Efficient Solution Techniques for Isogeometric Analysis

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High Performance Computing in Science and Engineering (HPCSE)

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The IGA team

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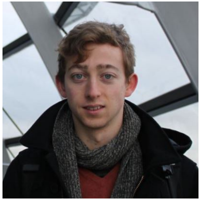
Roel Tielen (ASML)



Hugo Verhelst (TUD)

Andrzej Jaeschke (Łódź)

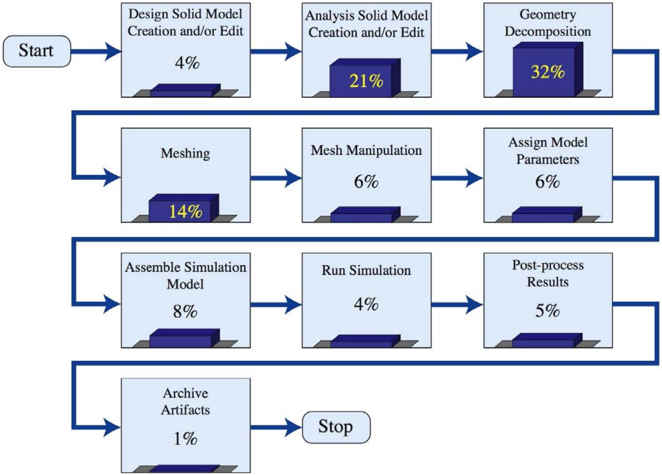
Collaborations

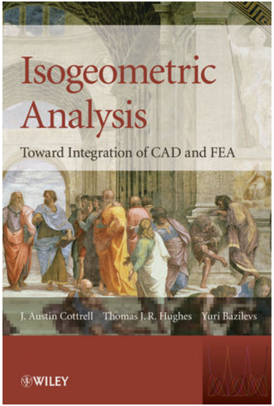
Göddeke (U Stuttgart), Elgeti/Helmig (RWTH Aachen, TU Vienna), Mantzaflaris (INRIA), Gauger (TU K'lautern), Jüttler (JKU), Simeon (TU K'lautern), ...

Funding

EU-H2020 MOTOR (GA 678727), NWO FlexFloat starting 2022 ($\Rightarrow$ apply by May 31st)

Isogeometric Analysis (IGA)





Ted Blacker, Sandia National Laboratories

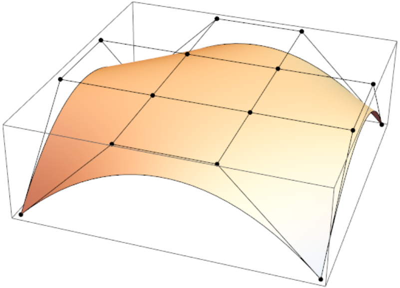
My personal 'top 3 features' of IGA

❶ Unified mathematical approach towards geometry modelling *and* PDE analysis

$$\mathbf{x}(\xi,\eta) = \sum_{i,j} \mathbf{x}_{i,j} N_i^p(\xi) N_j^q(\eta)$$

$$u(\xi,\eta) = \sum_{i,j} u_{i,j} N_i^p(\xi) N_j^q(\eta)$$

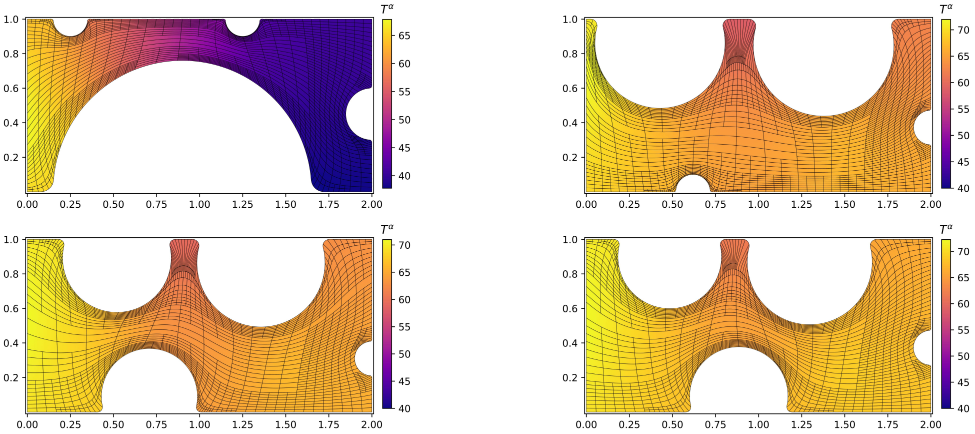
with B-spline basis functions N_i^p of order p.



- PoU, local support, non-negativity
- Geometry-preserving refinements
- Generic extension to higher order
- Operations can be expressed as SpMVs

My personal 'top 3 features' of IGA

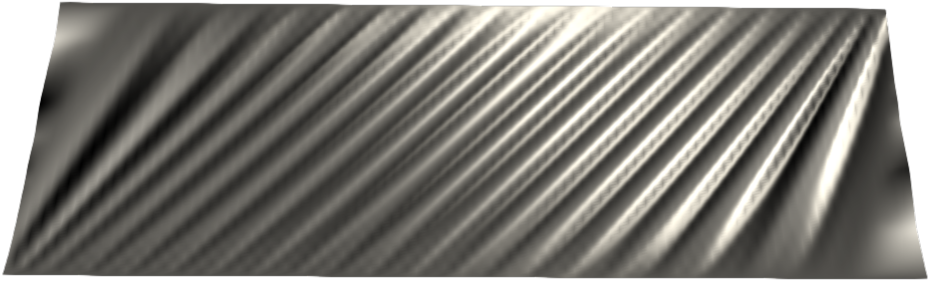
2. 'Meshing' + design optimization becomes one global optimization problem



J.P. Hinz, A. Jaeschke, M. Möller, C. Vuik (2021). The role of PDE-based parameterization techniques in gradient-based IGA shape optimization applications. CMAME 378, 10.1016/j.cma.2021.113685.

My personal 'top 3 features' of IGA

3. C^{p-1}-continuity enables direct simulation of higher-order PDEs



H.M. Verhelst, `https://github.com/gismo/gsKLShell` (v22.1)

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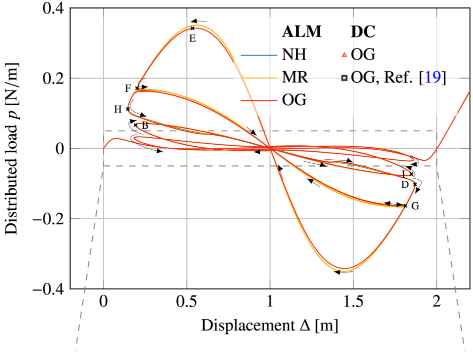
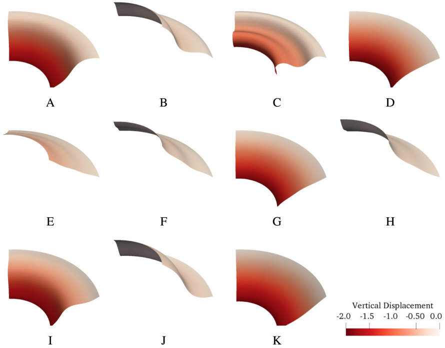
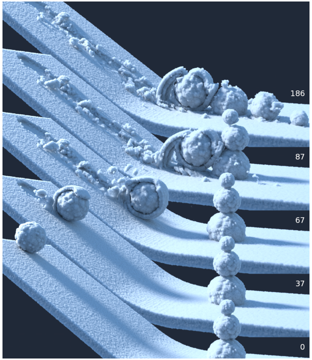


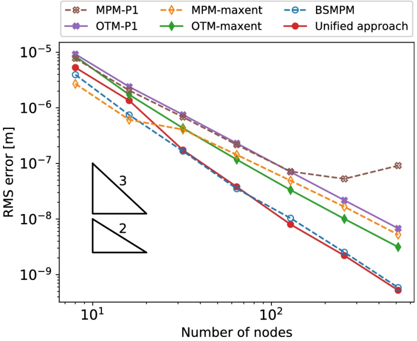


H.M. Verhelst, M. Möller, J.H. Den Besten, A. Mantzaflaris, and M.L. Kaminski (2021). Stretch-based hyperelastic material formulations for isogeometric Kirchhoff–Love shells with application to wrinkling. CAD, 139, 10.1016/j.cad.2021.103075.

My personal 'top 3 features' of IGA

3 C^{p-1}-continuity enables higher-order material point method





Left: Stomakhin et al. (2013). A material point method for snow simulation. ACM Trans. Graph. 32, 10.1145/2461912.2461948. *Right:* E. Wobbes, R. Tielen, M. Möller, and C. Vuik (2021). Comparison and unification of material-point and optimal transportation meshfree methods. Comput. Part. Mech., 8, 113-133, 10.1007/s40571-020-00316-7.

But ...

... IGA also has its challenges

- automatic BRep-CAD-to-VRep-analysis workflows
- efficient $C^{>0}$ multi-patch coupling
- efficient assembly of linear and multi-linear forms
- efficient solution of linear systems of equations
- ...

