CIME-EMS Summer School in Applied Mathematics

Splines and PDEs: Recent Advances
from Approximation Theory to Structured Numerical Linear Algebra

July 3 - July 7, 2017 - Cetraro

Efficient Formation of isogeometric matrices

Giancarlo Sangalli

joint work with Mattia Tani and Francesco Calabrò

July 7, 2017

k-method is the high-order isogeometric method

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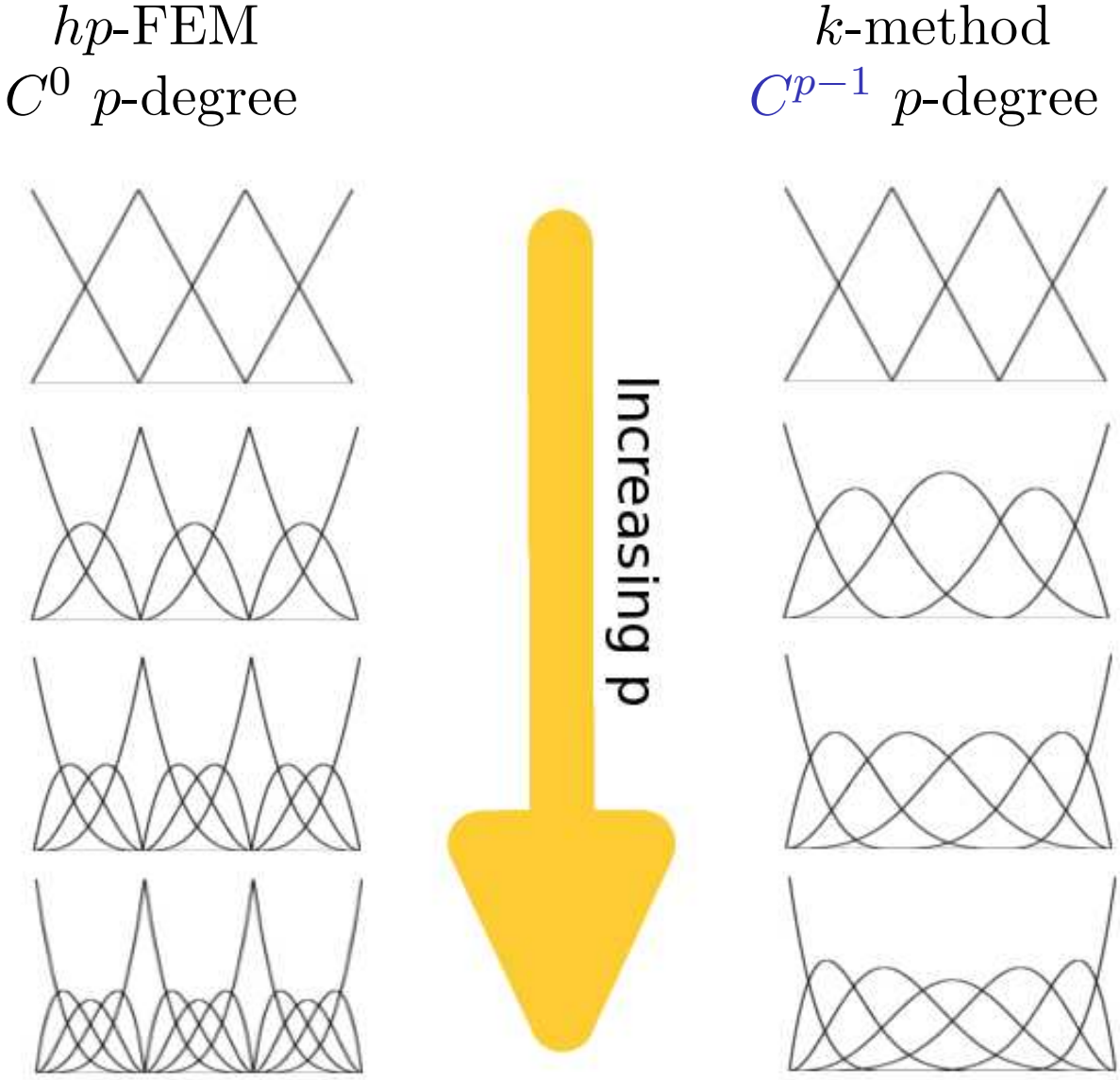

The k-method vs C^0 hp-FEM

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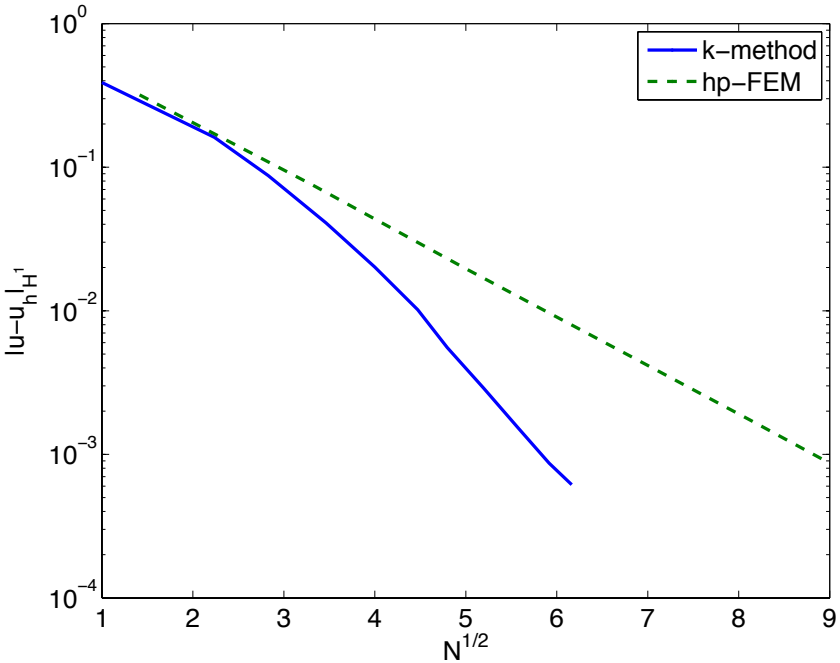

Approximation of $u(x) = x^{0.7} - x$.

The mesh is geometrically graded and the spline degree p is proportional to the number of elements for IGA. Mesh-size and degrees are optimally selected for hp-FEM.

Error is $|u - u_h|_{H^1} \leq C \exp\left(-b\sqrt{N}\right)$ in both cases, with larger b for IGA

[Buffa, Sangalli, and Schwab, 2014]

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The role of continuity in RBVMS modeling of turbulence

[Akkerman, Bazilevs, Calo, Hughes, and Hulshoff, 2008]

"We compared turbulent channel flow results using C^0 and C^1-continuous quadratic discretizations. Using a C^1-continuous quadratic basis yields more accurate mean flow and fluctuating quantities than C^0-continuous quadratic basis functions. We conclude that smooth NURBS basis functions have advantages over C^0-continuous finite elements in turbulent flow calculations."

