

Teoría de elementos finitos y su implementación

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Lecture 3: Convection-Diffusion-Reaction Equations

Stationary case:

$$\begin{aligned}\sigma u + (\beta \cdot \nabla)u - \epsilon \Delta u &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \partial\Omega\end{aligned}$$

- Reaction term $\sigma \in L^\infty(\Omega)$
- Convection field $\beta \in L^\infty(\Omega)^d$, $\operatorname{div} \beta \in L^\infty(\Omega)$
- Diffusion $\epsilon \in \mathbb{R}_{>0}$

For existence and uniqueness:

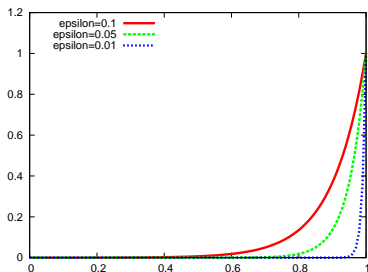
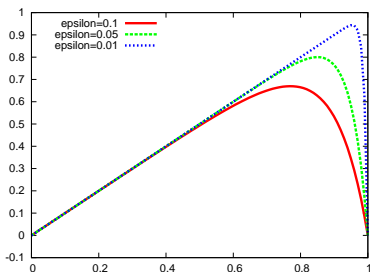
$$\sigma - \frac{1}{2} \operatorname{div} \beta \geq c \geq 0 \quad \text{a.e. in } \Omega$$

e.g., $\sigma \geq 0$ and $\operatorname{div} \beta = 0$.

3.1 Convection-Diffusion Equation in 1D

In interval $I = (0, 1)$ with diffusion parameter $\epsilon > 0$:

$$\begin{aligned} -\epsilon u'' + u' &= f \quad x \in I \\ u(0) &= u_0, \quad u(1) = u_1 \end{aligned}$$



Examples for $\epsilon \in \{0.1, 0.05, 0.01\}$ with $f = 1$ (left) and $f = 0$ (right):

- Boundary layers for $\epsilon \rightarrow 0$

Central differences for 1D convection-diffusion

- Central difference quotient for 1. derivatives (of 2. order) and 2. derivatives (of 2. order):

$$\begin{aligned}u'(x_i) &\approx \frac{1}{2h}(u_{i+1} - u_{i-1}) \\u''(x_i) &\approx \frac{1}{h^2}(u_{i+1} - 2u_i + u_{i-1}).\end{aligned}$$

- Linear system for approximate solution with $u_0 = u_N = 0$:

$$\begin{pmatrix} a & & & c & & \\ & \ddots & & & & \\ b & & \ddots & & & \\ & \ddots & & \ddots & & \\ & & \ddots & & \ddots & \\ & & & \ddots & & c \\ & & & & b & a \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ \vdots \\ \vdots \\ u_{N-1} \end{pmatrix} = F$$

with $a = 2\epsilon/h^2$, and $b = -\epsilon/h^2 - 1/(2h)$, and $c = -\epsilon/h^2 + 1/(2h)$.

- Diagonal elements a are always positive

$$a = \frac{2\epsilon}{h^2} > 0$$

- Off-diagonal elements b, c are negative for $h < 2\epsilon$:

$$b = -\frac{\epsilon}{h^2} - \frac{1}{2h} \leq c$$

$$c = -\frac{\epsilon}{h^2} + \frac{1}{2h} < 0$$

- But for $h > 2\epsilon$ we obtain positive off-diagonal elements:

$$c = -\frac{\epsilon}{h^2} + \frac{1}{2h} > 0$$

→ No M-matrix, no Discrete Maximum Principle (DMP) !