State of the art in IGA solvers

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Direct solvers

- Performance study [Collier *et al.* 2012]
- Refined IGA [Garcia *et al.* 2018]

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h-multigrid techniques

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Transient problems

- Parallel splitting solvers [Puzyrev et al. 2019]
- Space-time solvers [Langer et al 2016]
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- MGRIT-IGA [Tielen et al. 2021]

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Outline

1. Motivation and problem formulations
2. Part I: Multigrid methods for IGA
   - Introduction to h- and p-multigrid
   - ILUT smoother for single-patch IGA
   - Block-ILUT smoother for multi-patch IGA
3. Part II: Multigrid reduction in time (MGRIT)
   - Introduction to MGRIT
   - MGRIT-IGA
4. Conclusions

Model problems

Part I: Convection-diffusion-reaction equation (CDR-Eq)

$$
\begin{aligned}
-\nabla \cdot (\mathbb{D}\nabla u(\mathbf{x})) + \mathbf{v} \cdot \nabla u(\mathbf{x}) + r u(\mathbf{x}) &= f && \mathbf{x} \in \Omega \\
u(\mathbf{x}) &= g && \mathbf{x} \in \Gamma
\end{aligned}
$$

Part II: Heat equation (Heat-Eq)

$$
\begin{aligned}
\partial_t u(\mathbf{x}, t) - \kappa \Delta u(\mathbf{x}, t) &= f && \mathbf{x} \in \Omega,\ t \in [0, T] \\
u(\mathbf{x}, t) &= g && \mathbf{x} \in \Gamma,\ t \in [0, T] \\
u(\mathbf{x}, 0) &= u^0(\mathbf{x}) && \mathbf{x} \in \Omega
\end{aligned}
$$

d-dimensional connected Lipschitz domain $\Omega \subset \mathbb{R}^d$, its boundary $\Gamma = \partial\Omega$, load vector $f \in L^2(\Omega)$, Dirichlet boundary conditions g, diffusion tensor $\mathbb{D}$ and coefficient κ, resp., divergence-free velocity field $\mathbf{v}$, source term r, and u^0 initial conditions

Variational formulation

CDR-Eq: Find $u \in \mathcal{H}^1_g(\Omega)$ such that

$$a\,(w, u) = l(w) \qquad \forall w \in \mathcal{H}^1_0(\Omega)$$

Heat-Eq: Given $u^n \in \mathcal{H}^1_g(\Omega)$ find $u^{n+1} \in \mathcal{H}^1_g(\Omega)$ such that

$$\langle w, u^{n+1}\rangle + \Delta t\, k(w, u^{n+1}) = \langle w, u^n\rangle + l(w) \qquad \forall w \in \mathcal{H}^1_0(\Omega)$$

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with (bi-)linear forms defined as

$$a(w, u) := \int_\Omega \nabla w \cdot (\mathbb{D}\nabla u) + w\,(\mathbf{v} \cdot \nabla u + ru)\,\mathrm{d}\mathbf{x} \qquad \langle w, u\rangle := \int_\Omega w\,u\,\mathrm{d}\mathbf{x}$$

$$k(w, u) := \kappa \int_\Omega \nabla u \cdot \nabla u\,\mathrm{d}\mathbf{x} \qquad l(w) := \langle w, f\rangle$$

Algebraic equations

CDR-Eq: Find $u_{h,p} \in \mathcal{V}_{h,p}$ such that

$$\mathrm{A}_{h,p}\,\mathrm{u}_{h,p} = \mathrm{f}_{h,p}$$

Heat-Eq: Find $u_{h,p}^{n+1} \in \mathcal{V}_{h,p}$ such that

$$[\,\mathrm{M}_{h,p} + \Delta t\ \mathrm{K}_{h,p}]\ \mathrm{u}_{h,p}^{n+1} = \mathrm{M}_{h,p}\,\mathrm{u}_{h,p}^{n} + \mathrm{f}_{h,p}$$

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The unknown solution vector is given by

$$u_{h,p}^{n} = \sum_{j=1}^{N_b} \mathrm{u}_j^{n} \varphi_j(\mathbf{x}), \quad \text{where } \mathrm{u}_j^{n} \text{ is the basis coefficient corresponding to } \varphi_j \in \mathcal{V}_{h,p}$$

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and the system matrices and right-hand side vector are defined as

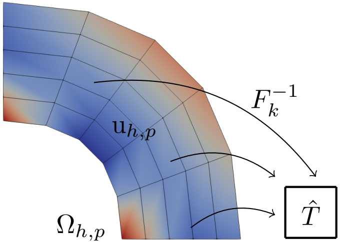
$$\mathrm{A}_{h,p} = \{a(\varphi_i, \varphi_j)\}_{i,j}, \quad \mathrm{K}_{h,p} = \{k(\varphi_i, \varphi_j)\}_{i,j}, \quad \mathrm{M}_{h,p} = \{\langle \varphi_i, \varphi_j \rangle\}_{i,j}, \quad \mathrm{f}_{h,p} = \{l(\varphi_i)\}_i$$

Ansatz spaces

FEA: element-wise 'pull-back'

$$\mathcal{V}_{h,p} = \{v \in C^0(\bar{\Omega}) : v|_{T_k} \in \mathbb{Q}_p \circ F_k^{-1}, \forall T_k \in \mathcal{T}_h$$
$$v|_\Gamma = 0\}$$

with $\mathbb{Q}_p$ the space of polynomials of degree p or less



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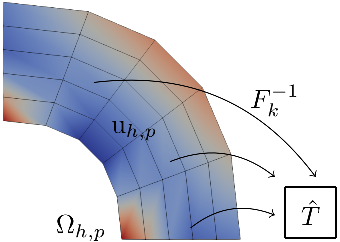

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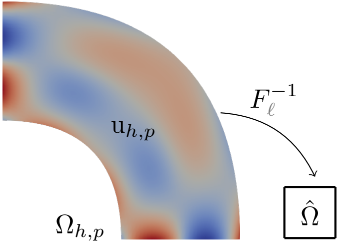
$$\mathcal{V}_{h,p} = \text{span}\{\hat{\varphi}_j \circ F_\ell^{-1}\}$$

with $\hat{\varphi}_j$ the j^{th} B-spline basis function



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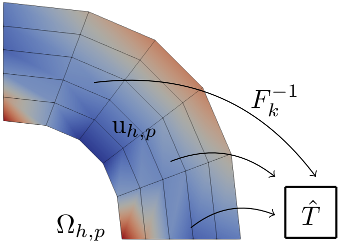

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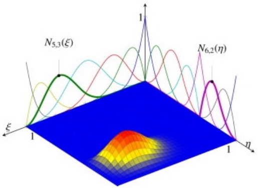
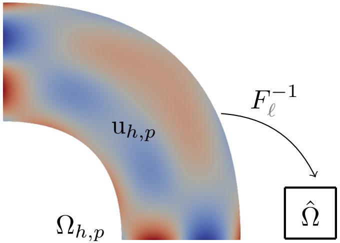
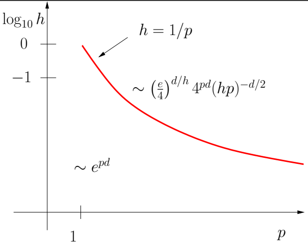
Think of IGA patches as macro elements





B-spline illustration taken from: H.Nguyen-XuanaLoc *et al.* (2014) 10.1016/j.tafmec.2014.07.008.

Condition number

<table>
<tr><th></th><th>SEM-NI</th><th>IGA-C^0</th><th>IGA-C^{p-1}</th></tr>
<tr><td>$\mathcal{K}(M)$</td><td>$\sim p^d$</td><td>$\sim p^{-d/2}4^{pd}$</td><td>
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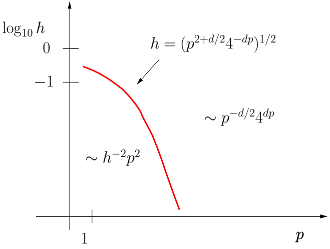
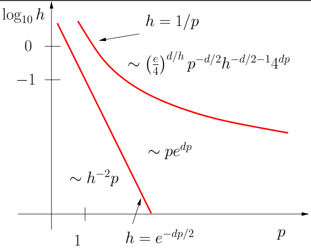
<tr><td>$\mathcal{K}(K)$</td><td>$\sim h^{-2}p^3$</td><td>
</td><td>
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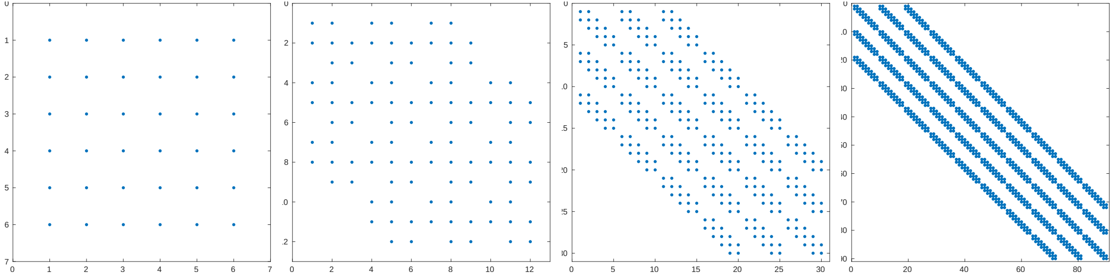
From: P. Gervasio, L. Dedè, O. Chanon, and A. Quarteroni (2020) 10.1007/s10915-020-01204-1.

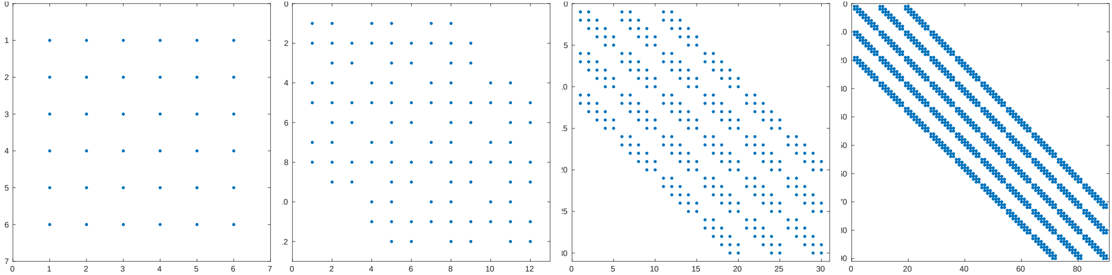
Sparsity pattern: 2d single patch, $p = 1$