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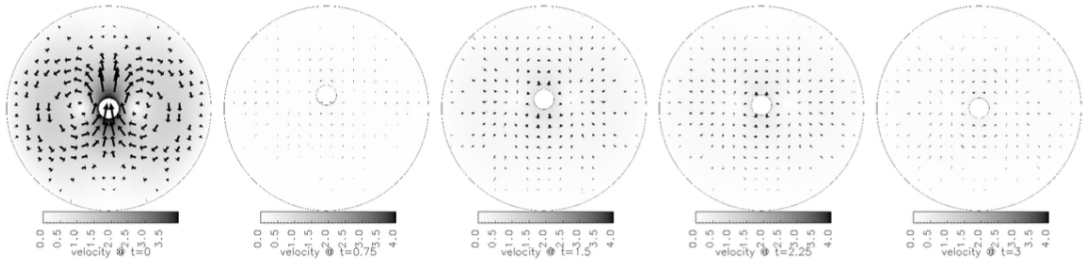
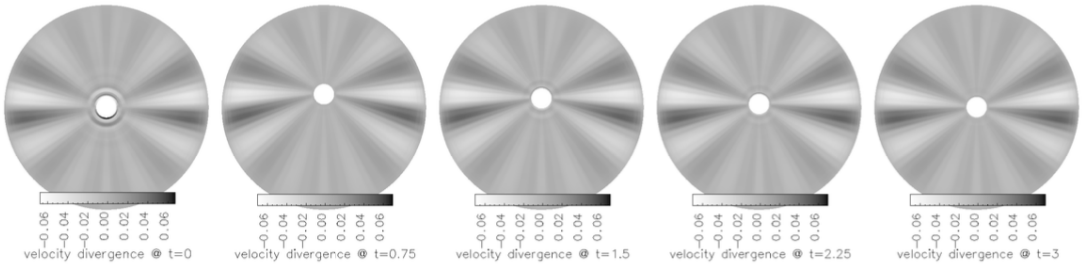
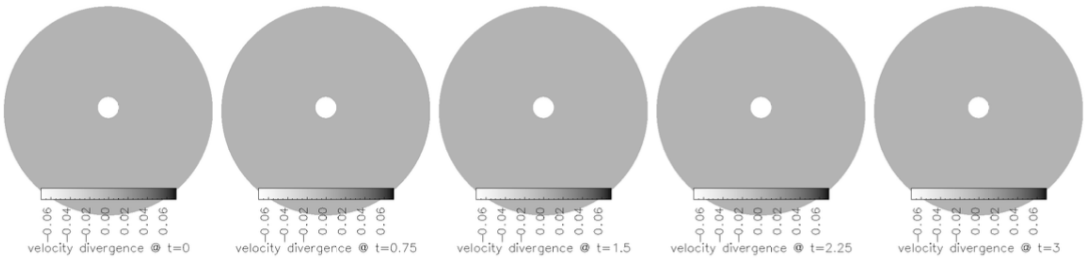
- structure-preserving



(a) Velocity snapshots computed with the RT discretization



(b) Divergence of the velocity computed with the TH discretization



(c) Divergence of the velocity computed with the RT discretization

"Div-conforming" k-method

[Buffa, de Falco, and Sangalli, 2011]

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Isogeometric Div-conforming B-splines for the Unsteady NS Eq.'s

[Evans and Hughes, 2013]

"... As incompressibility is satisfied pointwise, these semi-discretizations replicate the geometric structure of the unsteady Navier-Stokes equations and admit discrete balance laws for momentum, angular momentum, energy, vorticity, enstrophy, and helicity.... by combining the spectral-like properties of B-splines with the preservation of the geometric structure of the unsteady NS equations, our semi-discretization procedure may become a useful tool for both engineering analysis and the mathematical study of the unsteady NS equations. "

The k-method vs C^0 hp-FEM

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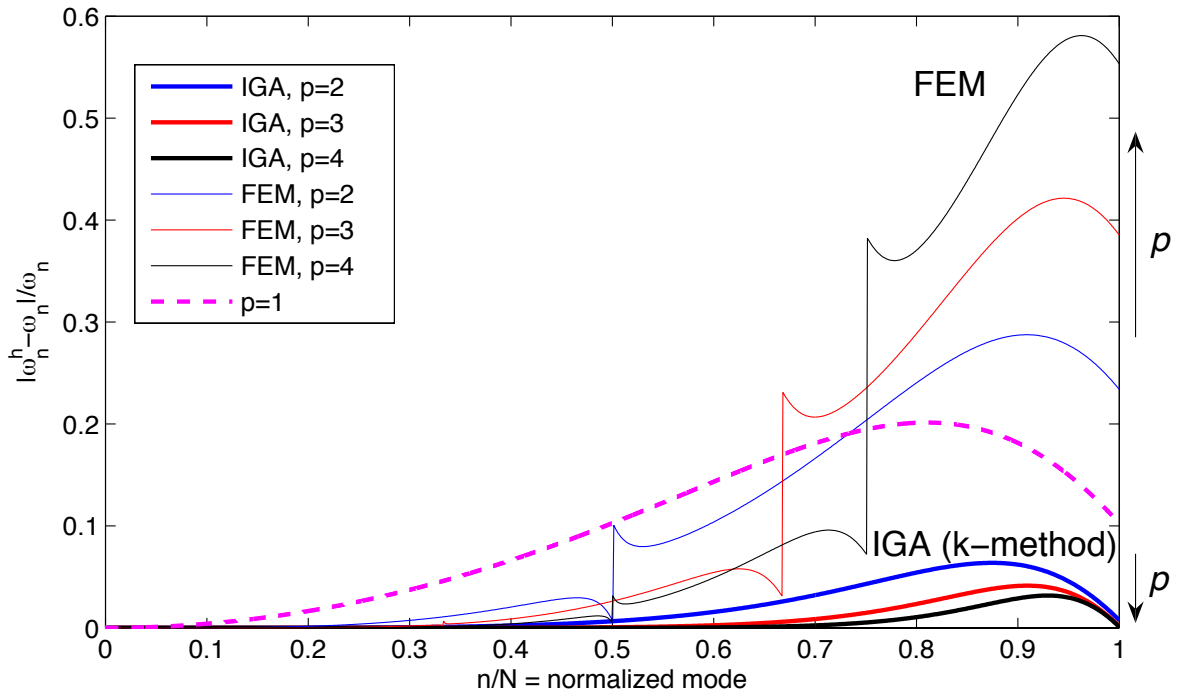
- improves the approximation of the spectrum



[Cottrell, Reali, Bazilevs, and Hughes, 2006; Hughes, Reali, and Sangalli, 2008]

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However in complex isogeometric simulation, e.g. VMS turbulence

[Bazilevs, Calo, Cottrell, Hughes, Reali, and Scovazzi, 2007]

"We found quadratic NURBS to give very significant accuracy advantages over linear elements. ... Cubics, on the other hand, increased cost considerably ... These remarks need to be qualified by the fact that our implementation of higher-order elements is not yet optimized in any way."

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"The cost of continuity..." [Collier, Pardo, Dalcin, Paszynski, and Calo, 2012]

"However this advantage comes at a cost which is not seen until looking in detail at the algorithms used to solve the resulting linear systems. In this case, we have shown that direct solvers require orders of magnitude more time and memory as continuity increases."

