Numerical Methods for Two-Phase Flows with Mass Transport

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Problem classes

- Fluid dynamics for Two-Phase (immiscible) incompressible flows: (Navier-Stokes Eqns. + surface tension effects)
- with mass transport (convection-diffusion eqn. + Henry interface condition)
- and surfactant transport (convection-diffusion eqn. on the surface)

applications:
- falling film (gas-liquid)
- rising bubble (liquid-liquid)
- taylor flow (gas-liquid)

Processes at (close to) the interface!
Standard (sharp interface) model for Two-Phase flows

Domains: $\Omega_1 = \Omega_1(t)$ and $\Omega_2 = \Omega_2(t)$

Interface: $\Gamma = \Gamma(t) = \partial \Omega_1 \cap \partial \Omega_2$

$\rho_i$: density in $\Omega_i$

$\mu_i$: viscosity in $\Omega_i$

$\tau$: surface tension coefficient

$D(w) = \nabla w + \nabla w^T$, $\sigma = -p \mathbf{I} + \mu D(w)$

$\kappa$: curvature

Navier-Stokes equations

\[
\begin{cases}
\rho_i(\mathbf{w}_t + (\mathbf{w} \cdot \nabla)\mathbf{w}) = \text{div}(\sigma) + \rho_i \mathbf{g} & \text{in } \Omega_i \\
\text{div} \mathbf{w} = 0 & \text{in } \Omega_i \\
[\sigma \mathbf{n}]_\Gamma = \tau \kappa \mathbf{n} + \nabla_\Gamma \tau, & \mathbf{[w]}_\Gamma = 0
\end{cases}
\]
Two-Phase Hydrodynamic Model

Standard (sharp interface) model for Two-Phase flows

Domains: \( \Omega_1 = \Omega_1(t) \) and \( \Omega_2 = \Omega_2(t) \)

Interface: \( \Gamma = \Gamma(t) = \partial \Omega_1 \cap \partial \Omega_2 \)

\( \rho_i \): density in \( \Omega_i \)
\( \mu_i \): viscosity in \( \Omega_i \)
\( \tau \): surface tension coefficient

\( D(w) = \nabla w + \nabla w^T, \sigma = -p I + \mu D(w) \)

\( \kappa \): curvature

Navier-Stokes equations

\[
\begin{cases}
\rho_i (w_t + (w \cdot \nabla)w) = \text{div} (\sigma) + \rho_i g & \text{in } \Omega_i \\
\text{div } w = 0 & \text{in } \Omega_i \\
\end{cases}
\]

for \( i = 1, 2 \)

\( [\sigma n]_\Gamma = \tau \kappa n + \nabla_\Gamma \tau, \quad [w]_\Gamma = 0. \)

How to identify the interface?
Interface capturing: Level set approach

\( \Gamma(t) = \) zero-level of a scalar function:
the level set function \( \varphi(x, t) \)

\[
\varphi(x, t) = \begin{cases} 
< 0 & \text{for } x \text{ in phase } \Omega_1 \\
> 0 & \text{for } x \text{ in phase } \Omega_2 \\
= 0 & \text{at the interface}
\end{cases}
\]

should be an “approximate signed distance function”.
\[
x(t) \in \Gamma(t) \Rightarrow \varphi(x(t), t) = 0.
\]

**Level set equation**

\[
\varphi_t + \mathbf{w} \cdot \nabla \varphi = 0 \quad \text{in } \Omega
\]
# Level set approach: Pros and Cons

## Eulerian vs. Lagrangian

Level set description allows us to stay in a purely **Eulerian** framework.

### Interface capturing (in contrast to interface tracking (e.g. ALE))

| + | no remeshing |
| + | topology changes (breakups, coalescence) and large deformations |
| − | interface description implicitly (interface is not meshed) |
| − | tracking of evolution of particles at or close to interface |

## Level set (in contrast to VOF)

| + | accuracy of (implicit) interface |
| − | no discrete mass conservation |
| (+) | signed distance property |
| − | signed distance property gets lost (re-initialization) |
## Level set approach: Pros and Cons

### Eulerian vs. Lagrangian

Level set description allows us to stay in a purely **Eulerian** framework.

