Space-time Finite Element Methods for Parabolic Evolution Problems
with Variable Coefficients

Ulrich Langer, Martin Neumüller, Andreas Schafelner

Johannes Kepler University, Linz

7 August 2018

Doctoral Program
Computational Mathematics
Numerical Analysis and Symbolic Computation

Der Wissenschaftsfonds.

Outline

- Introduction
- Space-time Variational Formulations
- Space-time Finite Element Methods
- Numerical Experiments
- Conclusions & Outlook

- Introduction
- Space-time Variational Formulations
- Space-time Finite Element Methods
- Numerical Experiments
- Conclusions & Outlook

A parabolic model problem

Let $\mathcal{Q} = \mathcal{Q}_T := \Omega \times (0,T)$ be our space-time cylinder and $\Sigma := \partial\Omega \times (0,T)$, $\Sigma_0 := \overline{\Omega} \times \{0\}$ and $\Sigma_T := \overline{\Omega} \times \{T\}$.
Then: Given f, g, ν and u_0, find u such that

$$\begin{aligned} \frac{\partial u}{\partial t}(x,t) - \operatorname{div}_x(\nu(x,t)\nabla_x u(x,t)) =& f(x,t), && (x,t) \in \mathcal{Q}, \\ u(x,t) =& g(x,t) = 0, && (x,t) \in \Sigma, \\ u(x,0) =& u_0(x) = 0, && x \in \overline{\Omega}, \end{aligned}$$

where ν is a given uniformly positive and bounded coefficient.

Examples: diffusion, heat-conduction and 2D eddy current.

References

Time-parallel methods:

Gander (2015): Historical overview on 50 years time-parallel methods

Space-time methods for parabolic evolution problems

Steinbach, Yang (2018): Overview on space-time methods.
Steinbach (2015): Theory for the limit case of our method

Space-time Variational Formulations I

(1) Line Variational Formulation and Vertical Method of Lines
  - ▷ discretize first in space, then in time

(2) Line Variational Formulation and Horizontal Method of Lines
  - ▷ discretize first in time, then in space

(3) Space-time Variational Formulation
  - ▷ discretize **all at once** on unstructured decompositions of the space-time cylinder
  - ▷ considered in this talk

Why?

Space-time Variational Formulations II

several ways to obtain wellposedness of the continuous problem

- Space-time v.f. in Sobolev spaces on the space-time cylinder, see, e.g., **Ladyšhenskaya**
  - $\exists!$ in $H^{k_x,k_t}(\mathcal{Q})$ + b.c.
- Space-time v.f. in Bochner spaces of abstract functions, see, e.g., Lions, Friedman
  - $\exists!$ in $H^{k_t}(0,T;H^{k_x}(\Omega))$ + b.c.

A (very) weak space-time variational formulation

Find $u \in H_0^{1,0}(\mathcal{Q})$ s.t.

$$a(u,v) = l(v) \qquad\qquad \forall v \in H_{0,\overline{0}}^{1,1}(\mathcal{Q}),$$

with

$$a(u,v) := -\int_{\mathcal{Q}} u(x,t)\ \partial_t v(x,t) + \nu(x,t) \nabla_x u(x,t) \cdot \nabla_x v(x,t)\ \mathrm{d}(x,t),$$

$$l(v) := \int_{\mathcal{Q}} f(x,t)\, v(x,t)\ \mathrm{d}(x,t) + \int_{\Omega} u_0(x)\, v(x,0)\ \mathrm{d}x.$$

Regularity results from Ladyžhenskaya et al

If $u_0 \in L_2(\Omega)$, $f \in L_{2,1}(Q_T) := \{v : \int_0^T \|v(\cdot,t)\|_{L_2(\Omega)}\,\mathrm{d}t < \infty\}$, and $0 < \underline{\nu} \leq \nu(x,t) \leq \overline{\nu}$, then there exist a unique generalized solution $u \in H_0^{1,0}(Q_T)$ that is a generalized solution in $V_{2,0}^{1,0}(Q_T)$.

For $\nu \equiv 1$, $f \in L_2(Q_T)$ and $u_0 \in H_0^1(\Omega)$, Ladyžhenskaya proved that the generalized solution u even belongs to space

$$H_0^{\Delta,1}(Q_T) = \{v \in H_0^1(Q_T) : \Delta_x v \in L_2(Q_T)\},$$

and continuously depends on t in the norm of the space $H_0^1(\Omega)$.