"Isogeometric Collocation: Cost Comparison with Galerkin Methods"

[Schillinger, Evans, Reali, Scott, and Hughes, 2013]

".. the total time for the formation and assembly of the global stiffness matrix of a given size takes ... almost two minutes for FEM and almost 1.5 hours in IGA (Galerkin)"

Fast formation/assembly of the system matrix

The model problem

$$\begin{aligned} -\nabla \cdot K \nabla \mathrm{u} &= \mathrm{f} \qquad \text{in } \Omega \subseteq \mathbb{R}^d,\ d = 2, 3 \\ \mathrm{u} &= 0 \qquad \text{in } \partial\Omega \end{aligned}$$

- d-dimensional scalar Poisson

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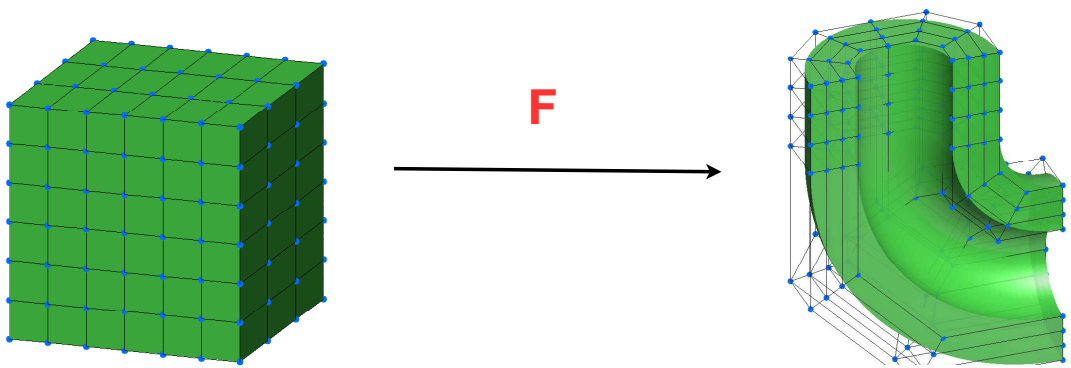

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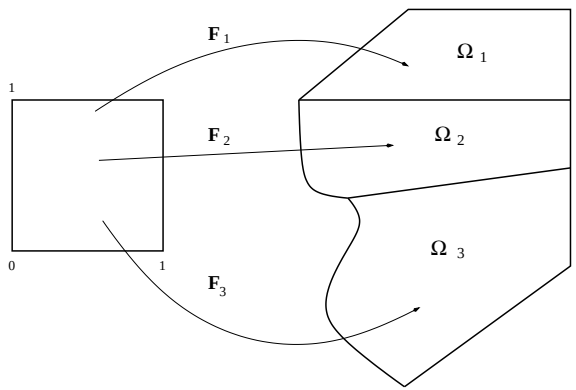

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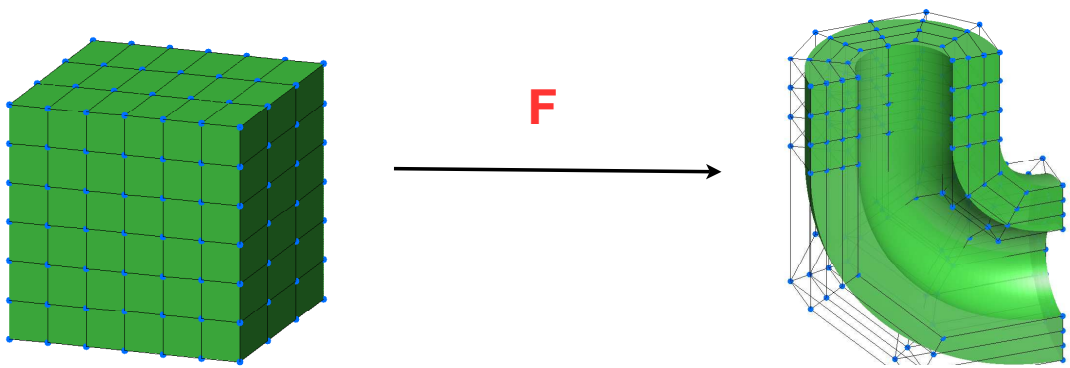

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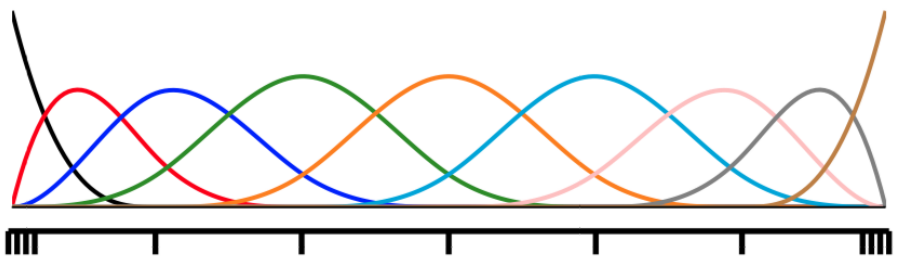

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- focus on Galerkin method

Isogeometric Galerkin matrices: element-wise quadrature

$$\mathbb{A}u = f$$

- The storage cost for $\mathbb{A}$ is $O(N_{\mathsf{DOF}} p^d)$ non-zero entries.

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- with element-wise assembling loop and element-wise standard Gaussian quadrature (SGQ): each elemental stiffness matrix has dimension $(p+1)^d \times (p+1)^d = O(p^{2d})$ and each entry is calculated by quadrature on $(p+1)^d = O(p^d)$ Gauss points. Total cost is $O(N_{\mathsf{EL}}p^{3d})$ that is $O(N_{\mathsf{DOF}}p^{3d})$.

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- The standard way to reduce the cost is to reduce the number of quadrature points, for example by reduced Gaussian [Adam, Hughes, Bouabdallah, Zarroug, and Maitournam, 2015; Schillinger, Hossain, and Hughes, 2014; Hillman, Chen, and Bazilevs, 2015]) or generalised Gaussian quadrature (GGQ) [Hughes, Reali, and Sangalli, 2010; Bremer, Gimbutas, and Rokhlin, 2010; Cheng, Rokhlin, and Yarvin, 1999; Ma, Rokhlin, and Wandzura, 1996] .

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Element-wise Gauss vs weighted quadrature (WQ)

Consider the mass matrix

$$\mathbb{M} = \{m_{\boldsymbol{i},\boldsymbol{j}}\} = \left\{ \int_{[0,1]^d} c(\boldsymbol{\zeta})\, B_{\boldsymbol{i}}(\boldsymbol{\zeta})\, B_{\boldsymbol{j}}(\boldsymbol{\zeta})\, d\boldsymbol{\zeta} \right\}$$

Gauss Quadrature (GQ) (or Generalized GQ)

$$m_{\boldsymbol{i},\boldsymbol{j}} \approx \mathfrak{Q}^{\mathrm{GQ}}(cB_{\boldsymbol{i}}B_{\boldsymbol{j}}) = \sum_{\boldsymbol{q}} w_{\boldsymbol{q}}^{\mathrm{GQ}} c(\boldsymbol{x}_{\boldsymbol{q}}^{\mathrm{GQ}}) B_{\boldsymbol{i}}(\boldsymbol{x}_{\boldsymbol{q}}^{\mathrm{GQ}}) B_{\boldsymbol{j}}(\boldsymbol{x}_{\boldsymbol{q}}^{\mathrm{GQ}})$$

weighted quadrature (WQ)

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Weighted Quadrature (WQ) for the mass matrix

We want to approximate the $(\boldsymbol{i}, \boldsymbol{j})$ entry of the mass matrix:

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- We incorporate the test function $B_{\boldsymbol{i}}(\boldsymbol{\zeta})$ into the integral measure; thus the quadrature rule $\mathfrak{Q}_{\boldsymbol{i}}^{\mathrm{WQ}}$, and in particular the weights $w_{\boldsymbol{q},\boldsymbol{i}}$, depend on $\boldsymbol{i}$.

