Streamline Diffusion Stabilization for mass transport in two phase incompressible flows

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Transport Processes at Fluidic Interfaces -
From Experimental to Mathematical Analysis, Aachen,
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Transport processes at fluidic interfaces
DFG SPP 1506

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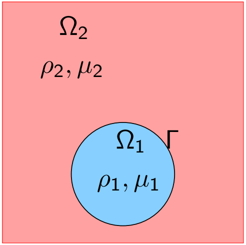
RWTH AACHEN UNIVERSITY

Overview

Overview

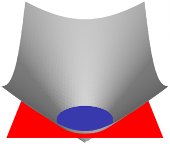
Background: Two phase flow (Navier-Stokes + level set)



$\Gamma(t)$ = zero-level of a scalar function:

the level set function $\varphi(x,t)$

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



Navier-Stokes equations coupled with level set equation

$$\begin{aligned} \rho(\varphi)\left(\frac{\partial}{\partial t}\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) - \operatorname{div}\left(\mu(\varphi)\,\mathbf{D}(\mathbf{u})\right) + \nabla p &= \rho(\varphi)\,g - \tau\,\kappa(\varphi)\,\delta_\Gamma \mathbf{n}_\Gamma \\ \operatorname{div}\mathbf{u} &= 0 \\ \varphi_t + \mathbf{u}\cdot\nabla\varphi &= 0 \end{aligned}$$

where ρ, μ and $\kappa, \delta_\Gamma, \mathbf{n}_\Gamma$ depend on φ

Mass transport

Mass transport equation

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c - \alpha \Delta c = 0 \qquad \text{in } \Omega_1 \cup \Omega_2,$$
$$[\![-\alpha \nabla c]\!] \cdot \mathbf{n} = 0 \qquad \text{on } \Gamma,$$
$$[\![\beta c]\!] = 0 \qquad \text{on } \Gamma.$$

$$\mathcal{V} \cdot \mathbf{n} = \mathbf{u} \cdot \mathbf{n} \qquad \text{on } \Gamma.$$
$$\mathrm{div}(\mathbf{u}) = 0 \qquad \text{in } \Omega$$

c: concentration,
α: piecewise constant diffusion coefficients,
β: piecewise constant Henry coefficients,
$\mathbf{u}$: convection velocity (from Navier Stokes)
$\mathcal{V}$: the interface velocity
Henry condition: discontinuity in c.

Numerical Aspects

Mass transport equation

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Numerical Challenges

- Level set to capture the interface
  $\Rightarrow$ Interface is not aligned with the mesh (might depend on time)
- concentration has discontinuities (approximation)
- problem is typically highly convection dominated (stability)
- time integration for moving interfaces

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Numerical Approaches

- Extended Finite Element space (XFEM)
- Nitsche-type technique to enforce Henry's law in a weak sense
- Streamline Diffusion Stabilization

Overview

Handling Discontinuities

Interface condition

We have the condition:

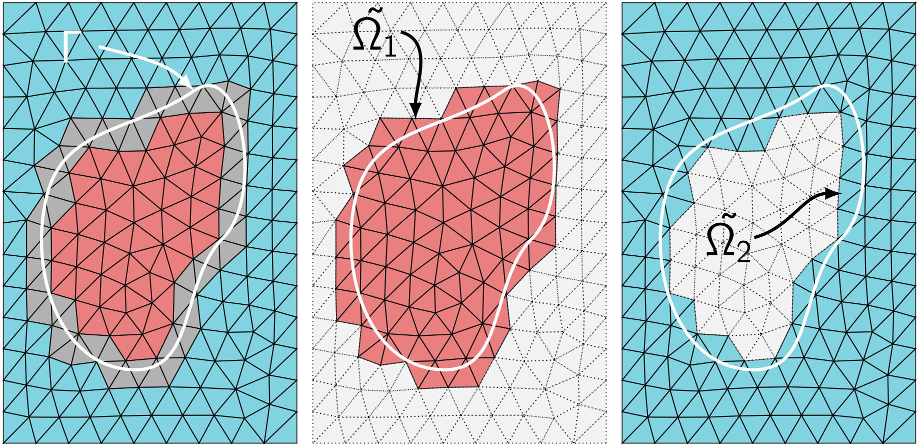
$$[\![\beta c]\!] = 0 \quad \text{at the interface } \Gamma$$