Maximal parabolic regularity

For the class of problems

$$\partial_t u - \underbrace{\operatorname{div}_x(\nu(x,t)\nabla_x u)}_{=\mathcal{L}u} = f$$

with $u_0 = 0$, we have *maximal parabolic regularity* if

$$\|\partial_t u\|_X + \|\mathcal{L}u\|_X \le C\|f\|_X,$$

where $X = L_p(0,T;L_q(\Omega)) = L_{p,q}(\mathcal{Q})$, $1 < p, q < \infty$.
For $p = q = 2$, we denote the space of such functions by

$$H^{\mathcal{L},1}(\mathcal{Q}) = \{v \in L_2(\mathcal{Q}) : \partial_t u \in L_2(\mathcal{Q}) \wedge \mathcal{L}u \in L_2(\mathcal{Q})\}.$$

Space-time FEM with time-upwind stabilization

The main idea:

- for each element K, define *individual* upwind test function

$$v_{h,t}(x,t) := v_h(x,t) + \boldsymbol{\theta_K h_K} \partial_t v_h(x,t), \text{ for all } (x,t) \in K,$$

  with θ_K positive parameter, and $h_K := diam(K)$,
- for each element K, multiply the PDE by $v_{h,t}(x,t)$,
- sum up over all elements K,
- proceed as usual, IbyP, etc.

Derivation of the FE scheme

Let $u \in H^{\mathcal{L},1}(\mathcal{Q})$ be the solution of our IBVP, i.e.

$$\partial_t u - \mathrm{div}_x(\nu \nabla_x u) = f \text{ in } L_2(K).$$

Multiplication of the **PDE** with $v_{h,t}$, integration over a single element K, and summing up over all elements yields

$$\sum_{K \in \mathcal{T}_h} \int_K \partial_t u (v_h + \theta_K \, h_K \partial_t v_h) \, \mathrm{d}(x,t)$$
$$+ \int_K \mathrm{div}_x(\nu \nabla_x u)(v_h + \theta_K \, h_K \partial_t v_h) \, \mathrm{d}(x,t)$$
$$= \sum_{K \in \mathcal{T}_h} \int_K f (v_h + \theta_K \, h_K \partial_t v_h) \, \mathrm{d}(x,t)$$

Derivation of the FE scheme (cont.)

The time derivative and the r.h.s. remain unchanged, IbyP wrt x on the div_x-term gives us

$$
\begin{aligned}
&\int_K \mathrm{div}_x(\nu \nabla_x u)(v_h + \theta_K\, h_K \partial_t v_h)\,\mathrm{d}(x,t) \\
&= \int_K (\nu \nabla_x u) \cdot \nabla_x v_h + \theta_K\, h_K (\nu \nabla_x u) \cdot \nabla_x\, (\partial_t v_h)\,\mathrm{d}(x,t) \\
&\quad - \int_{\partial K} (n_x \cdot (\nu \nabla_x u)) v_h + \theta_K\, h_K (n_x \cdot (\nu \nabla_x u)) \partial_t v_h\,\mathrm{d}s_{(x,t)}
\end{aligned}
$$

Derivation of the FE scheme (cont.)

We keep the volume integrals and take a closer look at the boundary terms. Summing again up gives

$$\sum_{K\in\mathcal{T}_h} \int_{\partial K} (n_x \cdot (\nu \nabla_x u))\, v_h \,\mathrm{d}s_{(x,t)} + \theta_K\, h_K \int_{\partial K} (n_x \cdot (\nu \nabla_x u))\, \partial_t v_h \,\mathrm{d}s_{(x,t)}$$

If u is sufficiently smooth, we have at a common edge/face/volume

$$(n_x \cdot (\nu \nabla_x u))\,\big|_K = \big(n_x' \cdot (\nu \nabla_x u)\big)\,\big|_{K'}$$

Derivation of the FE scheme (cont.)

Hence, the first integral vanishes at all *inner* edges/faces/volumes. Since $v_h|_\Sigma = 0$ and $n_x \equiv 0$ on Σ_0 and Σ_T, the first integral vanishes on the entire boundary $\partial\mathcal{Q} = \Sigma \cup \Sigma_0 \cup \Sigma_T$, i.e.,

$$\sum_{K \in \mathcal{T}_h} \int_{\partial K} (n_x \cdot (\nu \nabla_x u))\, v_h \,\mathrm{d}s_{(x,t)} = 0$$

The second boundary term however does not vanish, as in general $\theta_K \neq \theta_{K'}$ and $h_K \neq h_{K'}$ for $\overline{K} \cap \overline{K}' \neq \emptyset$.

