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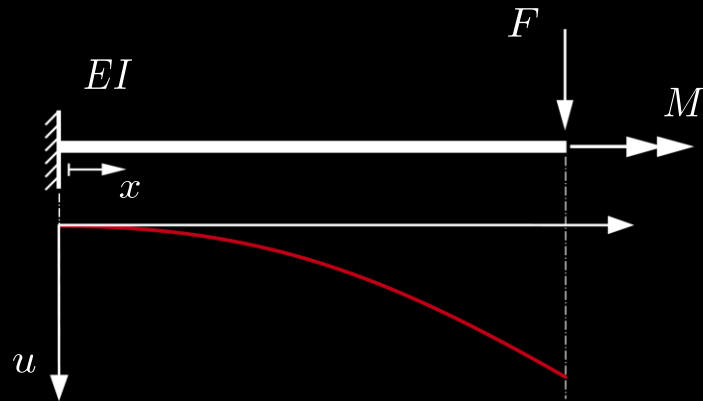
# Matrix-free isogeometric Galerkin method Karhunen-Loève approximation of random fields

Using tensor product splines, tensor contraction and interpolation based quadrature



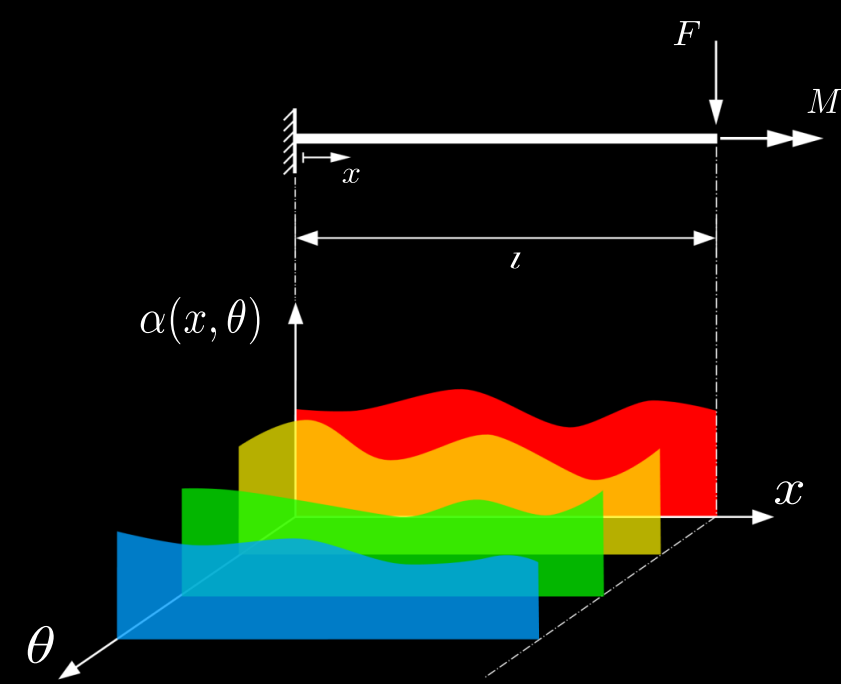
# Nondeterminism of (physical) systems

$$\mathcal{L}(x)u(x) = f(x) \text{ deterministic}$$



stochastic

$$\mathcal{L}(x, \theta)u(x, \theta) = f(x, \theta)$$



Most physical systems exhibit randomness, which, because of its lack of pattern or regularity, can not be explicitly captured by deterministic mathematical models