### Interface capturing (in contrast to interface tracking (e.g. ALE))

- **Pros**
  - no remeshing
  - topology changes (breakups, coalescence) and large deformations
  - interface description implicitly (interface is not meshed)
  - tracking of evolution of particles at or close to interface

- **Cons**
  - no discrete mass conservation

### Level set (in contrast to VOF)

- **Pros**
  - accuracy of (implicit) interface
  - signed distance property

- **Cons**
  - no discrete mass conservation
  - signed distance property gets lost

- **Note**
  - no corr. (1 b.),
  - single corr. (1 b.),
  - single corr. (2 b.),
  - multicom. corr. (2 b.)
Model: Navier-Stokes + level set equation

Navier-Stokes equations coupled with level set equation \((\tau = \text{const})\)

\[
\rho(\varphi) \left( w_t + (w \cdot \nabla)w \right) - \text{div} \left( \mu(\varphi) D(w) \right) + \nabla p = \rho(\varphi) g - \tau \kappa(\varphi) \delta_n \Gamma \nabla
\]

\[
\text{div} \ w = 0
\]

\[
\varphi_t + w \cdot \nabla \varphi = 0
\]

where \(\rho, \mu\) and \(\kappa, \delta, \Gamma, \nabla\) depend on \(\varphi\).
Model: Navier-Stokes + level set equation

Navier-Stokes equations coupled with level set equation \((\tau = \text{const})\)

\[
\begin{align*}
\rho(\varphi) \left( \mathbf{w}_t + (\mathbf{w} \cdot \nabla)\mathbf{w} \right) - \text{div} \left( \mu(\varphi) \mathbf{D}(\mathbf{w}) \right) + \nabla p &= \rho(\varphi) g - \tau \kappa(\varphi) \delta\Gamma \mathbf{n}_\Gamma \\
\text{div} \mathbf{w} &= 0 \\
\varphi_t + \mathbf{w} \cdot \nabla \varphi &= 0
\end{align*}
\]

where \(\rho, \mu\) and \(\kappa, \delta\Gamma, \mathbf{n}_\Gamma\) depend on \(\varphi\).

Additional equations

Surfactant transport (on the interface):

\[
s_t + \mathbf{w} \cdot \nabla \Gamma s - \mu \Gamma \Delta \Gamma s = f_\Gamma \quad \text{on } \Gamma
\]

Mass transport (discontinuity across the interface):

\[
\begin{align*}
u_t + \mathbf{w} \cdot \nabla u - \alpha \Delta u &= f \quad \text{in } \Omega_i \\
\left[ \alpha \frac{\partial u}{\partial n} \right] &= 0, \quad \left[ \beta u \right] = 0 \quad \text{on } \Gamma
\end{align*}
\]
Discretization background

Starting point

- Adaptive tetrahedral mesh for $\Omega = \Omega_1 \cup \Omega_2$
- Conforming finite elements:
  - P2-P1 Taylor-Hood elements (continuous)
  - P2 for level set (continuous)
  - P1 for mass/surfactants transport (continuous)
- Method of lines time integration (implicit euler, etc..)
Numerical Challenges

Key problems

- Multiscale phenomena close to the interface.
- Highly nonlinear couplings between $w$, $\varphi$, $f_\Gamma$, $c$, $c_\Gamma$.
- Interesting modeling aspects, e.g.: $\tau = \tau(c, c_\Gamma)$ (YZ) or coalescence (JB)
- Accurate resolution of unknown interface. Treatment of the level set equation (EL), volume correction (JB)
- Treatment of surface tension force (Laplace-Beltrami discretization)
- Treatment of discontinuous pressure
- Treatment of kinks in velocity (SG)
- Coupling of flow + interface dynamics + transport equations.
- Discretization of transport equation with (moving) discontinuities (CL)
- Discretization of transport equation on (moving) interface (JG) + (XZ)
- Efficiency/robustness of iterative solvers.
- High complexity: parallel solvers needed, (SG) + (PE)
- Higher order time integration (space-time formulation) (PE)
Interface force balance

