

Parallel Multipatch Space-Time IGA Solvers for Parabolic Initial-Boundary Value Problems

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Joint work with my collaborators

- Christoph Hofer (JKU, DK)
- Martin Neumüller (JKU, NuMa)
- Ioannis Toulopoulos (RICAM, CM4PDE)

Main results have just been published in

- [1] C. Hofer, U. Langer, M. Neumüller, I. Toulopoulos. Time-multipatch discontinuous Galerkin space-time isogeometric analysis of parabolic evolution problems. *ETNA*, 2018, v. 49, 126–150.
- [2] C. Hofer, U. Langer, M. Neumüller. Robust preconditioning for space-time isogeometric analysis of parabolic evolution problems. *[math.NA]*, 2018, [arXiv:1802.09277, arXiv.org](https://arxiv.org/abs/1802.09277).



Outline

1 Introduction

2 Time Multi-Patch Space-Time IgA

3 Space-Time Solvers

4 Conclusions & Outlooks

Parabolic Initial-Boundary Value Model Problem

Let us consider the IBVP problem: Find $u : \overline{Q} \rightarrow \mathbb{R}$ such that

$$\begin{aligned} \partial_t u - \Delta u &= f \quad \text{in} \quad Q := \Omega \times (0, T), \\ u = u_D &:= 0 \quad \text{on} \quad \Sigma := \partial\Omega \times (0, T), \\ u = u_0 & \quad \text{on} \quad \overline{\Sigma}_0 := \overline{\Omega} \times \{0\}, \end{aligned} \tag{1}$$

as the typical model problem for a linear parabolic evolution equation posed in the space-time cylinder $\overline{Q} = \overline{\Omega} \times [0, T]$.

Our space-time technology can be generalized to more general parabolic equations like

$$-\operatorname{div}_x(A(x, t)\nabla_x u) + b(x, t) \cdot \nabla_x u + c(x, t)\partial_t u + a(x, t)u = f,$$

eddy-current problems, non-linear problems etc.

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Standard Weak Space-Time Variational Formulation

Find $u \in H_0^{1,0}(Q)$ such that

$$a(u, v) = \ell(v) \quad \forall v \in H_{0,\bar{0}}^{1,1}(Q), \quad (2)$$

with the bilinear form

$$a(u, v) = - \int_Q u(x, t) \partial_t v(x, t) dxdt + \int_Q \nabla_x u(x, t) \cdot \nabla_x v(x, t) dxdt$$

and the linear form

$$\ell(v) = \int_Q f(x, t) v(x, t) dxdt + \int_\Omega u_0(x) v(x, 0) dx,$$

For solvability and regularity results, we refer to original papers by the Leningrad School of Mathematical Physics in the 50s, summarized in the monographs by [Ladyzhenskaya, Solonnikov & Uralceva \(1967\)](#) and [Ladyzhenskaya \(1973\)](#) !

Parabolic Solvability and Regularity Results

- If $f \in L_{2,1}(Q_T) := \{v : \int_0^T \|v(\cdot, t)\|_{L_2(\Omega)} dt < \infty\}$ and $u_0 \in L_2(\Omega)$, then there exists a unique generalized (weak) solution $u \in H_0^{1,0}(Q)$ of (2) that even belongs to $V_{2,0}^{1,0}(Q_T)$.
- If $f \in L_2(Q_T)$ and $u_0 \in H_0^1(\Omega)$, then the generalized solution u of (2) belongs to space $H_0^{\Delta,1}(Q_T) = W_{2,0}^{\Delta,1}(Q_T)$, and u continuously depends on t in the norm of the space $H_0^1(\Omega)$, where $W_{2,0}^{\Delta,1}(Q_T) = \{v \in H_0^1(Q_T) : \Delta_x v \in L_2(Q_T)\}$.
- Maximal parabolic regularity: $\partial_t u - \operatorname{div}_x(A(x, t)\nabla_x u) = f$

$$\|\partial_t u\|_X + \|\operatorname{div}_x(A(x, t)\nabla_x u)\|_X \leq C \|f\|_X,$$

where $X = L_p((0, T), L_q(\Omega)) = L_{p,q}(Q_T)$, $1 < p, q < \infty$, $u_0 = 0$, and $a = 0$, $b = 0$, $c = 1$.

Parabolic Solvability and Regularity Results

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- If $f \in L_2(Q_T)$ and $u_0 \in H_0^1(\Omega)$, then the generalized solution u of (2) belongs to space $H_0^{\Delta,1}(Q_T) = W_{2,0}^{\Delta,1}(Q_T)$, and u continuously depends on t in the norm of the space $H_0^1(\Omega)$, where $W_{2,0}^{\Delta,1}(Q_T) = \{v \in H_0^1(Q_T) : \Delta_x v \in L_2(Q_T)\}$.
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where $X = L_p((0, T), L_q(\Omega)) = L_{p,q}(Q_T)$, $1 < p, q < \infty$, $u_0 = 0$, and $a = 0$, $b = \mathbf{0}$, $c = 1$.

Some References to

Time-parallel methods:

Gander (2015): Nice historical overview on 50 years time-parallel method Parareal introduced by Lions, Maday, Turinici (2001)
Time-parallel multigrid: Hackbusch (1984),...,Vandewalle (1993),...,
Gander & Neumüller (2014): smart time-parallel multigrid,...,
Neumüller & Smears (2018), ...

Space-time methods for parabolic evolution problems:

Babuška & Janik (1989,1990), Behr (2008), Schwab & Stevenson (2009), Neumüller & Steinbach (2011), Neumüller (2013), Andreev (2013), Bank & Metti (2013), Mollet (2014), Urban & Patera (2014), Schwab & Stevenson (2014), Bank & Vassilevski (2014), Karabelas & Neumüller (2015), Langer & Moore & Neumüller (2016), Bank & Vassilevski & Zikatanov (2016), Larsson & Molteni (2017), Steinbach & Yang (2017), Langer & Neumüller & Schafelner (2018), ...

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References

Time-parallel methods:

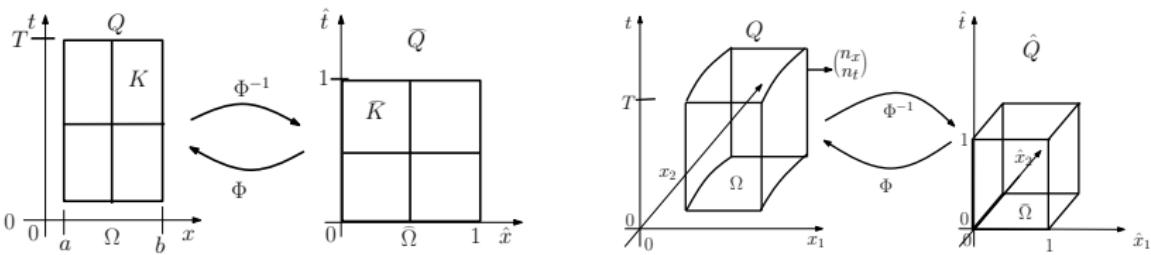
Gander (2015): Nice historical overview on 50 years time-parallel methods

Space-time methods for parabolic evolution problems:

Steinbach & Yang (2018): Nice overview on space-time methods in the space-time book that will be published in RSCAM by de Gruyter

Single-Patch Space-Time IgA: LMN'16

- [3] U. Langer, S. Moore, M. Neumüller. Space-time isogeometric analysis of parabolic evolution equations. *Comput. Methods Appl. Mech. Engrg.*, v. 306, pp. 342–363, 2016.



