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GESELLSCHAFT für ANGEWANDTE MATHEMATIK und MECHANIK e.V.
INTERNATIONAL ASSOCIATION of APPLIED MATHEMATICS and MECHANICS

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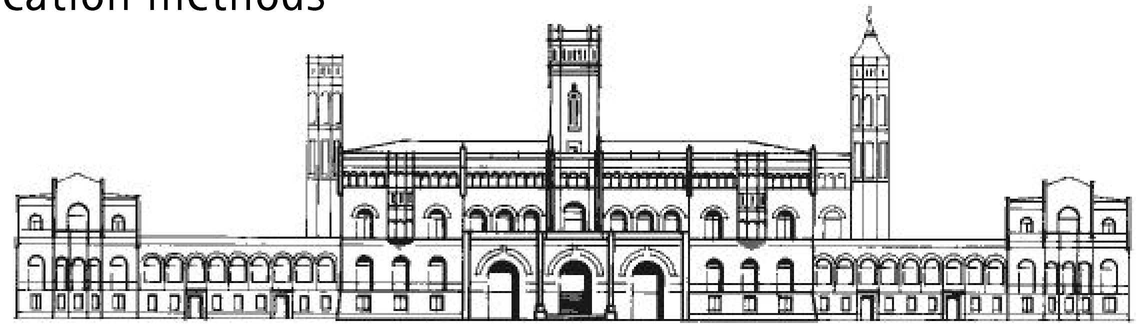
A fast and low-memory isogeometric Galerkin method for Karhunen-Loève series expansion of 3D random fields

A performance comparison to matrix-free isogeometric collocation methods



Random fields

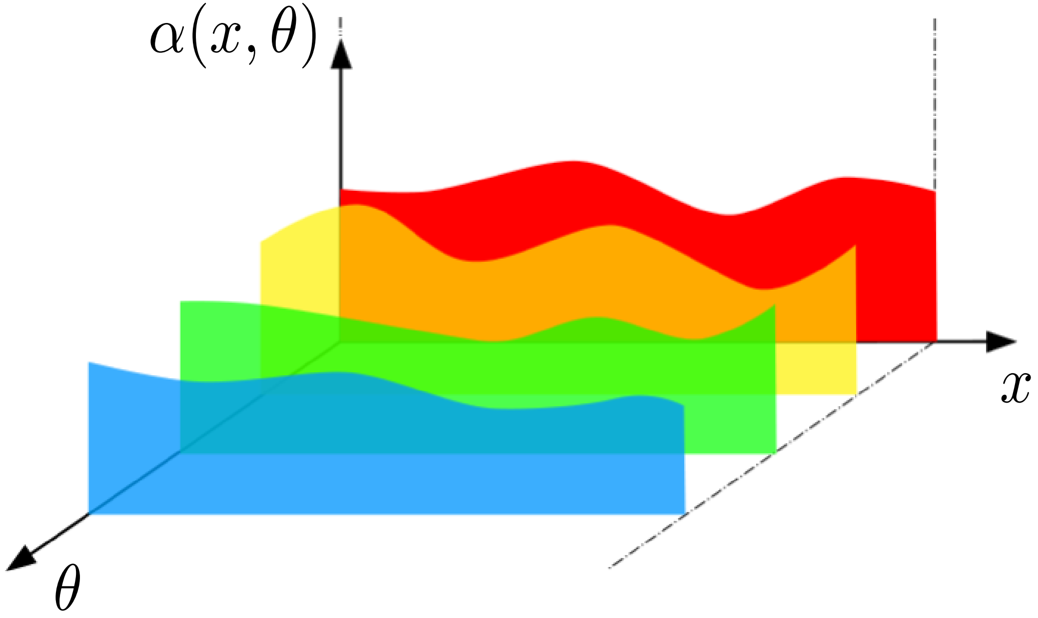
$$\alpha(\cdot,\theta)\ :\ \Theta \mapsto L^2(\mathcal{D})$$

Mean value

$$\mu(x) := \mathbb{E}\left[\alpha(x,\theta)\right]$$

Covariance function

$$\Gamma(x,x') := \mathbb{E}\left[(\alpha(x,\theta)-\mu(x))(\alpha(x',\theta)-\mu(x'))\right]$$



A **random field** is a collection of continuous deterministic functions on a bounded domain, called realizations, which are indexed by events in some sample set

Discretization by expansion

Numerical treatment of a continuous random field requires discretization in the stochastic space!

Decompose the random field into a sum of the mean and a finite linear combination of L^2 orthogonal functions weighted by uncorrelated stochastic random variables

$$\tilde{\alpha}_M(x,\theta) = \mu(x) + \sum_{i=1}^{M} f_i(x)\xi_i(\theta)$$

Karhunen-Loève expansion

$$T\phi_i = \lambda_i \phi_i, \qquad (T\phi)(x) = \int_{\mathcal{D}} \Gamma(x, x')\phi(x')\,\mathrm{d}x'$$

Hilbert-Schmidt operator
Karhunen (1947) and Loève (1948)

$$f_i(x) = \sqrt{\lambda_i}\phi_i(x)$$

$$\tilde{\alpha}_M(x, \theta) = \mu(x) + \sum_{i=1}^{M} f_i(x)\xi_i(\theta)$$

The Karhunen-Loève series expansion yields the **best** *M*-term linear approximation of the random field, in the sense that the total mean squared error is minimized

Karhunen, K. *Über lineare Methoden in der Wahrscheinlichkeitsrechnung. Suomalaisen Tiedeakatemian toimituks*, Helsinki, 1947.