IGA-C^0

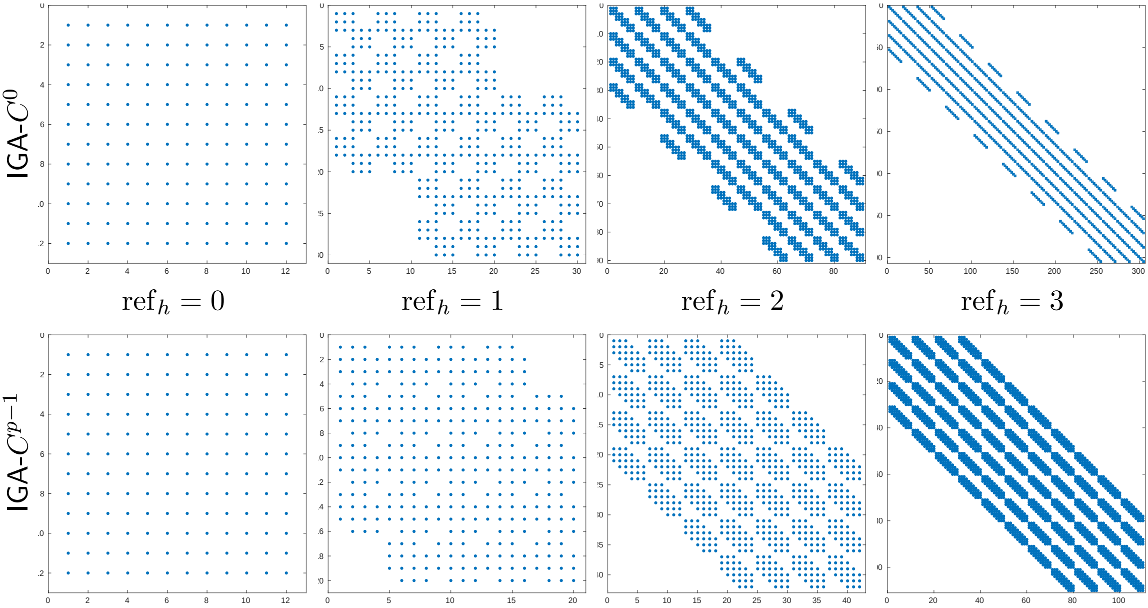


$\mathrm{ref}_h = 0$ $\qquad$ $\mathrm{ref}_h = 1$ $\qquad$ $\mathrm{ref}_h = 2$ $\qquad$ $\mathrm{ref}_h = 3$

IGA-C^{p-1}

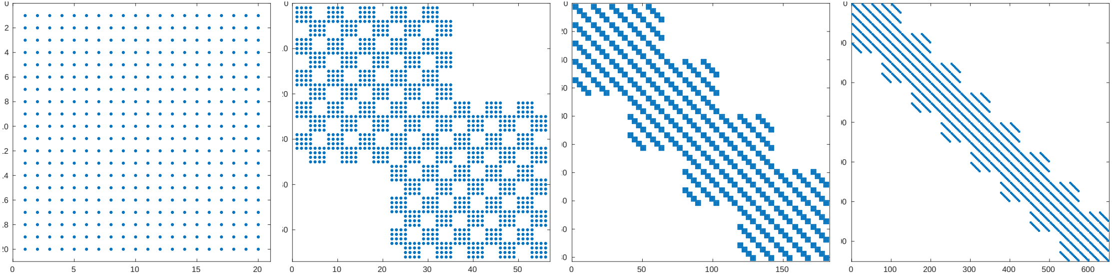


Sparsity pattern: 2d single patch, $p = 2$



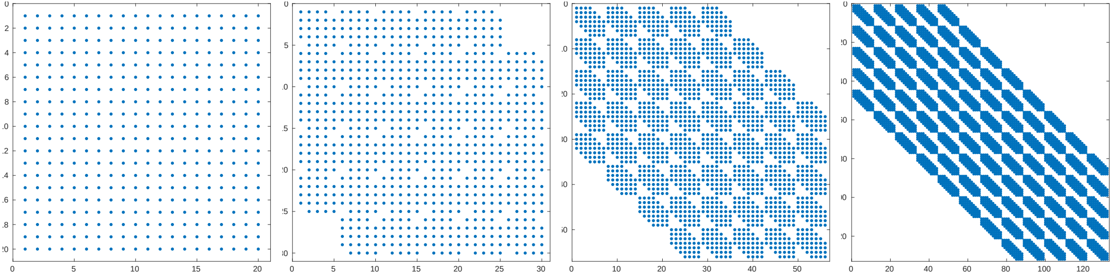
Sparsity pattern: 2d single patch, $p = 3$

IGA-C^0

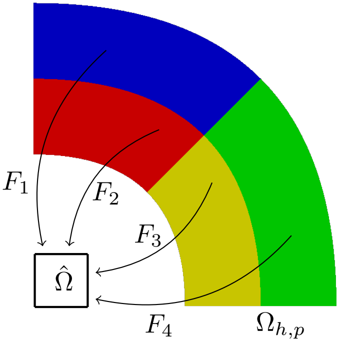


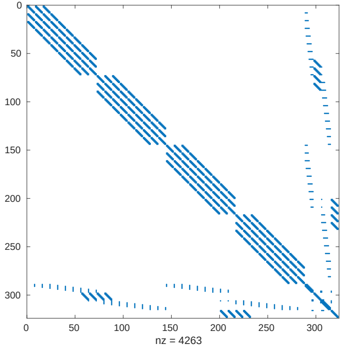
$\mathrm{ref}_h = 0$ $\mathrm{ref}_h = 1$ $\mathrm{ref}_h = 2$ $\mathrm{ref}_h = 3$

IGA-C^{p-1}



Sparsity pattern: 2d multi-patch IGA-C^{p-1}, $\mathrm{ref}_h = 3$





Four-patch geometry with C^0 coupling of conforming degrees of freedom.

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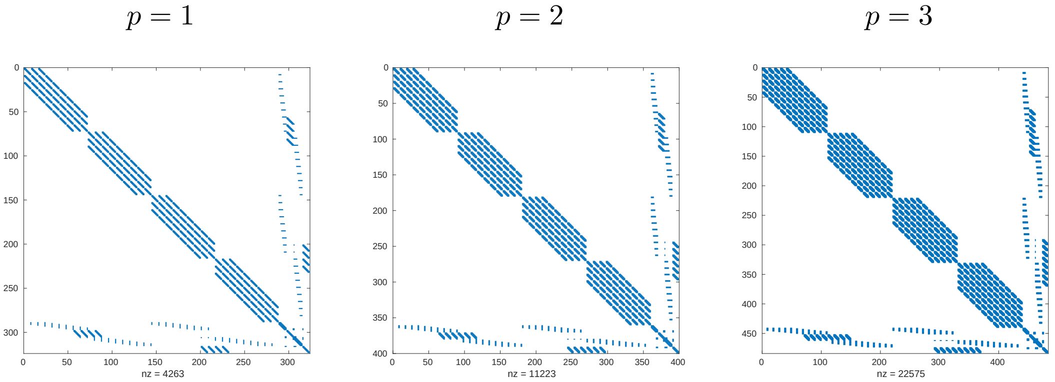
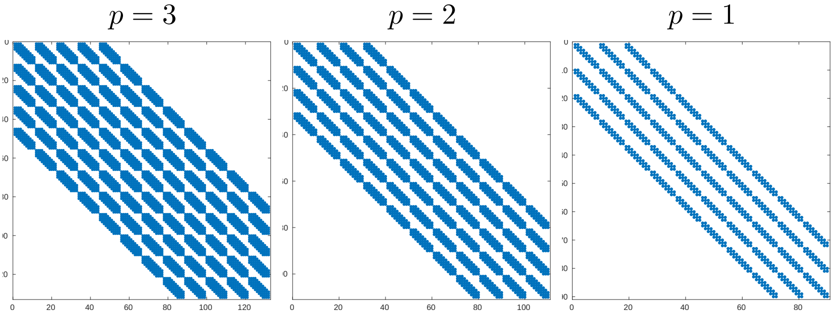
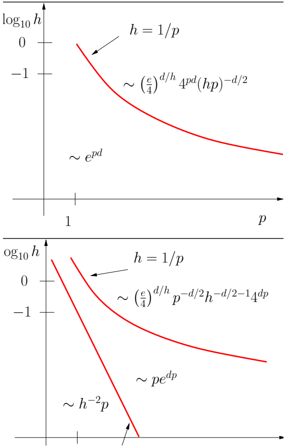


Four-patch geometry with C^0 coupling of conforming degrees of freedom.

Sketch of our solution strategy

- Coarsening in p reduces the stencil but not so much the number of unknowns
  - p-**multigrid with *direct* projection** $\mathcal{V}_{h,p} \searrow \mathcal{V}_{h,1}$
  - note that spaces are not nested $(\mathcal{V}_{h,p} \not\supset \mathcal{V}_{h,p-1} \not\supset \dots)$
  - **ILUT smoother** at single-patch level





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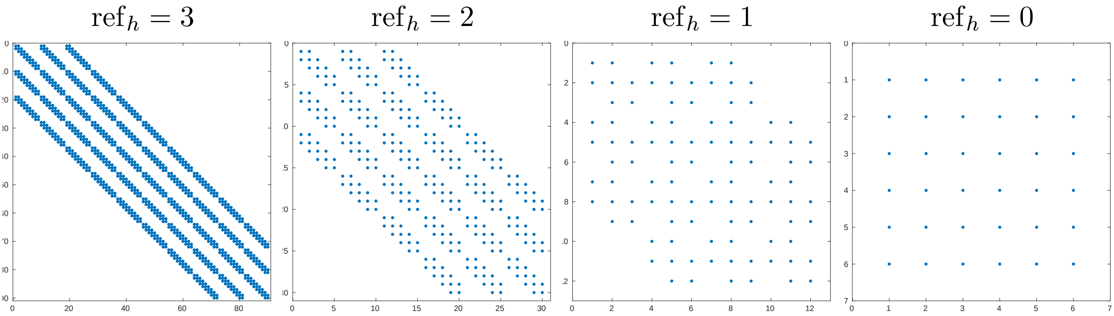

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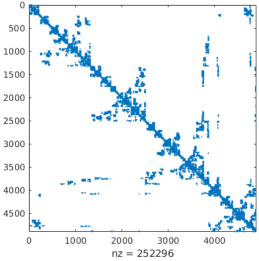
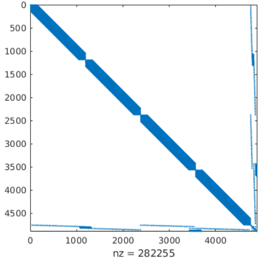
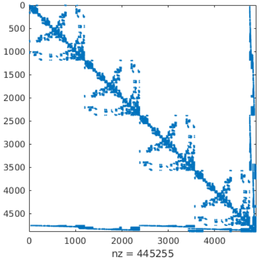
- Exploit the block structure of multi-patch topologies by using a ***block*-ILUT smoother**