Space-Time IgA paraphernalia: $Q \subset \mathbb{R}^{d+1}$; $d = 1$ (l) and $d = 2$ (r).

In this talk: Generalization to the multipatch case + Solvers !

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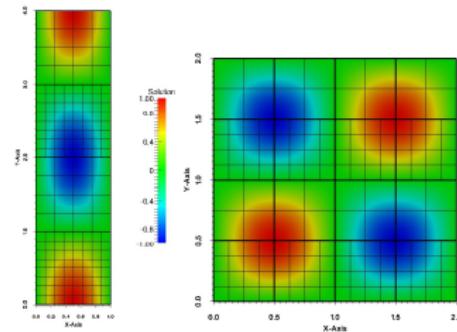
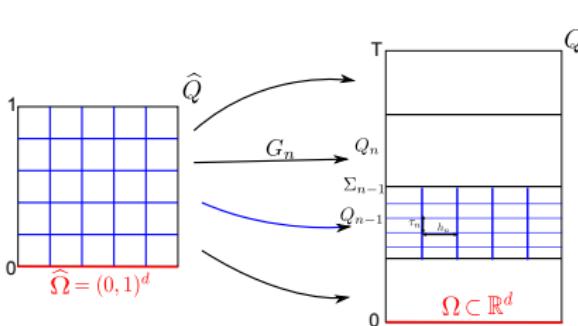
Time Multi-Patch Decomposition of Q

We decompose the space-time cylinder $Q = \Omega \times (0, T)$ into N non-overlapping space-time subcylinder

$Q_n = \Omega \times (t_{n-1}, t_n) = \Phi_n(\hat{Q})$, $n = 1, 2, \dots, N$, such that

$$\overline{Q} = \bigcup_{n=1}^N \overline{Q}_n$$

with the time faces $\Sigma_n = \overline{Q}_{n+1} \cap \overline{Q}_n = \Omega \times \{t_n\}$, $\Sigma_N = \Sigma_T$:



Time Multipatch dG IgA spaces V_{0h}

We look for an approximate solution u_h to the IBVP (2) in the globally discontinuous, but patch-wise smooth IgA (B-spline, NURBS) spaces

$$\begin{aligned} V_{0h} &= \{v_h \in H_0^{1,0}(Q) : v_h^n := v_h|_{Q_n} \in \mathbb{B}_{\Xi_n^{d+1}}(Q_n), n = 1, \dots, N\} \\ &= \{v_h \in L_2(Q) : v_h^n \in V_{0h}^n, n = 1, \dots, N\} = \text{span}\{\varphi_i\}_{i \in \mathcal{I}}, \\ V_{0h}^n &= \{v_h^n \in \mathbb{B}_{\Xi_n^{d+1}}(Q_n) : v_h^n = 0 \text{ on } \Sigma\} = \text{span}\{\varphi_{n,i}\}_{i \in \mathcal{I}_n} \end{aligned}$$

where $\mathbb{B}_{\Xi_n^{d+1}}(Q_n)$ is the smooth (depending on the polynomial degrees and multiplicity of the knots) IgA space corresponding to the knot vector

$$\Xi_n^{d+1} = \Xi_n^{d+1}(n_1^n, \dots, n_{d+1}^n; p_1^n, \dots, p_{d+1}^n) = \dots$$

Stable Time Multipatch dG IgA Scheme

Multiplying the PDE $\partial_t u - \Delta_x u = f$ by $v_h + \theta_n h_n \partial_t v_h$, integrating over Q_n , integrating by parts, summing over n , and using that the jumps $[[u]]$ across Σ_n are 0 at the solution $u \in H_0^{\Delta,1}(Q)$, we get the consistency identity

$$a_h(u, v_h) = \ell_h(v_h) \quad \forall v_h \in V_{0h},$$

where

$$\begin{aligned} a_h(u, v_h) &= \sum_{n=1}^N \int_{Q_n} (\partial_t u v_h + \theta_n h_n \partial_t u \partial_t v_h + \nabla_x u \nabla_x v_h + \theta_n h_n \nabla_x u \cdot \nabla_x \partial_t v_h) dx dt \\ &\quad + \sum_{n=1}^N \int_{\Sigma_{n-1}} [[u^{n-1}]] v_{h,+}^{n-1} dx, \\ \ell_h(v_h) &= \sum_{n=1}^N \int_{Q_n} f [v_h + \theta_n h_n \partial_t v_h] dx dt + \int_{\Sigma_0} u_0 v_{h,+}^0 dx. \end{aligned}$$

Stable Time Multipatch dG IgA Scheme

Multiplying the PDE $\partial_t u - \Delta_x u = f$ by $v_h + \theta_n h_n \partial_t v_h$, integrating over Q_n , integrating by parts, summing over n , and using that the jumps $[[u]]$ across Σ_n are 0 at the solution $u \in H_0^{\Delta,1}(Q)$, we get the multi-patch space-time scheme: Find $u_h \in V_{0h}$ such that

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

where

$$\begin{aligned} a_h(u_h, v_h) &= \sum_{n=1}^N \int_{Q_n} (\partial_t u_h v_h + \theta_n h_n \partial_t u_h \partial_t v_h + \nabla_x u_h \nabla_x v_h + \theta_n h_n \nabla_x u_h \cdot \nabla_x \partial_t v_h) dxdt \\ &\quad + \sum_{n=1}^N \int_{\Sigma_{n-1}} [[u_h^{n-1}]] v_{h,+}^{n-1} dx, \\ \ell_h(v_h) &= \sum_{n=1}^N \int_{Q_n} f [v_h + \theta_n h_n \partial_t v_h] dxdt + \int_{\Sigma_0} u_0 v_{h,+}^0 dx. \end{aligned}$$

Space-Time IgA Scheme and System of IgA Eqns

Hence, we look for the solution $u_h \in V_{0h}$ of the IgA scheme

$$a_h(u_h, v_h) = \ell_h(v_h) \quad \forall v_h \in V_{0h} \quad (3)$$

in the form of

$$u_h(x, t) = u_h(x_1, \dots, x_d, x_{d+1}) = \sum_{i \in \mathcal{I}} u_i \varphi_i(x, t)$$

where $\mathbf{u}_h := [u_i]_{i \in \mathcal{I}} \in \mathbb{R}^{N_h=|\mathcal{I}|}$ is the unknown solution vector of control points defined by the solution of the linear system

$$\mathbf{L}_h \mathbf{u}_h = \mathbf{f}_h \quad (4)$$

with huge, non-symmetric, but **positive definite** system matrix \mathbf{L}_h .

