Space-time XFEM for two-phase mass transport

Christoph Lehrenfeld

joint work with Arnold Reusken

EFEF, Prague, June 5-6th 2015
Two-phase flows
Two-phase flows
Two-phase flows

Fluid dynamics (within the phases $\Omega_i$)

- incompressible Navier Stokes equations $(w, p)$
- (mass and momentum conservation)

Mass transport (within the phases $\Omega_i$)

- convection diffusion equation $(u)$
- (species conservation)
Two-phase flows

Fluid dynamics (within the phases $\Omega_i$)
- incompressible Navier Stokes equations ($w, p$)
- (mass and momentum conservation)

Mass transport (within the phases $\Omega_i$)
- convection diffusion equation ($u$)
- (species conservation)

Interface conditions (on $\Gamma$)
- mass and mom. cons. (capillary forces) ($w, p$)
- species conservation and thermodyn. equil. ($u$)
Mass transport model

Mass transport equation

\[ \partial_t u + \mathbf{w} \cdot \nabla u - \alpha \Delta u = 0 \quad \text{in } \Omega_i(t), \ i = 1, 2, \]
\[ [-\alpha \nabla u \cdot \mathbf{n}] = 0 \quad \text{on } \Gamma(t), \]
\[ \text{⚠️} \ [\beta u] = 0 \quad \text{on } \Gamma(t), \text{ (Henry condition)} \]

(+ initial + boundary conditions)
\[ \alpha, \beta: \text{piecewise constant diffusion / Henry coefficients.} \]

Compatibility conditions on the velocity:

\[ \mathcal{V} \cdot \mathbf{n} = \mathbf{w} \cdot \mathbf{n} \quad \text{on } \Gamma(t), \quad \mathcal{V}: \text{interface velocity.}, \quad \text{div}(\mathbf{w}) = 0 \quad \text{in } \Omega \]

no relative velocity on \( \Gamma \),

incompressible flow
Description of the interface
Description of the interface

Level set function $\phi$

$\phi(x, t) \begin{cases} 
= 0, & x \in \Gamma(t), \\
< 0, & x \in \Omega_1(t), \\
> 0, & x \in \Omega_2(t).
\end{cases}$

$\phi$ describes position of the interface
Description of the interface

Level set function $\phi$

\[
\phi(x, t) = \begin{cases} 
0, & x \in \Gamma(t), \\
< 0, & x \in \Omega_1(t), \\
> 0, & x \in \Omega_2(t). 
\end{cases}
\]

$\phi$ describes position of the interface

Level set equation

\[
\partial_t \phi + w \cdot \nabla \phi = 0 \text{ in } \Omega, \text{ + i.c. & b.c.} \quad (*)
\]

$(*)$ describes the motion of the interface
Description of the interface

Level set function $\phi$

\[ \phi(x, t) \begin{cases} = 0, & x \in \Gamma(t), \\ < 0, & x \in \Omega_1(t), \\ > 0, & x \in \Omega_2(t). \end{cases} \]

$\phi$ describes position of the interface

Level set equation

\[ \partial_t \phi + \mathbf{w} \cdot \nabla \phi = 0 \text{ in } \Omega, + \text{ i.c. & b.c.} \quad (*) \]

(*) describes the motion of the interface

**Implicit** description of the interface (Euler)

**Unfitted** meshes
Numerical aspects

Mass transport equation

\[ \partial_t u + \mathbf{w} \cdot \nabla u - \alpha \Delta u = 0 \quad \text{in } \Omega_1(t) \cup \Omega_2(t), \]
\[ [-\alpha \nabla u] \cdot \mathbf{n} = 0 \quad \text{on } \Gamma(t), \]
\[ [[\beta u]] = 0 \quad \text{on } \Gamma(t). \]
Numerical aspects

Mass transport equation

\[
\begin{align*}
\partial_t u + \mathbf{w} \cdot \nabla u - \alpha \Delta u &= 0 \quad \text{in } \Omega_1(t) \cup \Omega_2(t), \\
[-\alpha \nabla u] \cdot \mathbf{n} &= 0 \quad \text{on } \Gamma(t), \\
[\beta u] &= 0 \quad \text{on } \Gamma(t).
\end{align*}
\]