Non-aligned mesh + standard polynomial FE space V_h
⇒ approximation quality reduces to

$$inf_{c_h \in V_h} \|c - c_h\|_{L^2} \leq \mathcal{O}(\sqrt{h})$$

Handling Discontinuities: Domain-wise cont. ansatz

$$V_h^\Gamma := V_h(\tilde{\Omega}_1) \cdot H^\Gamma \oplus V_h(\tilde{\Omega}_2) \cdot (1 - H^\Gamma)$$



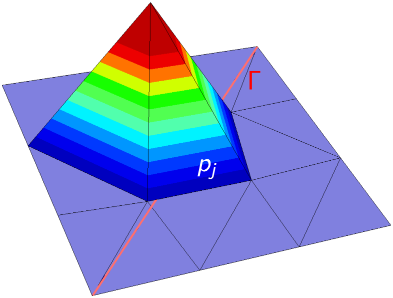
Handling Discontinuities: Add. ansatz functions (XFEM)

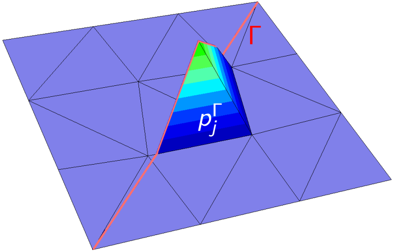
Remedy

Extend P_1 FE basis with discontinuous basis functions near Γ:

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

and use $V_h^\Gamma = V_h \oplus \{p_j^\Gamma\}$

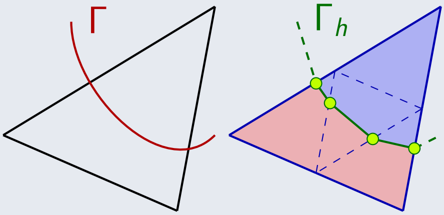




Handling Discontinuities: XFEM

Remarks

- In practice: Γ_h instead of Γ.
- $\dim(V_h^\Gamma)$ depends on Γ.
- New basis functions can have very small supports.
- other applications:
  [Belytschko (1999 ->)]: elasticity,
  [Hansbo (2002 ->)]: interf. probl.,
  [Reusken, Groß(2007 ->)]:
  twophase (Navier-) Stokes



XFEM for approximation

Enrichment: we use a P1X finite element space. This provides discontinuous ansatz functions, which **do not satisfy the interface condition**.

(+) approximation is optimal: $\mathcal{O}(h^2)$ in L^2-norm.

(-) discrete functions in V_h^Γ do not fulfill Henry's interface condition

Handling the non-conformity

Shifting interface condition: from f.e. space ...

The finite element space P1X does not incorporate the interface condition. Thus the variational formulation has to enforce it!

Handling the non-conformity: Nitsche XFEM

Shifting interface condition: from f.e. space to var. formulation

The finite element space P1X does not incorporate the interface condition. Thus the variational formulation has to enforce it! $\Longrightarrow$ Nitsche's method

Nitsche-XFEM formulation (no convection $\mathbf{u} = 0$)

Find $c_h \in V_h$, s.t.

(testing $-\alpha\Delta c_h$ with βv_h and applying part. int. on Ω_i)

$$A(c_h, v_h) \quad := \quad \sum_i \left\{ \int_{\Omega_i} \alpha\beta \nabla c_h \, \nabla v_h \, dx \right\} - \int_\Gamma [\![\alpha\partial_{\mathbf{n}} c_h \;\, \beta v_h]\!] \, dx$$

$$\frac{\partial}{\partial t}(\beta c_h, v_h)_{L^2} \quad + \quad A_h(c_h, v_h) = 0 \quad \forall \; v_h \in V_h$$

Handling the non-conformity: Nitsche XFEM

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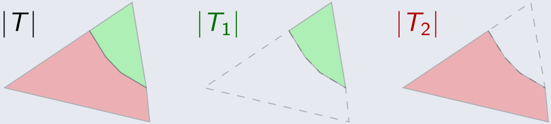
manipulating

$$-\int_\Gamma [\![\alpha \partial_{\mathbf{n}} c \;\, \beta v]\!] \, dx \quad \xrightarrow{[\![\beta c]\!]=0} \quad -\int_\Gamma \{\!\{\alpha \partial_{\mathbf{n}} c\}\!\} [\![\beta v]\!] \, dx$$

with $\{\!\{u\}\!\} := \kappa_1 u_1 + \kappa_2 u_2$,

$\kappa_i = \frac{|T_i|}{|T_1| + |T_2|}$, $\kappa_1 + \kappa_2 = 1$



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$$\frac{\partial}{\partial t}(\beta c_h, v_h)_{L^2} + A_h(c_h, v_h) = 0 \quad \forall\, v_h \in V_h$$

manipulating , symmetrizing

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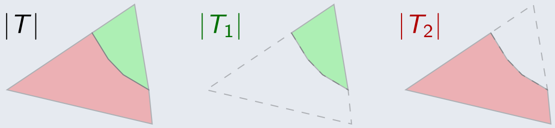