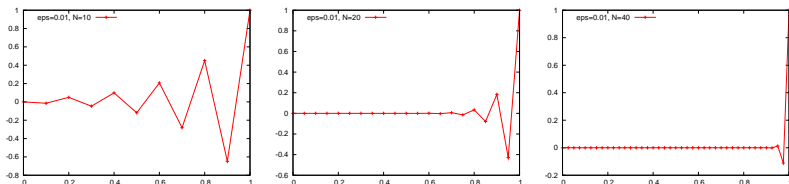
Good and bad news for central differences

Good properties:

- Formally of 2. order (in L^2 -norm).
- DMP if $h < 2\epsilon$

Bad properties:

- No DMP if $h \geq 2\epsilon$
- The violation of a DMP leads to strong numerical artefacts:
- In many practical applications $h < 2\epsilon$ is unfeasible, because often $\epsilon \sim 10^{-8} - 10^{-5}$.



$\epsilon = 0.01$ and $N = 10, 20, 40$ (from left to right)

Alternatives for FDM:

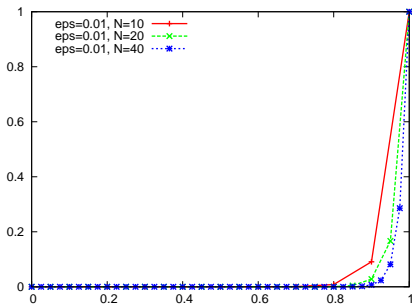
- Artificial diffusion
- Upwinding

Artificial diffusion

Idea: Ensure $\epsilon \geq 2h$ by changing to an augmented diffusion coefficient:

$$\epsilon_h := \max(2h, \epsilon)$$

Use ϵ_h instead of ϵ in the discrete equation.



Drawback: Very diffusive and only of 1. order in L^2 -norm.

Upwinding in 1D

Idea: Use one-sided difference quotient for the first derivatives instead of a central difference quotient:

$$u'(x_i) \approx \frac{1}{h}(U_i - U_{i-1})$$

Resulting linear system:

$$bU_{i-1} + aU_i + cU_{i+1} = f_i$$

With positive diagonal elements a and negative off-diagonal elements b, c :

$$\begin{aligned} a &= \frac{2\epsilon}{h^2} + \frac{1}{h} > 0 \\ b &= -\frac{\epsilon}{h^2} - \frac{1}{h} < 0 \\ c &= -\frac{\epsilon}{h^2} < 0 \end{aligned}$$

M-matrix

Upwinding in 1D (cont'd)

More general convection-diffusion-reaction equation with varying coefficients:

$$-\epsilon u'' + bu' + cu = f \quad x \in I$$

The difference quotient depends on the direction of the convective part:

$$u'(x_i) \approx \begin{cases} h^{-1}(U_i - U_{i-1}) & \text{if } b(x_i) > 0 \\ h^{-1}(U_{i+1} - U_i) & \text{if } b(x_i) < 0 \end{cases}$$

Leads to DMP in 1D.

3.2 Scalar convection-diffusion problems in multi-dimensions

- Convection-diffusion problem:

$$\begin{aligned}\sigma u + (\beta \cdot \nabla)u - \epsilon \Delta u &= f \\ u &= 0 \quad \text{on } \partial\Omega\end{aligned}$$

- Variational formulation in $V = H_0^1(\Omega)$:

$$u \in V : \quad A(u, \phi) = \langle f, \phi \rangle \quad \forall \phi \in V$$

with bilinear form:

$$A(u, \phi) := (\sigma u + (\beta \cdot \nabla)u, \phi) + (\epsilon \nabla u, \nabla \phi)$$

- Existence and uniqueness of solutions due to Lax-Milgram.

Existence and uniqueness for scalar convection-diffusion problem

Theorem

Let $\sigma, \nabla \cdot \beta \in L^\infty(\Omega)$ and $\epsilon > 0$. If there exists a constant c_0 , s.t.

$$\sigma - \frac{1}{2} \operatorname{div} \beta \geq c_0 \geq 0 \quad \text{a.e. in } \Omega$$

the variational formulation features for each $f \in L^2(\Omega)$ a unique solution $u \in H_0^1(\Omega)$.

