Streamline Diffusion Stabilization for mass transport in two phase incompressible flows

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Overview

Problem description

Presentation of the method

Parameter choice, theoretical results

Numerical Example

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

Γ(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

\[
\rho(\varphi) \left( \frac{\partial}{\partial t} \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) - \text{div} \left( \mu(\varphi) \mathbf{D} (\mathbf{u}) \right) + \nabla p = \rho(\varphi) \mathbf{g} - \tau \kappa(\varphi) \delta \mathbf{n} \Gamma \\
\text{div} \mathbf{u} = 0 \\
\varphi_t + \mathbf{u} \cdot \nabla \varphi = 0
\]

where \( \rho, \mu \) and \( \kappa, \delta \Gamma, \mathbf{n} \Gamma \) depend on \( \varphi \)
Mass transport equation

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

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

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

\[
\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega
\]

\[
\mathbf{V} \cdot \mathbf{n} = \mathbf{u} \cdot \mathbf{n} \quad \text{on } \Gamma.
\]

\[c: \text{ concentration},\]
\[\alpha: \text{ piecewise constant diffusion coefficients},\]
\[\beta: \text{ piecewise constant Henry coefficients},\]
\[\mathbf{u}: \text{ convection velocity (from Navier Stokes)}\]
\[\mathbf{V}: \text{ the interface velocity}\]

Henry condition: discontinuity in \(c\).
Numerical Aspects

Mass transport equation

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

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
## Numerical Aspects

### Mass transport equation

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

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

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

### Numerical Challenges

- Level set to capture the interface
  - 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

### Numerical Approaches

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

**Interface condition**

We have the condition:

\[ \llbracket \beta c \rrbracket = 0 \quad \text{at the interface } \Gamma \]

Non-aligned mesh + **standard polynomial** FE space \( V_h \)

⇒ approximation quality reduces to

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

\[ V_h^\Gamma := V_h(\tilde\Omega_1) \cdot H^\Gamma \oplus V_h(\tilde\Omega_2) \cdot (1 - H^\Gamma) \]
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 $V^\Gamma_h = V_h \oplus \{ p_j^\Gamma \}$
Handling Discontinuities: XFEM

Remarks

- In practice: \( \Gamma_h \) instead of \( \Gamma \).
- \( \text{dim}(V_{\Gamma h}) \) depends on \( \Gamma \).
- 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: \( O(h^2) \) in \( L^2 \)-norm.

(-) discrete functions in \( V_{\Gamma h} \) 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! ⇒ Nitsche’s method

Nitsche-XFEM formulation (no convection \( u = 0 \))

Find \( c_h \in V_h \), s.t.

\[
\text{(testing } - \alpha \Delta c_h \text{ with } \beta v_h \text{ and applying part. int. on } \Omega_i) \]

\[
A(c_h, v_h) := \sum_i \left\{ \int_{\Omega_i} \alpha \beta \nabla c_h \nabla v_h \, dx \right\} - \int_{\Gamma} [\alpha n \cdot c_h \beta v_h] \, dx
\]

\[
\frac{\partial}{\partial t} (\beta c_h, v_h)_{L^2} + A_h(c_h, v_h) = 0 \quad \forall \ v_h \in V_h
\]
Handling the non-conformity: Nitsche XFEM

Nitsche-XFEM formulation (no convection $u = 0$)

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

$$A(c_h, v_h) := \sum_i \left\{ \int_{\Omega_i} \alpha \beta \nabla c_h \nabla v_h \, dx \right\} - \int_\Gamma \{ \alpha \partial_n c_h \} [\beta v_h] \, dx$$

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

manipulating

$$- \int \{\alpha \partial_n c \, \beta v\} \, dx \quad [\beta c] = 0 \quad \Rightarrow \quad - \int \{\alpha \partial_n c\} [\beta v] \, dx$$

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

$$\kappa_i = \frac{|T_i|}{|T_1| + |T_2|}, \quad \kappa_1 + \kappa_2 = 1$$
Handling the non-conformity: Nitsche XFEM

Nitsche-XFEM formulation (no convection \( u = 0 \))

Find \( c_h \in V_h \), s.t.

\[
A(c_h, v_h) := \sum_i \left\{ \int_{\Omega_i} \alpha \beta \nabla c_h \nabla v_h \, dx \right\} - \int_{\Gamma} \{\{\alpha \partial_n c_h\}\} \{\beta v_h\} \, dx \\
- \int_{\Gamma} \{\{\alpha \partial_n v_h\}\} \{\beta c_h\} \, dx
\]

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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

with \( \{\{u\}\} := \kappa_1 u_1 + \kappa_2 u_2 \), \( |T| \)

\[
\kappa_i = \frac{|T_i|}{|T_1| + |T_2|}, \quad \kappa_1 + \kappa_2 = 1
\]

| \( T_1 \) | | \( T_2 \) |
Handling the non-conformity: Nitsche XFEM

Nitsche-XFEM formulation (no convection \( u = 0 \))

Find \( c_h \in V_h \), s.t.