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$$\frac{\partial}{\partial t}(\beta c_h, v_h)_{L^2} + A_h(c_h, v_h) = 0 \quad \forall \, v_h \in V_h$$

manipulating , symmetrizing , stabilizing ($\lambda_T > 0$).

with $\{\!\{u\}\!\} := \kappa_1 u_1 + \kappa_2 u_2$,

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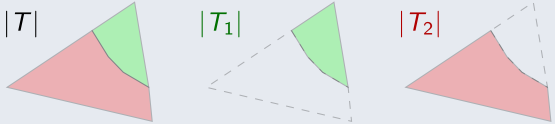

Handling large convection

Status

- Nitsche XFEM works fine for diffusion dominated problems.
- For high convection we get oscillations.
- Same situation as Standard FEM in one phase.

Handling large convection: SD Stabilization

Status

- Nitsche XFEM works fine for diffusion dominated problems.
- For high convection we get oscillations.
- Same situation as Standard FEM in one phase.

$\Rightarrow$ Stabilize in a similar way as in one phase!

Adding streamline diffusion consistently

Consistently add $$+\sum_{T\in\mathcal{T}_h}\int \mathrm{scal}\cdot\mathrm{res}\cdot(\mathbf{u}\cdot\nabla v)$$

This gives $$+\sum_{T^*\in\mathcal{T}_h^*}\int_{T^*}\beta\gamma_T\left(\partial_t c+\mathbf{u}\cdot\nabla c-\mathrm{div}(\alpha\nabla c)\right)\ (\mathbf{u}\cdot\nabla v)\ dx$$

which contains additional numerical diffusion in streamline direction!

Overview

How to choose γ_T and λ_T?

Discrete energy norm

$$\|v\|^2 := \bar{\alpha}|\sqrt{\beta}\, v|^2_{1,\Omega_1\cup\Omega_2} + \|\sqrt{\beta\gamma_T}\,\mathbf{u}\cdot\nabla v\|_0^2 + \lambda\bar{\alpha}\|[\![\beta v]\!]\|^2_{\frac{1}{2},h,\Gamma}$$

Choice of γ_T (convection stabilization)

Standard Streamline Diffusion choice (no direct dependence on domain):

$$\gamma_T \sim \begin{cases} h_T/\|\mathbf{u}\|_{\infty,T} & \text{if} \quad P_h^T > 1 \\ 0 & \text{if} \quad P_h^T \le 1 \end{cases} \qquad \text{with } P_h^T := \frac{1}{2}\|\mathbf{u}\|_{\infty,T} h_T/\bar{\alpha}$$

Choice of λ_T (interface stabilization)

$$\lambda_T = \begin{cases} c\|\mathbf{u}\|_{\infty,T} h_T/\bar{\alpha} & \text{if} \quad P_h^T \ge 1 \\ c & \text{if} \quad P_h^T < 1, \end{cases}$$

How to choose γ_T and λ_T?

Discrete energy norm

$$\|v\|^2 := \bar{\alpha}|\sqrt{\beta}\, v|^2_{1,\Omega_1\cup\Omega_2} + \|\sqrt{\beta\gamma_T}\,\mathbf{u}\cdot\nabla v\|_0^2 + \lambda\bar{\alpha}\|[\![\beta v]\!]\|^2_{\frac{1}{2},h,\Gamma}$$

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Choice of λ_T (interface stabilization)

$$\ldots + \sum_{T\in\mathcal{T}_h} const \cdot \left\{ \begin{array}{ccc} \|\mathbf{u}\|_{\infty,T} & \text{if} & P_h^T \geq 1 \\ \bar{\alpha}/h_T & \text{if} & P_h^T \leq 1 \end{array} \right\} \int_{\Gamma\cap T} [\![\beta c_h]\!][\![\beta v_h]\!]\, dx$$