Solution methods

Find $\{\lambda_h, \phi_h\} \in \mathbb{R}_0^+ \times \mathcal{S}_h$ such that

$$\int_{\mathcal{D}} \left(\int_{\mathcal{D}'} \Gamma(x, x')\phi_h(x')\,\mathrm{d}x' - \lambda\phi_h(x) \right) \psi_h(x)\,\mathrm{d}x = 0 \qquad \forall\, \psi_h \in \mathcal{S}_h \subset L^2(\mathcal{D})$$

Galerkin
$\mathcal{O}\left(N^2(p+1)^{3d}\right)$

Find $\{\lambda_h, \phi_h\} \in \mathbb{R}_0^+ \times \mathcal{S}_h$ such that

$$\int_{\mathcal{D}} \Gamma(x_i, x')\phi_h(x')\,\mathrm{d}x' - \lambda\phi_h(x_i) = 0 \qquad \forall\, x_i \in \mathcal{D}$$

Collocation
$\mathcal{O}\left(N^2(p+1)^{2d}\right)$

Atkinson, K.E. *The Numerical Solution of Integral Equations of the Second Kind.* Cambridge University Press, 1997.

Rahman, S., *A Galerkin isogeometric method for Karhunen–Loève approximation of random fields*; Comput. Methods Appl. Mech. Engrg. 338 (2018) 533–561

Jahanbin, R., Rahman S., *An isogeometric collocation method for efficient random field discretization*; Int. J. Numer. Methods Eng. 117 (2019) 344–369

Why splines?

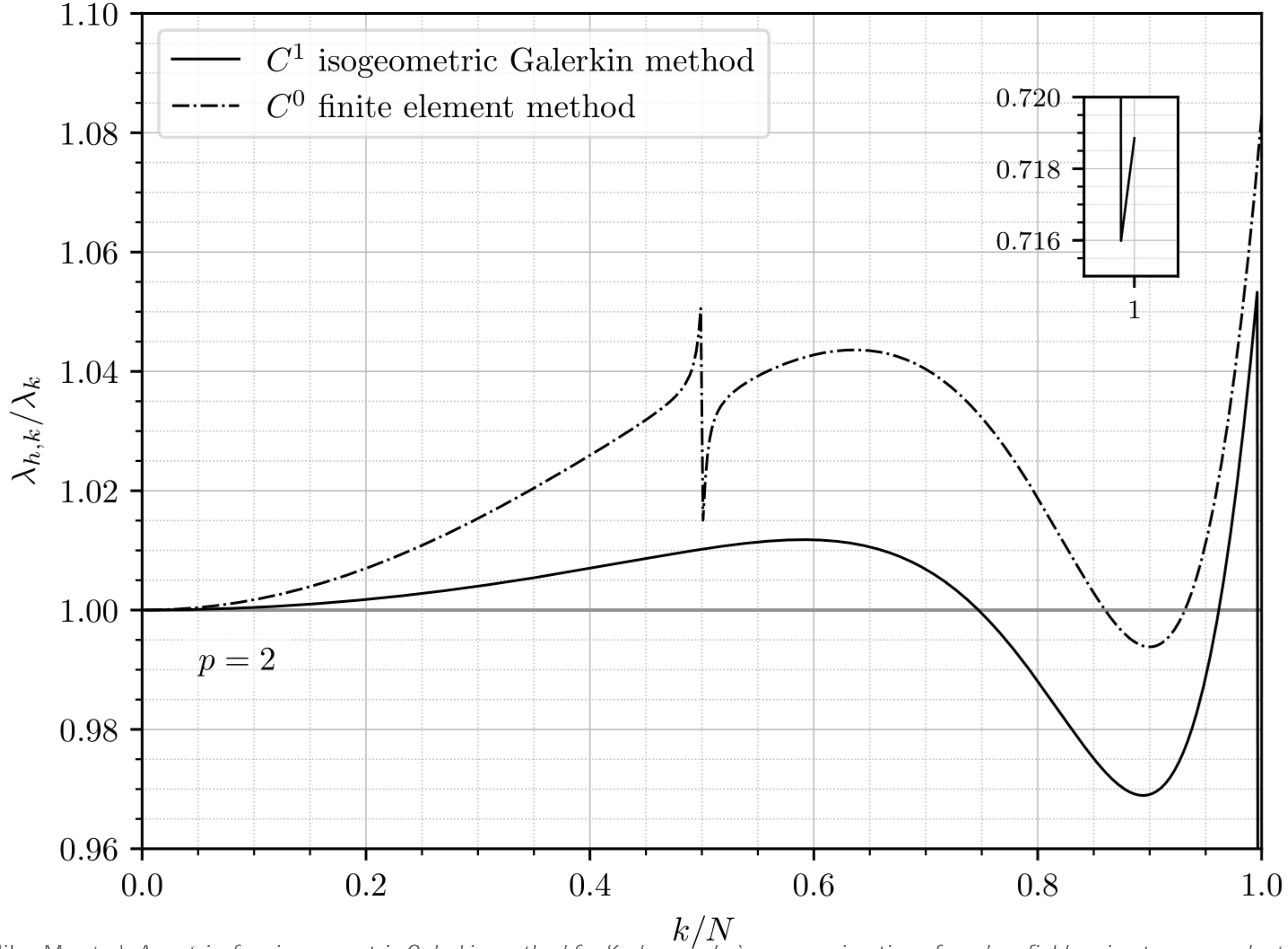


Figure 1
Accuracy of the eigenvalue spectra for Galerkin methods of different continuity and the exponential kernel

Splines possess better spectral approximation properties, which have been shown for a multitude of model equations and applies to integral eigenvalue problems as well

Mika, M., et al. *A matrix-free isogeometric Galerkin method for Karhunen–Loève approximation of random fields using tensor product splines, tensor contraction and interpolation based quadrature, CMAME (accepted)*

Numerical properties

$$\mathsf{A}\mathsf{v}_h = \lambda_h \mathsf{Z}\mathsf{v}_h$$

Generalized algebraic eigenvalue problem

Galerkin

+ monotonic convergence of the solution spectra
+ symmetric positive (semi-)definite system matrices
+ established stability and convergence analysis
– computationally intensive
– memory intensive

Collocation

+ computationally efficient
– non-symmetric system matrices
– no established stability and convergence analysis
– real-valued eigensolutions are not guaranteed
– memory intensive