Road Map of the Numerical Analysis

$$\|v_h\|_h^2 = \sum_{n=1}^N \left(\|\nabla_x v_h\|_{L_2(Q_n)}^2 + \theta_n h_n \|\partial_t v_h\|_{L_2(Q_n)}^2 + \frac{1}{2} \|[\![v_h]\!]^{n-1}\|_{L_2(\Sigma_{n-1})}^2 \right) + \frac{1}{2} \|v_h\|_{L_2(\Sigma_N)}^2$$

$$\|v\|_{h,*}^2 = \|v\|_h^2 + \sum_{n=1}^N (\theta_n h_n)^{-1} \|v\|_{L_2(Q_n)}^2 + \sum_{n=2}^N \|v_-^{n-1}\|_{L_2(\Sigma_{n-1})}^2$$

- **Coercivity:** $a_h(v_h, v_h) \geq \mu_c \|v_h\|_h^2, \quad \forall v_h \in V_{0h}, \quad \Rightarrow ! \Rightarrow \exists u_h \leftrightarrow \mathbf{u}_h: (4)$
- **Boundedness:** $|a_h(u, v_h)| \leq \mu_b \|u\|_{h,*} \|v_h\|_h, \quad \forall u \in V_{0h} + H_0^{\Delta,1}(Q), \forall v_h \in V_{0h}$,
- **Consistency:** $a_h(u, v_h) = \ell_h(v_h) \quad \forall v_h \in V_{0h}, u \in H_0^{1,0}(Q) \cap H^{\Delta,1}(Q): (2)$
- **GO:** $a_h(u - u_h, v_h) = 0 \quad \forall v_h \in V_{0h}$,
- **Cea-like:** $\|u - u_h\|_h \leq (1 + \mu_b/\mu_c) \inf_{v_h \in V_{0h}} \|u - v_h\|_{h,*} \leq \dots$
- **Convergence rates:** $\|u - u_h\|_h \leq ch^p \|u\|_{H^{p+1}(Q)}$

V_{0h} -Coercivity of the bilinear form $a_h(\cdot, \cdot)$

We now introduce the mesh-dependent norm

$$\|v_h\|_h^2 = \sum_{n=1}^N \left(\|\nabla_x v_h\|_{L_2(Q_n)}^2 + \theta_n h_n \|\partial_t v_h\|_{L_2(Q_n)}^2 + \frac{1}{2} \|[\![v_h]\!]^{n-1}\|_{L_2(\Sigma_{n-1})}^2 \right) + \frac{1}{2} \|v_h\|_{L_2(\Sigma_N)}^2.$$

Lemma (Coercivity / Ellipticity on V_{0h})

The bilinear form $a_h(\cdot, \cdot) : V_{0h} \times V_{0h} \rightarrow \mathbb{R}$ is V_{0h} -coercive wrt the norm $\|\cdot\|_h$, i.e., there exists a constant $\mu_c = 1/2$ such that

$$a_h(v_h, v_h) \geq \mu_c \|v_h\|_h^2, \quad \forall v_h \in V_{0h}. \quad (5)$$

provided that $\theta_n \leq c_{inv,0}^{-2}$, where $\|v_h\|_{L_2(\partial E)}^2 \leq c_{inv,0} h_n^{-1} \|v_h\|_{L_2(E)}^2$

This lemma immediately yields **uniqueness** and **existence** of the solution $u_h \in V_{0h}$ and $\mathbf{u}_h \in \mathbb{R}^{N_h}$ of (9) and (4), respectively.

Uniform Boundedness of $a_h(\cdot, \cdot)$ on $V_{0h,*} \times V_{0h}$

Let us introduce the space $V_{0h,*} = V_{0h} + H_0^{\Delta,1}(Q)$ equipped with the norm

$$\|v\|_{h,*} = \left(\|v\|_h^2 + \sum_{n=1}^N (\theta_n h_n)^{-1} \|v\|_{L_2(Q_n)}^2 + \sum_{n=2}^N \|v_-^{n-1}\|_{L_2(\Sigma_{n-1})}^2 \right)^{\frac{1}{2}}. \quad (6)$$

Lemma (Boundedness)

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

$$|a_h(u, v_h)| \leq \mu_b \|u\|_{h,*} \|v_h\|_h, \quad \forall u \in V_{0h,*}, \forall v_h \in V_{0h}, \quad (7)$$

with $\mu_b = \max(c_{inv,1} \theta_{max}, 2)$, where $\theta_{max} = \max_n \{\theta_n\} \leq c_{inv,0}^{-2}$. and $c_{inv,k} = c_{inv,k}(p)$ are constants in the inverse inequalities

$$\|\partial_t \partial_{x_i} v_h\|_{L_2(E)}^2 \leq c_{inv,1} h_n^{-2} \|\partial_{x_i} v_h\|_{L_2(E)}^2 \quad \text{and} \quad \|v_h\|_{L_2(\partial E)}^2 \leq c_{inv,0} h_n^{-1} \|v_h\|_{L_2(E)}^2.$$

Consistency and Galerkin orthogonality

Lemma (Consistency)

If the solution $u \in H_0^{1,0}(Q)$ of the variational problem (2) belongs to $H^{\Delta,1}(Q)$, then it satisfies the consistency identity

$$a_h(u, v_h) = \ell_h(v_h) \quad \forall v_h \in V_{0h}. \quad (8)$$

Lemma (Galerkin orthogonality)

If the solution $u \in H_0^{1,0}(Q)$ of the variational problem (2) belongs to $H^{\Delta,1}(Q)$, then the Galerkin orthogonality

$$a_h(u - u_h, v_h) = 0 \quad \forall v_h \in V_{0h}. \quad (9)$$

holds, where $u_h \in V_{0h}$ is the space-time dG IgA solution.

Cea-like Discretization Error Estimate

Theorem (Cea-like Estimate)

Let the exact solution u of (2) belong to $H_0^{1,0}(Q) \cap H^{\Delta,1}(Q)$, and let u_h be the solution of the space-time IgA scheme (9). Then we get

$$\|u - u_h\|_h \leq (1 + \frac{\mu_b}{\mu_c}) \inf_{v_h \in V_{0h}} \|u - v_h\|_{h,*}, \quad (10)$$

where $\|v\|_{h,*} = \left(\|v\|_h^2 + \sum_{n=1}^N (\theta_n h_n)^{-1} \|v\|_{L_2(Q_n)}^2 + \sum_{n=2}^N \|v_-^{n-1}\|_{L_2(\Sigma_{n-1})}^2 \right)^{\frac{1}{2}}$ and
 $\|v\|_h = \left(\sum_{n=1}^N \left(\frac{1}{2} \|\nabla_x v\|_{L^2(Q_n)}^2 + \theta_n h_n \|\partial_t v\|_{L^2(Q_n)}^2 + \frac{1}{2} \|[v]\|_{L^2(\Sigma_{n-1})}^2 \right) + \frac{1}{2} \|v\|_{L^2(\Sigma_N)}^2 \right)^{\frac{1}{2}}.$

Proof: $\|u - u_h\|_h \leq \|u - v_h\|_h + \|v_h - u_h\|_h$

$$\begin{aligned} \mu_c \|v_h - u_h\|_h^2 &\leq a_h(v_h - u_h, v_h - u_h) = a_h(v_h - u, v_h - u_h) \\ &\leq \mu_b \|u - v_h\|_{h,*} \|v_h - u_h\|_h \quad \square \end{aligned}$$

Approximation Error Estimate

Theorem (Approximation Theorem)