Results for SD-Nitsche-XFEM

Bilinear forms

A_h	:	diffusion + Nitsche
C	:	convection
S	:	SD stabilization integrals

Properties of $A_h + C + S$

- $A_h + C + S$ is stable (ellipticity w.r.t. discrete energy norm $\|\!|\cdot|\!\|$)
- $A_h + C + S$ is consistent
- control due to stabilization:
  - Control on streamline derivative (Streamline Diffusion)
  - Control on interface condition (Nitsche)
- optimal convergence, i.e.
  - $\mathcal{O}(h^{1\frac{1}{2}})$ in L^2 norm in convection dominated regime
  - $\mathcal{O}(h^2)$ in L^2 norm in diffusion dominated regime

Overview

Problem description

Presentation of the method

Parameter choice, theoretical results

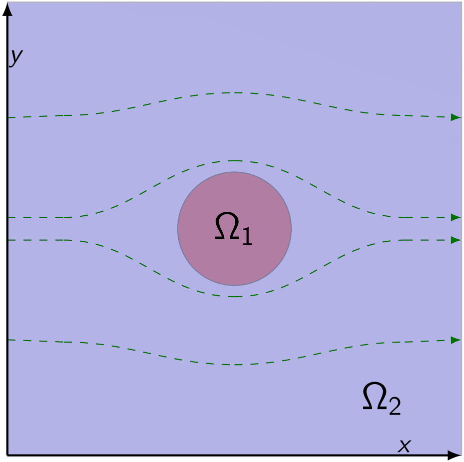
Numerical Example

Conclusion and Outlook

Setup: Flow around a cylinder

domain

- $\Omega = [0,2] \times [0,2] \times [0,1]$,
  $\Omega_1 := \left\{ (x-1)^2 + (y-1)^2 < R^2 \right\}$,
  $R = 0.25$



Setup: Flow around a cylinder

stationary interface + velocity

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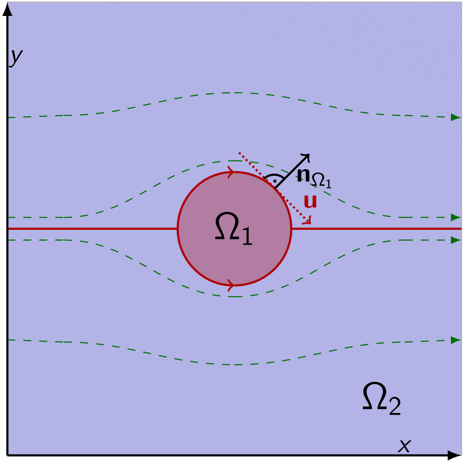

Setup: Flow around a cylinder

non-matching grid, bound. cond.

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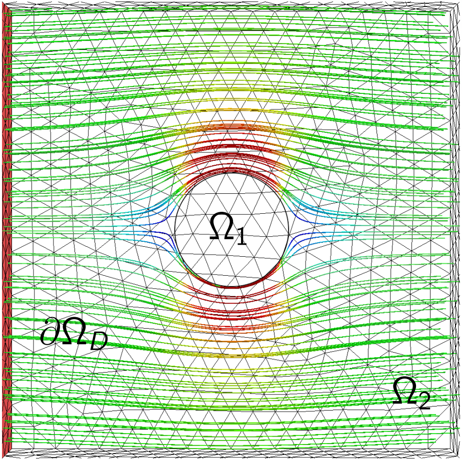
- $\Gamma \neq \Gamma(t)$, $\mathbf{u} \neq \mathbf{u}(t)$
- non-matching grid, $h \approx 0.1$
- Dirichlet b.c. at inflow $x = 0$
  natural b.c. else



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Henry jump condition

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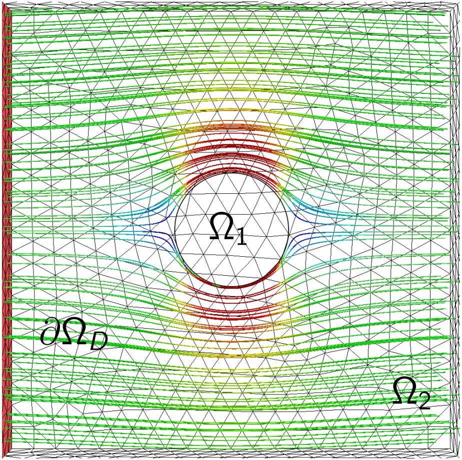
- Dirichlet b.c. at inflow $x = 0$
  natural b.c. else
- $(\beta_1, \beta_2) = (3, 1)$
- $(\alpha_1, \alpha_2) = (1, 2) \cdot 10^{-4}$