**Interface condition**

We have the condition:

\[
[\sigma n]_\Gamma = [(\mu D(w) + pl)n]_\Gamma = \tau \kappa n \quad (\nabla_\Gamma \tau)
\]

Typically:

\[
[p]_\Gamma \neq 0
\]

Non-aligned mesh + **standard polynomial** \( Q_h \)

\( \Rightarrow \) approximation quality reduces to

\[
\inf_{p_h \in Q_h} \| p - p_h \|_{L^2} \leq O(\sqrt{h})
\]
Handling Discontinuities: Domain-wise cont. ansatz

\[ Q^\Gamma_h := Q_h(\tilde{\Omega}_1) \cdot H^\Gamma \oplus Q_h(\tilde{\Omega}_2) \cdot (1 - H^\Gamma) \]
Handling Discontinuities: Add. ansatz functions (XFEM)

Remedy

Extend $P_1$ FE basis with discontinuous basis functions near $\Gamma$:

$$p_j^\Gamma := p_j \left( H_\Gamma(x) - H_\Gamma(x_j) \right), \quad H_\Gamma = \begin{cases} 1 & \text{in } \Omega_1 \\ 0 & \text{in } \Omega_2 \end{cases}$$

and use $Q_h^\Gamma = Q_h \oplus \{ p_j^\Gamma \}$
Handling (Pressure) Discontinuities: XFEM

Remarks

- In practice: $\Gamma_h$ instead of $\Gamma$.
- $\dim(Q_\Gamma^h)$ depends on $\Gamma$.
- New basis functions can have very small supports.
- Other applications:
  - [Belytschko (1999 ->)]: elasticity,
  - [Hansbo (2002 ->)]: interf. probl.,
  - Two-Phase Mass Transport

P2-P1-Taylor-Hood + XFEM for pressure

Enrichment: we use a P1X finite element space for the pressure space.

(+): pressure approximation is optimal: $O(h^2)$ in $L^2$-norm.
(-): no LBB-stability result for velocity-pressure pair $(V_h, Q_\Gamma^h)$ any more

Kinks in velocity field also need a "kink-version" XFEM!
Key components in DROPS:

- Hybrid level set technique for interface capturing
- Adaptive multilevel triangulations (tetrahedra) + Finite Elements (not aligned to the interface)
- Special quadrature techniques (discontinuous $\mu, \rho$)
- Discretization of localized force term $f_f$: Laplace-Beltrami
- Finite element space for discontinuous pressure: XFEM
- Special iterative solvers: robustness w.r.t. $h, \Delta t$, jumps in $\rho, (\mu)$
- MPI based parallelization (Institute for Scientific Computing)
- Surfactant transport equation: Interface FE method
- Mass transport equation: Nitsche-XFEM method
Some DROPS movies
Two-Phase mass transport: A movie
Two-Phase Mass Transport

Mass Transport Problem statement

Situation at the interface

\[ \Gamma(t), \Omega_1(t), \Omega_2(t) \]

discontinuous conc. 

\[ u_1 / u_2 = \beta_2 / \beta_1 \]

disc. normal derivative 

\[ \alpha_1 \partial u_1 / \partial n_1 = \alpha_2 \partial u_2 / \partial n_2 \]

sharp layers

moving interface
Situation at the interface

\[ \Omega_1 \quad \Gamma \quad \Omega_2 \]

discontinuous conc.
\[ \frac{u_1}{u_2} = \frac{\beta_2}{\beta_1} \]
Situation at the interface

- Discontinuous concentration:
  \[ u_1 / u_2 = \beta_2 / \beta_1 \]