Numerical approaches

- Extended finite element space (XFEM)
- Nitsche’s method to enforce (weakly) the Henry condition
- Space-time formulation for moving discontinuity
Approximation of discontinuous function, \( u \in H^{k+1}(\Omega_1 \cup \Omega_2) \)

space: \( V_h \) (Standard FE space, degree \( k \))

\[
\inf_{u_h \in V_h} \| u - u_h \|_{L^2(\Omega)} \leq c\sqrt{h}
\]
Approximation of discontinuous function, \( u \in H^{k+1}(\Omega_1 \cup \Omega_2) \)

Approximation space: 

\[
V_h^\Gamma = \mathcal{R}_1 V_h \oplus \mathcal{R}_2 V_h
\]

\[
\inf_{u_h \in V_h^\Gamma} \|u - u_h\|_{L^2(\Omega)} \leq c h^{k+1}
\]
"Extended" FEM (XFEM)

\[ V_h^\Gamma = \mathcal{R}_1 V_h \oplus \mathcal{R}_2 V_h \quad \iff \quad V_h^\Gamma = V_h \oplus V_h^x \]

Extend \( P_1 \) basis with discontinuous basis functions near \( \Gamma \):

\[ V_h^\Gamma = V_h \oplus \{ p_j^\Gamma \}, \quad p_j^\Gamma := \mathcal{R}^* p_j, \quad \mathcal{R}^* = \begin{cases} \mathcal{R}_1 & \text{if } x_j \text{ in } \Omega_2, \\ \mathcal{R}_2 & \text{if } x_j \text{ in } \Omega_1 \end{cases} \]
"Extended" FEM (XFEM)

\[ V_h^\Gamma = \mathcal{R}_1 V_h \oplus \mathcal{R}_2 V_h \quad \iff \quad V_h^\Gamma = V_h \oplus V_h^x \]

Extend \( P_1 \) basis with discontinuous basis functions near \( \Gamma \):

\[ V_h^\Gamma = V_h \oplus \{ p_j^\Gamma \}, \quad p_j^\Gamma := \mathcal{R}^* p_j, \quad \mathcal{R}^* = \left\{ \begin{array}{ll} \mathcal{R}_1 & \text{if } x_j \text{ in } \Omega_2, \\ \mathcal{R}_2 & \text{if } x_j \text{ in } \Omega_1 \end{array} \right. \]

Henry condition not respected.
FE Space is non-conforming!
## Implementation of the Henry condition

<table>
<thead>
<tr>
<th>Nitsche</th>
<th>(Henry condition in a weak sense)</th>
</tr>
</thead>
<tbody>
<tr>
<td>stationary problem ($\Gamma(t) = \Gamma$):</td>
<td></td>
</tr>
<tr>
<td>$-\alpha \Delta u + \mathbf{w} \cdot \nabla u = f$ in $\Omega_1 \cup \Omega_2$,</td>
<td></td>
</tr>
<tr>
<td>$[-\alpha \nabla u \cdot \mathbf{n}] = 0$ on $\Gamma$,</td>
<td></td>
</tr>
<tr>
<td>$[\beta u] = 0$ on $\Gamma$.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Discrete variational formulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a(u, v) := \sum_{i=1,2} \int_{\Omega_i} \beta (\alpha \nabla u \nabla v + \mathbf{w} \cdot \nabla u \ v) , dx$</td>
</tr>
<tr>
<td>+ Nitsche bilinear form $N_h(\cdot, \cdot)$ (Henry-condition in a weak sense)</td>
</tr>
</tbody>
</table>

$$N_h(u, v) = -\int_{\Gamma} \{\alpha \nabla u \cdot \mathbf{n}\} \{\beta v\} \, ds - \int_{\Gamma} \{\alpha \nabla v \cdot \mathbf{n}\} \{\beta u\} \, ds + \bar{\alpha} \lambda h^{-1} \int_{\Gamma} \{\beta u\} \{\beta v\} \, ds$$

$\lambda$: stab. parameter. Nitsche term for **consistency**, **symmetry** and **stability**.
Remarks on Nitsche-XFEM

discrete Nitsche-XFEM problem\(^1,2\):
Find \(u_h \in V^\Gamma_h\), such that
\[
a(u_h, v_h) + N_h(u_h, v_h) = f(v_h) \quad \forall v_h \in V^\Gamma_h.
\]