Proof.

Continuity:

$$\begin{aligned} |A(u, \phi)| &\leq \sigma \|u\| \|\phi\| + \epsilon \|\nabla u\| \|\nabla \phi\| + \|\beta\|_{L^\infty(\Omega)} \|\nabla u\| \|\phi\| \\ &\leq C_{\epsilon, \beta, \sigma} (\|u\| + \|\nabla u\|) (\|\phi\| + \|\nabla \phi\|) \end{aligned}$$

With Poincare inequality we obtain continuity.

Coercivity:

$$A(u, u) = (\sigma u + (\beta \cdot \nabla)u, u) + \epsilon \|\nabla u\|^2$$

Reformulation of the convective part:

$$\begin{aligned} ((\beta \cdot \nabla)u, u) &= \int_{\Omega} \nabla u \cdot (\beta u) \, dx \\ &= -(u, \operatorname{div}(\beta u)) + \int_{\partial\Omega} u^2 (\beta \cdot n) \\ &= -(u, (\operatorname{div} \beta)u) - (u, (\beta \cdot \nabla)u) \end{aligned}$$

Hence

$$((\beta \cdot \nabla)u, u) = -\frac{1}{2}(u, u \operatorname{div} \beta)$$

$$(\sigma u + (\beta \cdot \nabla)u, u) = ((\sigma - \frac{1}{2} \operatorname{div} \beta), u^2) \geq c_0 \|u\|^2$$

Therefore, we get for $c_0 > 0$:

$$A(u, u) \geq c_0 \|u\|^2 + \epsilon \|\nabla u\|^2 \geq \epsilon \|\nabla u\|^2$$

The conditions for Lax-Milgram are fulfilled.

Where is the problem for discrete (FE) schemes ?

- Lax-Milgram also applies to the discrete standard FE scheme.
- Existence and uniqueness of discrete solutions.
- Cea's Lemma:

$$\|u - u_h\| + \|\nabla(u - u_h)\| \leq \frac{\alpha_1}{\alpha_2} \inf_{v_h \in V_h} (\|u - v_h\| + \|\nabla(u - v_h)\|)$$

- But:

$$\frac{\alpha_1}{\alpha_2} = \frac{\sigma + \|\beta\|_{L^\infty(\Omega)} + \epsilon}{\min\{c_0, \epsilon\}} \sim \frac{1}{\epsilon} \quad \text{for small } \epsilon$$

- E.g., for P_1 -elements:

$$\|u - u_h\| + \|\nabla(u - u_h)\| \sim \frac{h}{\epsilon}$$

Large errors for small viscosities $\epsilon \ll 1$.

3.3 Standard Galerkin formulation

Standard Galerkin formulation: Seek $u_h \in V_h$ s.t.

$$A(u_h, \phi) = (f, \phi) \quad \forall \phi \in V_h$$

A priori estimate in the norm

$$\|u\|_\epsilon := (\epsilon \|\nabla u\|^2 + \|u\|^2)^{1/2}.$$

Theorem

Under the conditions of the previous Thm. and H^{r+1} -regularity of the solution u the P_r (or Q_r) FE solution of the CDR problem fulfills the following a priori estimate:

$$\|u - u_h\|_\epsilon \leq Ch^r |u|_{H^{r+1}(\Omega)}$$

with $C = C(\beta, \epsilon, \sigma, \Omega, \kappa)$.