- Discontinuous normal derivative:
  \[ \alpha_1 \frac{\partial u_1}{\partial n_1} = \alpha_2 \frac{\partial u_2}{\partial n_2} \]
Situation at the interface

Discontinuous concentration:
\[ u_1/u_2 = \beta_2/\beta_1 \]

Discontinuous normal derivative:
\[ \alpha_1 \frac{\partial u_1}{\partial n_1} = \alpha_2 \frac{\partial u_2}{\partial n_2} \]

Sharp layers
Two-Phase Mass Transport

Mass Transport Problem statement

Situation at the interface

![Diagram showing two phases with a moving interface \( \Gamma(t) \), discontinuous concentration \( u_1/u_2 = \beta_2/\beta_1 \), discontinuous normal derivative, sharp layers, and moving interface.]

- discontinuous conc. \( u_1/u_2 = \beta_2/\beta_1 \)
- disc. normal derivative \( \alpha_1 \frac{\partial u_1}{\partial n_1} = \alpha_2 \frac{\partial u_2}{\partial n_2} \)
- sharp layers
- moving interface \( \Gamma(t) \)
Mass transport

Mass transport equation

\[
\frac{\partial u}{\partial t} + w \cdot \nabla u - \alpha \Delta u = 0 \quad \text{in} \, \Omega_1 \cup \Omega_2,
\]

\[
[-\alpha \nabla u] \cdot n = 0 \quad \text{on} \, \Gamma,
\]

\[
[\beta u] = 0 \quad \text{on} \, \Gamma.
\]

\[
\mathcal{V} \cdot n = w \cdot n \quad \text{on} \, \Gamma.
\]

\[
\text{div}(w) = 0 \quad \text{in} \, \Omega
\]

\(u\): concentration,
\(\alpha\): piecewise constant diffusion coefficients,
\(\beta\): piecewise constant Henry coefficients,
\(w\): convection velocity (from Navier Stokes)
\(\mathcal{V}\): the interface velocity
Henry condition: discontinuity in \(u\).
Numerical Aspects

Mass transport equation

\[
\frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u - \alpha \Delta u = 0 \quad \text{in } \Omega_1(t) \cup \Omega_2(t),
\]

\[
[-\alpha \nabla u] \cdot \mathbf{n} = 0 \quad \text{on } \Gamma(t),
\]

\[
[\beta u] = 0 \quad \text{on } \Gamma(t).
\]
Numerical Aspects

Mass transport equation

\[
\frac{\partial u}{\partial t} + w \cdot \nabla u - \alpha \Delta u = 0 \quad \text{in} \ \Omega_1(t) \cup \Omega_2(t),
\]

\[
[-\alpha \nabla u] \cdot n = 0 \quad \text{on} \ \Gamma(t),
\]

\[
\llbracket \beta u \rrbracket = 0 \quad \text{on} \ \Gamma(t).
\]

Numerical Challenges

▶ Level set to capture the interface
  ⇒ Interface is not aligned with the mesh (might depend on time)
▶ concentration has discontinuities (approximation)
▶ time integration for (non-matched) moving interfaces
▶ problem is typically highly convection dominated (stability)
Numerical Aspects

Numerical Challenges

- Level set to capture the interface
  ⇒ Interface is not aligned with the mesh (might depend on time)
- Concentration has discontinuities (approximation)
- Time integration for (non-matched) moving interfaces
- Problem is typically highly convection dominated (stability)

Numerical Approaches

- Extended Finite Element space (XFEM)
- Space-time formulation on each time slab
- Nitsche-type technique to enforce Henry’s law in a weak sense
- (Space-time Streamline Diffusion) Stabilization
Anisotropic Spaces; \( Q = Q_1 \cup Q_2 \)

\[
V_\beta = \{ u \in L^2(Q) \mid u_i \in H^{1,0}(Q_i), \; i = 1, 2, \; u|_{\partial \Omega} = 0, \; [\beta u]_{\Gamma^*} = 0 \}
\]

\[
W_\beta = \{ v \in V_\beta \mid \frac{\partial v}{\partial t} \in H^{1,0}_0(Q)' \}.
\]
Space-time weak formulation II