# Random fields

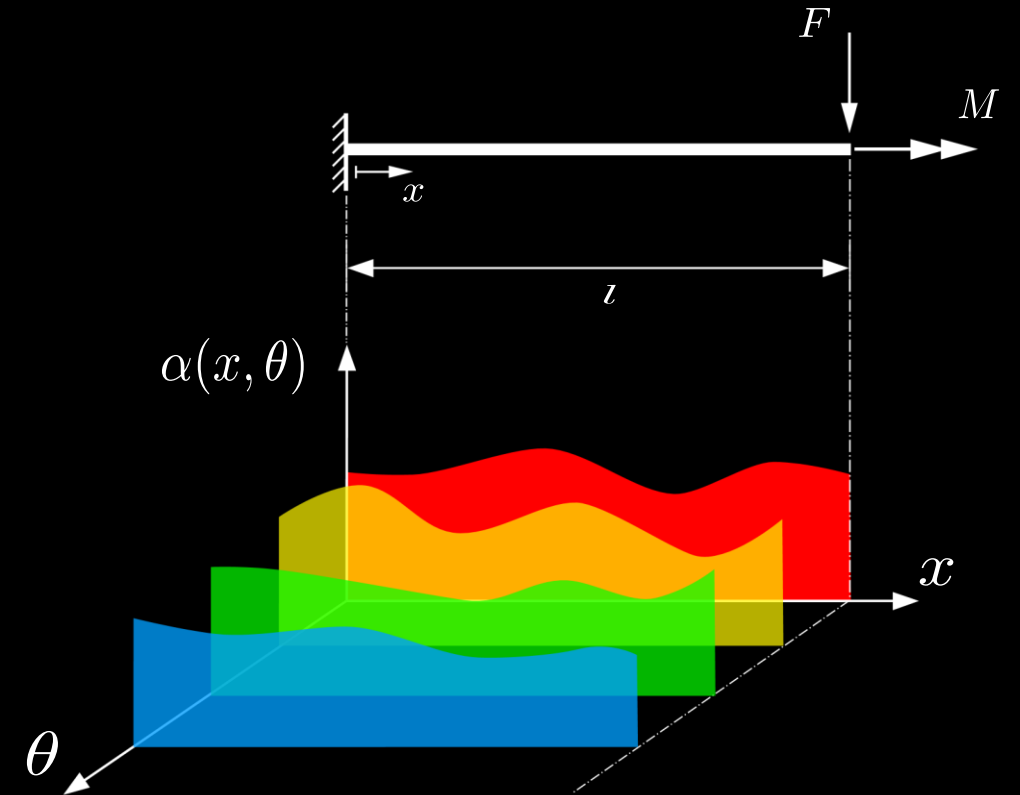
$$\alpha(\cdot, \theta) : \Theta \mapsto L^2(\mathcal{D})$$