Let $p_n + 1 \geq \ell_n \geq 2$ and $p_n + 1 \geq m_n \geq 1$ be integers, and let $u \in L_2(Q)$ such that the restriction $u^n := u|_{Q_n}$ belongs to $H^{\ell_n, m_n}(Q_n)$ for $n = 1, \dots, N$. Then there exists a quasi-interpolant $\Pi_h u \in V_{0h}$ such that

$$\begin{aligned} \|u - \Pi_h u\|_{h,*}^2 &= \left(\sum_{n=1}^N \left(\|\nabla_x(u - \Pi_h^n u)\|_{L_2(Q_n)}^2 + \theta_n h_n \|\partial_t(u - \Pi_h^n u)\|_{L_2(Q_n)}^2 \right. \right. \\ &\quad \left. \left. + \frac{1}{2} \|\llbracket (u - \Pi_h u)^{n-1} \rrbracket\|_{L_2(\Sigma_{n-1})}^2 \right) + \frac{1}{2} \|u - \Pi_h^N u\|_{L_2(\Sigma_N)}^2 \right) \\ &\quad + \sum_{n=1}^N \frac{1}{\theta_n h_n} \|u - \Pi_h^n u\|_{L_2(Q_n)}^2 + \sum_{n=2}^N \|(u - \Pi_h^{n-1} u)_-^{n-1}\|_{L_2(\Sigma_{n-1})}^2 \\ &\leq \sum_{n=1}^N \left(C_n \left(h_n^{2(\ell_n-1)} + \theta_n h_n^{2\ell_n-1} + h_n^{2m_n-1} + \theta_n h_n^{2m_n-1} \right) \|u\|_{H^{\ell_n, m_n}(Q_n)}^2 \right) \\ &\leq \sum_{n=1}^N \left(\tilde{C}_n \left(h_n^{2(\ell_n-1)} + h_n^{2(m_n-\frac{1}{2})} \right) \|u\|_{H^{\ell_n, m_n}(Q_n)}^2 \right) \end{aligned}$$

A priori Discretization Error Estimate

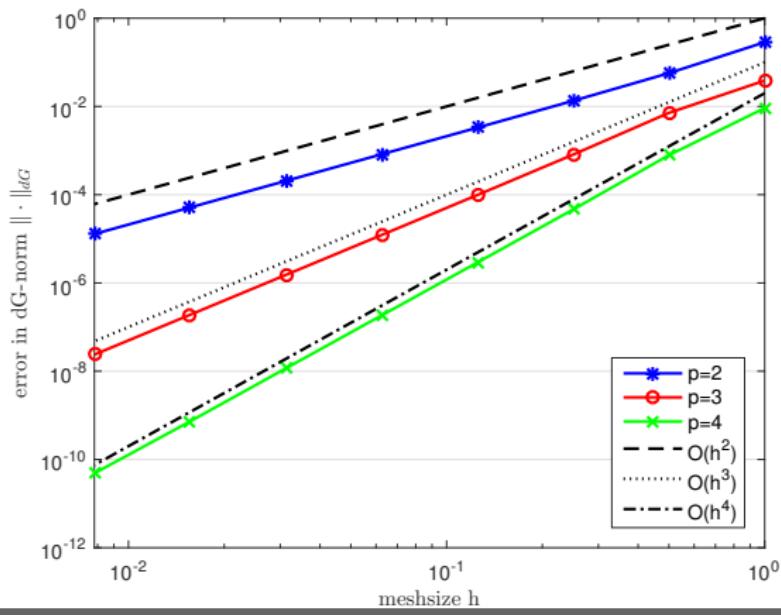
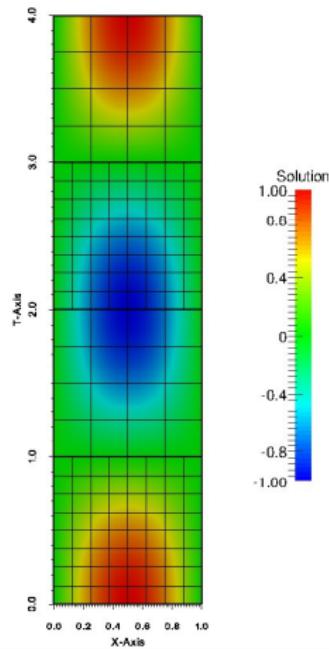
Theorem (A priori Discretization Error Estimate)

$$\|u - u_h\|_h \leq \left(1 + \frac{\mu_b}{\mu_c}\right) \sum_{n=1}^N \left(\tilde{C}_n \left(h_n^{2(\ell_n-1)} + h_n^{2(m_n-\frac{1}{2})} \right) \|u\|_{H^{\ell_n, m_n}(Q_n)}^2 \right)^{1/2}$$

We remark that for the case of highly smooth solutions, i.e., $p+1 \leq \min(\ell_n, m_n)$, the above estimate takes the form

$$\begin{aligned} \|u - u_h\|_h &\leq C \sum_{n=1}^N h_n^p \|u\|_{H^{p+1,p+1}(Q_n)} \\ &\leq C h^p \|u\|_{H^{p+1,p+1}(Q)} \end{aligned}$$

where the last estimate holds if $u \in H^{p+1,p+1}(Q)$ and $h = \max\{h_n\}$ is assumed.

(sp cG, mp dG) IgA for $d = 1$ and $p = 2, 3, 4$ 

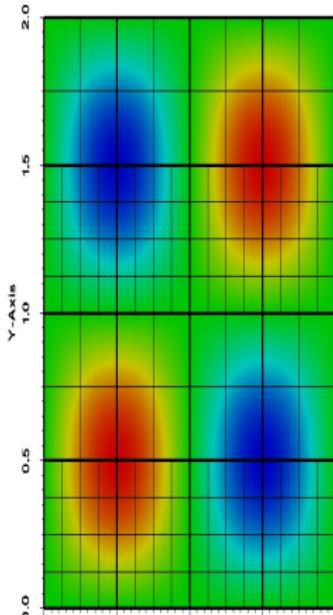
(sp cG, mp dG) IgA for $d = 1$ and $p = 2, 3, 4$

Error in the dG-norm and convergence rate for the exact solution

$$u(x, t) = \sin(\pi x) \sin\left(\frac{\pi}{2}(t + 1)\right)$$

and for B-Spline degrees 2, 3 and 4

refinement	$p = 2$		$p = 3$		$p = 4$	
	error	eoc	error	eoc	error	eoc
0	2.85633E-02	-	3.85617E-02	-	9.18731E-03	-
1	5.68232E-02	2.33	7.15551E-03	2.43	7.87619E-04	3.54
2	1.34212E-02	2.08	8.11296E-04	3.14	4.62549E-05	4.09
3	3.30721E-03	2.02	9.84754E-05	3.04	2.90675E-06	3.99
4	8.23704E-04	2.01	1.22142E-05	3.01	1.84067E-07	3.98
5	2.05716E-04	2.00	1.52376E-06	3.00	1.16139E-08	3.99
6	5.14138E-05	2.00	1.90375E-07	3.00	7.29917E-10	3.99
7	1.28522E-05	2.00	2.37936E-08	3.00	4.85647E-11	3.91

(mp cG, mp dG) IgA for $d = 1$ and $p = 2, 3$ 

ref.	$p = 2$		$p = 3$	
	error	eoc	error	eoc
0	0.0724164	-	0.00679753	-
1	0.0155074	2.22	0.000845039	3.01
2	0.00357715	2.12	0.000101469	3.06
3	0.000858059	2.06	1.24268e-05	3.03
4	0.000210051	2.03	1.53787e-06	3.01
5	5.19582e-05	2.02	1.91282e-07	3.01
6	1.29204e-05	2.01	2.38512e-08	3.00

Outline

1 Introduction

2 Time Multi-Patch Space-Time IgA

3 Space-Time Solvers

4 Conclusions & Outlooks

One huge system of IgA equations

Once the basis is chosen, the IgA scheme (9) can be rewritten as a huge system of algebraic equations of the form

$$\mathbf{L}_h \mathbf{u}_h = \mathbf{f}_h \quad (11)$$

for determining the vector $\mathbf{u}_h = ((u_{1,i})_{i \in \mathcal{I}_1}, \dots, (u_{N,i})_{i \in \mathcal{I}_N}) \in \mathbb{R}^{N_h}$ of the control points of the IgA solution

$$u_h(x, t) = \sum_{i \in \mathcal{I}_n} u_{n,i} \varphi_{n,i}(x, t), \quad (x, t) \in \overline{Q}_n, \quad n = 1, \dots, N,$$

solving the IgA scheme (9). The system matrix \mathbf{L}_h is the usual Galerkin (stiffness) matrix, and \mathbf{f}_h is the rhs (load) vector.
The matrix \mathbf{L}_h is non-symmetric, but positive definite !