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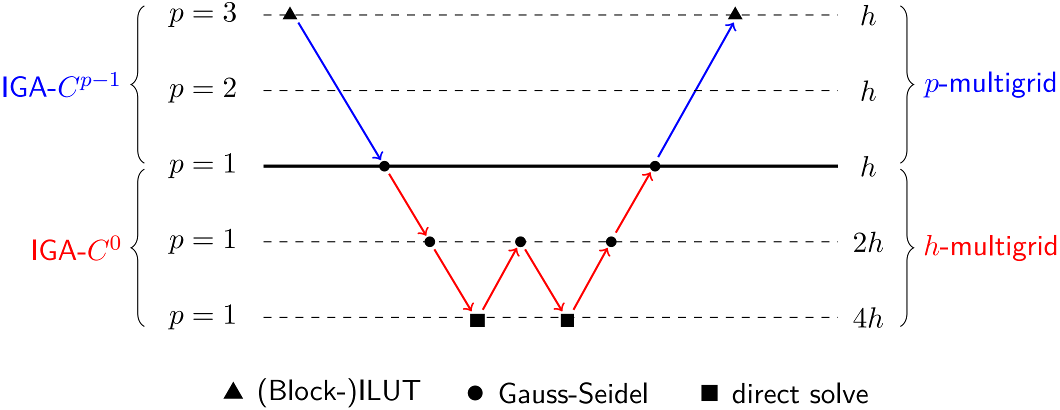
- robust with respect to h, p, N_p, and 'the PDE'
- computational efficient throughout all problem sizes
- applicable to locally refined THB-splines
- good spatial solver for transient problems (Part II)

The complete multigrid cycle



The complete multigrid algorithm – the outer p-multigrid part

1. Starting from $\mathrm{u}_{h,p}^{(0,0)}$ apply ν_1 pre-smoothing steps:

$$\mathrm{u}_{h,p}^{(0,m)} := \mathrm{u}_{h,p}^{(0,m-1)} + \mathrm{S}_{h,p}\left(\mathrm{f}_{h,p} - \mathrm{A}_{h,p}\,\mathrm{u}_{h,p}^{(0,m-1)}\right), \quad m = 0, 1, \ldots, \nu_1$$

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The complete multigrid algorithm – the inner h-multigrid part

3.1. Starting from $\mathrm{u}_{h,1}^{(k,0)}$ apply ν_1 pre-smoothing steps:

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3.2. Restrict the residual onto $\mathcal{V}_{2h,1}$:

$$\mathrm{r}_{2h,1} = \mathrm{I}_{h,1}^{2h,1}\left(\mathrm{f}_{h,1} - \mathrm{A}_{h,1}\,\mathrm{u}_{h,1}^{(k,\nu_1)}\right), \quad \mathrm{I}_{h,1}^{2h,1} \text{ linear interpolation}$$

3.3. Solve the residual equation by applying h-multigrid recursively or the coarse-grid solver:

$$\mathrm{A}_{2h,1}\,\mathrm{e}_{2h,1} = \mathrm{r}_{2h,1}$$

3.4. Project the error onto $\mathcal{V}_{h,1}$ and update the solution:

$$\mathrm{u}_{h,1}^{(k,\nu_1)} := \mathrm{u}_{h,1}^{(k,\nu_1)} + \mathrm{I}_{2h,1}^{h,1}\left(\mathrm{e}_{2h,1}\right), \quad \mathrm{I}_{2h,1}^{h,1} := \frac{1}{2}\left(\mathrm{I}_{h,1}^{2h,1}\right)^{\top}$$

3.5. Apply ν_2 post-smoothing steps as in 3.1. to obtain $\mathrm{u}_{h,1}^{(k+1,0)} := \mathrm{u}_{h,1}^{(k,\nu_1+\nu_2)}$ and repeat steps 3.1.–3.5. according to the h-multigrid cycle (V- or W-cycle).

Multigrid components

	h-multigrid	p-multigrid
restriction operator	$\mathrm{I}_{h,1}^{2h,1}$ linear interpolation	$\mathrm{I}_{h,1}^{h,p} := \mathrm{M}_{h,p}^{-1}\,\mathrm{M}_{h,1,p}$
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smoothing operator	incomplete LU factorization of $\mathrm{A}_{h,p} \approx \mathrm{L}_{h,p}\,\mathrm{U}_{h,p}$, whereby all elements smaller than 10^{-13} are dropped and the amount of non-zero entries per row are kept constant	

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$\mathrm{A}_{h,p}$ operator	rediscretization	

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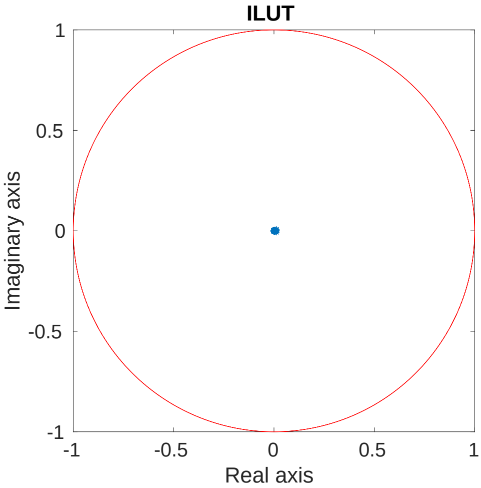
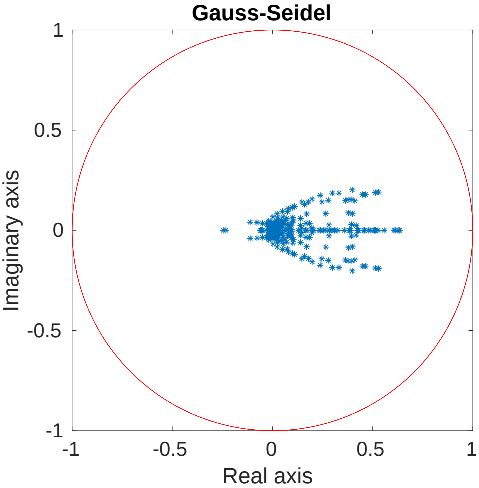
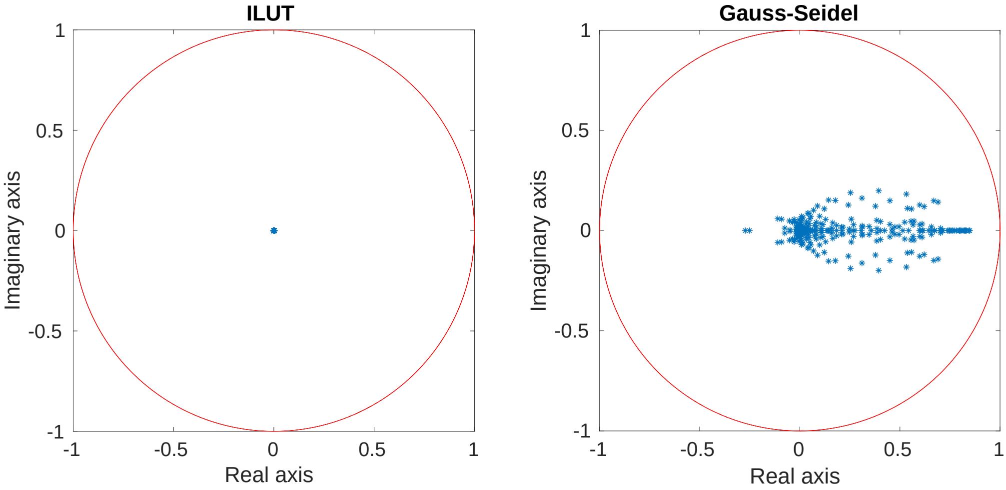
Spectrum of the iteration matrix: Poisson on quarter annulus, $p = 2$





R. Tielen, M. Möller, D. Göddeke, and C. Vuik (2020) p-multigrid methods and their comparison to h-multigrid methods within Isogeometric Analysis. CMAME 372, 10.1016/j.cma.2020.113347.

Spectrum of the iteration matrix: Poisson on quarter annulus, $p = 3$



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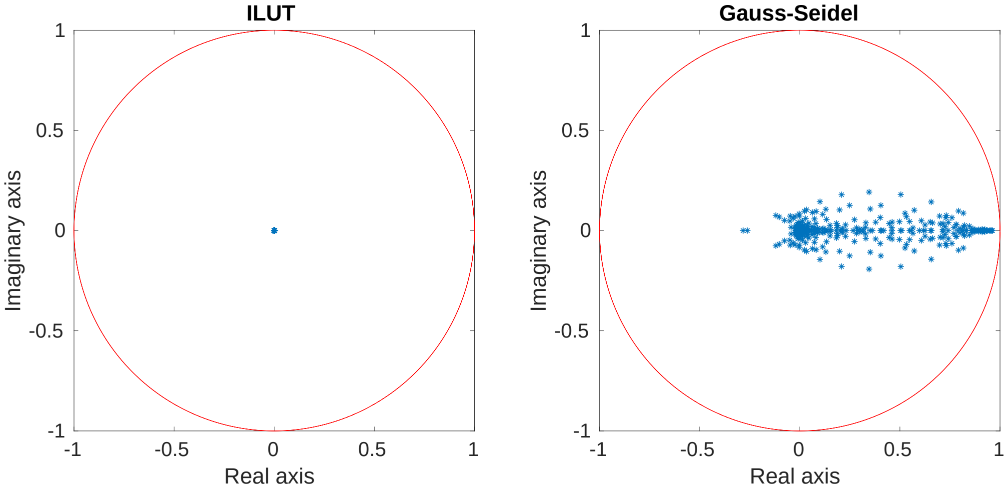
Spectrum of the iteration matrix: Poisson on quarter annulus, $p = 4$