Well-posed weak formulation [Gross/Reusken 11]

Determine $u \in W_\beta$ with $u(\cdot, 0) = 0$ such that

$$\frac{\partial u}{\partial t}(v) - \int_Q u \mathbf{w} \cdot \nabla v \, dx \, dt + \sum_{i=1}^{2} \int_{Q_i} \alpha_i \nabla u_i \cdot \nabla v \, dx \, dt = \int_Q f v \, dx \, dt$$

for all $v \in H_{0,0}^1(Q) \neq V_\beta$

Remarks:

- Space-time (n+1 dimensional) formulation
- Trial functions are discontinuous across $\Gamma_*$, test functions are not
- Condition $[\beta u]_{\Gamma} = 0$ essential condition in space $W_\beta$
Nitsche-DG-XFEM discretization

Space-time FE

\( I_n = (t_{n-1}, t_n], \ Q^n = \Omega \times I_n. \quad V_n : \text{standard FE space on } \Omega. \)

\[
W_n := \left\{ v : Q^n \to \mathbb{R} \mid v(x, t) = \phi_0(x) + t\phi_1(x), \ \phi_0, \phi_1 \in V_n \right\}
\]

\[
W := \left\{ v : Q \to \mathbb{R} \mid v|_{Q^n} \in W_n \right\} \quad \text{(space-time FE)}.
\]
Approximating discontinuities

Space-time FE $\Rightarrow$ Space-time XFEM

$$Q_{i}^{n} := \bigcup_{t \in I_n} \Omega_{i}(t), \quad R_{i}^{n} : \text{restriction to } Q_{i}^{n}$$

$$W_{n}^{\Gamma} := R_{1}^{n} W_{n} \oplus R_{2}^{n} W_{n}, \quad W^{\Gamma*} := \{v : Q \rightarrow \mathbb{R} \mid v|_{Q^n} \in W_{n}^{\Gamma}\}$$
Two-Phase Mass Transport  Space-time approach

Bilinear forms (within time slab $Q^n$)

**Conforming part (strong form + part. int. on diffusion)**

$$a^n(u, v) = \sum_{i=1}^{2} \int_{Q^n_i} \left( \frac{\partial u_i}{\partial t} + w \cdot \nabla u_i \right) \beta_i v_i + \alpha_i \beta_i \nabla u_i \cdot \nabla v_i \, dx \, dt$$
Bilinear forms (within time slab $Q^n$)

**Conforming part (strong form + part. int. on diffusion)**

$$a^n(u, v) = \sum_{i=1}^{2} \int_{Q^n_i} \left( \frac{\partial u_i}{\partial t} + w \cdot \nabla u_i \right) \beta_i v_i + \alpha_i \beta_i \nabla u_i \cdot \nabla v_i \, dx \, dt$$

**Discontinuous Galerkin Upwind w.r.t. time:**

$$d^n(u, v) = \int_{\Omega} \beta(\cdot, t_n)[u]^{n-1} v^{n-1} \, dt$$
Bilinear forms (within time slab $Q^n$) I

**Conforming part (strong form + part. int. on diffusion)**

$$a^n(u, v) = \sum_{i=1}^{2} \int_{Q^n_i} \left( \frac{\partial u_i}{\partial t} + \mathbf{w} \cdot \nabla u_i \right) \beta_i v_i + \alpha_i \beta_i \nabla u_i \cdot \nabla v_i \, dx \, dt$$

**Discontinuous Galerkin Upwind w.r.t. time:**

$$d^n(u, v) = \int_{\Omega} \beta(\cdot, t_n)[u]^{n-1} v^{n-1} \, dt$$

**Henry interface condition**

$$W_n^\Gamma \not\subset W_\beta \quad \text{(non-conformity)}$$

$$\Rightarrow \text{enforce condition}[\![\beta u]\!]_{\Gamma^*} = 0 \text{ only weakly} \quad \text{(Nitsche)}$$
Bilinear forms (within time slab $Q^n$) II