A high-order matrix-free IBQ-Galerkin

IBQ-Galerkin
$$\mathcal{O}\left(N_{\text{iter}} \cdot \tilde{N}^2\right)$$

- Interpolation based quadrature (IBQ) using tensor product B-splines and tensor contraction (inspired by sum factorization techniques)
- Computational cost is independent of polynomial order (enables high-order)
- Scalable and memory inexpensive by a matrix-free formulation of the matrix-vector product

Bressan, A., Takacs. S. *Sum factorization techniques in Isogeometric Analysis.* Computer Methods in Applied Mechanics and Engineering, 352:437–460, August 2019.
Mika, M., et al. *A matrix-free isogeometric Galerkin method for Karhunen–Loève approximation of random fields using tensor product splines, tensor contraction and interpolation based quadrature,* CMAME *(accepted)*

New isogeometric Galerkin method

Search in $\mathcal{S}_h \subset L^2(\mathcal{D})$ where $\mathcal{S}_h := \operatorname{span}\left\{ \frac{B_\mathsf{i}(\hat{x})}{\sqrt{\det \mathrm{D}F(\hat{x})}} \right\}_{\mathsf{i}\in\mathcal{I}}$

$$\mathsf{A}_{\mathsf{ij}} = \int_{\mathcal{D}} \int_{\mathcal{D}'} \hat{\Gamma}(\hat{x}, \hat{x}') B_\mathsf{i}(\hat{x}) B_\mathsf{j}(\hat{x}') \sqrt{\det \mathrm{D}F(\hat{x}) \det \mathrm{D}F(\hat{x}')}\, \mathrm{d}\hat{x}\, \mathrm{d}\hat{x}'$$

$$\mathsf{A}\mathsf{v}_h = \lambda_h \mathsf{Z}\mathsf{v}_h$$

Generalized algebraic eigenvalue problem

$$\mathsf{Z}_{\mathsf{ij}} = \int_{\mathcal{D}} B_\mathsf{i}(\hat{x}) B_\mathsf{j}(\hat{x})\, \mathrm{d}\hat{x} = \mathsf{Z}_d \otimes \cdots \otimes \mathsf{Z}_1 \quad \text{where} \quad \mathsf{Z}_k = \int_0^1 B_{i_k,p_k}(\hat{x}_k) B_{j_k,p_k}(\hat{x}_k)\, \mathrm{d}\hat{x}_k$$

Integrated exactly up machine precision using Gauss-Legendre quadrature rule with (p+1) quadrature points per element

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Interpolation based quadrature

IBQ–Galerkin

$$\mathcal{O}\left(N_{\text{iter}} \cdot \tilde{N}^2\right)$$

$$\mathsf{A}_{\mathsf{ij}} = \int_{\mathcal{D}} \int_{\mathcal{D}'} \hat{\Gamma}(\hat{x},\hat{x}') \sqrt{\det \mathrm{D}F(\hat{x}) \det \mathrm{D}F(\hat{x}')}\, B_{\mathsf{i}}(\hat{x}) B_{\mathsf{j}}(\hat{x}')\, \mathrm{d}\hat{x}\, \mathrm{d}\hat{x}'$$

$$G(\hat{x},\hat{x}') := \hat{\Gamma}(\hat{x},\hat{x}') \sqrt{\det \mathrm{D}F(\hat{x}) \det \mathrm{D}F(\hat{x}')}$$

Interpolation i.e. at Greville abscissae

$$\tilde{G}(\hat{x}_{\mathsf{m}},\hat{x}'_{\mathsf{n}}) := \sum_{\mathsf{k},\mathsf{l} \in \tilde{\mathcal{I}}} \tilde{\mathsf{G}}_{\mathsf{kl}} \tilde{B}_{\mathsf{k}}(\hat{x}_{\mathsf{m}}) \tilde{B}_{\mathsf{l}}(\hat{x}'_{\mathsf{n}}) = \tilde{\mathsf{B}}^{\top} \tilde{\mathsf{G}} \tilde{\mathsf{B}}$$

$$\tilde{\mathsf{A}}_{\mathsf{ij}} = \int_{\mathcal{D}} \int_{\mathcal{D}'} \tilde{G}(\hat{x},\hat{x}')\, B_{\mathsf{i}}(\hat{x}) B_{\mathsf{j}}(\hat{x}')\, \mathrm{d}\hat{x}\, \mathrm{d}\hat{x}'$$

$$\tilde{\mathsf{A}}_{\mathsf{ij}} = \sum_{\mathsf{k},\mathsf{l} \in \tilde{\mathcal{I}}} \tilde{\mathsf{G}}_{\mathsf{kl}} \int_{\mathcal{D}} \tilde{B}_{\mathsf{k}}(\hat{x}) B_{\mathsf{i}}(\hat{x})\, \mathrm{d}\hat{x} \int_{\mathcal{D}'} \tilde{B}_{\mathsf{l}}(\hat{x}') B_{\mathsf{j}}(\hat{x}')\, \mathrm{d}\hat{x}'$$

$$\tilde{\mathsf{A}}_{\mathsf{ij}} = \sum_{\mathsf{k},\mathsf{l} \in \tilde{\mathcal{I}}} \tilde{\mathsf{G}}_{\mathsf{kl}} \mathsf{M}_{\mathsf{ki}} \mathsf{M}_{\mathsf{lj}}$$

$$\mathsf{M}_{\mathsf{ki}} = \mathsf{M}_d \otimes \cdots \otimes \mathsf{M}_1 \quad \text{where}$$

$$\mathsf{M}_k = \int_0^1 \tilde{B}_{i_k,\tilde{p}_k}(\hat{x}_k) B_{j_k,p_k}(\hat{x}_k)\, \mathrm{d}\hat{x}_k$$

Integrated exactly up machine precision using Gauss-Legendre quadrature rule with (p+1) quadrature points per element