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Numerical examples

#1: Poisson's equation on a quarter annulus domain with radii 1 and 2

	$p=2$		$p=3$		$p=4$		$p=5$	
	ILUT	GS	ILUT	GS	ILUT	GS	ILUT	GS
$h=2^{-6}$	4	30	3	62	3	176	3	491
$h=2^{-7}$	4	29	3	61	3	172	3	499
$h=2^{-8}$	5	30	3	60	3	163	3	473
$h=2^{-9}$	5	32	3	61	3	163	3	452

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Numerical examples

#2: CDR equation with $\mathbb{D} = \begin{pmatrix} 1.2 & -0.7 \\ -0.4 & 0.9 \end{pmatrix}$, $\mathbf{v} = (0.4, -0.2)^\top$, and $r = 0.3$ on the unit square domain

	$p = 2$		$p = 3$		$p = 4$		$p = 5$	
	ILUT	GS	ILUT	GS	ILUT	GS	ILUT	GS
$h = 2^{-6}$	5	–	3	–	3	–	4	–
$h = 2^{-7}$	5	–	3	–	4	–	4	–
$h = 2^{-8}$	5	–	3	–	3	–	4	–
$h = 2^{-9}$	5	–	4	–	3	–	4	–

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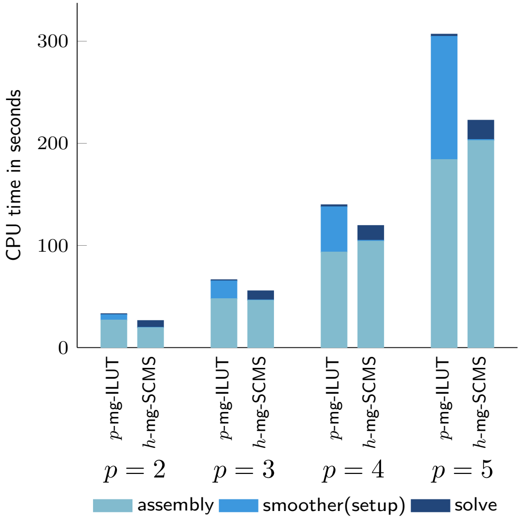
Computational efficiency: p- vs. h-multigrid



Comparison with h-multigrid method with subspace corrected mass smoother [Takacs, 2017]

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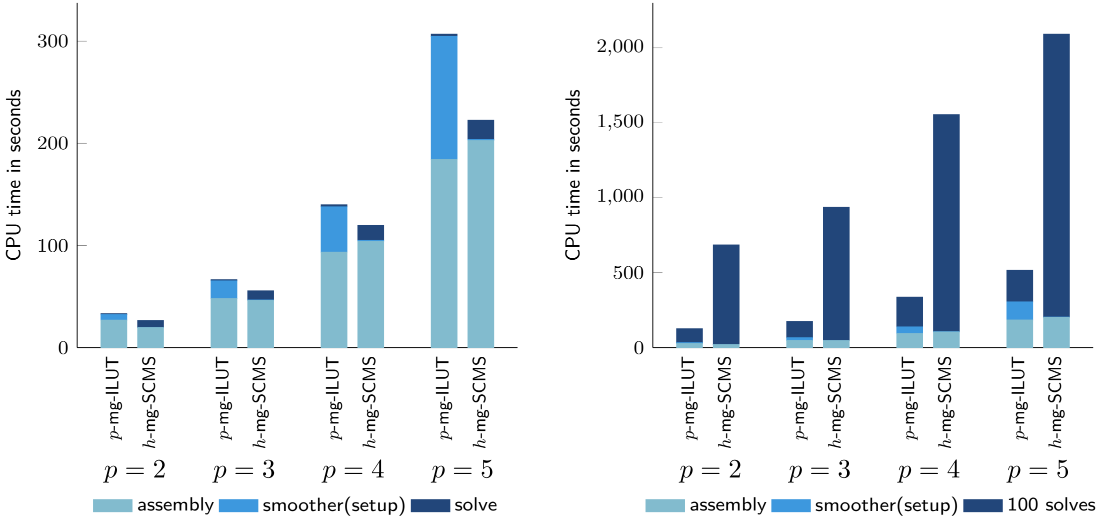
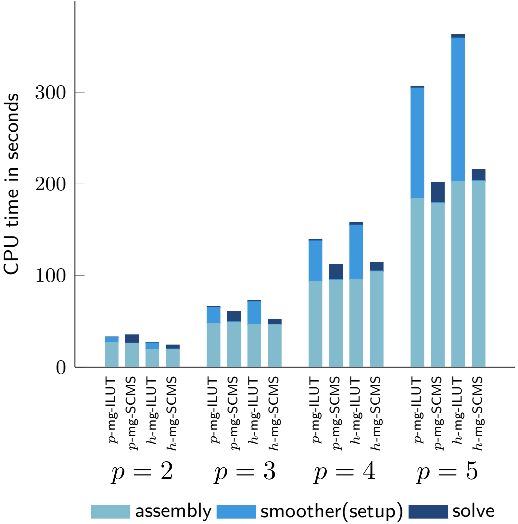
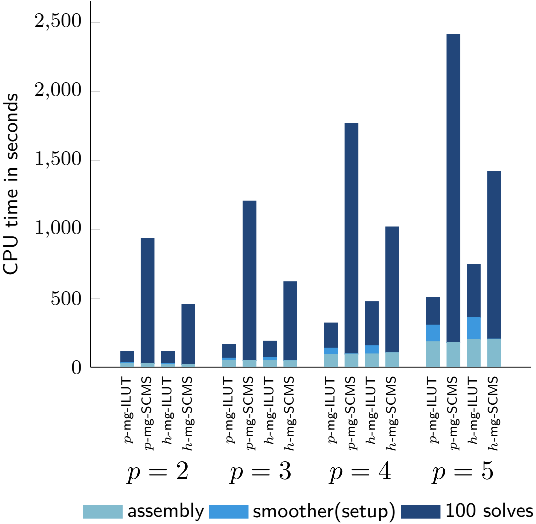


Comparison with h-multigrid method with subspace corrected mass smoother [Takacs, 2017]

Computational efficiency: $\{h, p\}$-*multigrid* + $\{$*ILUT,SCMS*$\}$-*smoother*

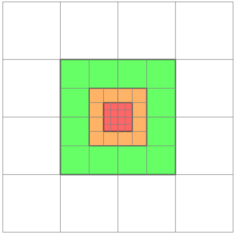


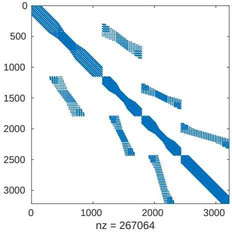


Numerical examples: *THB splines*

#3: Poisson's equation on the unit square domain

	$p=2$		$p=3$		$p=4$		$p=5$	
	ILUT	GS	ILUT	GS	ILUT	GS	ILUT	GS
$h=2^{-4}$	6	17	8	47	7	177	10	1033
$h=2^{-5}$	6	16	7	44	8	182	7	923
$h=2^{-6}$	6	17	5	43	6	201	12	1009





R. Tielen, M. Möller, D. Göddeke, and C. Vuik (2020) p-multigrid methods and their comparison to h-multigrid methods within Isogeometric Analysis. CMAME 372, 10.1016/j.cma.2020.113347.

Block ILUT

Exact LU decomposition of the block matrix A

$$\begin{bmatrix} \mathrm{A}_{11} & & & \mathrm{A}_{\Gamma 1} \\ & \ddots & & \vdots \\ & & \mathrm{A}_{N_p N_p} & \mathrm{A}_{\Gamma N_p} \\ \mathrm{A}_{1\Gamma} & \cdots & \mathrm{A}_{N_p \Gamma} & \mathrm{A}_{\Gamma\Gamma} \end{bmatrix} = \begin{bmatrix} \mathrm{L}_1 & & & \\ & \ddots & & \\ & & \mathrm{L}_{N_p} & \\ \mathrm{B}_1 & \cdots & \mathrm{B}_{N_p} & \mathrm{I} \end{bmatrix} \begin{bmatrix} \mathrm{U}_1 & & & \mathrm{C}_1 \\ & \ddots & & \vdots \\ & & \mathrm{U}_{N_p} & \mathrm{C}_{N_p} \\ & & & \mathrm{S} \end{bmatrix},$$

with

$$\mathrm{A}_{\ell\ell} = \mathrm{L}_\ell \, \mathrm{U}_\ell, \qquad \mathrm{B}_\ell = \mathrm{A}_{\ell\Gamma} \, \mathrm{U}_\ell^{-1}, \qquad \mathrm{C}_\ell = \mathrm{L}_\ell^{-1} \, \mathrm{A}_{\Gamma\ell}, \qquad \mathrm{S} = \mathrm{A}_{\Gamma\Gamma} - \sum_{\ell=1}^{N_p} \mathrm{B}_\ell \, \mathrm{C}_\ell$$

Block ILUT

Approximate LU decomposition of the block matrix A

$$\begin{bmatrix} \mathrm{A}_{11} & & & \mathrm{A}_{\Gamma 1} \\ & \ddots & & \vdots \\ & & \mathrm{A}_{N_p N_p} & \mathrm{A}_{\Gamma N_p} \\ \mathrm{A}_{1\Gamma} & \cdots & \mathrm{A}_{N_p \Gamma} & \mathrm{A}_{\Gamma\Gamma} \end{bmatrix} \approx \begin{bmatrix} \tilde{\mathrm{L}}_1 & & & \\ & \ddots & & \\ & & \tilde{\mathrm{L}}_{N_p} & \\ \tilde{\mathrm{B}}_1 & \cdots & \tilde{\mathrm{B}}_{N_p} & \mathrm{I} \end{bmatrix} \begin{bmatrix} \tilde{\mathrm{U}}_1 & & & \tilde{\mathrm{C}}_1 \\ & \ddots & & \vdots \\ & & \tilde{\mathrm{U}}_{N_p} & \tilde{\mathrm{C}}_{N_p} \\ & & & \tilde{\mathrm{S}} \end{bmatrix},$$

with

$$\mathrm{A}_{\ell\ell} = \mathrm{L}_\ell \, \mathrm{U}_\ell, \qquad \mathrm{B}_\ell = \mathrm{A}_{\ell\Gamma} \, \mathrm{U}_\ell^{-1}, \qquad \mathrm{C}_\ell = \mathrm{L}_\ell^{-1} \, \mathrm{A}_{\Gamma\ell}, \qquad \mathrm{S} = \mathrm{A}_{\Gamma\Gamma} - \sum_{\ell=1}^{N_p} \mathrm{B}_\ell \, \mathrm{C}_\ell$$