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  - a-priori (they do not depend on $\boldsymbol{i}$) as suitable interpolation points,
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Each matrix row is computed independently: "embarrassingly parallel"

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- How to select the quadrature points $\boldsymbol{x}_{\boldsymbol{q}}$? how many?
- How to compute the weights $w_{\boldsymbol{q},\boldsymbol{i}}$ relative to $B_{\boldsymbol{i}}$?

Weighted Quadrature

Exactness conditions:

$$\mathfrak{Q}_{\boldsymbol{i}}^{\mathrm{WQ}}(B_{\boldsymbol{j}}(\cdot)) = \int_{[0,1]^d} B_{\boldsymbol{i}}(\boldsymbol{\zeta})\, B_{\boldsymbol{j}}(\boldsymbol{\zeta})\, d\boldsymbol{\zeta} \qquad \forall\, \boldsymbol{j}$$

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- If c is constant, then $\mathfrak{Q}_{\boldsymbol{i}}^{\mathrm{WQ}}(c(\cdot)B_{\boldsymbol{j}}(\cdot)) =: \tilde{m}_{\boldsymbol{i},\boldsymbol{j}} = m_{\boldsymbol{i},\boldsymbol{j}}$.
- For non-constant c, the new mass matrix is nonsymmetric in general ($\tilde{m}_{\boldsymbol{i},\boldsymbol{j}} \neq \tilde{m}_{\boldsymbol{j},\boldsymbol{i}}$).
- optimal accuracy follows from

$$\sup_{v_h = \sum_{\boldsymbol{i}} v_{\boldsymbol{i}} B_{\boldsymbol{i}}} \frac{\int_{[0,1]^d} c\, w\, v_h \;-\; \sum_{\boldsymbol{i}} v_{\boldsymbol{i}} \mathfrak{Q}_{\boldsymbol{i}}^{\mathrm{WQ}}(c\, w)}{\|v_h\|_{L^2}} \leq C h^{p+1} |c\, w|_{\mathcal{H}^{p+1}_{\mathrm{bent}}}$$

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We impose that

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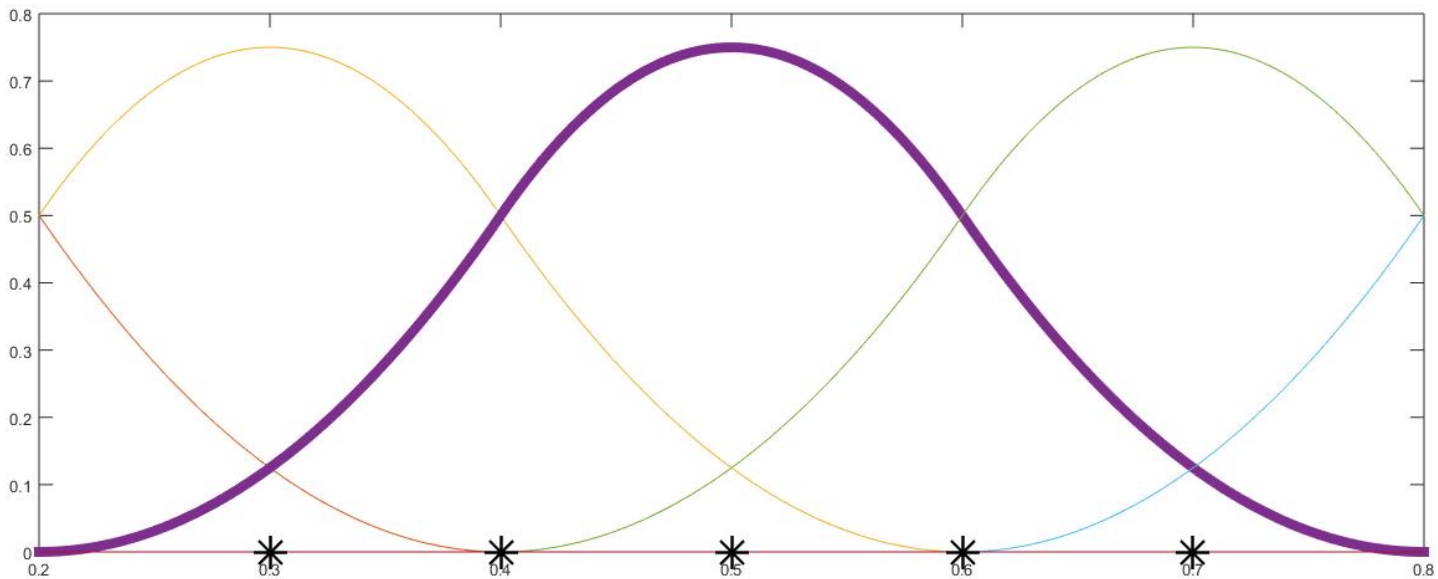

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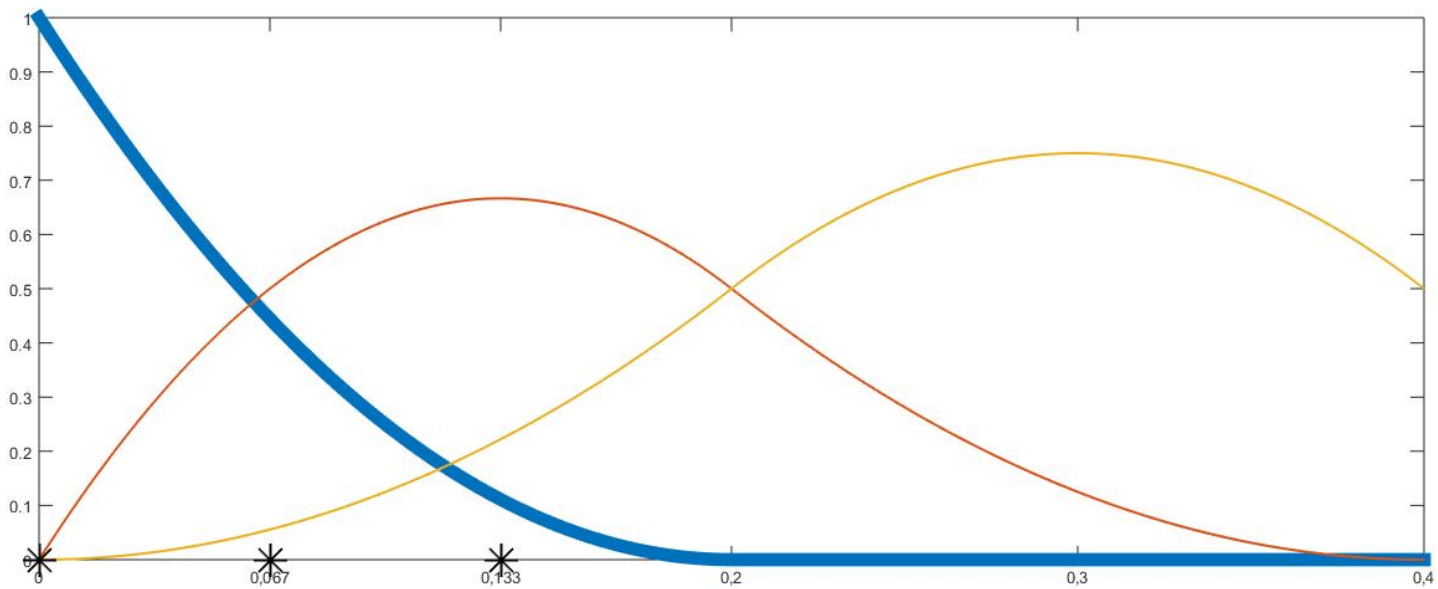