The approximation error is entirely due to the interpolation error

Matrix-free isogeometric collocation

Matrix-free Collocation

$$\mathcal{O}\left(N_{\text{iter}} \cdot N^2 (p+1)^d\right)$$

$$\mathsf{A}_{\mathsf{ij}} = \int_{\mathcal{D}} \Gamma(x_{\mathsf{i}}, x') R_{\mathsf{j}}(x') \mathrm{d}\hat{x}' \quad \text{and} \quad \mathsf{Z}_{\mathsf{ij}} = R_{\mathsf{j}}(x'_{\mathsf{i}}) := \mathsf{P}^\top \mathsf{LUQ}^\top$$

$$\{R_{\mathsf{j}}(x)\}_{\mathsf{j} \in \mathcal{I}}$$

NURBS space

Collocated at the Cartesian product Greville abscissae $\{\mathsf{x}_{\mathsf{i}}\}_{\mathsf{i} \in \mathcal{I}}$

$$\mathsf{A}\mathsf{v}_h = \lambda_h \mathsf{Z}\mathsf{v}_h$$

Generalized algebraic eigenvalue problem

Algorithm 1 Matrix-free evaluation of the matrix-vector product $\mathsf{v}' \mapsto \mathsf{A}'\mathsf{v}'$ emerging from collocation

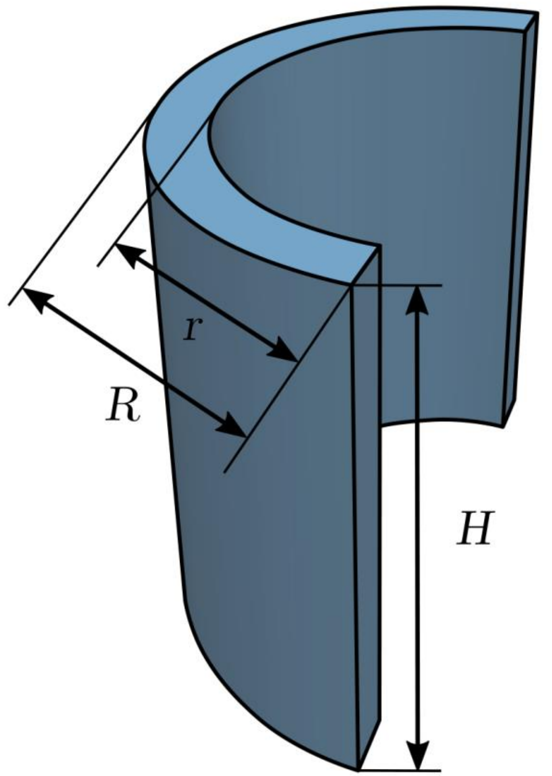
Input: $v_{\mathsf{j}} \in \mathbb{R}^N$, $D_{\mathsf{ki}} \in \mathbb{R}^{(N_e \cdot N_q) \times N}$, $P_{\mathsf{ij}}, Q_{\mathsf{ij}}, U_{\mathsf{ij}}, L_{\mathsf{ij}} \in \mathbb{R}^{N \times N}$, $J_{\mathsf{k}} \in \mathbb{R}^{N_e \cdot N_q}$, $W_{\mathsf{k}} \in \mathbb{R}^{N_e \cdot N_q}$

Output: $v'_{\mathsf{i}} \in \mathbb{R}^N$

1: $Y_{\mathsf{k}} \leftarrow R_{\mathsf{jk}} v_{\mathsf{j}}$ ▷ Interpolation of v_{j} at quadrature points
2: $Y'_{\mathsf{k}} \leftarrow Y_{\mathsf{k}} \odot J_{\mathsf{k}} \odot W_{\mathsf{k}}$ ▷ Scaling of entries at quad. points
3: $Z_{\mathsf{l}} \leftarrow \Gamma_{\mathsf{lk}} Y'_{\mathsf{k}}$ ▷ Row-wise evaluation without forming Γ
4: $v'_{\mathsf{i}} \leftarrow Q_{\mathsf{it}} U^{-1}_{\mathsf{tr}} L^{-1}_{\mathsf{rs}} P_{\mathsf{sj}} v_{\mathsf{j}}$ ▷ Backsolve using pivoted LU of Z

Jahanbin, R., Rahman S., *An isogeometric collocation method for efficient random field discretization*; Int. J. Numer. Methods Eng. 117 (2019) 344–369

Model problem



$r = 8$
$R = 10$
$H = 15$

$b = 0.5$
$L = 10$

Example 1

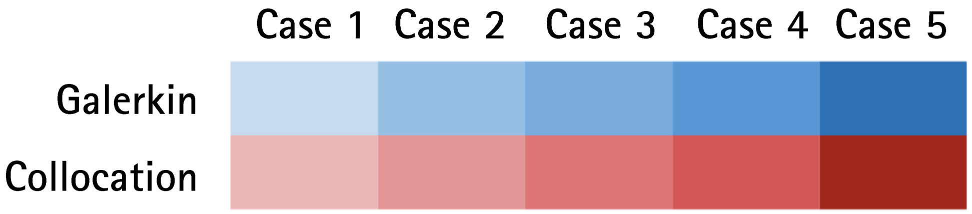
The exponential (rough) kernel and five different cases of *h*-refined solution and interpolation spaces

Example 2

The Gaussian (smooth) kernel and five different cases of *k*-refined solution and interpolation spaces

Reference solution

Standard isogeometric Galerkin with $p = 2$ and $N = 6642$ and an execution time of ~17 hours