Nitsche method for Henry condition:

$$- \int_{Q^n} \beta \text{div} (\alpha \nabla u) v \, dx$$
Bilinear forms (within time slab $Q^n$) II

Nitsche method for Henry condition:

$$- \int_{Q^n} \beta \text{div}(\alpha \nabla u) v \, dx = \int_{Q^n} \alpha \beta \nabla u \nabla v \, dx - \int_{\partial Q^n} \left( \begin{array}{c} \alpha \nabla u \\ 0 \end{array} \right) \cdot (\mathbf{n}^*) \, v \, ds$$
Bilinear forms (within time slab $Q^n$) II

Nitsche method for Henry condition:

$$- \int_{Q^n} \beta \text{div}(\alpha \nabla u) v \, dx = \int_{Q^n} \alpha \beta \nabla u \nabla v \, dx - \int_{\partial Q^n} \begin{pmatrix} \alpha \nabla u \\ 0 \end{pmatrix} \cdot (n^*) v \, ds$$

$$= \ldots - \int_{\Gamma^*_n} \nu \alpha \nabla u \cdot n \beta v \, ds$$

$$\nu = \frac{1}{\sqrt{1 + (w \cdot n)^2}}: \int_{t_{n-1}}^{t_n} \int_{\Gamma_n} f \, ds \, dt = \int_{\Gamma^*_n} \nu f \, ds,$$
Bilinear forms (within time slab $Q^n$) II

Nitsche method for Henry condition:

$$- \int_{Q^n} \beta \text{div}(\alpha \nabla u) v \, dx = \int_{Q^n} \alpha \beta \nabla u \nabla v \, dx - \int_{\partial Q^n} \left( \frac{\alpha \nabla u}{0} \right) \cdot (n^*) \, v \, ds$$

$$= \ldots - \int_{\Gamma^*_n} \nu \alpha \nabla u \cdot n \beta v \, ds$$

$$\rightarrow \ldots - \sum_{i=1}^{2} \int_{\Gamma^*_n} \nu \{ \alpha \nabla u \cdot n \} \Gamma^*_n [\beta v]_{\Gamma^*_n} \, ds$$

$$= \ldots - \int_{\Gamma^*_n} \nu \{ \alpha \nabla u \cdot n \} \Gamma^*_n [\beta v]_{\Gamma^*_n} \, ds$$

with $\{ \cdot \}_{\Gamma^*_n}$ suitable volume weighted average.

$$\nu = \frac{1}{\sqrt{1 + (w \cdot n)^2}}: \int_{t^n}^{t_{n-1}} \int_{\Gamma_n} f \, ds \, dt = \int_{\Gamma^*_n} \nu f \, ds,$$
Bilinear forms (within time slab $Q^n$) II

Nitsche method for Henry condition:

\[- \int_{Q^n} \beta \text{div}(\alpha \nabla u) \nu \, dx = \int_{Q^n} \alpha \beta \nabla u \nabla \nu \, dx - \int_{\partial Q^n} \left( \frac{\alpha \nabla u}{0} \right) \cdot (n^*) \nu \, ds \]

\[= \ldots - \int_{\Gamma^*_n} \nu \alpha \nabla u \cdot n \beta \nu \, ds \]

\[\rightarrow \ldots - \sum_{i=1}^{2} \int_{\Gamma^*_n} \nu \{\alpha \nabla u \cdot n\} \Gamma^*_n [\beta \nu]_{\Gamma^*_n} \, ds \]

\[= \ldots - \int_{\Gamma^*_n} \nu \{\alpha \nabla u \cdot n\} \Gamma^*_n [\beta \nu]_{\Gamma^*_n} ds \quad \text{(A)} \]

