface

We consider the problem (1)-(2) in the domain $\Omega = (0,1)^3$, which contains two subdomains $\Omega_1 := \{(x,y,z) \in \Omega : z < 0.341\}$ and $\Omega_2 := \Omega \setminus \Omega_1$, with the coefficients $\alpha = (\alpha_1, \alpha_2) := (1,2)$, $\beta = (\beta_1, \beta_2) := (2,1)$ and a velocity field $\mathbf{w} := (y(1-z), x, 0)^T$. The exact solution is chosen as

$$u(x,y,z,t) := \begin{cases} \exp(-t)\cos(\pi x)\cos(2\pi y) a z(z+b) & \text{in } \Omega_1, \\ \exp(-t)\cos(\pi x)\cos(2\pi y) z(z-1) & \text{in } \Omega_2, \end{cases} \tag{7}$$

where the constants a and b are determined from the interface condtions (2). For the spatial discretization, we create a uniform grid with mesh size $h = \frac{1}{N}$ ($N = 8, 16, 32$) then refine the elements near the interface two times further. The semi-discretization $u_h(t)$ is approximated by $u_h^*(t)$ using the implicit Euler time-stepping scheme with a (sufficiently small) time step size $\Delta t = 10^{-4}$. In Table 1, the errors $\|u_h^*(T) - u(T)\|_{L^2}$ for $T = 0.15$ are displayed, which are consistent with the theoretical bound $\mathcal{O}(h^2)$ given in theorem 1. For a *stationary* elliptic problem the bound[3] $\|[\beta u_h]\|_{L^2(\Gamma)} \leq c h^{1\frac{1}{2}} \|u\|_{2,\Omega_1\cup\Omega_2}$ holds. For the *time dependent* case we were not able to derive a theoretical bound for this error quantity. The errors $\|[\beta u_h^*]\|_{L^2(\Gamma)}$ are given in Table 2, which seems to behave like $\mathcal{O}(h)$. The numerical solution for $N = 16$ at $T = 0.15$ in the plane $x = 0.25$ is shown in Figure 1. To investigate the time discretization

N	$\|u_h^*(T) - u(T)\|_{L^2}$	factor	order
8	0.00738506	-	-
16	0.00202308	3.65	1.87
32	0.0005228	3.87	1.95

Table 1: Planar interface: Spatial discretization error in L^2-norm and convergence order at $T = 0.15$

N	$\|[\beta u_h^*(T)]\|_{L^2(\Gamma)}$	factor	order
8	$1.565e-4$	-	-
16	$7.975e-05$	1.96	0.972
32	$3.900e-05$	2.05	1.03

Table 2: Planar interface: L^2-norm of the jump $[\beta u_h^*(T)]_\Gamma$ and convergence order at $T = 0.15$

error, we use a fixed mesh with $N = 16$ and compute a reference solution $u_h^*(t)$ with $\Delta t = 10^{-4}$ in the time interval $[0, 0.2]$. The Euler discretization with time step $\Delta t = \frac{T}{n}$ results in approximations $u_h^n(T)$ of $u_h^*(T)$. For the cases $n = 5, 10, 20$ the temporal errors in the L^2-norm are given in Table 3. We observe the expected first order of convergence in Δt.

4.2 Experiment with a nonstationary interface

We consider the problem (1)-(2) in the unit cube Ω and with $\Omega_1(0)$ a sphere of radius $R = 0.2$ centered at the barycenter of Ω. This sphere is moved in with constant velocity $\mathbf{w} = (0,1,0)^T$, i.e.,

n	$\|u_h^n - u_h^*(0.2)\|_{L^2}$	factor	order
5	$1.254e-05$	-	-
10	$6.092e-06$	2.06	1.04
20	$3.011e-06$	2.02	1.02

Table 3: Planar interface: Time discretization error in L^2 norm and convergence order at $T = 0.2$

N	$\|u_h^*(T) - u(T)\|_{L^2}$	factor	order
16	0.00490676	-	-
32	0.00121142	4.05	2.018
64	0.000310616	3.9	1.963

Table 4: Moving interface: Spatial discretization error in L^2-norm and convergence order at $T = 0.1$

$\Omega_1(t) = \Omega_1(0) + t\mathbf{w}$. Let $d(x,t)$ be the distance from the point $x \in \Omega$ to the center of $\Omega_1(t)$. We take the piecewise quadratic solution

$$u(x,t) := \begin{cases} \alpha_2\big(d(x,t)^2 - R^2\big) + 0.1 \cdot \beta_2 & \text{in } \Omega_1, \\ \alpha_1\big(d(x,t)^2 - R^2\big) + 0.1 \cdot \beta_1 & \text{in } \Omega_2, \end{cases} \tag{8}$$

with coefficients $(\alpha_1, \alpha_2) := (1, 5)$, $(\beta_1, \beta_2) := (2, 1)$. As the XFEM space now is time dependent, we discretize the problem first in time using the implicit Euler method with the time step size $\Delta t = 10^{-4}$. The resulting convection-diffusion-reaction problem is discretized with the Nitsche method. We use a uniform grid with the mesh size $h = \frac{1}{N}$, where $N = 16, 32, 64$. The errors $\|u_h^*(T) - u(T)\|_{L^2}$ for $T = 0.1$ are displayed in Table 4 with the expected convergence order 2.

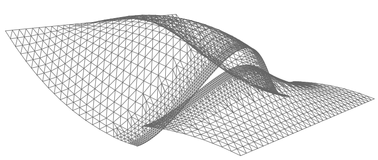

Figure 1: Planar interface: Numerical solution at $T = 0.15$ in the plane $x = 0.25$.

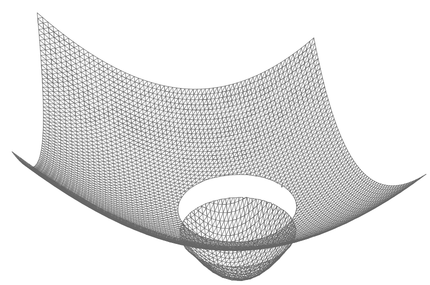

Figure 2: Moving interface: Numerical solution at $T = 0.1$ in the plane $x = 0.5$.

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