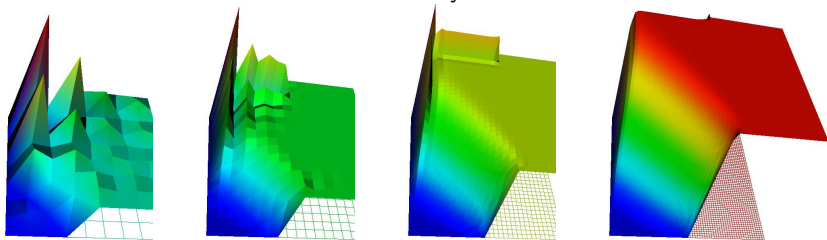
This is not satisfactory because e.g. for $r = 1$:

$$\|\nabla(u - u_h)\| \sim \frac{h}{\epsilon} |u|_{H^2(\Omega)}$$

and $\lim_{\epsilon \rightarrow 0} |u|_{H^2(\Omega)} = \infty$.

Instabilities of the pure Galerkin formulation

- Diffusion coefficient $\epsilon = 0.01$, convection $\beta = (1, 1)^T$.
- The Galerkin formulation stabilizes only on sufficient fine meshes:



- No DMP

$$\text{if } h > \frac{\epsilon}{2|\beta|} \implies \text{unphysical oscillations}$$

- Convergence for P_1 (or Q_1) elements of pure Galerkin:

$$\|\nabla(u - u_h)\| \sim \frac{h}{\epsilon} |u|_{H^2(\Omega)}$$

- Galerkin formulation of first order term is equivalent to central difference scheme.

- Similar strategies as for FD are possible with FEM: Adding the term

$$(h\nabla u_h, \nabla \phi)$$

to the bilinear form $A(\cdot, \cdot)$.

- Diffusion in streamline direction only: Adding

$$(h(\beta \cdot \nabla) u_h, (\beta \cdot \nabla) \phi)$$

Only 1. order !

- Accuracy of 1. order methods can be worse than pure Galerkin (see Brooks & Hughes)

Numerical schemes for convection-diffusion-reaction problems

- Still challenging for dominating convection, i.e. $\|\beta\| \gg \epsilon$.
- Apperance of interior and boundary layers, small subregions with large gradients
- Width of layers are often smaller than the mesh size.
- Then, sufficient resolution of sharp gradients are not possible.
- Spurious nonphysical oszillations.
- Extensive research in the last decades.

3.4 Stabilized finite elements

$$A(u, \phi) := (\sigma u + (\beta \cdot \nabla)u, \phi) + (\epsilon \nabla u, \nabla \phi)$$

- Stabilized form:

$$u_h \in V_h : \quad A(u_h, \phi) + S_h(u_h, \phi) = \langle F_h, \phi \rangle \quad \forall \phi \in V_h$$

- Such stabilization is called **fully consistent**, if the strong solution u still fulfills the discrete equation.
- Pure Galerkin formulation for

$$S_h(u_h, \phi) = 0 \quad \text{and} \quad F_h = F$$

- Several choices are possible, e.g.
 - SUPG: Streamline upwind Petrov Galerkin
 - LPS: Local projection stabilization
 - EOS: edge oriented stabilization / IP: interior penalty
 - SOLD: Spurious Oscillation at Layer Disminishing methods
 - DG: Discontinuous Galerkin

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3.4.1 Streamline Upwind Petrov Galerkin (SUPG)

- Add a diffusion term in direction of the streamlines, i.e. β

$$((\beta \cdot \nabla)u_h, (\beta \cdot \nabla)\phi)$$

- choose a clever weighting s.t. a balance of sufficient diffusion and accuracy is obtained:

$$\sum_{T \in \mathcal{T}_h} \delta_T ((\beta \cdot \nabla)u_h, (\beta \cdot \nabla)\phi)_T$$

- Introduce further consistency terms:

$$\sum_{T \in \mathcal{T}_h} \delta_T (\sigma u_h + (\beta \cdot \nabla)u_h - \epsilon \Delta u_h, (\beta \cdot \nabla)\phi)_T$$

- No additional diffusion in crosswind direction.