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convection domination

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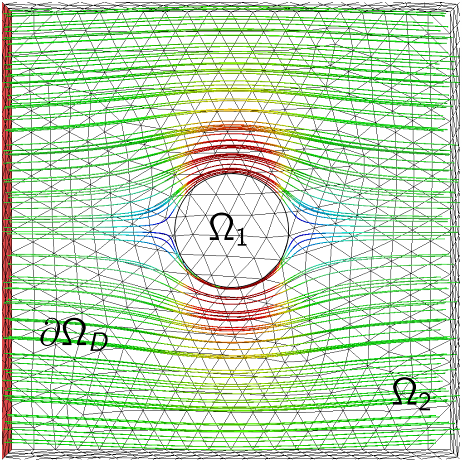

Setup: Flow around a cylinder

parabolic boundary layers

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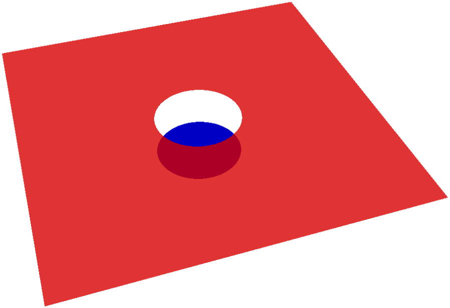
- $(\beta_1, \beta_2) = (3, 1)$
- $(\alpha_1, \alpha_2) = (1, 2)\cdot 10^{-4}$, $|\mathbf{u}| = (0, \sim \mathcal{O}(1)) \Rightarrow P_D \sim (0, \mathbf{10^3})$
- non-fitting initial conditions $c\big|_{t=0} = (0, 0.05)$



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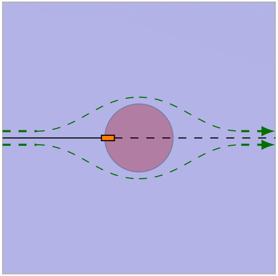
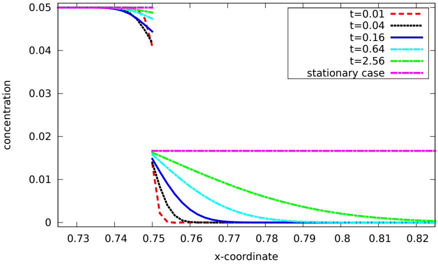
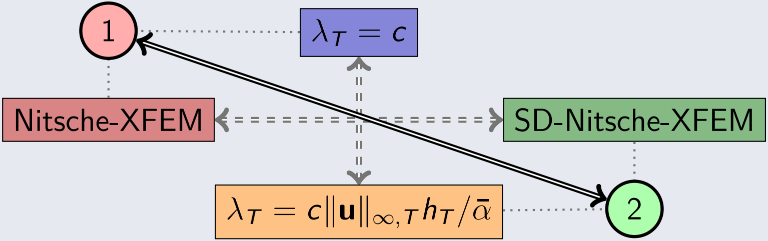
  $c\big|_{t=0} = (0, 0.05)$
  $\Rightarrow$ *parabolic* boundary layers
  $(O(\sqrt{\alpha t}))$





Compared methods

Comparing volume terms (↔) and Nitsche penalty scaling (↕)

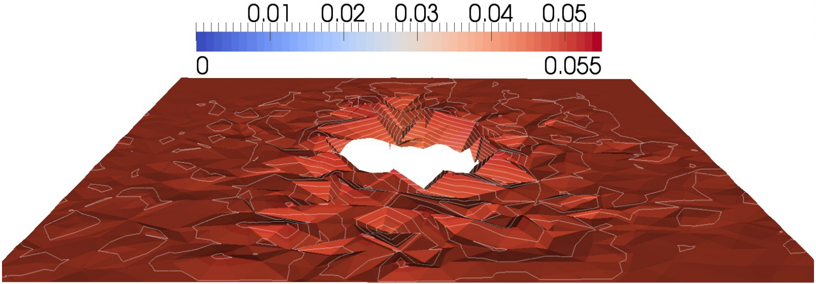


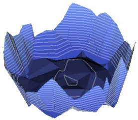
Time integration

Methods can be combined with the method of lines as the interface is stationary. Here, a simple implicit Euler, i.e. $\delta_t c = \frac{1}{\Delta t}(u^{n+1} - u^n)$, with very small time steps ($\Delta t = 10^{-4}$) is used.