\[\rightarrow - \int_{\Gamma^*_n} \nu \{\alpha \nabla \nu \cdot n\} \Gamma^*_n [\beta u]_{\Gamma^*_n} ds \quad \text{(B)} + \lambda h_n^{-1} \int_{\Gamma^*_n} \nu [\beta u]_{\Gamma^*_n} [\beta \nu]_{\Gamma^*_n} ds, \quad \text{(C)} \]

with $\{\cdot\}_{\Gamma^*_n}$ suitable volume weighted average. $\lambda > 0$: stabilization parameter and $\nu = 1/\sqrt{1 + (w \cdot n)^2}$: $\int_{t^{n-1}}^{t^n} \int_{\Gamma_n} f \, ds \, dt = \int_{\Gamma^*_n} \nu f \, ds$.

$N^n_{\Gamma^*_n}(c, \nu) := \text{(A)} + \text{(B)} + \text{(C)}$
Nitsche-DG-XFEM variational problem

**global bilinearforms**

\[ a(u, v) = \sum_{n=1}^{N} a^n(u, v), \]  
\[ d(u, v), \quad N_{\Gamma^*}(u, v). \]

**Discrete problem**

Determine \( U \in W_{\Gamma^*} \) such that

\[ B(U, V) = f(V) \quad \text{for all} \quad V \in W_{\Gamma^*}, \]
\[ B(U, V) := a(U, V) + d(U, V) + N_{\Gamma^*}(U, V). \]
Nitsche-DG-XFEM variational problem

**global bilinearforms**

\[ a(u, v) = \sum_{n=1}^{N} a^n(u, v), \quad \text{similarly:} \quad d(u, v), \quad N_{\Gamma^*}(u, v). \]

**Discrete problem**

Determine \( U \in W^{\Gamma^*} \) such that

\[
B(U, V) = f(V) \quad \text{for all} \quad V \in W^{\Gamma^*},
\]

\[
\]

Still allows for time stepping, i.e. solving time slab by time slab!
Error analysis (results)

**Theorem**

*Error analysis for linear (space+time) FE*

\[ \| (u - U)(\cdot, t_N) \|_{L^2(\Omega^N)} \leq c(h^2 + \Delta t^2). \]
Error analysis (results)

Theorem

Error analysis for linear (space+time) FE

\[ \| (u - U)(\cdot, t_N) \|_{L^2(\Omega^N)} \leq c(h^2 + \Delta t^2). \]

Remark:

for standard space-time DG [V. Thomee] (no Nitsche, no XFEM):

\[ \| (u - U)(\cdot, t_N) \|_{L^2(\Omega^N)} \leq c(h^2 + \Delta t^3) \]

Concept of V. Thomee needs tensor product decomposition of the spaces which we don’t have for moving interfaces.
Numerical experiment

Numerical example in (1+1)D

Diffusion dominates, periodic boundary conditions, artificial source terms
Discretization error (temporal convergence)

This indicates: \( \| (U - u)(\cdot, t_N) \|_{L^2(\Omega)} \sim \Delta t^3 \) if \( h \) sufficiently small.
Discretization error (spatial convergence)

This indicates: \( \|(U - u)(\cdot, t_N)\|_{L^2(\Omega)} \sim h^2 \) if \( \Delta t \) sufficiently small.
Two-Phase Mass Transport Space-time approach

Numerical example (continued): Non-planar interface

This indicates: \( \|(U - u)(\cdot, t_N)\|_{L^2(\Omega)} \sim \Delta t^3 \Delta t^2 \) if \( h \) sufficiently small.