Let us replace L_ℓ and U_ℓ by their (local) ILUT factorizations (compute in parallel!)

$$\mathrm{A}_{\ell\ell} \approx \tilde{\mathrm{L}}_\ell \, \tilde{\mathrm{U}}_\ell, \qquad \tilde{\mathrm{B}}_\ell = \mathrm{A}_{\ell\Gamma} \, \tilde{\mathrm{U}}_\ell^{-1}, \qquad \tilde{\mathrm{C}}_\ell = \tilde{\mathrm{L}}_\ell^{-1} \, \mathrm{A}_{\Gamma\ell}, \qquad \tilde{\mathrm{S}} = \mathrm{A}_{\Gamma\Gamma} - \sum_{\ell=1}^{N_p} \tilde{\mathrm{B}}_\ell \, \tilde{\mathrm{C}}_\ell$$

. I.C.L. Nievinski et al. Parallel implementation of a two-level algebraic ILU(k)-based domain decomposition preconditioner, TEMA (São Carlos) 19(1), Jan-Apr 2018

Numerical examples: *Block-ILUT vs. global ILUT*

#1: Poisson's equation on the quarter annulus domain with radii 1 and 2

	$p=2$ # patches			$p=3$ # patches			$p=4$ # patches			$p=5$ # patches		
	4	16	64	4	16	64	4	16	64	4	16	64
$h=2^{-5}$	3(5)	4(7)	4(9)	3(5)	3(7)	4(11)	2(4)	2(6)	4(–)	2(4)	2(6)	–(–)
$h=2^{-6}$	3(5)	3(5)	4(7)	3(5)	3(7)	4(10)	3(6)	2(7)	3(11)	3(5)	3(7)	3(10)
$h=2^{-7}$	3(5)	3(5)	3(5)	3(5)	3(6)	3(8)	3(5)	2(6)	3(10)	–(5)	6(7)	3(11)

Numbers in parentheses correspond to global ILUT

R. Tielen, M. Möller, and C. Vuik (2022) A block ILUT smoother for multipatch geometries in Isogeometric Analysis, To appear in: Geometric Challenges in Isogeometric Analysis, Springer INdAM Series.

Numerical examples: *Block-ILUT vs. global ILUT*

#2: CDR equation with $\mathbb{D} = \begin{pmatrix} 1.2 & -0.7 \\ -0.4 & 0.9 \end{pmatrix}$, $\mathbf{v} = (0.4, -0.2)^\top$, and $r = 0.3$ on the unit square domain

	$p=2$ # patches			$p=3$ # patches			$p=4$ # patches			$p=5$ # patches		
	4	16	64	4	16	64	4	16	64	4	16	64
$h=2^{-5}$	4(6)	4(8)	7(11)	3(6)	3(9)	5(15)	2(6)	3(8)	5(15)	2(5)	2(7)	4(14)
$h=2^{-6}$	4(6)	4(7)	5(8)	3(6)	3(8)	4(10)	3(7)	3(9)	4(13)	3(7)	3(8)	3(13)
$h=2^{-7}$	4(6)	4(6)	4(7)	3(6)	3(7)	3(8)	2(7)	3(7)	3(10)	4(6)	3(8)	3(12)

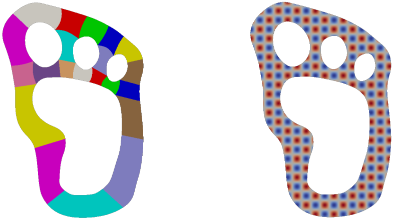
Numbers in parentheses correspond to global ILUT

R. Tielen, M. Möller, and C. Vuik (2022) A block ILUT smoother for multipatch geometries in Isogeometric Analysis, To appear in: Geometric Challenges in Isogeometric Analysis, Springer INdAM Series.

Numerical examples: *Block-ILUT vs. global ILUT*

#4: Poisson's equation on the Yeti footprint

	$p=2$		$p=3$		$p=4$		$p=5$	
	block	global	block	global	block	global	block	global
$h=2^{-3}$	4	5	2	4	2	4	2	4
$h=2^{-4}$	4	8	3	5	3	5	2	4
$h=2^{-5}$	4	8	3	6	3	5	3	5



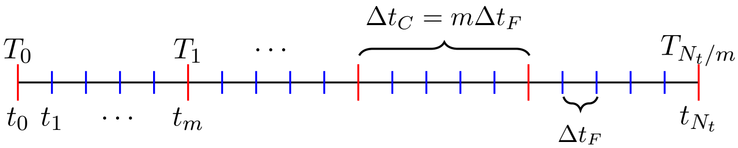
R. Tielen, M. Möller, and C. Vuik (2022) A block ILUT smoother for multipatch geometries in Isogeometric Analysis, To appear in: Geometric Challenges in Isogeometric Analysis, Springer INdAM Series.

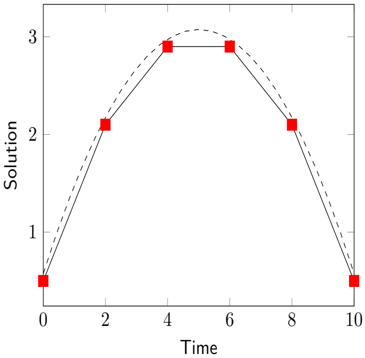
Outline

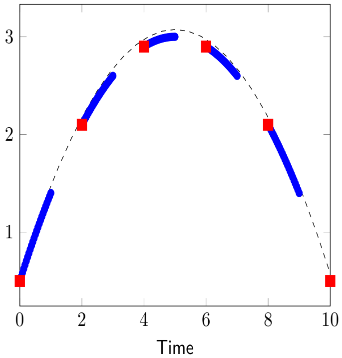
1. Motivation and problem formulations
2. Part I: Multigrid methods for IGA
   - Introduction to h- and p-multigrid
   - ILUT smoother for single-patch IGA
   - Block-ILUT smoother for multi-patch IGA
3. Part II: Multigrid reduction in time (MGRIT)
   - Introduction to MGRIT
   - MGRIT-IGA
4. Conclusions

- robust with respect to h, p, N_p, and 'the PDE'
- computational efficient throughout all problem sizes
- applicable to locally refined THB-splines
- Good spatial solver for transient problems (Part II)

Part II: Multigrid reduction in time (MGRIT)







S. Friedhoff, et al. A Multigrid-in-Time Algorithm for Solving Evolution Equations in Parallel, 16^{th} Copper Mountain Conference on Multigrid Methods 2013.

Sketch of the MGRIT algorithm

Heat-Eq: Find $u_{h,p}^{n+1} \in \mathcal{V}_{h,p}$ such that

$$[\,\mathrm{M}_{h,p} + \Delta t_F\ \mathrm{K}_{h,p}]\ \mathrm{u}_{h,p}^{n+1} = \mathrm{M}_{h,p}\,\mathrm{u}_{h,p}^{n} + \mathrm{f}_{h,p}$$

S. Friedhoff, et al. A Multigrid-in-Time Algorithm for Solving Evolution Equations in Parallel, 16^{th} Copper Mountain Conference on Multigrid Methods 2013.

Sketch of the MGRIT algorithm

Heat-Eq: Find $u_{h,p}^{n+1} \in \mathcal{V}_{h,p}$ such that

$$[\,\mathrm{M}_{h,p} + \Delta t_F\ \mathrm{K}_{h,p}]\ \mathrm{u}_{h,p}^{n+1} = \mathrm{M}_{h,p}\,\mathrm{u}_{h,p}^{n} + \mathrm{f}_{h,p}$$

Writing out the above two-level scheme for all time levels yields

$$\mathrm{A}_{h,p}\,\mathrm{U}_{h,p} = \begin{bmatrix} \mathrm{I}_{h,p} & & & \\ -\Psi_{h,p}\,\mathrm{M}_{h,p} & \mathrm{I}_{h,p} & & \\ & \ddots & \ddots & \\ & & -\Psi_{h,p}\,\mathrm{M}_{h,p} & \mathrm{I}_{h,p} \end{bmatrix} \begin{bmatrix} \mathrm{u}_{h,p}^{0} \\ \mathrm{u}_{h,p}^{1} \\ \vdots \\ \mathrm{u}_{h,p}^{N_t} \end{bmatrix} = \Delta t_F \begin{bmatrix} \Psi_{h,p}\,\mathrm{f}_{h,p} \\ \Psi_{h,p}\,\mathrm{f}_{h,p} \\ \vdots \\ \Psi_{h,p}\,\mathrm{f}_{h,p} \end{bmatrix}$$

with

$$\Psi_{h,p} = [\,\mathrm{M}_{h,p} + \Delta t_F\ \mathrm{K}_{h,p}]^{-1}$$

S. Friedhoff, et al. A Multigrid-in-Time Algorithm for Solving Evolution Equations in Parallel, 16^{th} Copper Mountain Conference on Multigrid Methods 2013.

Sketch of the MGRIT algorithm, cont'd

Reordering of $\mathrm{A}_{h,p}$ into (F)ine and (C)oarse time levels yields

$$\begin{bmatrix} \mathrm{A}_{FF} & \mathrm{A}_{FC} \\ \mathrm{A}_{CF} & \mathrm{A}_{CC} \end{bmatrix} = \begin{bmatrix} \mathrm{I}_F & 0 \\ \mathrm{A}_{CF}\,\mathrm{A}_{FF}^{-1} & \mathrm{I}_C \end{bmatrix} \begin{bmatrix} \mathrm{A}_{FF} & 0 \\ 0 & \mathrm{S} \end{bmatrix} \begin{bmatrix} \mathrm{I}_F & \mathrm{A}_{FF}^{-1}\,\mathrm{A}_{FC} \\ 0 & \mathrm{I}_C \end{bmatrix}$$

S. Friedhoff, et al. A Multigrid-in-Time Algorithm for Solving Evolution Equations in Parallel, 16^{th} Copper Mountain Conference on Multigrid Methods 2013.