Nitsche-XFEM, $\lambda_T = c$

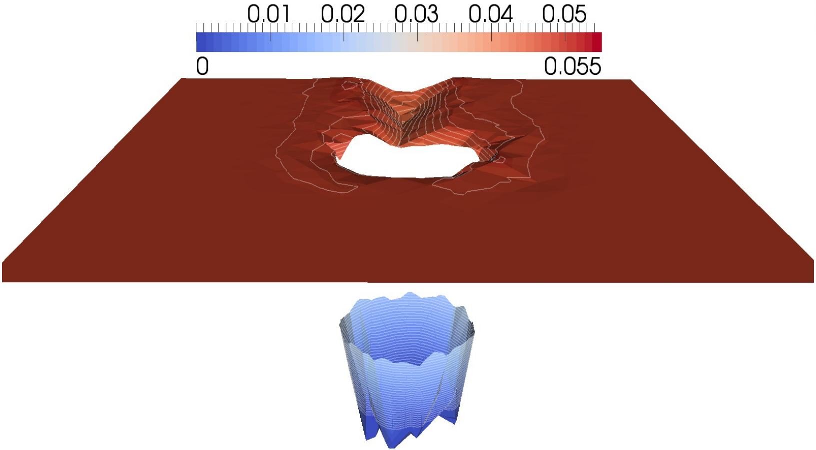
1





$$\|[\![\beta c_h]\!]\|_{L^2(\Gamma_h)}\Big|_{t=1} \approx 4.5 \cdot 10^{-2}$$

SD-Nitsche-XFEM, 2 $\lambda_T = c\|\mathbf{u}\|_{\infty,T} h_T / \bar{\alpha}$



$$\|[\![\beta c_h]\!]\|_{L^2(\Gamma_h)}\Big|_{t=1} \approx 2.3 \cdot 10^{-3}$$

Overview

Conclusion and Outlook

Main Ingredients

- Discontinuous Approximations due to XFEM
- Nitsche to deal with interf. cond. and non-conforming disc. space
- Streamline Diffusion Stabilization to allow for convection dominated flows
- Adaptations to Nitsche penalty parameter λ_T

Next steps

- Time integration for moving interfaces
  - Space time finite element formulation for diffusion-dominated regime
  - Space time Streamline Diffusion Stabilization formulation
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Thanks to:

- the German Science Foundation (DFG), for the money
- **you**, for your attention!

Error estimates for SD-Nitsche-XFEM

error estimates

$$|||v|||^2 := \bar{\alpha}|\sqrt{\beta}\,v|^2_{1,\Omega_1\cup\Omega_2} + \|\sqrt{\beta\gamma_T}\,\mathbf{u}\cdot\nabla v\|^2_0 + \lambda\bar{\alpha}\|[\![\beta v]\!]\|^2_{\frac{1}{2},h,\Gamma}$$

$$|||c - c_h||| \leq c(\sqrt{\bar{\alpha}} + \sqrt{|\mathbf{u}|_\infty h})h\|c\|_{2,\Omega_1\cup\Omega_2}$$

Diffusion dominates

$$|c - c_h|_{1,\Omega_1\cup\Omega_2} \leq c \cdot h\|c\|_{2,\Omega_1\cup\Omega_2}$$

$$\|[\![c_h]\!]\|_{\frac{1}{2},h,\Gamma} \leq c \cdot h^{\frac{3}{2}}\|c\|_{2,\Omega_1\cup\Omega_2}$$

Convection dominates

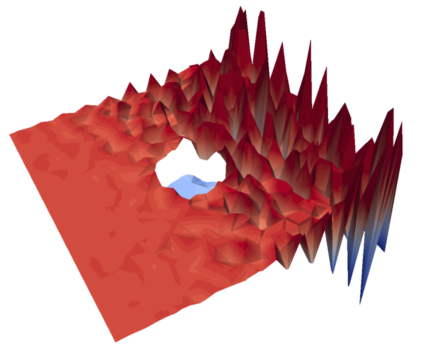
$$\|\mathbf{u}\cdot\nabla(c - c_h)\|_{L^2(\Omega)} \leq c \cdot h\|c\|_{2,\Omega_1\cup\Omega_2}$$

$$\|[\![c_h]\!]\|_{\frac{1}{2},h,\Gamma} \leq c \cdot h^{\frac{3}{2}}\|c\|_{2,\Omega_1\cup\Omega_2}$$