SUPG for convection-diffusion problems

- Idea: Add a consistent diffusion term in direction of the flow:

$$S_h(u_h, \phi) := \sum_{T \in \mathcal{T}_h} (\sigma u_h + (\beta \cdot \nabla) u_h - \epsilon \Delta u_h, \delta_h(\beta \cdot \nabla) \phi)_T$$

$$\langle F_h, \phi \rangle := \langle F, \phi \rangle + \sum_{T \in \mathcal{T}_h} (f, \delta_h(\beta \cdot \nabla) \phi)_T$$

- SUPG is fully consistent: The strong solution u fulfills the discrete equation.
- The parameter δ_h is mesh size dependent, $\delta_T := \delta_h|_T$.

Coercivity of the SUPG stabilization form

For P_1 elements (u_h cell-wise linear):

$$S_h(u_h, u_h) = \sum_{T \in \mathcal{T}_h} (\sigma u_h + (\beta \cdot \nabla) u_h - \epsilon \Delta u_h, \delta_T (\beta \cdot \nabla) u_h)_T$$

Cell-wise estimation:

$$\begin{aligned} & (\sigma u_h + (\beta \cdot \nabla) u_h - \epsilon \Delta u_h, \delta_T (\beta \cdot \nabla) u_h)_T \\ = & \delta_T \|(\beta \cdot \nabla) u_h\|_T^2 + (\sigma u_h, \delta_T (\beta \cdot \nabla) u_h)_T \\ \geq & \delta_T \|(\beta \cdot \nabla) u_h\|_T^2 - \|\sigma u_h\|_T \delta_T \|(\beta \cdot \nabla) u_h\|_T \\ \geq & \delta_T \|(\beta \cdot \nabla) u_h\|_T^2 - \frac{\delta_T}{2} \|\sigma u_h\|_T^2 - \frac{\delta_T}{2} \|(\beta \cdot \nabla) u_h\|_T^2 \end{aligned}$$

We obtain the coercivity property:

$$S_h(u_h, u_h) \geq \frac{1}{2} \sum_{T \in \mathcal{T}_h} \delta_T (\|(\beta \cdot \nabla) u_h\|_T^2 - \|\sigma u_h\|_T^2)$$

Coercivity of the SUPG bilinear form

For P_1 elements (u_h cell-wise linear):

$$\begin{aligned} & A(u_h, u_h) + S_h(u_h, u_h) \\ \geq & c_0 \|u_h\|^2 + \epsilon \|\nabla u_h\|^2 + \frac{1}{2} \sum_{T \in \mathcal{T}_h} \delta_T (\|(\beta \cdot \nabla) u_h\|_T^2 - \|\sigma u_h\|_T^2) \\ \geq & c' \|u_h\|^2 + \epsilon \|\nabla u_h\|^2 + \frac{1}{2} \sum_{T \in \mathcal{T}_h} \delta_T \|(\beta \cdot \nabla) u_h\|_T^2 \end{aligned}$$

with

$$c' = \|\sigma(1 - \delta_h/2) - \tfrac{1}{2} \operatorname{div} \beta\|_{L^\infty(\Omega)}$$

By Lax-Milgramm we obtain:

Theorem

Under the condition that $\delta_h \leq 1$ and

$$\operatorname{div} \beta \leq \sigma \quad \text{a.e.}$$

the SUPG formulation of the convection-diffusion-reaction system with P_1 elements has a unique discrete solution $u_h \in P_1(\mathcal{T}_h)$.

Optimal choice for δ_T

Local Peclet number

$$Pe|_T := \frac{h_T \|\beta\|_{L^\infty(T)}}{\epsilon}$$

$Pe|_T > 1/2$: convection dominated region

$$\delta_T := \frac{h_T}{\|\beta\|_{L^\infty(T)}}$$

$Pe|_T \leq 1/2$: diffusion dominated region

$$\delta_T := \frac{h_T^2}{\epsilon}$$

Or

$$\delta_T := \min \left(\frac{h_T}{\|\beta\|_{L^\infty(T)}}, \frac{h_T^2}{\epsilon}, \frac{1}{\sigma} \right)$$