With sufficiently fine quadrature we reobtain \( \|(U - u)(\cdot, t_N)\|_{L^2(\Omega)} \sim \Delta t^3 \).
Remark on 3+1 dimensions

**Quadrature in (3+1)D**

- Triangulation consists of prism-4 elements
- Decompose prism-4 into four pentatopes (simplex-4)
- Decompose cut-pentatopes into uncut pentatopes (approximation of $\Gamma_*$)
- 4D quadrature on uncut pentatopes

(!) For realistic problems quadrature limits convergence to $O(\Delta t^2)$

**Implementation and numerical results**

- First implementation in 3+1 dimensions exists
- At least second order convergence is validated
- For simple examples even third order is observed
## Conclusion

### Interface capturing and consequences

- Level-set approach, Eulerian frame
- Non-matching interface needs special care for space discretization
- Moving discontinuities needs special care for time discretization

### Discretization concepts

- (Domain-)piecewise continuous approximation + XFEM
- Nitsche(-XFEM) for interface conditions
- Space-time FEM with (P1) Discontinuous Galerkin in time.
  
  \[
  \text{space-time integrals} \implies \text{Composite quadrature in (n+1) D}
  \]
Conclusion

Interface capturing and consequences

- Level-set approach, Eulerian frame
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Discretization concepts

- (Domain-)piecewise continuous approximation + XFEM
- Nitsche(-XFEM) for interface conditions
- Space-time FEM with (P1) Discontinuous Galerkin in time.
  
  \[ \text{space-time integrals} \Rightarrow \text{Composite quadrature in } (n+1)D \]
Decomposition into simplices

The reference element can be decomposed into simplices

- \((1 + 1)\): \(\hat{Q}\) is a square → 2 triangles
- \((2 + 1)\): \(\hat{Q}\) is a (regular) prism → 3 tetrahedra
- \((3 + 1)\): \(\hat{Q}\) is a (regular) prism-4 → 4 pentatopes

The reference prism-4 \(\hat{Q}\)

![Diagram of a reference prism-4 element with vertices labeled X, Y, Z, and T.](image)
### Decomposition into simplices

The reference element can be decomposed into simplices

- \((1 + 1): \hat{Q}\) is a square \(\rightarrow 2\) triangles
- \((2 + 1): \hat{Q}\) is a (regular) prism \(\rightarrow 3\) tetrahedra
- \((3 + 1): \hat{Q}\) is a (regular) prism-4 \(\rightarrow 4\) pentatopes

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The reference prism-4 \(\hat{Q}\) and it’s decomposition
Decomposition into simplices

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The reference prism-4 \( \hat{Q} \) and it’s decomposition

Consider the quadrature problem on \((n+1)\)-simplex!
Slicing the pentatope

(Non-degenerates) Case 1:

<table>
<thead>
<tr>
<th>cut pentatope</th>
<th>(irregular) prism-4 + pentatope</th>
</tr>
</thead>
<tbody>
<tr>
<td>↓ (decomposition)</td>
<td>4 pentatopes + 1 pentatope</td>
</tr>
</tbody>
</table>

interface

1 tetrahedra
Slicing the pentatope

(Non-degenerated) Case 2:

- Cut pentatope
  - (irregular) hypertriangle
  - (decomposition)
  - 6 pentatopes
- Interface
  - Prism-3 \(\rightarrow\) 3 tetrahedra

- (irregular) prism-4
  - 4 pentatopes
Slicing the pentatope

(Non-degerenated) Case 2:

Cut pentatope

(irregular) hypertriangle + (irregular) prism-4

↓ (decomposition)

6 pentatopes + 4 pentatopes

Interface

prism-3 → 3 tetrahedra

Step 4: Decomposition into one-phase (n+1)-simplices and n-simplices!
(Non-degenerated) Case 2:

<table>
<thead>
<tr>
<th>cut pentatope</th>
<th>(irregular) hypertriangle \downarrow \text{(decomposition)} \uparrow 6 pentatopes</th>
<th>(irregular) prism-4 \downarrow 4 pentatopes</th>
</tr>
</thead>
<tbody>
<tr>
<td>interface</td>
<td>prism-3 \rightarrow 3 tetrahedra</td>
<td></td>
</tr>
</tbody>
</table>

Step 4: Decomposition into one-phase (n+1)-simplices and n-simplices!
Decomposition of the hypertriangle into 6 pentatopes