The space-time FE scheme

Find $u_h \in V_{0h} := \{v \in C(\overline{Q}) : v(x_K(\cdot)) \in \mathbb{P}_p(K),\ v|_{\overline{\Sigma}\cup\overline{\Sigma}_0} = 0\}$:

$$a_h(u_h, v_h) = l_h(v_h), \quad \forall v_h \in V_{0h}, \tag{1}$$

where

$$\begin{aligned} a_h(u_h, v_h) := \sum_{K\in\mathcal{T}_h} \int_K &\partial_t u_h\, v_h + \theta_K h_K\, \partial_t u_h\, \partial_t v_h \,\mathrm{d}(x,t) \\ &+ \int_K (\nu\nabla_x u_h)\cdot\nabla_x v_h + \theta_K h_K\,(\nu\nabla_x u_h)\cdot\nabla_x(\partial_t v_h)\,\mathrm{d}(x,t) \\ &- \int_{\partial K} \theta_K h_K\ (n_x\cdot(\nu\nabla_x u_h))\ \partial_t v_h\ \mathrm{d}s_{(x,t)}, \\ l_h(v_h) := \sum_{K\in\mathcal{T}_h} \int_K &f\,(v_h + \theta_K h_K \partial_t v_h)\,\mathrm{d}(x,t). \end{aligned}$$

Ellipticity = Stability

Definition 3.1 (Mesh dependent norm).

$$\|v_h\|_h^2 := \sum_{K\in\mathcal{T}_h} \left[\|\nu^{1/2}\nabla_x v_h\|^2_{L_2(K)} + \theta_K h_K \|\partial_t v_h\|^2_{L_2(K)}\right] + \frac{1}{2}\|v_h\|^2_{L_2(\Sigma_T)}.$$

Lemma 3.2 (Coercivity on the FE space).

There exits a constant μ_a such that

$$a_h(v_h, v_h) \geq \mu_a \|v_h\|_h^2, \quad \forall v_h \in V_{0h},$$

with $\mu_a = \min_{K\in\mathcal{T}_h}\left\{1 - c_{I,\mathrm{div}_x}\sqrt{\frac{\overline{\nu}_K\theta_K}{4h_K}}\right\} \geq \frac{1}{2}$ *for* $\theta_K \leq \frac{h_K}{c^2_{I,\mathrm{div}_x}\overline{\nu}_K}$,
i.e., $\mu_a = \frac{1}{2}$ *for* $\theta_K = \frac{h_K}{c^2_{I,\mathrm{div}_x}\overline{\nu}_K}$.

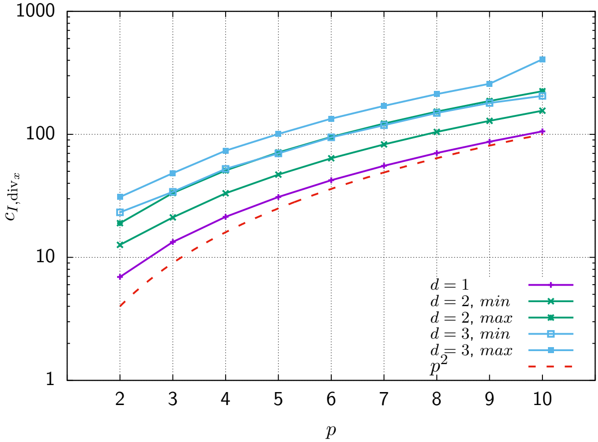
The constant c_{I,div_x}

- the constant c_{I,div_x} comes from the *inverse inequality*

  $$\|\operatorname{div}_x(\nu w_h)\|_{L_2(K)} \leq c_{I,\mathrm{div}_x} h_K^{-1} \|\nu w_h\|_{L_2(K)}, \forall w_h \in W_h|_K,$$

  with $W_h|_K := \{w_h : w_h = \nabla_x v_h, v_h \in V_{0h}|_K\}$ and $\nu \in W^1_\infty(\mathcal{T}_h)$,
- c_{I,div_x} is independent of h_K, but depends on polynomial degree p and the dimension d,
- c_{I,div_x} is **computable!**
  - to be precise, we can compute a *sharp* lower bound for $c_{I,\mathrm{div}_x} h_K^{-1}$

The constant c_{I,div_x}



Values of c_{I,div_x} on the coarsest triangulation of the $d+1$ hypercube.

Boundedness

Definition 3.3.

$$\|v\|_{h,*}^2 = \|v\|_h^2 + \sum_{K\in\mathcal{T}_h} \left[(\theta_K h_K)^{-1}\|v\|_{L_2(K)}^2 + \theta_K h_K |v|_{H^2(K)}^2\right]$$

Lemma 3.4.