Sketch of the MGRIT algorithm, cont'd

Reordering of $\mathrm{A}_{h,p}$ into (F)ine and (C)oarse time levels yields

$$\begin{bmatrix} \mathrm{A}_{FF} & \mathrm{A}_{FC} \\ \mathrm{A}_{CF} & \mathrm{A}_{CC} \end{bmatrix} = \begin{bmatrix} \mathrm{I}_F & 0 \\ \mathrm{A}_{CF}\,\mathrm{A}_{FF}^{-1} & \mathrm{I}_C \end{bmatrix} \begin{bmatrix} \mathrm{A}_{FF} & 0 \\ 0 & \mathrm{S} \end{bmatrix} \begin{bmatrix} \mathrm{I}_F & \mathrm{A}_{FF}^{-1}\,\mathrm{A}_{FC} \\ 0 & \mathrm{I}_C \end{bmatrix}$$

with block-diagonal fine-level system matrix

$$\mathrm{A}_{FF} = \mathrm{I}_{N_t/m,N_t/m} \otimes \underbrace{\begin{pmatrix} \mathrm{I}_{h,p} & & & \\ -\Psi_{h,p}\,\mathrm{M}_{h,p} & \mathrm{I}_{h,p} & & \\ & \ddots & \ddots & \\ & & -\Psi_{h,p}\,\mathrm{M}_{h,p} & \mathrm{I}_{h,p} \end{pmatrix}}_{m\times m \text{ blocks}}$$

S. Friedhoff, et al. A Multigrid-in-Time Algorithm for Solving Evolution Equations in Parallel, 16^{th} Copper Mountain Conference on Multigrid Methods 2013.

Sketch of the MGRIT algorithm, cont'd

Reordering of $\mathrm{A}_{h,p}$ into (F)ine and (C)oarse time levels yields

$$\begin{bmatrix} \mathrm{A}_{FF} & \mathrm{A}_{FC} \\ \mathrm{A}_{CF} & \mathrm{A}_{CC} \end{bmatrix} = \begin{bmatrix} \mathrm{I}_F & 0 \\ \mathrm{A}_{CF}\,\mathrm{A}_{FF}^{-1} & \mathrm{I}_C \end{bmatrix} \begin{bmatrix} \mathrm{A}_{FF} & 0 \\ 0 & \mathrm{S} \end{bmatrix} \begin{bmatrix} \mathrm{I}_F & \mathrm{A}_{FF}^{-1}\,\mathrm{A}_{FC} \\ 0 & \mathrm{I}_C \end{bmatrix}$$

with block-diagonal fine-level system matrix

$$\mathrm{A}_{FF} = \mathrm{I}_{N_t/m,N_t/m} \otimes \underbrace{\begin{pmatrix} \mathrm{I}_{h,p} & & & \\ -\Psi_{h,p}\,\mathrm{M}_{h,p} & \mathrm{I}_{h,p} & & \\ & \ddots & \ddots & \\ & & -\Psi_{h,p}\,\mathrm{M}_{h,p} & \mathrm{I}_{h,p} \end{pmatrix}}_{m\times m \text{ blocks}}$$

and the Schur complement $\mathrm{S} = \mathrm{A}_{CC} - \mathrm{A}_{CF}\,\mathrm{A}_{FF}^{-1}\,\mathrm{A}_{FC}$

S. Friedhoff, et al. A Multigrid-in-Time Algorithm for Solving Evolution Equations in Parallel, 16^{th} Copper Mountain Conference on Multigrid Methods 2013.

Sketch of the MGRIT algorithm, cont'd

Approximate the Schur complement

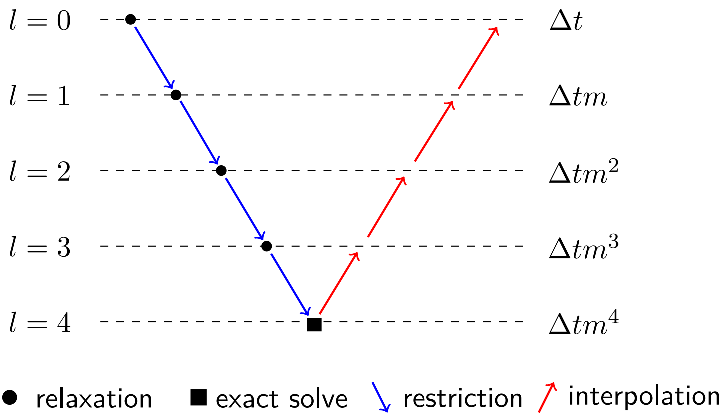
$$\mathrm{S} = \begin{bmatrix} \mathrm{I} & & & \\ -(\Psi_{h,p}\,\mathrm{M}_{h,p})^m & \mathrm{I} & & \\ & \ddots & \ddots & \\ & & -(\Psi_{h,p}\,\mathrm{M}_{h,p})^m & \mathrm{I} \end{bmatrix} \approx \begin{bmatrix} \mathrm{I} & & & \\ -\Phi_{h,p}\,\mathrm{M}_{h,p} & \mathrm{I} & & \\ & \ddots & \ddots & \\ & & -\Phi_{h,p}\,\mathrm{M}_{h,p} & \mathrm{I} \end{bmatrix}$$

with *coarse integrator*

$$\Phi_{h,p} = \left[\,\mathrm{M}_{h,p} + \Delta t_C\ \mathrm{K}_{h,p}\right]^{-1}$$

S. Friedhoff, et al. A Multigrid-in-Time Algorithm for Solving Evolution Equations in Parallel, 16^{th} Copper Mountain Conference on Multigrid Methods 2013.

The MGRIT-IGA V-cycle



MGRIT-IGA implementation

G+Smo: Geometry plus Simulation Modules

- open-source cross-platform IGA library written in C++
- dimension-independent code development using templates
- building on Eigen C++ library for linear algebra

XBraid: Parallel Multigrid in Time

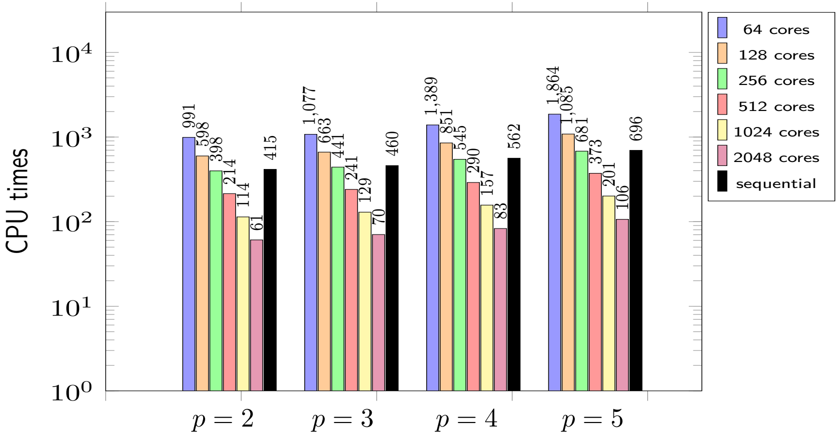
- open-source implementation of the optimal-scaling multigrid solver in MPI/C with C++ interface
- extendable by overloading callback functions

Try it yourself

`https://github.com/gismo/gismo/tree/xbraid/extensions/gsXBraid`

Numerical examples: *Strong scaling of MGRIT-IGA*

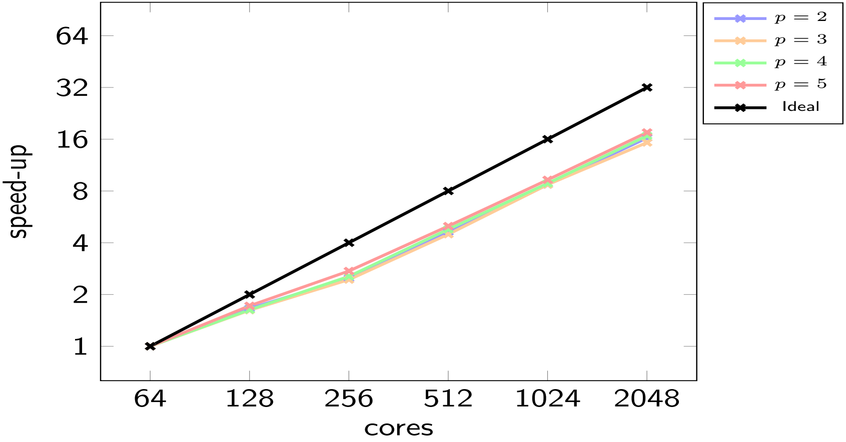
#5: Heat-Eq with $h = 2^{-6}$ spatial resolution solved for $N_t = 10.000$ time steps with backward Euler method on 128 Xeon Gold 6130 CPUs (2.10GHz, 96GB, 16 cores)



R. Tielen, M. Möller, and C. Vuik (2022) Combining p-multigrid and multigrid reduction in time methods to obtain a scalable solver for isogeometric analysis, SN Appl. Sci. 410.1007/s42452-022-05043-7.

Numerical examples: *Speed-up of MGRIT-IGA*

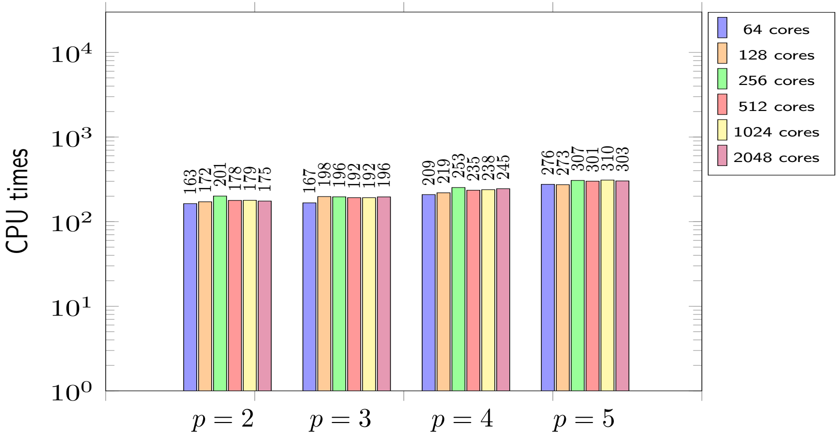
#5: Heat-Eq with $h = 2^{-6}$ spatial resolution solved for $N_t = 10.000$ time steps with backward Euler method on 128 Xeon Gold 6130 CPUs (2.10GHz, 96GB, 16 cores)



R. Tielen, M. Möller, and C. Vuik (2022) Combining p-multigrid and multigrid reduction in time methods to obtain a scalable solver for isogeometric analysis, SN Appl. Sci. 410.1007/s42452-022-05043-7.