Color-coding of the different cases in Example 1 and Example 2

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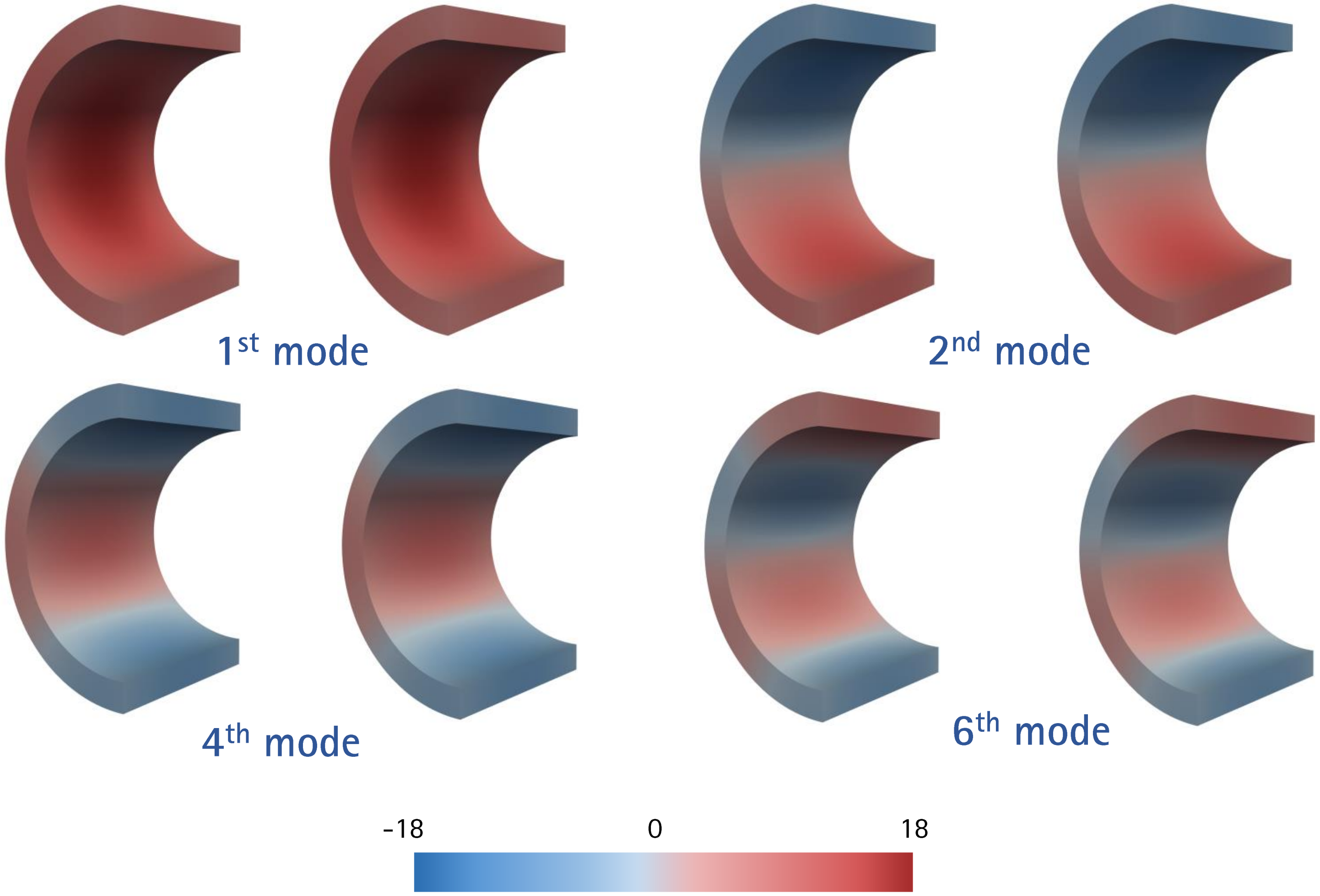
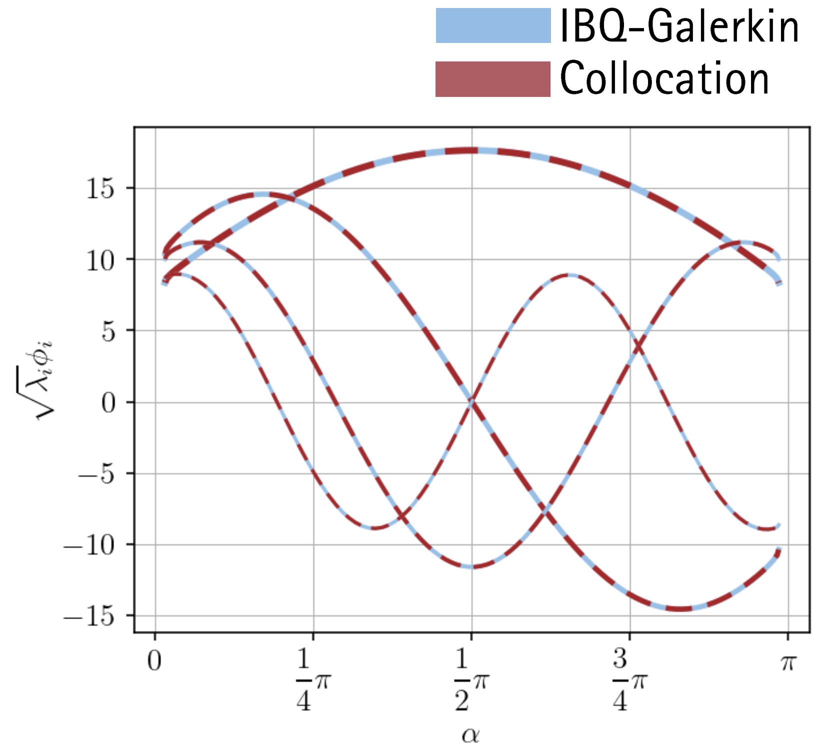
Example 1