Exponential layers

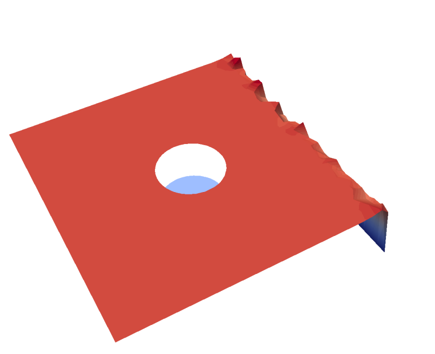
$c|_{x=2} = 0$, i.e. "non-fitting" Dirichlet b.c. $\Rightarrow$ exp. layers.
$P_D \approx 100$

Nitsche-XFEM



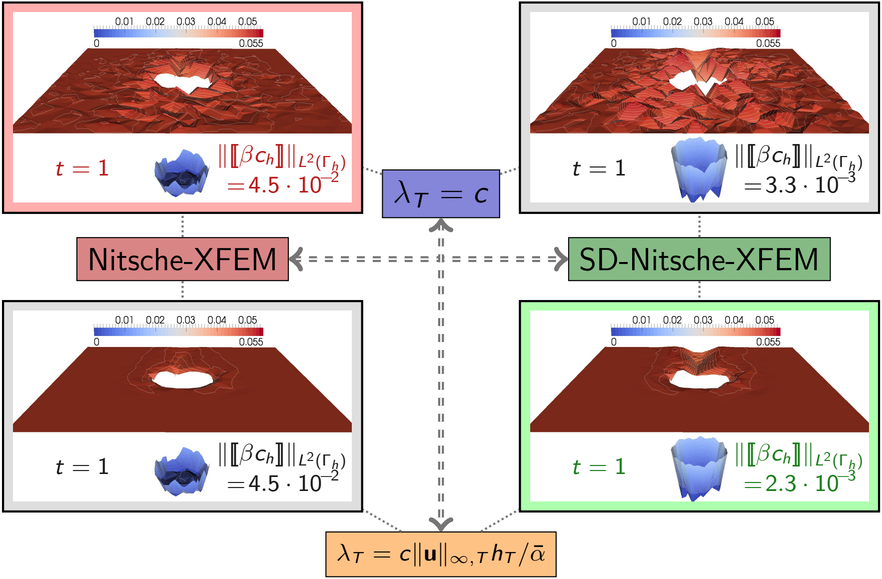
$||[\![\beta c_h]\!]||_{L^2(\Gamma_h)}\big|_{t=1} = 6.0 \cdot 10^{-3}$

SD-Nitsche-XFEM



$||[\![\beta c_h]\!]||_{L^2(\Gamma_h)}\big|_{t=1} = 3.1 \cdot 10^{-9}$

Comparison to intermediate methods



Results for Nitsche-XFEM (pure diffusion)

Properties of A_h(pure diffusion)

One can show with $\lambda_T = const(\mathcal{O}(1))$ suff. large

- A_h is stable (ellipticity on V_h w.r.t. a “disc. energy norm”)
- A_h is consistent
- semi-discretization of

$$\frac{\partial}{\partial t}c - \Delta c = f \quad + \text{interf.} + \text{init.} + \text{bound. cond.}$$

gives optimal convergence (2nd order) [Reusken,Nguyen].

Results for Nitsche-XFEM (diffusion dominates)

$$C(c_h, v_h) = \sum_i \left\{ \int_{\Omega_i} \beta \ \mathbf{u} \cdot \nabla c_h \, v_h \, dx \right\}$$

Properties of $A_h + C$(diffusion dominates)

One can show with $\lambda_T = const(\mathcal{O}(1))$ suff. large

- $A_h + C$ is stable (ellipticity on V_h w.r.t. a "disc. energy norm")
- $A_h + C$ is consistent
- semi-discretization of

$$\frac{\partial}{\partial t} c + \mathbf{u} \cdot \nabla c - \Delta c = f \quad + \text{interf.} + \text{init.} + \text{bound. cond.}$$

gives optimal convergence (2nd order) [Reusken,Nguyen].