The bilinear form $a_h(\,.\,,\,.\,)$ *is uniformly bounded on* $V_{0h,*} \times V_{0h}$*, i.e.,*

$$|a_h(u, v_h)| \le \mu_b \|u\|_{h,*}\,\|v_h\|_h,$$

where $V_{0h,*} := V_{0h} + H^2(\mathcal{T}_h) \cap H_0^{1,0}(\mathcal{Q})$*, and* $\mu_b = \max_{K\in\mathcal{T}_h}\left\{2(1+\theta_K h_K^{-1} c_{Tr}^2 \frac{\overline{\nu}_K^2}{\underline{\nu}_K}), 2c_{Tr}^2\overline{\nu}_K^2, 2 + c_{I,1}^2, 1 + (c_{I,\nu}\theta_K)^2\right\}^{1/2}$ *that is bounded provided that* $\theta_K = \mathcal{O}(h_K)$*.*

A Cea-like estimate

Lemma 3.5.

Let $u \in V_0 \cap H^2(\mathcal{T}_h)$ be the exact solution, and $u_h \in V_{0h}$ the solution of the finite element scheme (1). *Then there holds the Cea-like estimate*

$$\|u - u_h\|_h \leq \left(1 + \frac{\mu_b}{\mu_a}\right) \inf_{v_h \in V_{0h}} \|u - v_h\|_{h,*}$$

Remark.

We can again weaken the assumptions on u, in particular, it is enough to require $u \in H^{\mathcal{L},1}(\mathcal{Q})$.

An a prior error estimate I

Theorem 3.6.

Let s and k be positive integers with $s \in [2, p+1]$ and $k > (d+1)/2$. Furthermore, let $u \in V_0 \cap H^k(\mathcal{Q}) \cap H^s(\mathcal{T}_h)$ be the exact solution, and $u_h \in V_{0h}$ the solution of the finite element scheme (1). Then there holds the a priori error estimate

$$\|u - u_h\|_h \leq c \Big(\sum_{K \in \mathcal{T}_h} h_K^{2(s-1)} |u|^2_{H^s(K)} \Big)^{1/2}. \qquad (2)$$

An a prior error estimate II

Remark.

- $u \in H^k(\mathcal{Q})$ with $k > (d+1)/2$ is a rather strong assumption
- needed because of Lagrange Interpolant Π_h
- can be weakened → Duan et al. have shown

$$\|\nabla(v - I_h v)\|_{L_2(\mathcal{Q})} \leq C \sum_{i=1}^{M} h_i^{s_i - 1} \|v\|_{H^{s_i}(\mathcal{Q}_i)},$$

for $v \in H^{\mathbf{s}}(\mathcal{T}(\mathcal{Q}))$ with $\mathbf{s} = (s_1, \ldots, s_M)$ and

$$H^{\mathbf{s}}(\mathcal{T}(\mathcal{Q})) := \{v \in L_2(\mathcal{Q}) : v|_{\mathcal{Q}_i} \in H^{s_i}(\mathcal{Q}_i), \text{ for all } i = 1, \ldots, M\}$$

Numerical Experiments

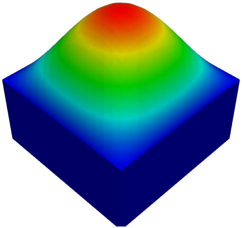
Key information

- Space-time FEM was implemented with MFEM,
- Linear systems were solved by means of *hypre*,
- Meshes generated by NETGEN (2D, 3D) and **Karabelas & Neumüller** (4D),
- Tests were performed on RADON1,
- c_{I,div_x} was computed numerically,
- Convergence rates in L_2-norm and $\|\,.\,\|_h$-**norm**.

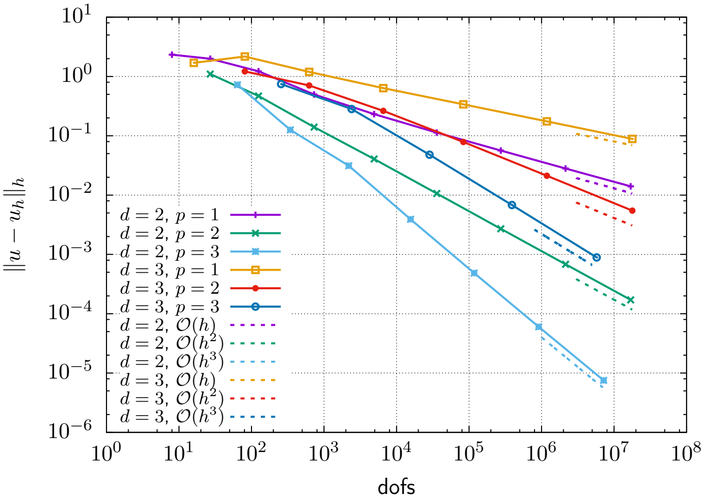
Example 4.1 (Smooth solution, uniform coefficient).