\[
A_h(c_h, v_h) := \sum_i \left\{ \int_{\Omega_i} \alpha \beta \nabla c_h \nabla v_h \, dx \right\} - \int_{\Gamma} \left\{ \alpha \partial_n c_h \right\} \left[ \left[ \beta v_h \right] \right] \, dx \\
- \int_{\Gamma} \left\{ \alpha \partial_n v_h \right\} \left[ \left[ \beta c_h \right] \right] \, dx + \int_{\Gamma} \frac{\alpha \lambda T_h}{h_T} \left[ \beta c_h \right] \left[ \beta v_h \right] \, dx
\]

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

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

with \( \left\{ u \right\} := \kappa_1 u_1 + \kappa_2 u_2 \),

\[
\kappa_i = \frac{|T_i|}{|T_1| + |T_2|}, \quad \kappa_1 + \kappa_2 = 1
\]

\( T \) \quad \( T_1 \) \quad \( T_2 \)
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.

Adding streamline diffusion consistently:

\[ \sum_{T \in T_h} \int_T \text{scal} \cdot \text{res} \cdot (u \cdot \nabla v) \]

This gives:

\[ \sum_{T^{\ast} \in T^{\ast}_h} \int_{T^{\ast}} \beta \gamma \left( \partial_t c + u \cdot \nabla c - \text{div} (\alpha \nabla c) \right) (u \cdot \nabla v) \, dx \]

which contains additional numerical diffusion in streamline direction!
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.

⇒ Stabilize in a similar way as in one phase!

Adding streamline diffusion consistently

Consistently add \[ + \sum_{T \in \mathcal{T}_h} \int_{T} \text{scal} \cdot \text{res} \cdot (u \cdot \nabla v) \]

This gives \[ + \sum_{T^* \in \mathcal{T}^*_h} \int_{T^*} \beta \gamma_T (\partial_t c + u \cdot \nabla c - \text{div}(\alpha \nabla c)) \ (u \cdot \nabla v) \ dx \]

which contains additional numerical diffusion in streamline direction!
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How to choose $\gamma_T$ and $\lambda_T$?

**Discrete energy norm**

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

**Choice of $\gamma_T$ (convection stabilization)**

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

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

**Choice of $\lambda_T$ (interface stabilization)**

$$\lambda_T = \begin{cases} 
    c \|u\|_{\infty,T} h_T/\bar{\alpha} & \text{if } P_h^T \geq 1 \\
    c & \text{if } P_h^T < 1,
\end{cases}$$
How to choose $\gamma_T$ and $\lambda_T$?

**Discrete energy norm**

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

**Choice of $\gamma_T$ (convection stabilization)**

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

\[ \gamma_T \sim \begin{cases} h_T/\|u\|_{\infty,T} & \text{if } P_h^T > 1 \\ 0 & \text{if } P_h^T \leq 1 \end{cases} \]

with $P_h^T := \frac{1}{2} \|u\|_{\infty,T} h_T/\bar{\alpha}$

**Choice of $\lambda_T$ (interface stabilization)**

\[ \ldots + \sum_{T \in \mathcal{T}_h} \text{const} \cdot \begin{cases} \|u\|_{\infty,T} & \text{if } P_h^T \geq 1 \\ \bar{\alpha}/h_T & \text{if } P_h^T \leq 1 \end{cases} \int_{\Gamma \cap T} [\beta c_h] [\beta v_h] \, dx \]
## Results for SD-Nitsche-XFEM

### Bilinear forms

<table>
<thead>
<tr>
<th>$A_h$</th>
<th>diffusion + Nitsche</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C$</td>
<td>convection</td>
</tr>
<tr>
<td>$S$</td>
<td>SD stabilization integrals</td>
</tr>
</tbody>
</table>

### 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.
  - $\mathcal{O}(h^{1.5})$ in $L^2$ norm in convection dominated regime
  - $\mathcal{O}(h^2)$ in $L^2$ norm in diffusion dominated regime
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Setup: Flow around a cylinder

**domain**

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

Setup: Flow around a cylinder

stationary interface + velocity

- $\Omega = [0, 2] \times [0, 2] \times [0, 1]$, 
  $\Omega_1 := \{(x - 1)^2 + (y - 1)^2 < R^2\}$, 
  $R = 0.25$
- $\Gamma \neq \Gamma(t), u \neq u(t)$
Setup: Flow around a cylinder

- **non-matching grid, bound. cond.**
  - $\Omega = [0, 2] \times [0, 2] \times [0, 1]$,
  - $\Omega_1 := \{(x-1)^2 + (y-1)^2 < R^2\}$, $R = 0.25$
  - $\Gamma \neq \Gamma(t)$, $u \neq u(t)$
  - non-matching grid, $h \approx 0.1$
  - Dirichlet b.c. at inflow $x = 0$
  - natural b.c. else
Setup: Flow around a cylinder