System Matrix \mathbf{L}_h

The Galerkin matrix \mathbf{L}_h can be rewritten in the block form

$$\mathbf{L}_h = \begin{pmatrix} \mathbf{A}_1 & & & \\ -\mathbf{B}_2 & \mathbf{A}_2 & & \\ & -\mathbf{B}_3 & \mathbf{A}_3 & \\ & & \ddots & \ddots \\ & & & -\mathbf{B}_N & \mathbf{A}_N \end{pmatrix},$$

with the matrices

$$\mathbf{A}_n := \mathbf{M}_{n,x} \otimes \mathbf{K}_{n,t} + \mathbf{K}_{n,x} \otimes \mathbf{M}_{n,t} \text{ for } n = 1, \dots, N,$$

$$\mathbf{B}_n := \tilde{\mathbf{M}}_{n,x} \otimes \mathbf{N}_{n,t} \text{ for } n = 2, \dots, N.$$

Parallel Space-Time Multigrid Solvers

Solve

$$\mathbf{L}_h \mathbf{u}_h = \mathbf{f}_h, \quad \text{with} \quad \mathbf{L}_h = \begin{pmatrix} \mathbf{A}_1 & & & \\ -\mathbf{B}_2 & \mathbf{A}_2 & & \\ & \ddots & \ddots & \\ & & -\mathbf{B}_N & \mathbf{A}_N \end{pmatrix}$$

by the time-parallel MGM proposed by Gander & Neumüller ('16):

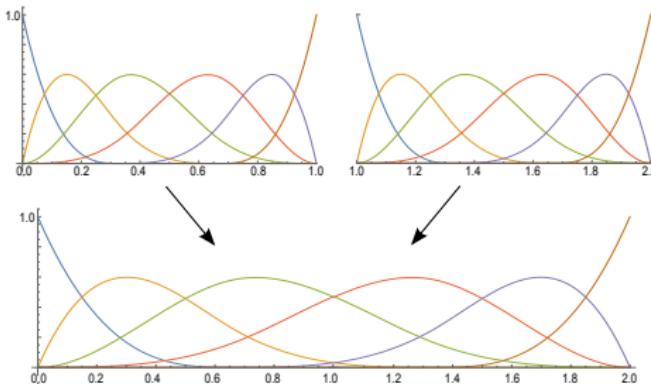
Ingredients:

- Time-Restriction and Prolongation
- Smoother

Time-Restriction

Two time-slabs are restricted to a single time-slab.

Assumption: Same basis on each slab.



Smoother

Inexact damped block Jacobi smoother:

$$\mathbf{u}_h^{(k+1)} = \mathbf{u}_h^{(k)} + \omega_t \mathbf{D}_h^{-1} \left[\mathbf{f}_h - \mathbf{L}_h \mathbf{u}_h^{(k)} \right] \quad \text{for } k = 1, 2, \dots$$

with $\omega_t = \frac{1}{2}$ and $\omega_t = \frac{1}{2} \mathbf{D}_h := \text{diag}\{\mathbf{A}_n\}_{n=1,\dots,N}$

- Parallel w.r.t. time
- Replace \mathbf{D}_h^{-1} by multigrid $\widehat{\mathbf{D}}_h^{-1}$ w.r.t space \rightarrow parallel in space

Parallel Solver Studies for $d = 3$ and $p = 1$

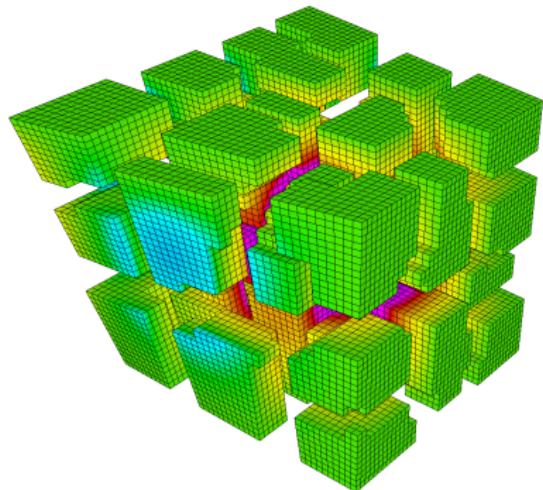
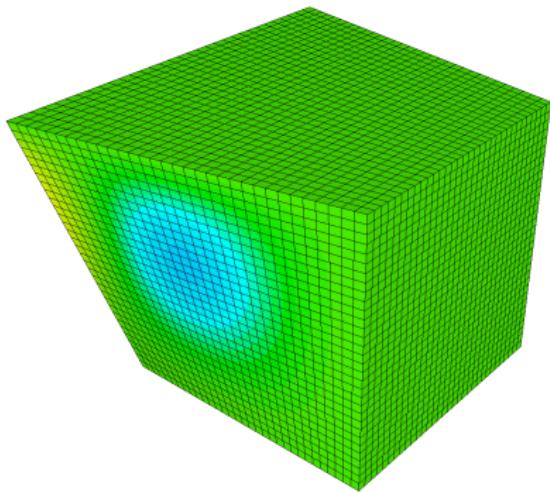


Figure: Computational spatial domain Ω decomposed into 4096 elements (left) and distributed over 32 processors (right). The IgA solution $u_h(x, t) \approx u(x, t) = \sin(\pi x_1) \sin(\pi x_2) \sin(\pi x_3) \sin(\pi t)$ is plotted at $t = 0.5$.