Consider space-time cylinder $\mathcal{Q} = (0,1)^{d+1}$, $\nu \equiv 1$ and choose the exact solution

$$u(x,t) = \prod_{i=1}^{d} \sin(x_i \pi) \sin(t\pi).$$



Example 4.1: Solution for $d = 2$


10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
$\|u - u_h\|_h$
$d = 2,\ p = 1$
$d = 2,\ p = 2$
$d = 2,\ p = 3$
$d = 3,\ p = 1$
$d = 3,\ p = 2$
$d = 3,\ p = 3$
$d = 2,\ \mathcal{O}(h)$
$d = 2,\ \mathcal{O}(h^2)$
$d = 2,\ \mathcal{O}(h^3)$
$d = 3,\ \mathcal{O}(h)$
$d = 3,\ \mathcal{O}(h^2)$
$d = 3,\ \mathcal{O}(h^3)$
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
10^{8}
dofs

Example 4.1.

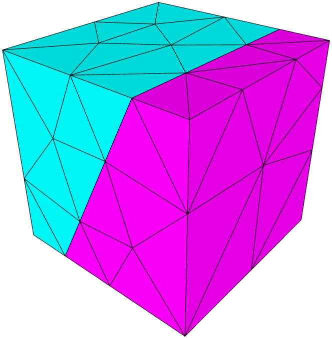
Example 4.2 (Smooth solution, discont. coefficient).

Consider space-time cylinder $\mathcal{Q} = (0,1)^{d+1}$, space-time dependent coefficient

$$\nu(x,t) = \begin{cases} 1 \times 10^2, & \text{for } 2x_1 - t < \frac{1}{2}, \\ 7 \times 10^5, & \text{for } 2x_1 - t > \frac{1}{2}, \end{cases}$$

and choose the smooth solution

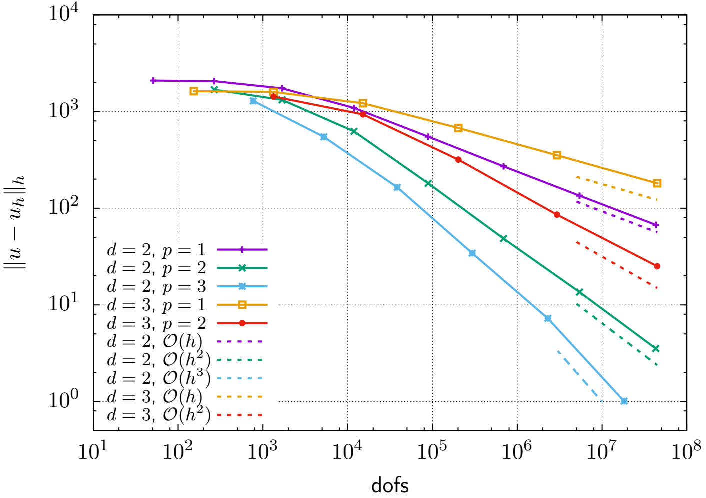
$$u(x,t) = \begin{cases} \sin\left(9\pi\left(2x_1 - t - \frac{1}{2}\right)^2 (x_1 - x_1^2)\right) \times \sin(4\pi t) \prod_{i=2}^{d} \sin(\pi x_i), & \text{for } 2x_1 - t \le \frac{1}{2}, \\ \sin\left(40\pi\left(2x_1 - t - \frac{1}{2}\right)^2 (x_1 - x_1^2)(t - t^2)\right) \times \prod_{i=2}^{d} \sin(\pi x_i), & \text{otherwise}, \end{cases}$$



(a)

(b)

(a) Initial mesh for $d = 2$; (b) Inital mesh for $d = 3$, sliced in t direction



10^4
10^3
10^2
10^1
10^0
$\|u - u_h\|_h$
$d = 2,\ p = 1$
$d = 2,\ p = 2$
$d = 2,\ p = 3$
$d = 3,\ p = 1$
$d = 3,\ p = 2$
$d = 2,\ \mathcal{O}(h)$
$d = 2,\ \mathcal{O}(h^2)$
$d = 2,\ \mathcal{O}(h^3)$
$d = 3,\ \mathcal{O}(h)$
$d = 3,\ \mathcal{O}(h^2)$
10^1 10^2 10^3 10^4 10^5 10^6 10^7 10^8
dofs

Example 4.2.