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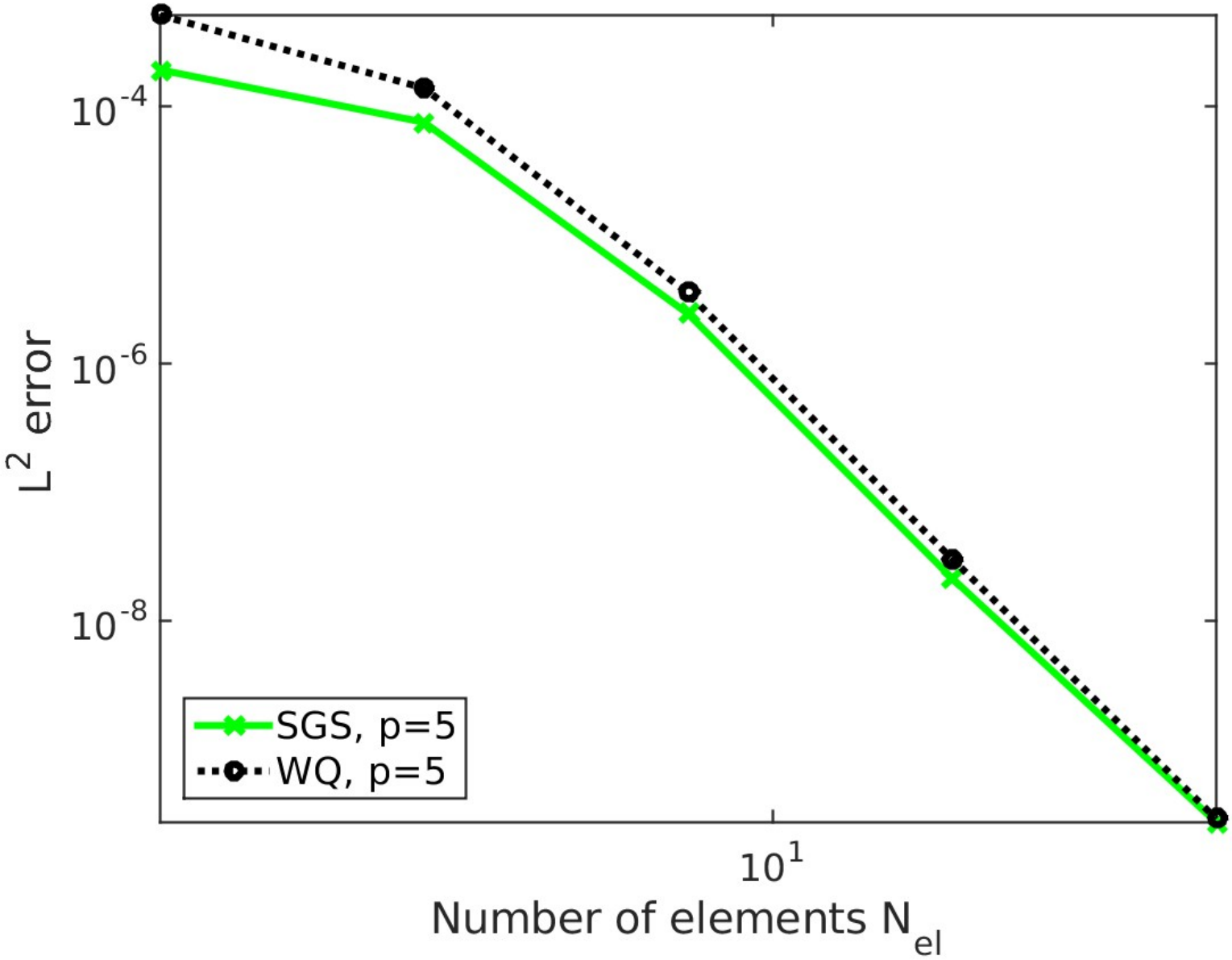
- The total number of quadrature points is $\approx 2^d N_{\mathsf{DOF}}$.

Convergence plot

Thick quarter of ring domain.



Assembly algorithm for the mass matrix

Using sum-factorization approach and matrix-tensor products.

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for $\boldsymbol{i} = 1, \ldots, N_{\mathsf{DOF}}$

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$\quad$ **for** $l = 1, \ldots, d$

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$\quad$ **end**

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- The inner loop is repeated N_{DOF} and perform $O(p)$ (BLAS level 3) operations to compute $O(p^d)$ results: total $O(N_{\mathsf{DOF}} p^{d+1})$ FLOPS