Parallel Solver Studies for $d = 3$ and $p = 1$

Convergence results in the $\|\cdot\|_h$ -norm for the regular solution

$$u(x, t) = \sin(\pi x_1) \sin(\pi x_2) \sin(\pi x_3) \sin(\pi t)$$

as well as iteration numbers and solving times for the parallel space-time multigrid preconditioned GMRES method on Vulcan

N	overall dof	$\ u - u_h\ _h$	eoc	c_x	c_t	cores	iter	time [s]
1	1 125	3.56223E-01	-	1	1	1	1	0.03
2	13 122	1.77477E-01	1.01	1	2	2	13	1.87
4	176 868	8.86255E-02	1.00	1	4	4	15	21.47
8	2 587 464	4.42868E-02	1.00	4	8	32	15	100.48
16	39 546 000	2.21376E-02	1.00	32	16	512	17	94.32
32	618 246 432	1.10675E-02	1.00	256	32	8192	17	162.90
64	9 777 365 568	5.53340E-03	1.00	2048	64	131072	17	211.33

Parallel Solver Studies for $d = 3$ and $p = 1$

Convergence results in the norm $\|\cdot\|_h$ for the low regularity solution

$$u(x, t) = \cos(\beta x_1) \cos(\beta x_2) \cos(\beta x_3)(1 - t)^\alpha \in H^{s, \alpha + \frac{1}{2} - \varepsilon}(Q),$$

with $\alpha = 0.75$ and $\beta = 0.3$, for an arbitrary $s \geq 2$ and for an arbitrary small $\varepsilon > 0$, as well as iteration numbers and solving times for the parallel space-time multigrid preconditioned GMRES method on Vulcan BlueGene/Q at LLNL

N	overall dof	$\ u - u_h\ _h$	eoc	c_x	c_t	cores	iter	time [s]
1	1 125	1.58022E-02	-	1	1	1	1	0.03
2	13 122	8.88627E-03	0.83	1	2	2	13	2.00
4	176 868	5.41668E-03	0.71	1	4	4	15	21.48
8	2 587 464	3.33881E-03	0.70	4	8	32	15	100.57
16	39 546 000	2.05545E-03	0.70	32	16	512	17	94.43
32	618 246 432	1.25859E-03	0.71	256	32	8192	17	171.83
64	9 777 365 568	7.65921E-04	0.72	2048	64	131072	17	211.49

New Space-Time Multigrid Solver / Preconditioner

Utilizing the tensor product structure

$$\mathbf{A} = \mathbf{A}_n = \mathbf{K}_t \otimes \mathbf{M}_x + \mathbf{M}_t \otimes \mathbf{K}_x,$$

to construct a cheap approximation $\widehat{\mathbf{A}}^{-1}$ to \mathbf{A}^{-1} , i.e., $\widehat{\mathbf{D}}^{-1}$ to \mathbf{D}^{-1} :

- $\mathbf{K}_t \neq \mathbf{K}_t^T$, $\mathbf{M}_t \neq \mathbf{M}_t^T$
- \mathbf{K}_t and \mathbf{M}_t are small ("1d" - matrices) compared to \mathbf{K}_x and \mathbf{M}_x ("1d, 2d, 3d" - SPD-matrices).
- Idea: Perform decomposition of $\mathbf{M}_t^{-1}\mathbf{K}_t$
 - 1 Fast Diagonalization: $\mathbf{M}_t^{-1}\mathbf{K}_t = \mathbf{X}\mathbf{D}\mathbf{X}^{-1}$, $\mathbf{X}, \mathbf{D} \in \mathbb{C}^{n_t \times n_t}$
 - 2 Complex-Schur: $\mathbf{M}_t^{-1}\mathbf{K}_t = \mathbf{Q}\mathbf{T}\mathbf{Q}^*$, $\mathbf{Q}, \mathbf{T} \in \mathbb{C}^{n_t \times n_t}$
 - 3 Real-Schur: $\mathbf{M}_t^{-1}\mathbf{K}_t = \mathbf{Q}\mathbf{T}\mathbf{Q}^T$, $\mathbf{Q}, \mathbf{T} \in \mathbb{R}^{n_t \times n_t}$
 - 4 Ref.: Sangalli & Tani (2016), Tani (2017) for elliptic BVP

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Fast Diagonalization

Eigenvalue decomposition $\mathbf{M}_t^{-1} \mathbf{K}_t = \mathbf{X} \mathbf{D} \mathbf{X}^{-1}$, i.e. $\mathbf{K}_t \mathbf{X} = \mathbf{M}_t \mathbf{X} \mathbf{D}$

- $\mathbf{D} = \text{diag}(\lambda_i)$, $\lambda_i \in \mathbb{C}$ (Eigenvalues)
- $\mathbf{X} \in \mathbb{C}^{n_t \times n_t}$ (Eigenvectors), $\mathbf{X}^{-1} \neq \mathbf{X}^*$!

Defining $\mathbf{Y} := (\mathbf{M}_t \mathbf{X})^{-1}$ gives

- $\mathbf{M}_t = \mathbf{Y}^{-1} \mathbf{X}^{-1}$
- $\mathbf{K}_t = \mathbf{Y}^{-1} \mathbf{D} \mathbf{X}^{-1}$

Hence, we obtain

$$\begin{aligned}\mathbf{A}^{-1} &= (\mathbf{K}_t \otimes \mathbf{M}_x + \mathbf{M}_t \otimes \mathbf{K}_x)^{-1} \\ &= ((\mathbf{Y}^{-1} \otimes \mathbf{I}) \cdot (\mathbf{D} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x) \cdot (\mathbf{X}^{-1} \otimes \mathbf{I}))^{-1} \\ &= (\mathbf{X} \otimes \mathbf{I}) \cdot \underbrace{(\mathbf{D} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)^{-1}}_{\text{diag}((\mathbf{K}_x + \lambda_i \mathbf{M}_x)^{-1})} \cdot (\mathbf{Y} \otimes \mathbf{I})\end{aligned}$$

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Solver for $\mathbf{K}_x + \lambda_i \mathbf{M}_x$

- Case 1: $\lambda_i \in \mathbb{R}^+$:
 - $\mathbf{K}_x + \lambda_i \mathbf{M}_x \dots$ SPD matrix \rightsquigarrow solvers available, e.g., DD, MG
- Case 2: $\lambda_i = \alpha_i + \beta_i i \in \mathbb{C}$, $\alpha_i > 0$:
 - $(\mathbf{K}_x + \lambda_i \mathbf{M}_x)^H \neq \mathbf{K}_x + \lambda_i \mathbf{M}_x$
 - Rewrite as symmetric, indefinite problem:

$$\bar{\mathbf{A}}_i := \begin{pmatrix} \mathbf{K}_x + \alpha_i \mathbf{M}_x & \beta \mathbf{M}_x \\ \beta \mathbf{M}_x & -(\mathbf{K}_x + \alpha_i \mathbf{M}_x) \end{pmatrix}$$

■ Robust preconditioner¹: $\text{cond}_1(P_i^{-1} \bar{\mathbf{A}}_i) \lesssim \sqrt{2}$

$$P_i := \begin{pmatrix} \mathbf{K}_x + (\alpha_i + |\beta_i|) \mathbf{M}_x & 0 \\ 0 & \mathbf{K}_x + (\alpha_i + |\beta_i|) \mathbf{M}_x \end{pmatrix}$$

■ $\mathbf{K}_x + (\alpha_i + |\beta_i|) \mathbf{M}_x$ is a SPD matrix \rightsquigarrow DD, MG

¹W. Zulehner, SIAM J. Matrix Anal. & Appl., 32(2), 536–560, 2011

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- Robust preconditioner¹ $\text{cond}_2(P_i^{-1} \bar{\mathbf{A}}_i) \leq \sqrt{2}$:

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-
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Numerical Tests

- Parallel application for each $i = 1, \dots, n_t$
- Unfortunately, $\text{cond}_2(\mathbf{X}) \gg 1$ (Eigenvectors)
- Reliable approximation $\hat{\mathbf{A}}$ only for small n_t .