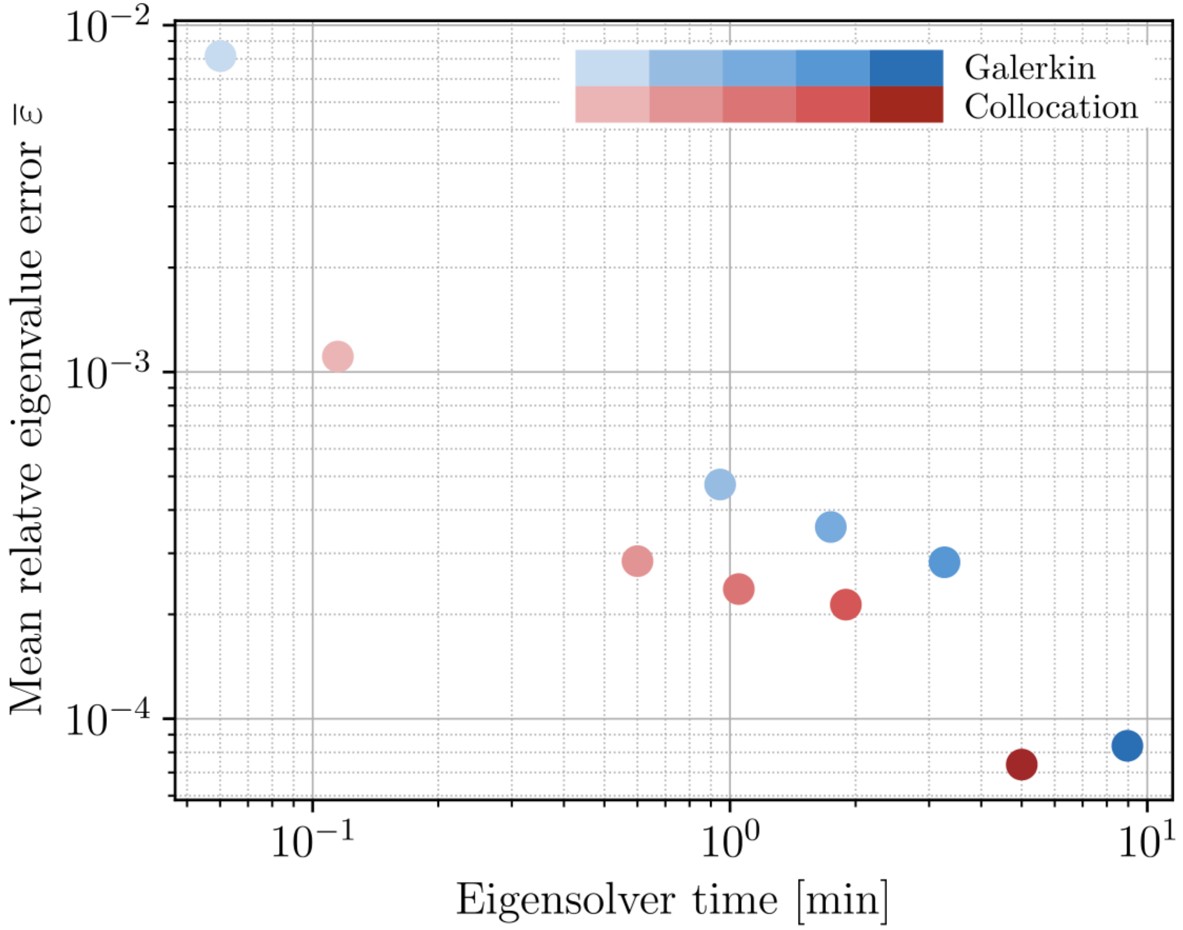
IBQ-Galerkin Collocation IBQ-Galerkin Collocation





Line plot at the mid-planes along the circumferential direction

Example 1



Mean relative error in the first $N = 20$ eigenvalues

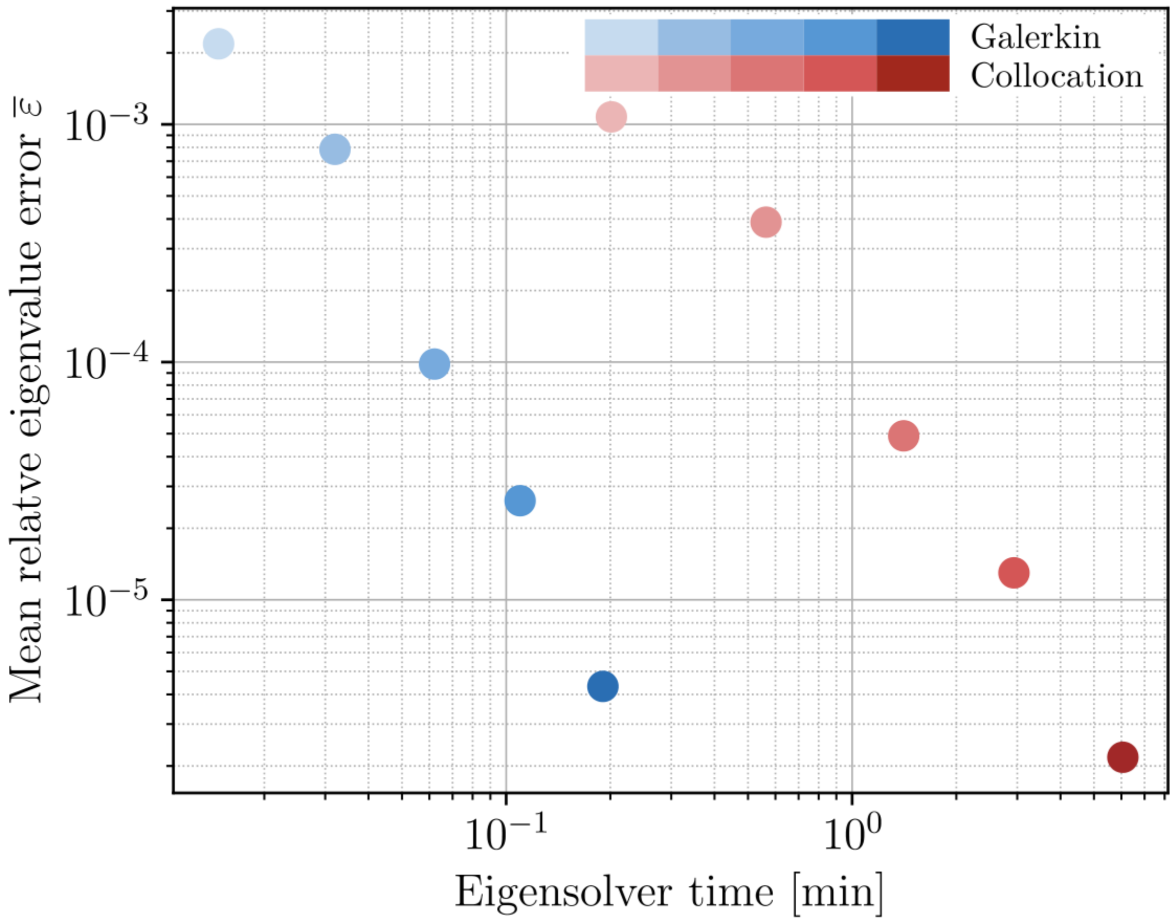
$$\bar{\varepsilon} := \frac{1}{N} \sum_{i=1}^{N} \frac{|\lambda_{\mathrm{ref},i} - \lambda_i|}{\lambda_{\mathrm{ref},i}}$$