A priori estimate for SUPG

$$\|u\|_h^2 := \sigma \|u\|^2 + \epsilon \|\nabla u\|^2 + \sum_{T \in \mathcal{T}_h} \delta_T \|(\beta \cdot \nabla) u\|_T^2$$

Theorem

Under the smoothness assumption $u \in H^{r+1}(\Omega)$ it holds for P_r -elements

$$\|u - u_h\|_h \leq C \sum_{T \in \mathcal{T}_h} a_T h_T^r |u|_{H^{r+1}(T)}$$

with $a_T := (\epsilon + h_T \|\beta\|_{L^\infty(T)} + h_T^2 \sigma)^{1/2}$.

E.g. for P_1 - or Q_1 -elements:

$$\|\nabla(u - u_h)\| \sim \left(1 + \frac{h}{\epsilon}\right)^{1/2} h |u|_{H^2}$$

plus additional control about streamline derivative.

For pure Galerkin remember: $\|\nabla(u - u_h)\| \sim h/\epsilon$.

- Aim: Bound the discretization error by a multiple of

$$H_h(u) := \sum_{T \in \mathcal{T}_h} a_T h_T^r |u|_{H^{r+1}(T)}$$

- Splitting the error in **interpolation error** and **projection error**:

$$u - u_h = (u - I_h u) + (I_h u - u_h)$$

- The **interpolation error** $\eta_h = u - I_h u$ is properly bounded by standard interpolation results:

$$\|u_h - I_h u\|_h \leq CH_h(u)$$

- The **projection error** $\xi_h := I_h u - u_h \in V_h$ can be bounded by help of the coercivity:

$$\alpha_2^{-1} \|\xi_h\|_h^2 \leq A(\xi_h, \xi_h) + S_h(\xi_h, \xi_h)$$

- Use Galerkin orthogonality:

$$A(u - u_h, \xi_h) + S_h(u - u_h, \xi_h) = 0$$

$$\begin{aligned}
\alpha_2^{-1} \|\xi_h\|_h^2 &\leq A(\xi_h, \xi_h) - A(u - u_h, \xi_h) \\
&\quad + S_h(\xi_h, \xi_h) - S_h(u - u_h, \xi_h) \\
&= A(I_h u - u, \xi_h) + S_h(I_h u - u, \xi_h)
\end{aligned}$$

- Individual bounds

$$\begin{aligned}
|A(\eta_h, \xi_h)| &\leq H_h(u) \|\xi_h\|_h \\
|S_h(\eta_h, \xi_h)| &\leq H_h(u) \|\xi_h\|_h
\end{aligned}$$

- e.g. for the Galerkin terms arising in $A(\eta_h, \xi_h)$:

$$\begin{aligned}
|(\sigma \eta_h, \xi_h)| &\leq \sigma^{1/2} \|\eta_h\| \|\xi_h\|_h \\
|((\beta \cdot \nabla) \eta_h, \xi_h)| &= (\eta_h, (\beta \cdot \nabla) \xi_h) \\
&\leq \delta_h^{-1/2} \|\eta_h\| \|\xi_h\|_h \\
|\epsilon(\nabla \eta_h, \nabla \xi_h)| &\leq \epsilon^{1/2} \|\nabla \eta_h\| \|\xi_h\|_h
\end{aligned}$$

- With a priori bounds on $\|\eta_h\|$, $\|\nabla\eta_h\|$:

$$\begin{aligned}
A(-\eta_h, \xi_h) &\leq \underbrace{\left(\sigma^{1/2} \|\eta_h\| + \delta_h^{-1/2} \|\eta_h\| + \epsilon^{1/2} \|\nabla\eta_h\| \right)}_{(\sigma^{1/2}h + \delta_h^{-1/2}h + \epsilon^{1/2})h^r |u|_{H^{r+1}}} \|\xi_h\|_h \\
&\leq H_h(u) \|\xi_h\|_h
\end{aligned}$$