Example 4.3 (Adaptivity).

Choose space-time cylinder $\mathcal{Q} = (0,1)^3$, $\nu \equiv 1$, and exact solution

$$u(x,t) = (x_1^2 - x_1)(x_2^2 - x_2)(t^2 - t)e^{-100\left((x_1-t)^2+(x_2-t)^2\right)}$$

An error indicator

We use the residual-based error indicator by Steinbach & Yang (2017)

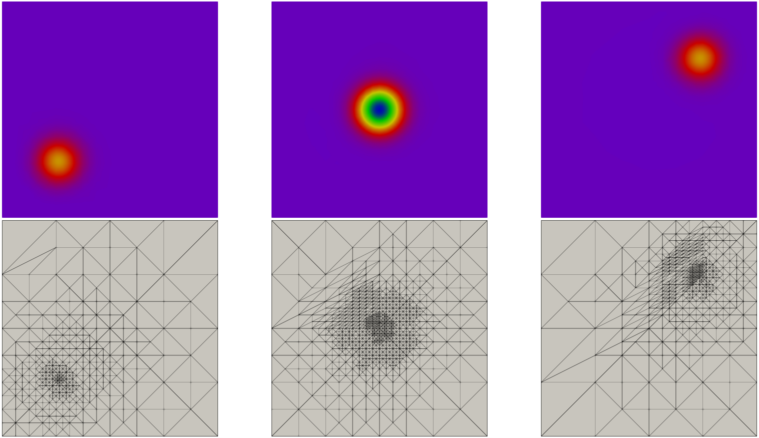
$$\eta_K := \left(h_K^2 \|R_h(u_h)\|^2_{L_2(K)} + h_K \|J_h(u_h)\|^2_{L_2(\partial K)} \right)^{1/2},$$

where

$$\begin{aligned} R_h(u_h) &:= f + \operatorname{div}_x(\nu \nabla_x u_h) - \partial_t u_h && \text{in } K, \\ J_h(u_h) &:= [\nu \nabla_x u_h]_e && \text{on } e \subset \partial K, \end{aligned}$$

with maximum marking strategy, i.e., **MARK** $K \in \mathcal{T}_h$ if

$$\eta_K \geq \sigma \max_{K \in \mathcal{T}_h} \eta_K$$

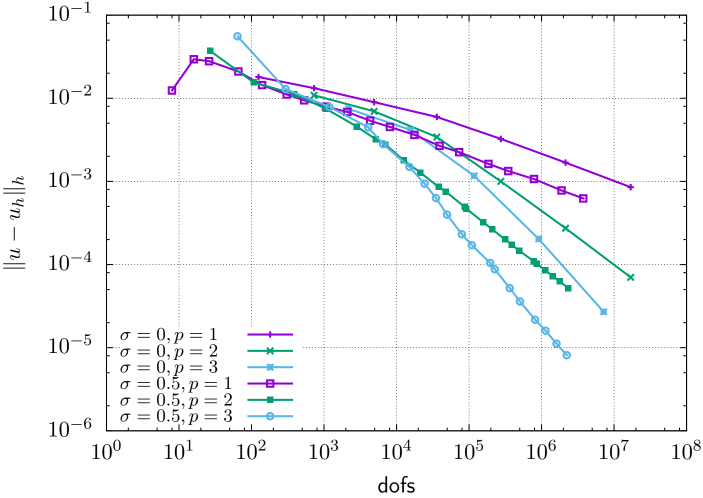


(a) (b) (c)

Plot and mesh at (a) $t = 0.25$, (b) $t = 0.5$, (c) $t = 0.75$

(a) (b) (c)