Example 1 The exponential (rough) kernel and five different cases of *h*-refined solution and interpolation spaces ($p = 2$)

	Case 1	Case 2	Case 3	Case 4	Case 5
h	2.857	1.719	1.556	1.423	1.142
N	1050	2108	2800	3772	5625
$\tilde{N}$	1980	8990	12210	16770	28294

h mesh size in the solution and interpolation mesh
N number of degrees of freedom (dof) in the solution space
$\tilde{N}$ number of dof in the interpolation space (IBQ-Galerkin only)

Example 2



Mean relative error in the $N = 20$ first eigenvalues

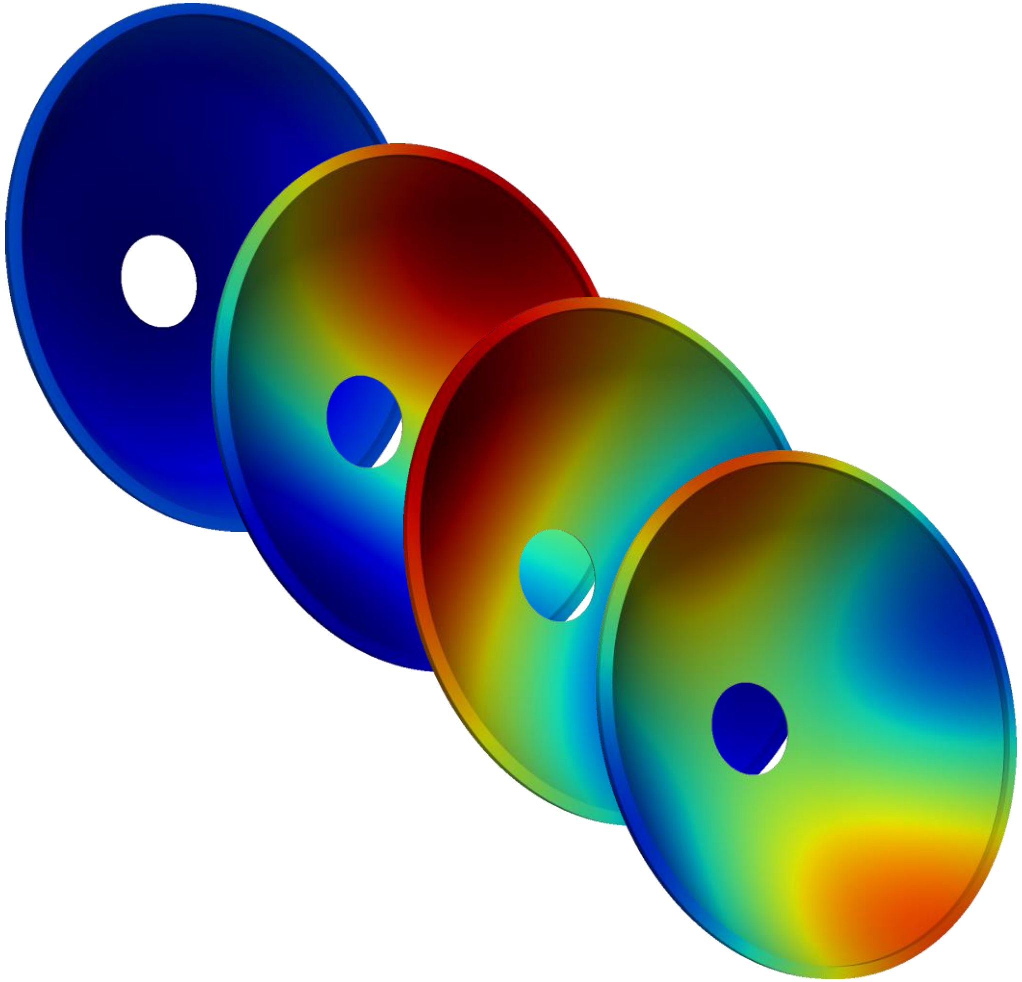
$$\bar{\varepsilon} := \frac{1}{N} \sum_{i=1}^{N} \frac{|\lambda_{\mathrm{ref},i} - \lambda_i|}{\lambda_{\mathrm{ref},i}}$$

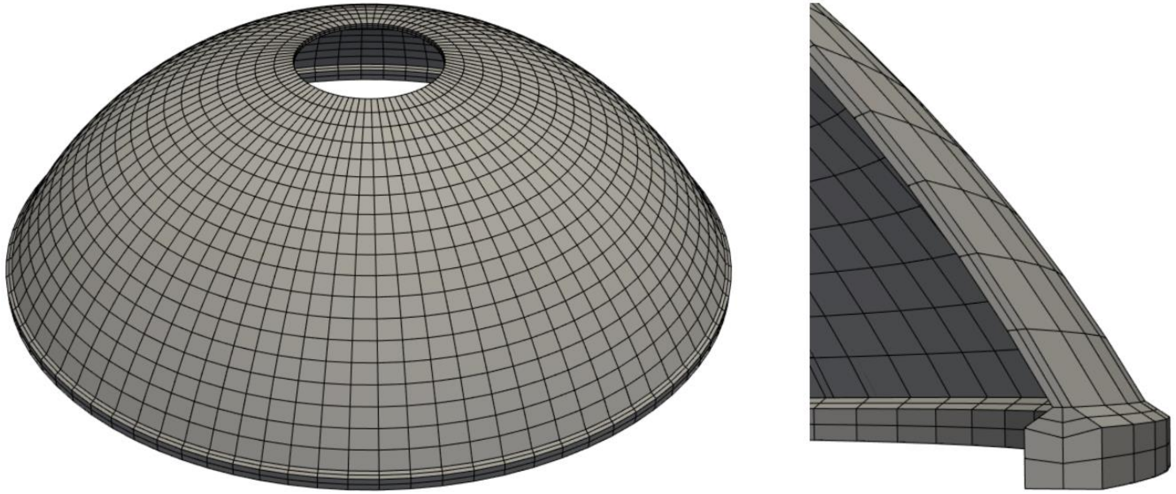
Example 2 The Gaussian (smooth) kernel and five different cases of *k*-refined solution and interpolation spaces ($h = 2.857$)