With standard ideas from the analysis of non-conforming FEM:
\[
\|u - u_h\|_{L^2(\Omega)} \leq c h^{k+1} \|u\|_{H^{k+1}(\Omega_{1,2})} \quad \text{(as in the one-phase case)}
\]

Nitsche-XFEM for convection-diffusion

Nitsche-XFEM and convection stabilization

Nitsche-XFEM with dominant convection with Streamline-Diffusion stabilization\(^3\):

Nitsche-XFEM and convection stabilization

Nitsche-XFEM with dominant convection with Streamline-Diffusion stabilization:\(^3\):

Nitsche-XFEM

SD-Nitsche-XFEM

Treatment of moving interfaces?

Formulation in space-time

Avoid taking differences across the interface!

Divide phases by means of a space-time variational formulation
Space-time finite element space

Divide space-time domain into slabs (discont. FE, \( \Rightarrow \) time stepping scheme)

\[
I_n = (t_{n-1}, t_n], \quad Q^n = \Omega \times I_n, \quad W := \{ v : Q \to \mathbb{R} \mid v|_{Q^n} \in W_n \}
\]
Space-time finite element space

**Space-time FE space (no XFEM)**

Divide space-time domain into slabs (discont. FE, ⇒ time stepping scheme)

\[ I_n = (t_{n-1}, t_n], \quad Q^n = \Omega \times I_n, \quad W := \{ v : Q \to \mathbb{R} \mid v|_{Q^n} \in W_n \} \]

**Finite element space with tensor-product-structure**

\[ W_n := \{ v : Q^n \to \mathbb{R} \mid v(x, t) = \phi_0(x) + t\phi_1(x), \quad \phi_0, \phi_1 \in V_n \}. \]
Enrichment of the space-time FE space:

\[ W_n^{\Gamma} = W_n \oplus W_n^x \]

By design

Good approximation properties

FE space is non-conforming w.r.t. Henry condition
Discrete formulation

components (sketch)

1. space-time interior (consistency to PDE inside the phases)
2. continuity (consistency in time) $\Rightarrow$ upwind in time
3. Henry condition $\Rightarrow$ Nitsche
Discrete formulation

Discrete formulation: Find \( u \in W_{\Gamma}^{\Gamma^*} \), s.t. \( 1 + 2 + 3 = 0 \) \( \forall \ v \in W_{\Gamma}^{\Gamma^*} \)

1. **consistency to PDE within the phases**

\[
\sum_{i=1}^{2} \int_{Q_i^n} \left( \partial_t u_i + \mathbf{w} \cdot \nabla u_i \right) \beta_i v_i + \alpha_i \beta_i \nabla u_i \cdot \nabla v_i - \beta_i f v_i \, dx \, dt
\]

2. **upwind in time**

\[
\int_{\Omega} \beta \left( u_+ (t_{n-1}) - u(t_{n-1}) \right) v_+ (t_{n-1}) \, dx
\]

3. **Nitsche (Henry condition in a weak sense)**

\[
\int_{t_{n-1}}^{t_n} \left( - \int_{\Gamma(t)} \left\{ \alpha \nabla u \cdot \mathbf{n} \right\} [\beta v] \, ds - \int_{\Gamma(t)} \left\{ \alpha \nabla v \cdot \mathbf{n} \right\} [\beta u] \, ds + \bar{\alpha} \lambda h_T^{-1} \int_{\Gamma(t)} [\beta u] [\beta v] \, ds \right) \, dt
\]
Error analysis (linear in space and time)

Error bounds Space-Time Nitsche-XFEM DG\(^4\)

\[ \| (u - u_h)(\cdot, T) \|_{-1} \leq c(h^2 + \Delta t^2). \]

Numerical experiments \((1D)^4\) and \((3D)^6\) (Test cases with piecewise smooth solutions)

\[ \| (u - u_h)(\cdot, T) \|_{L^2} \leq c(h^2 + \Delta t^3). \]

Example two-phase flow
Linear systems

Condition of (space-time) Nitsche-XFEM \( (\kappa (A)) \)

| support of XFEM basis functions arbitrarily small. | \( \implies \) system matrix \( A \) arbitrarily ill-conditioned. |

\[
\kappa (\nabla^{-1} A) \leq c^{-2}, \quad c \neq c (\Gamma)
\]

Proven for stationary case 6.