$n_t - p$	$p = 2$	$p = 3$	$p = 4$	$p = 5$	$p = 6$	$p = 7$	$p = 8$
2	64	309	362	766	1706	3907	9501
4	481	1036	3037	9419	41959	39323	73946
8	2869	16118	39693	74370	180054	472758	1e+06
16	34332	188263	463148	1e+06	6e+06	3e+07	1e+08
32	701306	2e+06	1e+07	6e+07	4e+08	7e+09	1e+10
64	5e+07	4e+07	3e+08	3e+09	6e+10	3e+11	1e+12
128	2e+08	1e+09	1e+10	3e+11	2e+13	5e+13	4e+14

Table: condition number of $\mathbf{X} : \theta = 0.01$ and $|t_{i+1} - t_i| = 0.1$.

Complex Schur decomposition

The complex Schur decomposition gives $\mathbf{M}_t^{-1} \mathbf{K}_t = \mathbf{Q} \mathbf{T} \mathbf{Q}^*$

- $\mathbf{T} = \text{upperTriag}(T_{ij}) \in \mathbb{C}$, $T_{ii} = \lambda_i$ (Eigenvalues)
- $\mathbf{Q} \in \mathbb{C}^{n_t \times n_t}$ with $\mathbf{Q}^{-1} = \mathbf{Q}^* \rightarrow \text{cond}_2(\mathbf{Q}) = 1$.

Again, by defining $\mathbf{Y} := (\mathbf{M}_t \mathbf{Q}^*)^{-1}$, we obtain

- $\mathbf{M}_t = \mathbf{Y}^{-1} \mathbf{Q}$
- $\mathbf{K}_t = \mathbf{Y}^{-1} \mathbf{T} \mathbf{Q}$.

Hence, we have

$$\begin{aligned}\mathbf{A}^{-1} &= (\mathbf{M}_x \otimes \mathbf{K}_t + \mathbf{K}_x \otimes \mathbf{M}_t)^{-1} \\ &= (\mathbf{Q}^* \otimes \mathbf{I}) \cdot (\mathbf{T} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x)^{-1} \cdot (\mathbf{Y} \otimes \mathbf{I})\end{aligned}$$

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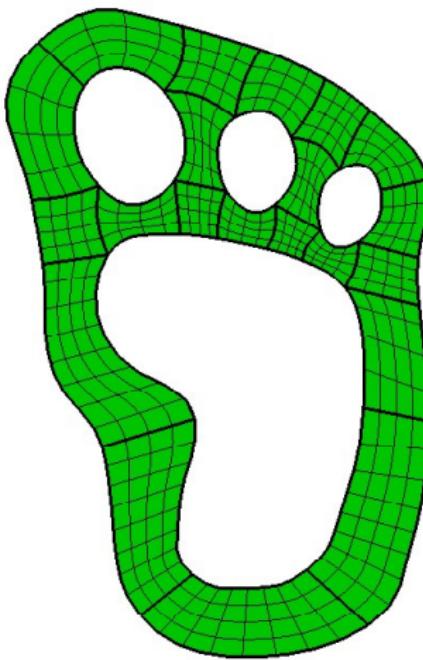
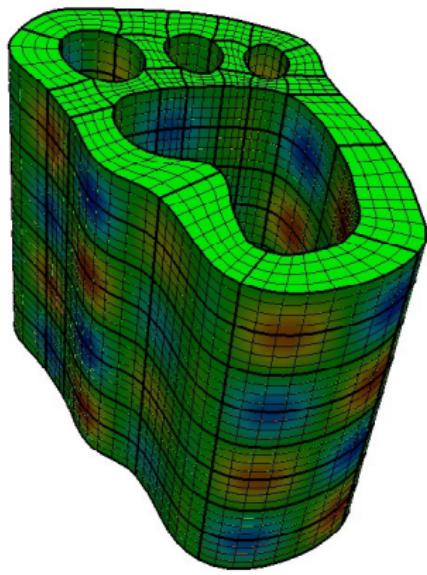
Complex Schur decomposition (cont.)

$\mathbf{T} \otimes \mathbf{M}_x + \mathbf{I} \otimes \mathbf{K}_x$ has the following structure

$$\begin{pmatrix} \mathbf{K}_x + \lambda_1 \mathbf{M}_x & T_{12} \mathbf{M}_x & \dots \\ 0 & \mathbf{K}_x + \lambda_2 \mathbf{M}_x & T_{23} \mathbf{M}_x \\ \vdots & 0 & \ddots & T_{n_t-1 n_t} \mathbf{M}_x \\ 0 & \dots & 0 & \mathbf{K}_x + \lambda_{n_t} \mathbf{M}_x \end{pmatrix}$$

- Application is done staggered
- $\mathbf{K}_x + \lambda_i \mathbf{M}_x$ has the same structure as in the diagonal case.
- **Real Schur decomposition** works similar
~ only real arithmetic.

YETI-footprint: Space mp cG & time mp dG IgA



Numerical Tests: Spatial Solver: $\mathbf{K}_x + \lambda_i \mathbf{M}_x$

- $\lambda_i \in \mathbb{C}$
- MinRes method with tolerance $\varepsilon = 10^{-8}$
- $(\mathbf{K}_x + (\alpha_i + |\beta_i|) \mathbf{M}_x)^{-1} \rightsquigarrow$ Direct solver

Maximum number of iterations for $i = 1, \dots, n_t$.

ref. x and t	$p = 2$	$p = 3$	$p = 4$	$p = 5$	$p = 6$
1	18	22	22	22	22
2	20	22	22	22	21
3	22	22	22	21	21
4	22	22	22	21	21
5	22	22	22	20	22

Numerical Tests: Sparse Direct Solver

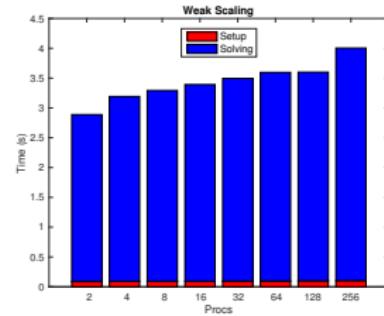
- Degree $p_x, p_t = (3, 3)$; $\theta = 0.01$ and $|t_i - t_{i-1}| = 0.1$
- $\bar{A}_i \rightsquigarrow$ MinRes with $\varepsilon = 10^{-4}$ (It. ≤ 10).
- $(\mathbf{K}_x + (\alpha_i + |\beta_i|)\mathbf{M}_x)^{-1} \rightsquigarrow$ Direct solver
- Direct Solver: PARDISO
- Tolerance Multigrid $\varepsilon = 10^{-8}$

#dofs	ref	#slabs	MG-It	Direct		Diag	
				Setup	Solving	Setup	Solving
15950	2 3	2	7	1.9	0.7	0.04	2.3
97020	3 3	4	7	38.6	8.5	0.3	19.4
665720	4 3	8	7	1008	94.6	3.7	183.8
#dofs	ref	#slabs	MG-It	C-Schur		R-Schur	
15950	2 3	2	7	0.05	2.4	0.04	1.3
97020	3 3	4	7	0.5	19.9	0.3	11.1
665720	4 3	8	7	5.4	187.3	3.7	108.0

Numerical Tests: Parallelization in time - Real Schur

- Degree $p_x, p_t = (3, 3)$, refinement $r_x, r_t = (2, 3)$
- $\theta = 0.01$ and $|t_i - t_{i-1}| = 0.1$;
- $(\mathbf{K}_x + (\alpha_i + |\beta_i|)\mathbf{M}_x)^{-1} \rightsquigarrow$ Direct solver
- Direct Solver: PARDISO
- Tolerance $\varepsilon = 10^{-8}$
- #slabs = #Processors.