**Henry jump condition**

- $\Omega = [0, 2] \times [0, 2] \times [0, 1]$, $\Omega_1 := \{(x-1)^2 + (y-1)^2 < R^2\}$, $R = 0.25$
- $\Gamma \neq \Gamma(t), \ u \neq u(t)$
- non-matching grid, $h \approx 0.1$
- Dirichlet b.c. at inflow $x = 0$
  - natural b.c. else
- $(\beta_1, \beta_2) = (3, 1)$
- $(\alpha_1, \alpha_2) = (1, 2) \cdot 10^{-4}$
Setup: Flow around a cylinder

convection domination

- \( \Omega = [0, 2] \times [0, 2] \times [0, 1] \),
  \( \Omega_1 := \{(x-1)^2 + (y-1)^2 < R^2\} \),
  \( R = 0.25 \)
- \( \Gamma \neq \Gamma(t), \; u \neq u(t) \)
- non-matching grid, \( h \approx 0.1 \)
- Dirichlet b.c. at inflow \( x = 0 \)
  natural b.c. else
- \((\beta_1, \beta_2) = (3, 1)\)
- \((\alpha_1, \alpha_2) = (1, 2) \cdot 10^{-4},\)
  \(|u| = (0, \sim O(1)) \Rightarrow P_D \sim (0, 10^3)\)
**Setup: Flow around a cylinder**

**parabolic boundary layers**

- \( \Omega = [0, 2] \times [0, 2] \times [0, 1] \)
- \( \Omega_1 := \{(x-1)^2 + (y-1)^2 < R^2\} \)
- \( R = 0.25 \)
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- Dirichlet b.c. at inflow \( x = 0 \)
- natural b.c. else
- \( (\beta_1, \beta_2) = (3, 1) \)
- \( (\alpha_1, \alpha_2) = (1, 2) \cdot 10^{-4} \)
- \( |u| = (0, \sim \mathcal{O}(1)) \Rightarrow P_D \sim (0, 10^3) \)
- non-fitting initial conditions
  \( c \big|_{t=0} = (0, 0.05) \)
**Numerical Example**

**Setup: Flow around a cylinder**

- **parabolic boundary layers**
  - $\Omega = [0, 2] \times [0, 2] \times [0, 1]$,
  - $\Omega_1 := \{(x - 1)^2 + (y - 1)^2 < R^2\}$,
  - $R = 0.25$
  - $\Gamma \neq \Gamma(t), \ u \neq u(t)$
  - non-matching grid, $h \approx 0.1$
  - Dirichlet b.c. at inflow $x = 0$
    - natural b.c. else
  - $(\beta_1, \beta_2) = (3, 1)$
  - $(\alpha_1, \alpha_2) = (1, 2) \cdot 10^{-4}$,
    - $|u| = (0, \sim \mathcal{O}(1)) \Rightarrow P_D \sim (0, 10^3)$
  - non-fitting initial conditions
    - $c|_{t=0} = (0, 0.05)$
    - $\Rightarrow$ parabolic boundary layers
      - $\mathcal{O}(\sqrt{\alpha t})$
Numerical Example

Compared methods

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

\[ \lambda_T = c \]

Nitsche-XFEM

SD-Nitsche-XFEM

\[ \lambda_T = c \| \mathbf{u} \|_{\infty, T} h_T / \bar{\alpha} \]

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,

\[ \lambda_T = c \]

\[ \left\| \left[ \beta c_h \right] \right\|_{L^2(\Gamma_h)} \bigg|_{t=1} \approx 4.5 \cdot 10^{-2} \]
SD-Nitsche-XFEM,

\[ \lambda_T = c \| u \|_\infty, T h_T / \bar{\alpha} \]

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

Next steps

- Time integration for moving interfaces
  - Space time finite element formulation for diffusion-dominated regime
  - Space time Streamline Diffusion Stabilization formulation
- Application to realistic two-phase mass transport problems

Thanks to:
- the German Science Foundation (DFG), for the money
- you, for your attention!
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Error estimates for SD-Nitsche-XFEM

**error estimates**

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

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

**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. ⇒ exp. layers.

\[ P_D \approx 100 \]

Nitsche-XFEM

SD-Nitsche-XFEM

\[ \left\| \left[ \beta c_h \right] \right\|_{L^2(\Gamma_h)} \bigg|_{t=1} = 6.0 \cdot 10^{-3} \]

\[ \left\| \left[ \beta c_h \right] \right\|_{L^2(\Gamma_h)} \bigg|_{t=1} = 3.1 \cdot 10^{-9} \]
Comparison to intermediate methods

\[ t = 1 \]
\[ \| \beta_{ch} \|_{L^2(\Gamma_h)} = 4.5 \cdot 10^{-2} \]

\[ t = 1 \]
\[ \| \beta_{ch} \|_{L^2(\Gamma_h)} = 4.5 \cdot 10^{-2} \]

\[ \lambda_T = c \parallel u \parallel_{\infty, T h_T / \bar{\alpha}} \]

Nitsche-XFEM

SD-Nitsche-XFEM
Results for Nitsche-XFEM (pure diffusion)

Properties of $A_h$ (pure diffusion)

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

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

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

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 \( \lambda_T = \text{const}(\mathcal{O}(1)) \) 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

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

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