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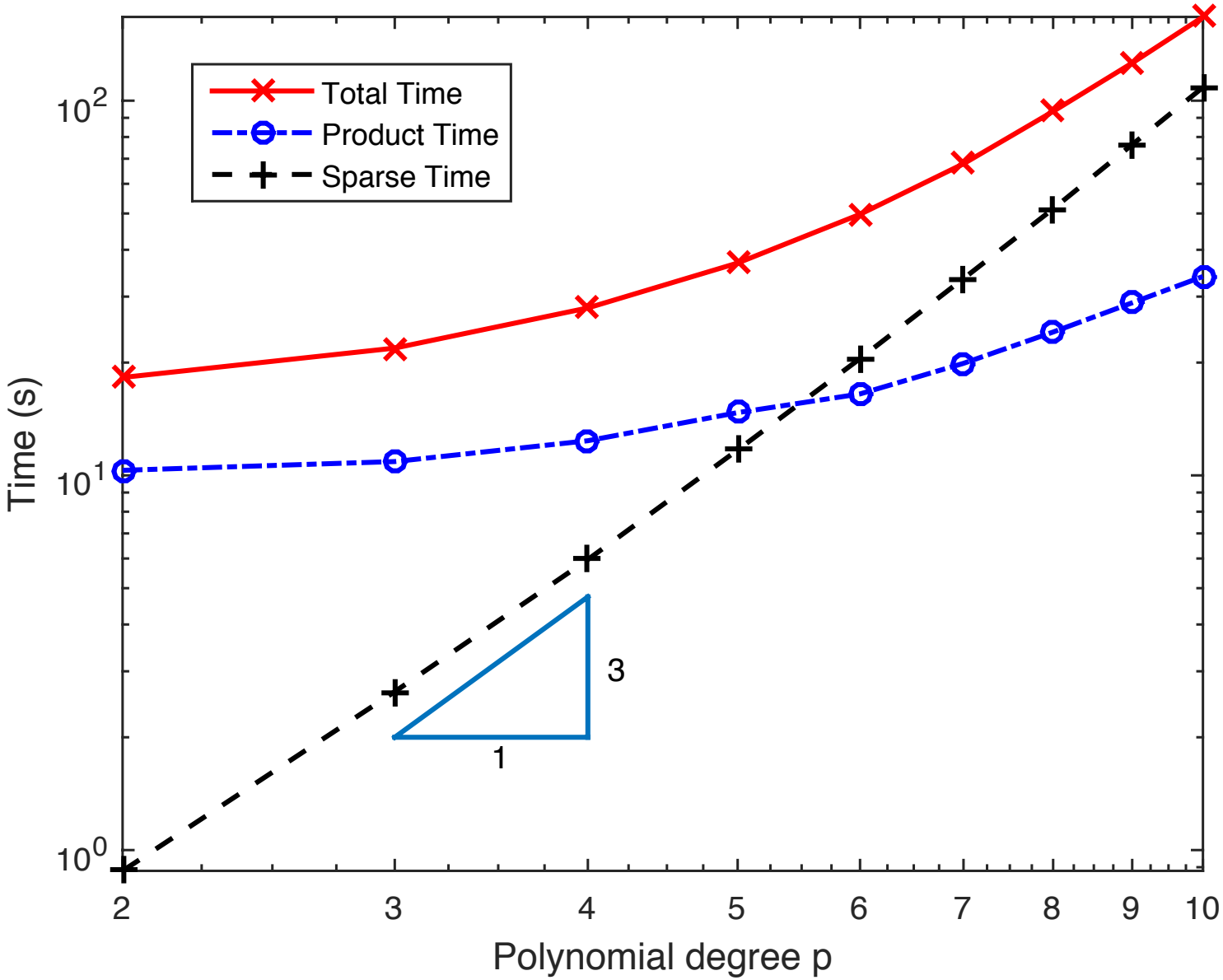
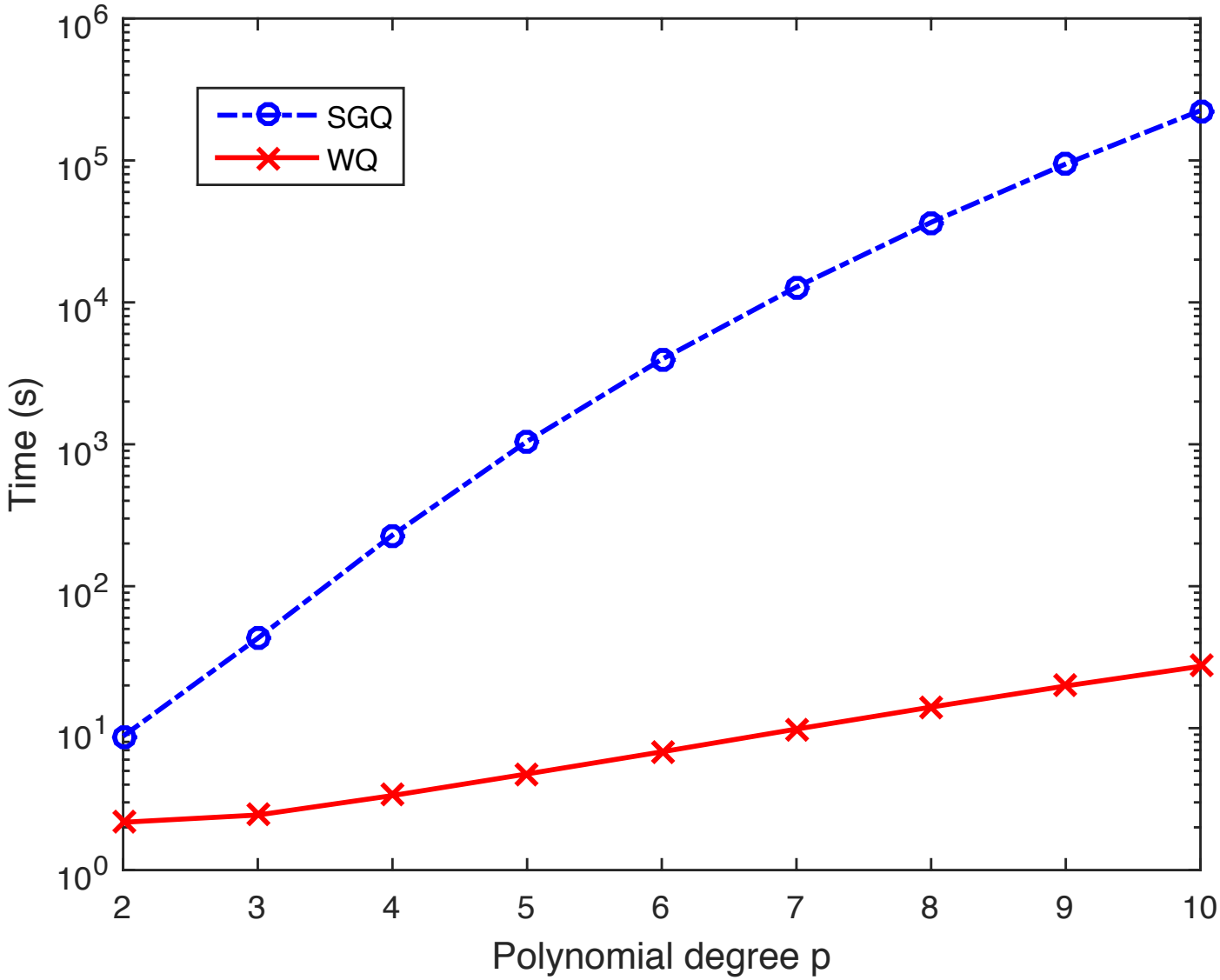
Assembly time ($\Omega = [0,1]^3$, $N_{\mathsf{EL}} = 40^3$)



Mass matrix assembly time: WQ vs. Geopdes 3.0

$$\Omega = [0,1]^3,\ N_{\mathsf{EL}} = 20^3.$$



SGQ: $O(N_{\mathsf{DOF}}\, p^{3d})$ FLOPS WQ: $O(N_{\mathsf{DOF}}\, p^{d+1})$ FLOPS

Weighted Quadrature for the stiffness matrix

$$
\begin{aligned}
k_{\boldsymbol{i},\boldsymbol{j}} &= \int_{[0,1]^d} \nabla B_{\boldsymbol{i}}(\boldsymbol{\zeta})^T \mathbf{c}(\boldsymbol{\zeta}) \nabla B_{\boldsymbol{j}}(\boldsymbol{\zeta}) \, d\boldsymbol{\zeta} \\
&= \sum_{\alpha,\beta=1}^{d} \int_{[0,1]^d} c_{\alpha,\beta}(\boldsymbol{\zeta}) \, \partial_\alpha B_{\boldsymbol{i}}(\boldsymbol{\zeta}) \, \partial_\beta B_{\boldsymbol{j}}(\boldsymbol{\zeta}) \, d\boldsymbol{\zeta} \\
&\approx \sum_{\alpha,\beta=1}^{d} \mathfrak{Q}^{\mathrm{WQ}}_{\alpha,\beta,\boldsymbol{i}} \left(c_{\alpha,\beta}(\cdot) \partial_\beta B_{\boldsymbol{j}}(\cdot) \right);
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Exactness conditions

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\mathfrak{Q}^{\mathrm{WQ}}_{\alpha,\beta,\boldsymbol{i}} (\partial_\beta B_{\boldsymbol{j}}(\cdot)) = \int_{[0,1]^d} \partial_\alpha B_{\boldsymbol{i}}(\boldsymbol{\zeta}) \, \partial_\beta B_{\boldsymbol{j}}(\boldsymbol{\zeta}) \, d\boldsymbol{\zeta} \qquad \forall \, \boldsymbol{j}
$$