Evolution of the mesh at (a) $t = 0.25$, (b) $t = 0.5$, (c) $t = 0.75$

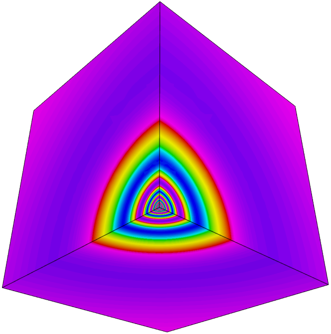


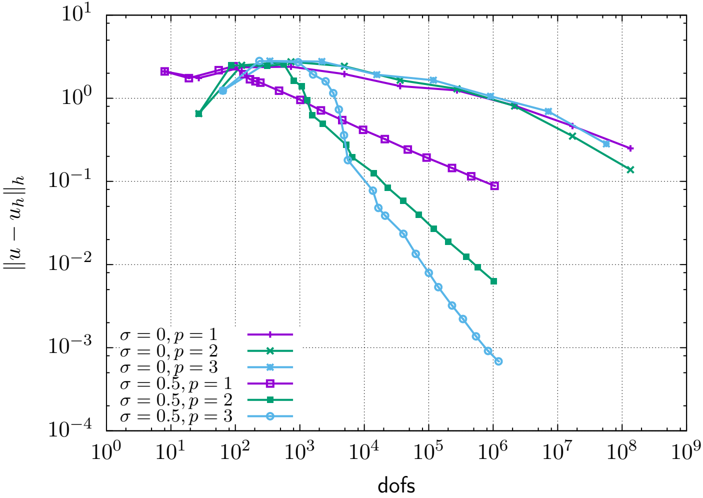
Example 4.3 Error rates for $d = 2$.

Example 4.4 (Adaptivity II).

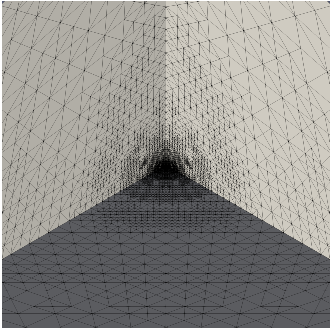
Choose space-time cylinder $\mathcal{Q} = (0,1)^3$, $\nu \equiv 1$, and exact solution

$$u(x,t) = \sin\left(\frac{1}{\frac{1}{10\pi} + \sqrt{x_1^2 + x_2^2 + t^2}}\right)$$





Example 4.4 Error rates for $d = 2$.

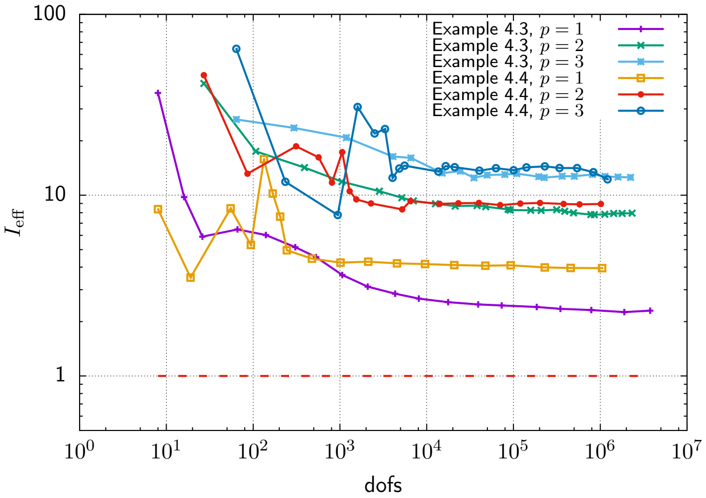


(a)

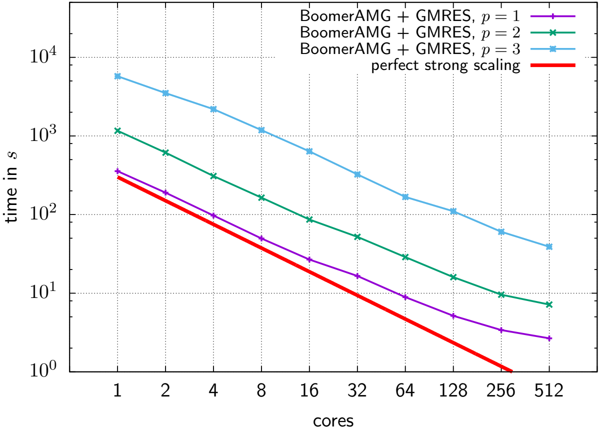
(b)

(a) Mesh at the origin $(0, 0, 0)$ after 13 adaptive refinements; (b) Evolution of the mesh in the origin over 13 adaptive refinements.