- The other term $|S_h(\eta_h, \xi_h)|$ is bounded as well:

$$|S_h(\eta_h, \xi_h)| \leq \left(\sum_{T \in \mathcal{T}_h} \delta_T \|\sigma\eta_h + (\beta \cdot \nabla)\eta_h - \epsilon\Delta\eta_h\|_T^2 \right)^{1/2} \|\xi_h\|_h$$

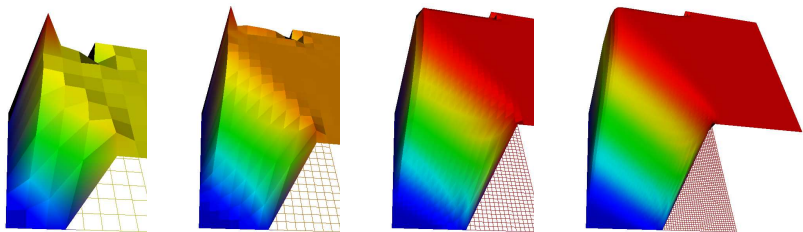
For $r = 1$ we deduce e.g.

$$\begin{aligned}
\delta_T^{1/2} \|\epsilon\Delta\eta_h\|_T &\leq \delta_T^{1/2} \|\epsilon\Delta u\|_T \\
&\leq \delta_T^{1/2} \epsilon |u|_{H^2(T)} \\
&\leq h_T \epsilon^{1/2} |u|_{H^2(T)}
\end{aligned}$$

For $r > 1$ an inverse estimate is needed.

Effect of SUPG stabilization

- Diffusion $\epsilon = 0.01$, convection $\beta = (1, 1)^T$.
- The SUPG formulation stabilizes much earlier.
- Over- and undershoots still remain on coarse meshes:



- Unphysical oscillations still are problematic (positivity of physical quantities, shocks in compressible flows, deterioration of nonlinear problems)

- ① Troublesome in the parabolic case (details below)
- ② Computation of second derivatives necessary for $r \geq 2$ and Q_1 -elements on arbitrary quadrilateral (or hexahedral) elements.
- ③ In the context of optimization: discretization and optimization do not commute.

3.4.2 SUPG for parabolic problems

- Time-dependent convection-diffusion system:

$$\begin{aligned}\partial_t u + (\beta \cdot \nabla) u - \epsilon \Delta u &= f && \text{in } \Omega \\ u &= 0 && \text{on } \partial\Omega \\ u|_{t=0} &= u_0 && \text{in } \Omega\end{aligned}$$

- Variational form:

$$(\partial_t u, \phi) + A(u, \phi) = (f, \phi)$$

with L^2 -scalar product (\cdot, \cdot) in space-time.

- Add consistent SUPG term:

$$S_h(u, \phi) := \sum_{T \in \mathcal{T}_h} \delta_T (\partial_t u + (\beta \cdot \nabla) u - \epsilon \Delta u, (\beta \cdot \nabla) \phi)_T$$

- The term $(\partial_t u, (\beta \cdot \nabla) \phi)$ is troublesome for discrete time derivative.

SUPG with an implicit Euler

With time step $\tau := t_n - t_{n-1}$:

$$(\tau^{-1}u_n, \phi) + ((\beta \cdot \nabla)u, \phi) + (\epsilon \nabla u, \nabla \phi) + \sum_{T \in \mathcal{T}_h} \delta_T (\tau^{-1}u_n + (\beta \cdot \nabla)u + \dots, (\beta \cdot \nabla)\phi)_T = (\tau^{-1}u_{n-1}, \phi) + \dots$$

- Not only the mass matrix scales with $1/\tau$.
- **Additional terms** may become dominant for small τ .

Remedy 1 in practise:

- Suppress the **blue** consistency terms.
- No optimal convergence analysis.

Remedy 2 in practise:

- Use different stabilization: LPS, EOS, ...