Weighted Quadrature for the stiffness matrix

- For $d = 2$, two of the exactness conditions read:

$$\mathfrak{Q}^{\mathrm{WQ}}_{1,1,\boldsymbol{i}}(\partial_1 B_{\boldsymbol{j}}(\cdot)) = \int_{[0,1]^2} \partial_1 B_{\boldsymbol{i}}(\boldsymbol{\zeta})\, \partial_1 B_{\boldsymbol{j}}(\boldsymbol{\zeta})\, d\boldsymbol{\zeta}$$

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- We take 4 univariate WQ rules (per direction).

$$\mathfrak{Q}_i^{(0,0)}\left(B_j(\cdot)\right) = \int_0^1 B_i(\zeta) B_j(\zeta) d\zeta \qquad \mathfrak{Q}_i^{(1,0)}\left(B_j(\cdot)\right) = \int_0^1 B'_i(\zeta) B_j(\zeta) d\zeta$$

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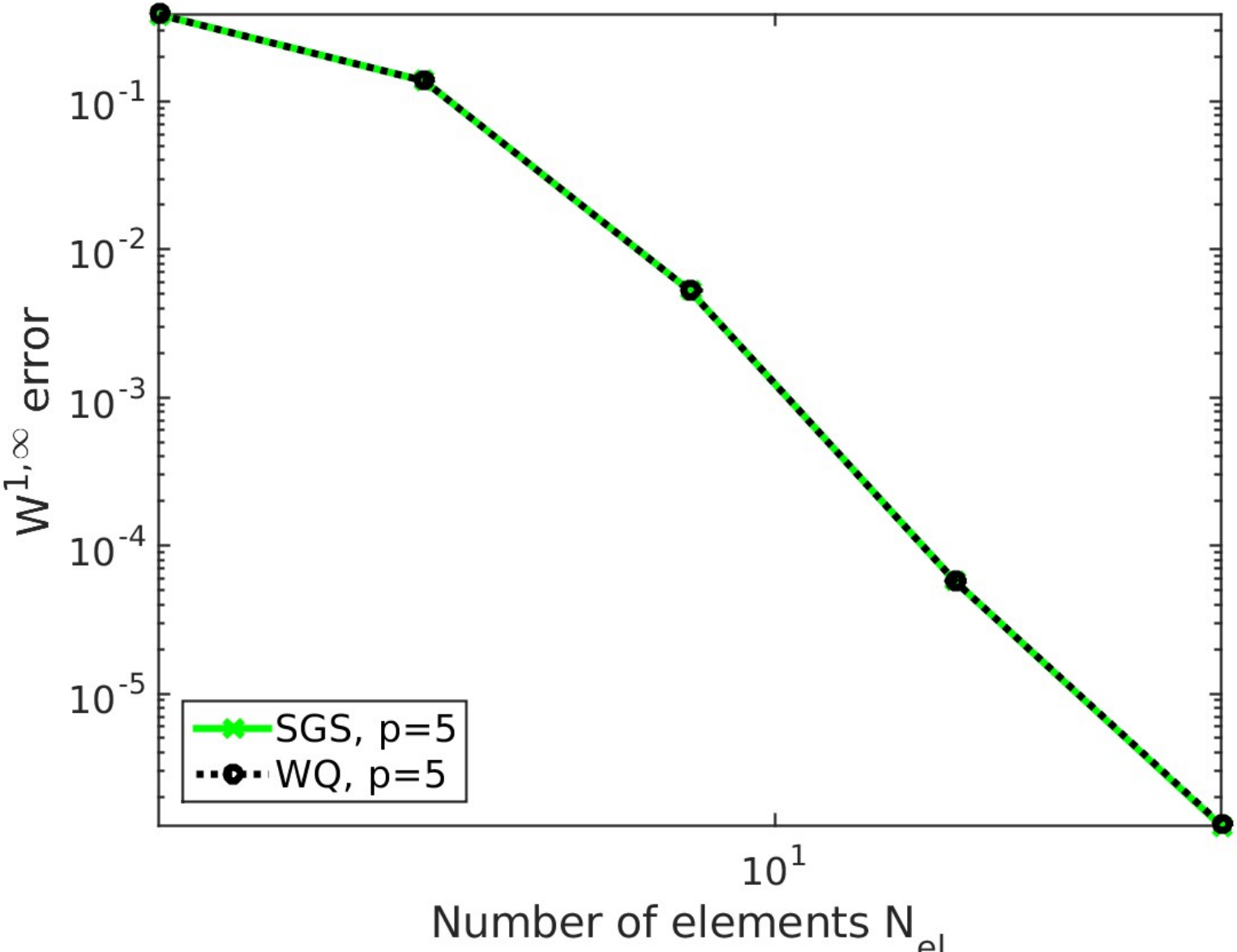
- These 4 univariate rules are the building blocks we use to define the rules $\mathfrak{Q}^{\mathrm{WQ}}_{\alpha,\beta,\boldsymbol{i}}$ (also for $d > 2$). For example:

$$\mathfrak{Q}^{\mathrm{WQ}}_{1,1,\boldsymbol{i}} = \mathfrak{Q}^{(1,1)}_{i_1} \otimes \mathfrak{Q}^{(0,0)}_{i_2} \qquad \mathfrak{Q}^{\mathrm{WQ}}_{1,2,\boldsymbol{i}} = \mathfrak{Q}^{(1,0)}_{i_1} \otimes \mathfrak{Q}^{(0,1)}_{i_2}$$