Numerical examples: *Weak scaling of MGRIT-IGA*

#5: Heat-Eq with $h = 2^{-6}$ spatial resolution solved for $N_t = \text{cores}/64 \cdot 1.000$ time steps with backward Euler method on 128 Xeon Gold 6130 CPUs (2.10GHz, 96GB, 16 cores)



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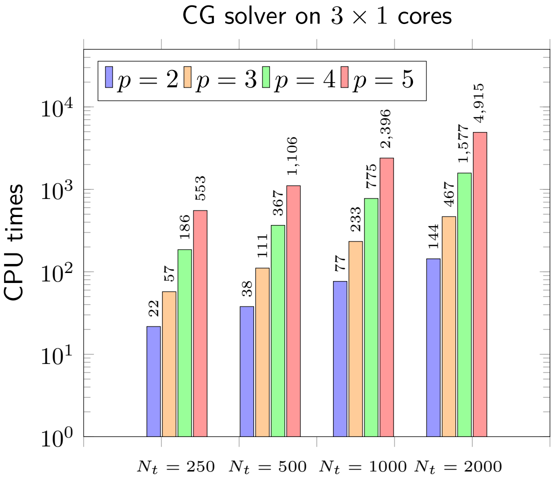
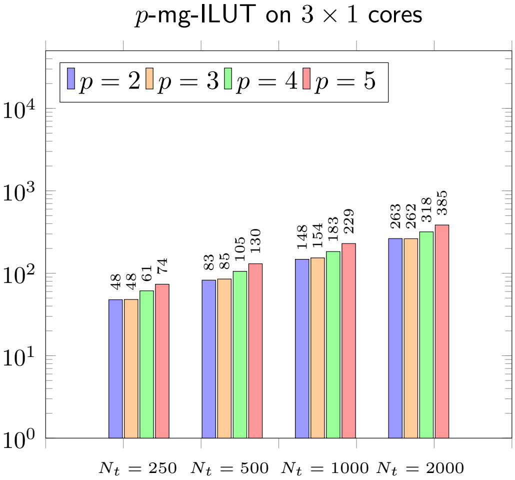
Do we really need p-multigrid or would a standard solver be good enough?

R. Tielen, M. Möller, and C. Vuik (2022) Combining p-multigrid and multigrid reduction in time methods to obtain a scalable solver for isogeometric analysis, SN Appl. Sci. 410.1007/s42452-022-05043-7.

Do we really need p-multigrid or would a standard solver be good enough?

No!





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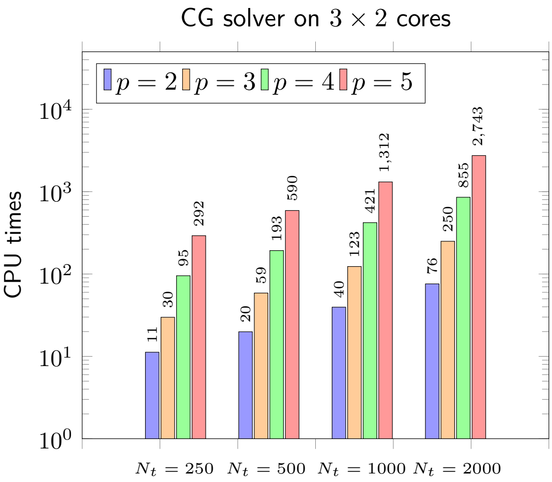

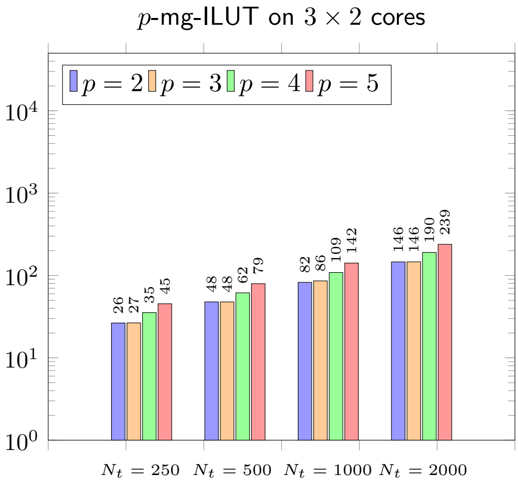

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Conclusion

MGRIT-IGA + p-multigrid with (block-)ILUT smoother

- robust with respect to h, p, N_p, and 'the PDE'
- computational efficient throughout all problem sizes
- applicable to locally refined THB-splines
- good strong and weak scaling in no. of cores and N_t

Conclusion

MGRIT-IGA + p-multigrid with (block-)ILUT smoother

- robust with respect to h, p, N_p, and 'the PDE'
- computational efficient throughout all problem sizes
- applicable to locally refined THB-splines
- good strong and weak scaling in no. of cores and N_t

What's next?

- MGRIT-IGA with THB-splines and adaptive refinement in time
- extension to nonlinear PDEs and higher-order time integrators

Further reading

R.Tielen, M. Möller, D. Göddeke and C. Vuik (2020) *p-multigrid methods and their comparison to h-multigrid methods within isogeometric analysis*, CMAME, 372.

R. Tielen, M. Möller and C. Vuik (2021) *A direct projection to low-order level for p-multigrid methods in isogeometric analysis*, Proc. ENUMATH 2019.

R. Tielen, M. Möller and C. Vuik (2022) *A block ILUT smoother for multipatch geometries in Isogeometric Analysis*, Geometric Challenges in Isogeometric Analysis, Springer INdAM Series.

R. Tielen, M. Möller and C. Vuik (2022) *Combining p-multigrid and multigrid reduced in time methods to obtain a scalable solver for Isogeometric Analysis*, SN Applied Sciences 4:163.

Thank you for your attention!

Reduction factors

Error reduction factors:

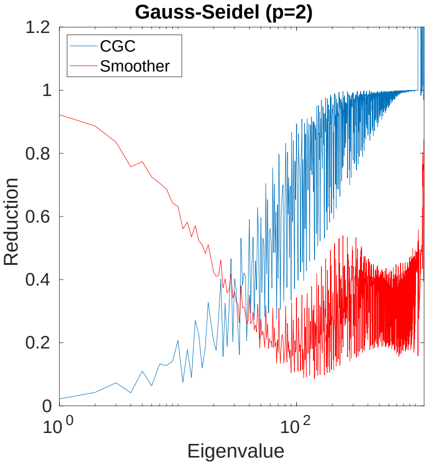
$$r^{\mathcal{S}}(\mathbf{v}) = \frac{|\mathcal{S}(\mathbf{v})|}{|\mathbf{v}|} \qquad r^{CGC}(\mathbf{v}) = \frac{|CGC(\mathbf{v})|}{|\mathbf{v}|}$$

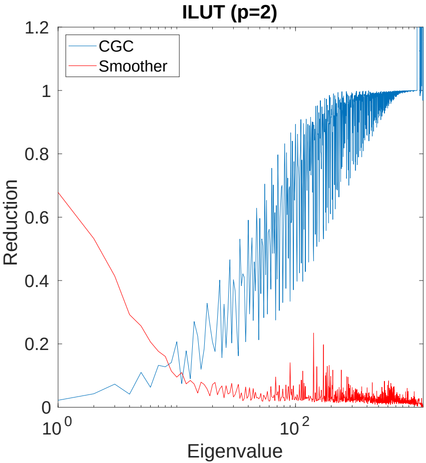
where $\mathcal{S}(\cdot)$ and $CGC(\cdot)$ denote a smoothing step and coarse grid correction applied on $\mathbf{v}$, respectively.

Here $(\mathbf{v}_i)$ are the generalized eigenvectors which satisfy:

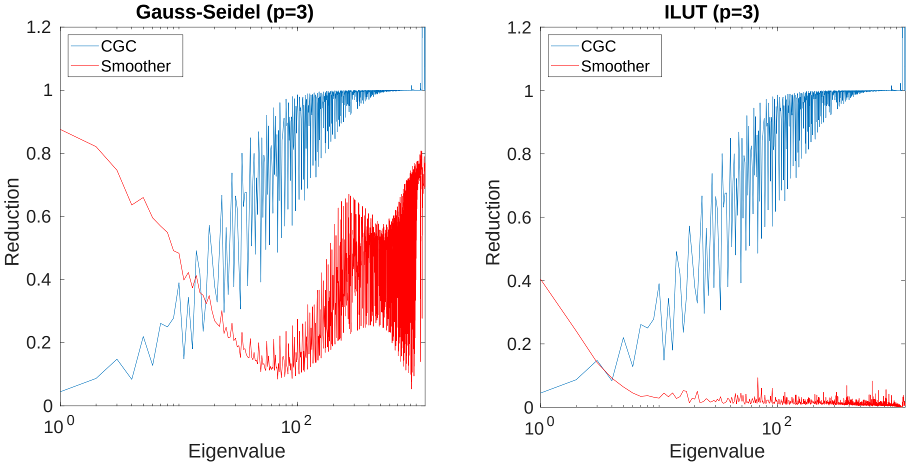
$$\mathbf{A}_{h,p}\mathbf{v}_i = \lambda_i {\mathbf{M}^{\mathbf{C}}}_{h,p}\mathbf{v}_i, \qquad i = 1, \ldots, N_{dof}$$

Reduction factors





Reduction factors



Reduction factors