#dofs	#slabs	MG-It.	Setup	Solving
48510	2	7	0.088	2.8
97020	4	7	0.092	3.1
194040	8	7	0.093	3.2
388080	16	7	0.093	3.3
776160	32	7	0.094	3.4
1552320	64	7	0.096	3.5
3104640	128	7	0.100	3.5
6209280	256	7	0.104	3.9



Parallelization in Space & Time – Complex Schur

- Spatial domain YETI-Footprint (84 patches)
- Degree $p_x, p_t = (3, 3)$, $\theta = 0.01$ and $t \in [0, 4]$
- Parallel MG as preconditioner/solver for spatial problems

#dofs	refs	#sl.	C_{total}	C_x	C_t	it	Setup	Solving
42028	1	4	2	1	2	6	0.37	431.4
84056	1	8	4	1	4	6	0.39	441.4
193368	2	8	16	4	4	6	0.90	292.5
386736	2	16	32	4	8	7	0.46	345.3
1092784	3	16	128	16	8	7	0.55	360.8
2185568	3	32	256	16	16	7	0.72	326.7
4371136	3	64	512	16	32	7	0.80	358.3

Parallelization in Space & Time – Real Schur

- Spatial domain YETI-Footprint (84 patches)
- Degree $p_x, p_t = (3, 3)$, $\theta = 0.01$ and $t \in [0, 4]$
- Parallel MG as preconditioner/solver for spatial problems

#dofs	refs	#sl.	C_{total}	C_x	C_t	it	Setup	Solving
42028	1	4	2	1	2	9	0.37	316.1
84056	1	8	4	1	4	9	0.39	322.2
193368	2	8	16	4	4	10	0.42	241.3
386736	2	16	32	4	8	10	0.44	245.7
1092784	3	16	128	16	8	11	0.53	267.2
2185568	3	32	256	16	16	11	0.54	270.6
4371136	3	64	512	16	32	11	0.76	296.9

Parallelization in Space & Time – Real Schur

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#dofs	refs	#sl.	c_{total}	c_x	c_t	it	Setup	Solving	serial	$c_t = 1$
42028	1	4	2	1	2	9	0.37	316.1	0.59	36.1
84056	1	8	4	1	4	9	0.39	322.2	1.06	71.9
193368	2	8	16	4	4	10	0.42	241.3	1.02	45.7
386736	2	16	32	4	8	10	0.44	245.7	1.86	90.9
1092784	3	16	128	16	8	11	0.53	267.2	1.79	91.1
2185568	3	32	256	16	16	11	0.54	270.6	3.41	179.8
4371136	3	64	512	16	32	11	0.76	296.9	6.53	377.8

Numerical Tests: Parallelization in Space & Time

- **Alternative Version** – non-symmetric IETI-DP for \mathbf{A}_n
- Spatial domain Ω : 4×4 square grid
- Degree $p_x, p_t = (3, 3)$, $\theta = 0.01$ and $|t_i - t_{i-1}| = 0.1$.
- GMRes-IETI-DP in the smoother (3 Iterations).
- Coarsening only in time!

#dofs	ref x	#sl.	C_{total}	C_x	C_t	It.	Setup	Solving
23276	2	4	2	1	2	8	5.7	22.3
46552	2	8	4	1	4	8	6.9	29.5
93104	2	16	8	1	8	8	8.3	36.6
267696	3	16	32	4	8	8	9.7	44.5
535392	3	32	64	4	16	8	11.3	54.0
1774432	4	32	256	16	16	7	9.6	82.5
3548864	4	64	512	16	32	10	11.6	185.3

Outline

1 Introduction

2 Time Multi-Patch Space-Time IgA

3 Space-Time Solvers

4 Conclusions & Outlooks

Conclusions & Ongoing Work & Outlook

- Space-time IgA: space singlepatch cG and time-multipatch dG
- Space-time IgA: space multipatch cG and time-multipatch dG
- Space-time IgA: Fast generation via tensor techniques
- Space-time IgA: Fast parallel solvers
- Functional a posteriori estimates and THB-Spline adaptivity
 - ⇒ joint work with S. Matculevich and S. Repin
 - ⇒ talk by Svetlana Matculevich on Thursday !
- space-time multipatch dG IgA + adaptivity + fast generation + efficient parallel solvers ???
- Adaptive Space-Time FEM
 - ⇒ talk by Andreas Schafelner on Tuesday !

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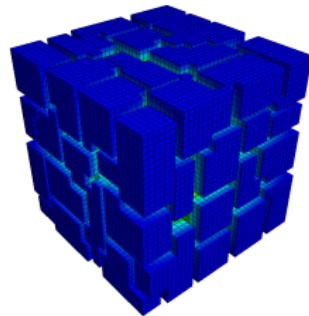
Numerical Results: Parallel Solution for $p = 1$

2d fixed spatial domain $\Omega = (0, 1)^2$ yielding $Q = \Omega \times (0, T) = (0, 1)^3$

Exact solution: $u(x, t) = \sin(\pi x_1) \sin(\pi x_2) \sin(\pi t)$

Figure shows space-time decomposition with 64 subdomains

Table shows parallel performance of the parallel AMG hypre preconditioned GMRES stopped after the relative residual error reduction by 10^{-10} !



Dofs	$\ u - u_h\ _{L_2(Q)}$	Rate	iter	time [s]	cores
8	3.65528e-01	-	1	0.01	1
27	9.39008e-02	1.961	2	0.01	1
125	2.32674e-02	2.013	6	0.01	1
729	5.75635e-03	2.015	15	0.07	64
4 913	1.43198e-03	2.007	16	0.14	64
35 937	3.57217e-04	2.003	19	0.40	64
274 625	8.92171e-05	2.001	24	1.04	1 024
2 146 689	2.22941e-05	2.001	29	3.65	1 024
16 974 593	5.57231e-06	2.000	36	21.40	1 024
135 005 697	1.39293e-06	2.000	50	36.26	8 192
1 076 890 625	3.48206e-07	2.000	63	156.50	16 384

This example was computed on the supercomputer Vulcan BlueGene/Q in Livermore by M. Neumüller.

Supercomputing Results on Vulcan: (3+1)D, $p = 1$

3d fixed spatial domain $\Omega = (0, 1)^3$ yielding $Q = \Omega \times (0, T) = (0, 1)^4$

Exact solution: $u(x, t) = \sin(\pi x_1) \sin(\pi x_2) \sin(\pi x_3) \sin(\pi t)$

Table shows parallel performance of the parallel AMG hypre preconditioned GMRES stopped after the relative residual error reduction by 10^{-6} !

dofs	$\ u - u_h\ _{L_2(Q)}$	rate	iter	time [s]	cores
16	2.61353e-01	-	1	0.01	1
81	7.24784e-02	1.85	2	0.01	1
625	1.75301e-02	2.05	6	0.02	16
6 561	4.32537e-03	2.02	8	0.06	16
83 521	1.07679e-03	2.01	10	0.61	512
1 185 921	2.68823e-04	2.00	12	2.25	512
17 850 625	6.71720e-05	2.00	15	15.92	16 384
276 922 881	1.67895e-05	2.00	21	53.78	16 384
4 362 470 401	4.19714e-06	2.00	30	186.42	65 536

THANK YOU VERY MUCH !