Optimal preconditioning for stationary case 6.

After transformation \( u \to \beta^{-1} u \):

\[
A \simeq (A_{ss} 0 0 A_{xx}) \simeq (A_{ss} 0 0 D A_{xx}) \simeq (W_{ss} MG 0 0 D A_{xx})
\]

\[
W \kappa (W^{-1} A) \simeq 1 \quad 6 \text{C.L., A. Reusken, 2014, subm. to Num. Math}
\]
Condition of (space-time) Nitsche-XFEM ($\kappa(A)$)

- support of XFEM basis functions arbitrarily small.
- $\implies$ system matrix $A$ arbitrarily ill-conditioned.

Diagonal preconditioning ($\kappa(D_A^{-1}A)$)

- Observation: $\kappa(D_A^{-1}A) \leq ch^{-2}$, $c \neq c(\Gamma)$
- Proven for stationary case\(^6\).

\(^6\)C.L., A. Reusken, 2014, subm. to Num. Math
Linear systems

Condition of (space-time) Nitsche-XFEM ($\kappa(A)$)

- Support of XFEM basis functions arbitrarily small.
- $\implies$ System matrix $A$ arbitrarily ill-conditioned.

Diagonal preconditioning ($\kappa(D^{-1}_A A)$)

- Observation: $\kappa(D^{-1}_A A) \leq ch^{-2}$, $c \neq c(\Gamma)$
- Proven for stationary case \footnote{C.L., A. Reusken, 2014, subm. to Num. Math}.

Optimal preconditioning for stationary case \footnote{C.L., A. Reusken, 2014, subm. to Num. Math}

- After transformation $u \rightarrow \beta^{-1} u$:
  \[ A \approx \begin{pmatrix} A^{ss} & 0 \\ 0 & A^{xx} \end{pmatrix} \approx \begin{pmatrix} A^{ss} & 0 \\ 0 & D_A^{xx} \end{pmatrix} \approx \begin{pmatrix} W^{ss} & 0 \\ 0 & D_A^{xx} \end{pmatrix} \]
  \[ \kappa(W^{-1} A) \approx 1 \]
Two-phase mass transport: solutions are discontinuous across moving interfaces (Henry condition).

Interface is described implicitly (level set method).
Grid is not aligned to the interface.
Two-phase mass transport: solutions are discontinuous across moving interfaces (Henry condition).

Interface is described implicitly (level set method).
Grid is not aligned to the interface.

Extended FE space for the approx. of discontinuities
Nitsche’s method for Henry condition
Space-time formulation for moving interfaces
Two-phase mass transport: solutions are **discontinuous** across **moving interfaces** (Henry condition).

Interface is described **implicitly** (level set method).

Grid is **not aligned** to the interface.

**Extended FE space** for the approx. of discontinuities

**Nitsche’s method** for Henry condition

**Space-time formulation** for moving interfaces

Numerical integration on implicitly described domains with **new decomposition rules in 4D**.

**Preconditioning of Nitsche-XFEM:**

diagonal precond., optimal precond. (Block+MG)
Outlook

Higher order time integration for two-phase Stokes with moving interfaces:
- Jumps in pressure (no time derivative),
- kinks in velocity.

Extended FE space for velocity and pressure

Nitsche’s method for velocity

Space-time formulation for moving interfaces

(Higher order) quadrature strategies for implicit domains.

Linear solvers for (Nitsche)-XFEM:
Space-time discr., Higher order discr., Stokes, ...
Thank you for your attention!

Questions?
Numerical integration on implicit domains

Integration on one element (prism)

Require integrals of the form:

\[
\int_{Q^n_{T,1}} f \, dx \quad \int_{Q^n_{T,2}} f \, dx \quad \int_{\Gamma^*,n_T} f \, dx
\]

Implicit representation of \( \Gamma^* \) (zero level of \( \phi \)), no explicit parametrization

strategy: Find approximation \( \Gamma^*_h \) with explicit parametrization

requires new decomposition rules in four dimensions\(^6\).