	Case 1	Case 2	Case 3	Case 4	Case 5
p	2	3	4	5	6
N	1050	1628	2340	3198	4214
$\tilde{N}$	1080	1672	2400	3276	4312

p polynomial order of the solution and interpolation space
N number of degrees of freedom (dof) in the solution space
$\tilde{N}$ number of dof in the interpolation space (IBQ-Galerkin only)

Further high-order example





High-order multi-patch example

Polynomial degree $p = 16$

Smooth Gaussian kernel

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In conclusion

Matrix-free Galerkin using IBQ

+ **computationally efficient**
+ **memory efficient**
+ symmetric positive (semi-)definite system matrices
+ monotonic convergence of the solution spectra
+ good outlook for stability and convergence analysis

– marginally suboptimal for rough kernels

Matrix-free Collocation

+ computationally efficient
+ **memory efficient**
+ slightly more optimal for rough kernels

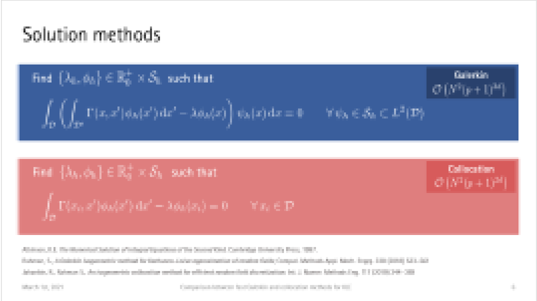
– non-symmetric system matrices

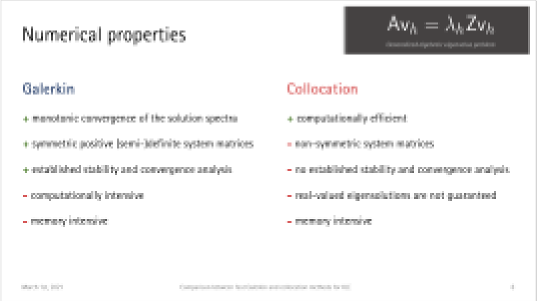
– real-valued eigensolutions are not guaranteed

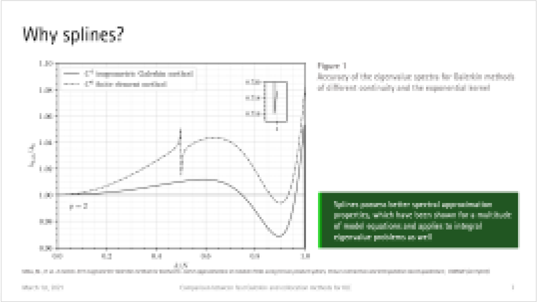
– no established stability and convergence analysis

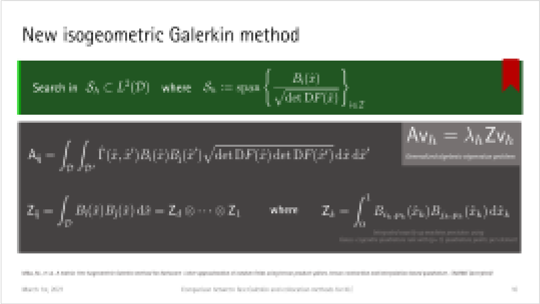
The matrix-free Galerkin using IBQ achieves computational and memory efficiency without sacrificing its advantageous properties.

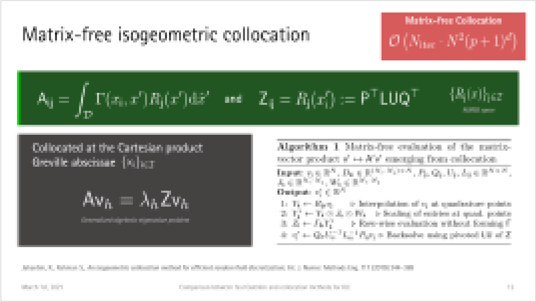
Discussion

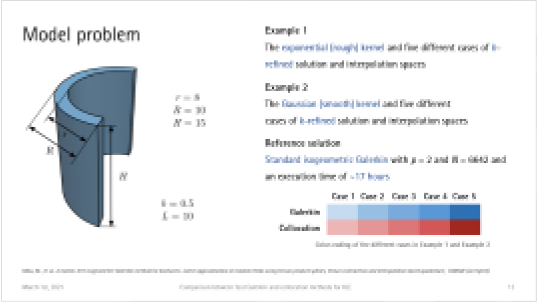


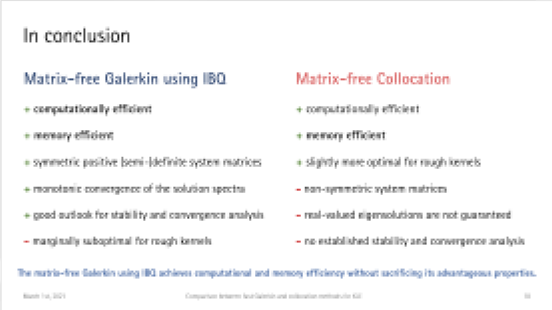












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