Efficiency index

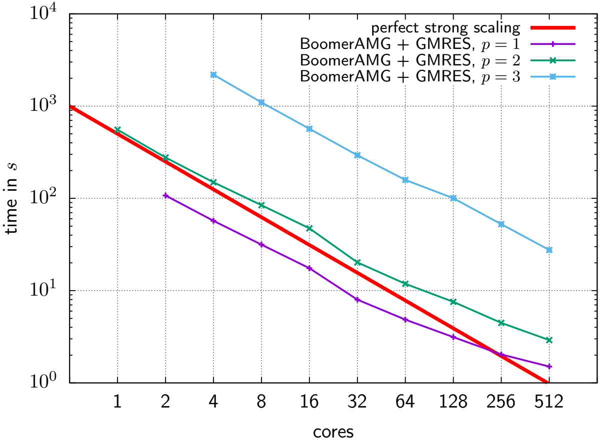


Strong scaling I



Example 4.1 with $d = 3$ and $\sim 4 - 5 \times 10^6$ dofs.

Strong scaling II



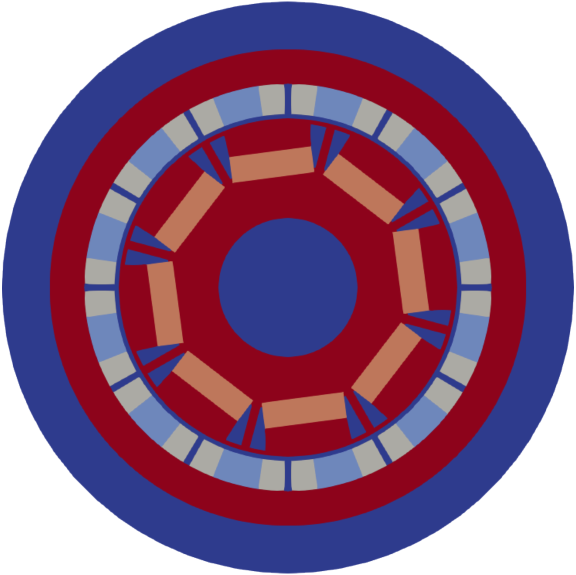
Example 4.2 with $d = 3$ and $\sim 3 - 14 \times 10^6$ dofs.

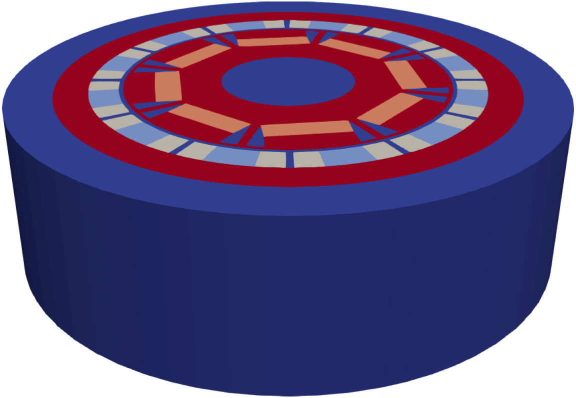
Conclusions

- **stability** of the FE scheme provided that $\theta_K = \mathcal{O}(h_K)$,
- we *compute* the **optimal** $\boldsymbol{\theta_K}$,
- we proved an **a priori estimate** for $\|\,.\,\|_h$,
- the numerical experiments are in accordance with the theory,
- fully *parallel* space-time FEM.

Outlook

- application to more complex domains, e.g., cross-section of an electrical motor,
- a posteriori error estimators for AFEM (adaptivity),
- improve the solving of the huge linear system (preconditioning),
- combine AFEM with Nested Iterations,
- **main future goal:** *non-linear parabolic problems* and *eddy-current problems* (electrical engineering).





[1] Karabelas, E., and Neumüller, M.
Generating admissible space-time meshes for moving domains in d+1-dimensions.
Tech. Rep. 07, Institute of Computational Mathematics, Johannes Kepler University Linz, 2015.

[2] Ladyženskaya, O. A.
The boundary value problems of mathematical physics, vol. 49 of *Applied Mathematical Sciences*.
Springer-Verlag, New York, 1985.
Translated from the Russian by Jack Lohwater [Arthur J. Lohwater].

[3] Langer, U., Moore, S., and Neumüller, M.
Space-time isogeometric analysis of parabolic evolution problems.
Comput. Methods Appl. Mech. Engrg. 306 (2016), 342–363.

[4] Langer, U., Neumüller, M., and S., A.
Space-time finite element methods for parabolic evolution problems with variable coefficients.
In Revision.

[5] Steinbach, O.
Space-time finite element methods for parabolic problems.
Comput. Methods Appl. Math. 15, 4 (2015), 551–566.

[6] Steinbach, O., and Yang, H.
Comparison of algebraic multigrid methods for an adaptive space-time finite-element discretization of the heat equation in 3d and 4d.
Numerical Linear Algebra with Applications 25, 3 (2018), 2018;25:e2143.

Thank you!