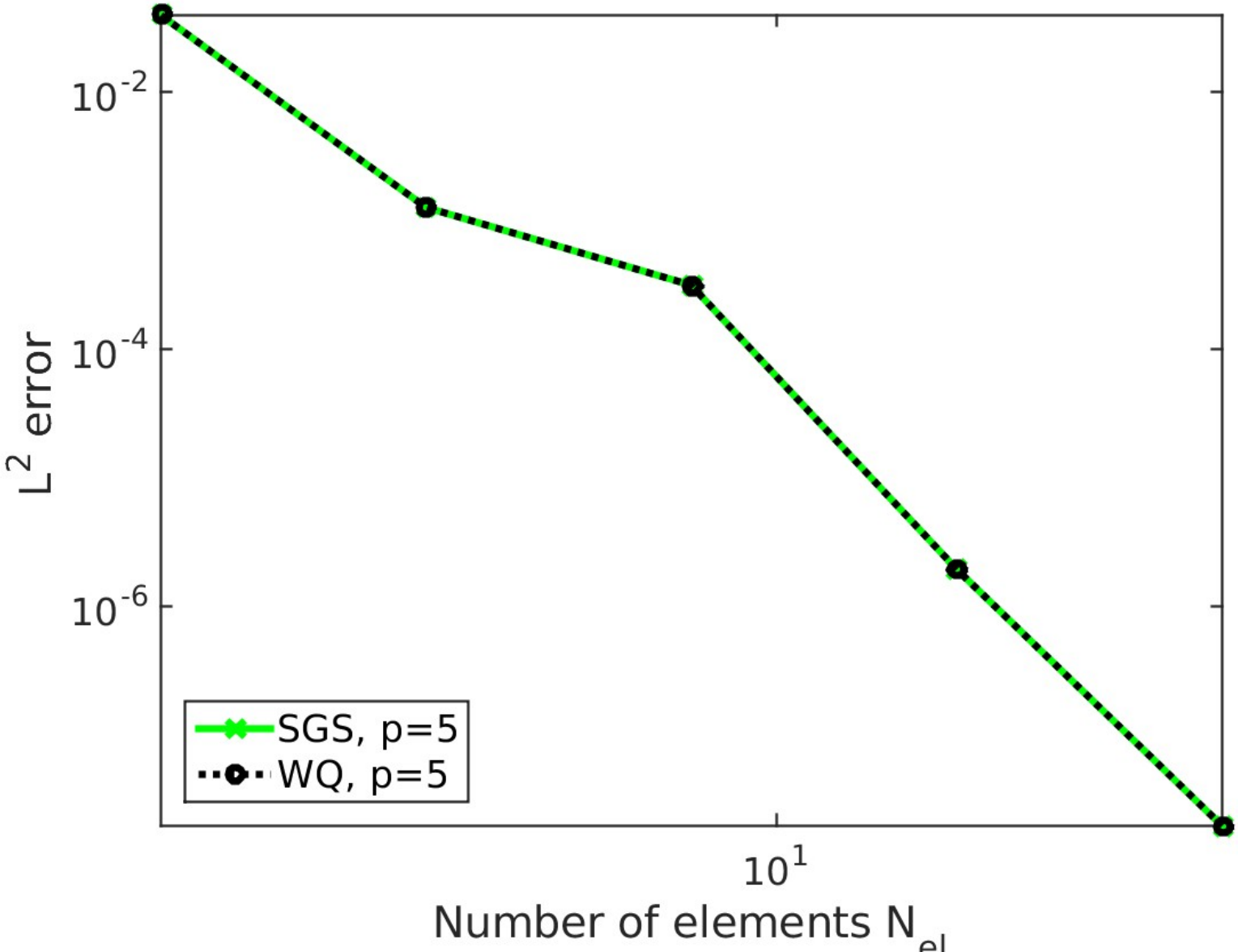
Convergence plot 1D: $W^{1,\infty}$ norm

Thick quarter of ring domain.



Convergence plot 1D: L^2 norm

Thick quarter of ring domain.



A matrix-free implementation

We only want to compute matrix-vector products with the mass matrix $\widetilde{\mathcal{M}}$:

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Let $u = (u_1, \ldots, u_{N_{DOF}}) \in \mathbb{R}^{N_{\mathsf{DOF}}}$. Since $\mathfrak{Q}_{\boldsymbol{i}}^{\mathrm{WQ}}(\cdot)$ is a linear functional, we have

$$\left(\widetilde{\mathcal{M}}u\right)_{\boldsymbol{i}} = \mathfrak{Q}_{\boldsymbol{i}}^{\mathrm{WQ}}\left(c(\cdot)u_h(\cdot)\right) = \sum_{\boldsymbol{q}} w_{\boldsymbol{iq}}\, c(x_{\boldsymbol{q}})\, u_h(x_{\boldsymbol{q}}),$$

where

$$u_h(\xi) = \sum_{\boldsymbol{j}} u_{\boldsymbol{j}} \hat{B}_{\boldsymbol{j}}(\xi)$$

A matrix-free implementation

$$\left(\widetilde{\mathcal{M}}u\right)_{\boldsymbol{i}} = \sum_{\boldsymbol{q}\in\mathcal{Q}} w_{\boldsymbol{iq}}\, c(x_{\boldsymbol{q}})\, u_h(x_{\boldsymbol{q}}), \qquad |\mathcal{Q}| = O(N_{\mathsf{DOF}})$$

The Setup

- Weights and basis spline values for univariate spaces.
- Coefficient values $c(x_{\boldsymbol{q}})$.

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The Setup

- Weights and basis spline values for univariate spaces.
  Negligible memory and cost.
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The Product

1. Given $u \in \mathbb{R}^{N_{\mathsf{DOF}}}$, compute $u_h(x_{\boldsymbol{q}})$ for every $\boldsymbol{q}$.
2. Compute $c(x_{\boldsymbol{q}}) \cdot u_h(x_{\boldsymbol{q}})$ for every $\boldsymbol{q}$.
3. Compute $\sum_{\boldsymbol{q}} w_{\boldsymbol{iq}}\, c(x_{\boldsymbol{q}})\, u_h(x_{\boldsymbol{q}})$ for every $\boldsymbol{i}$.

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   $O(N_{\mathsf{DOF}}\, p)$ FLOPS exploiting the tensor structure.
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A matrix-free implementation

	Standard WQ	Matrix-free WQ
Allocated memory	$O(N_{\mathsf{DOF}}\, p^d)$	$O(N_{\mathsf{DOF}})$
Setup cost	$O(N_{\mathsf{DOF}}\, p^{d+1}) + \mathrm{EV}$	EV
Product cost	$O(N_{\mathsf{DOF}}\, p^d)$	$O(N_{\mathsf{DOF}}\, p)$

EV = Cost of coefficient evaluation on $O(N_{\mathsf{DOF}})$ points

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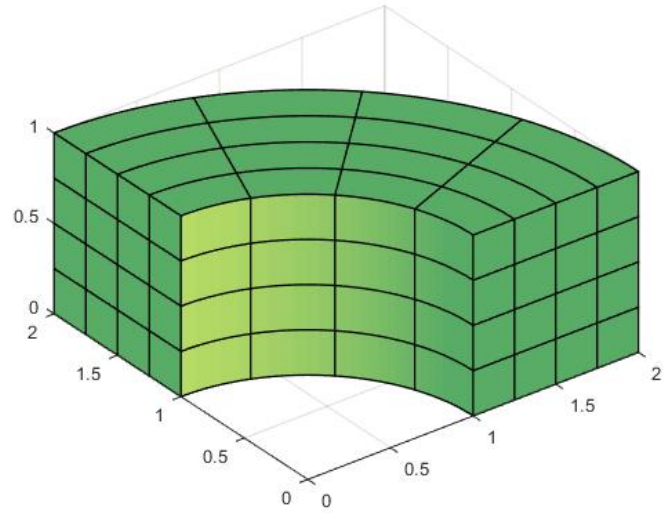
- Analogous for the matrix-free stiffness matrix $\mathcal{A}$.
- Can be coupled with a $p-$robust preconditioner to solve iteratively the system $\mathcal{A}x = b$ ☞ yesterday Mattia Tani talk.

Standard WQ (S-WQ) vs. Matrix-free WQ (MF-WQ)

$N_{\mathsf{EL}} = 64^3$



	Setup Time		Product Time	
	MF-WQ	S-WQ	MF-WQ	S-WQ
$p = 2$	1.28	72.79	0.04	0.05
$p = 3$	1.30	89.06	0.05	0.14
$p = 4$	1.36	112.52	0.05	0.34
$p = 5$	1.58	174.19	0.06	0.58

Conclusions

It is possible to form and solve high-order isogeometric Galerkin k-method is an efficient way, but this is beyond standard FE routines.

- with row-loop and WQ: calculating the matrix entries is faster than saving it in a sparse matrix (MATLAB `sparse`)
- with Fast Diagonalization direct solver as preconditioner: CPU time for the preconditioner setup+application is less than CPU time for the residual calculation in CG

Current work in Pavia is on:

- matrix-free approach
- dealing with "bad" geometries ($\sup_\Omega \kappa(J_F) \gg 1$).
- develop all this for NS

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