Mean value

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

Covariance function

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



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

# Covariance functions

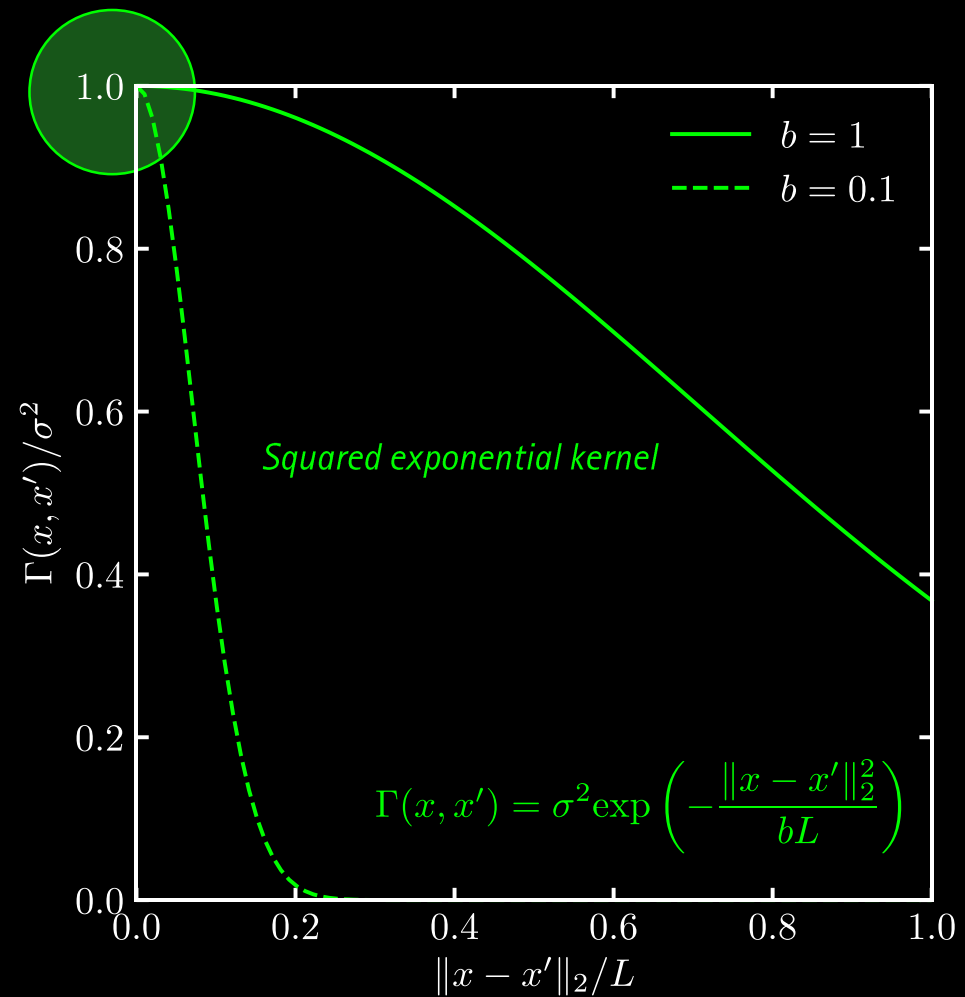
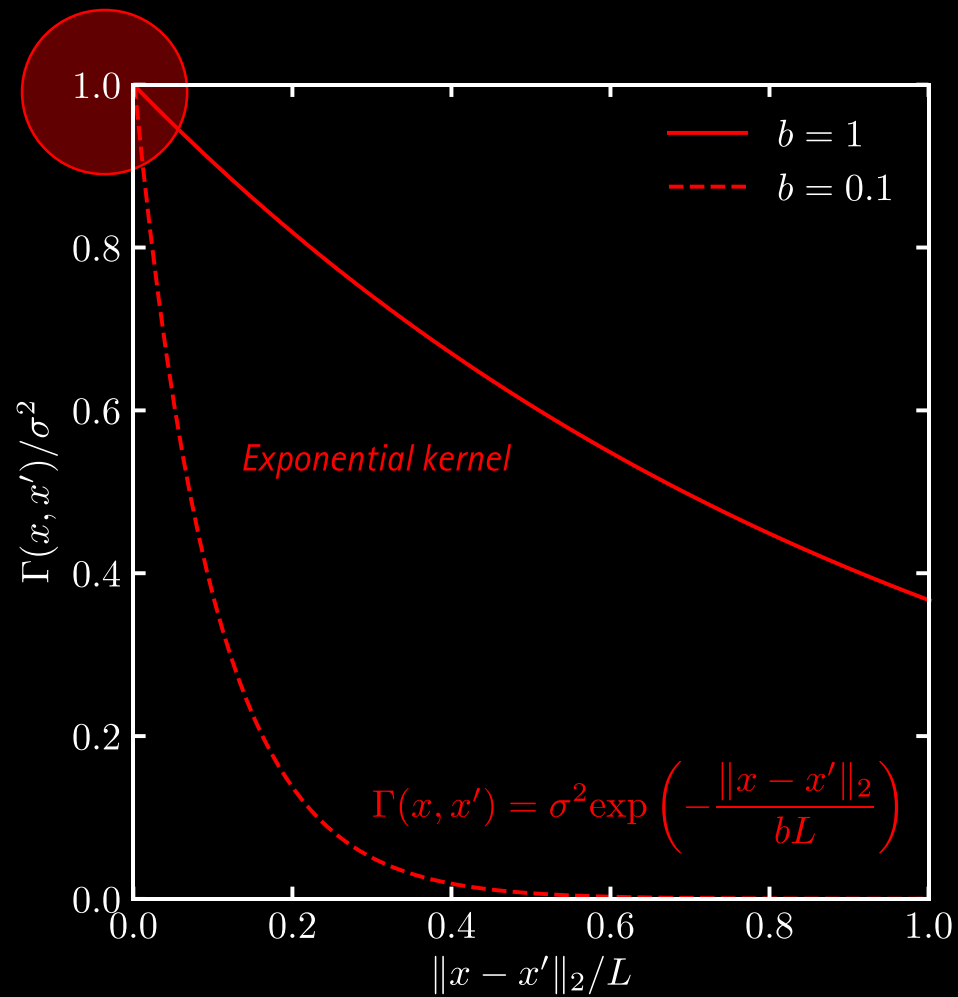


Figure 1: Common covariance functions (kernels), i.e. **exponential covariance function** (left) and **squared exponential covariance function** (right)

# Random field discretization

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

$$T\phi_i = \lambda_i\phi_i, \quad (T\phi)(x) = \int_{\mathcal{D}} \Gamma(x, x')\phi(x') dx'$$

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

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

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

# Solution of the integral eigenvalue problem

- A range of different methods for IEVP has been proposed in the literature<sup>1</sup>
- Recently an **isogeometric Galerkin method** has been proposed<sup>2</sup>

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

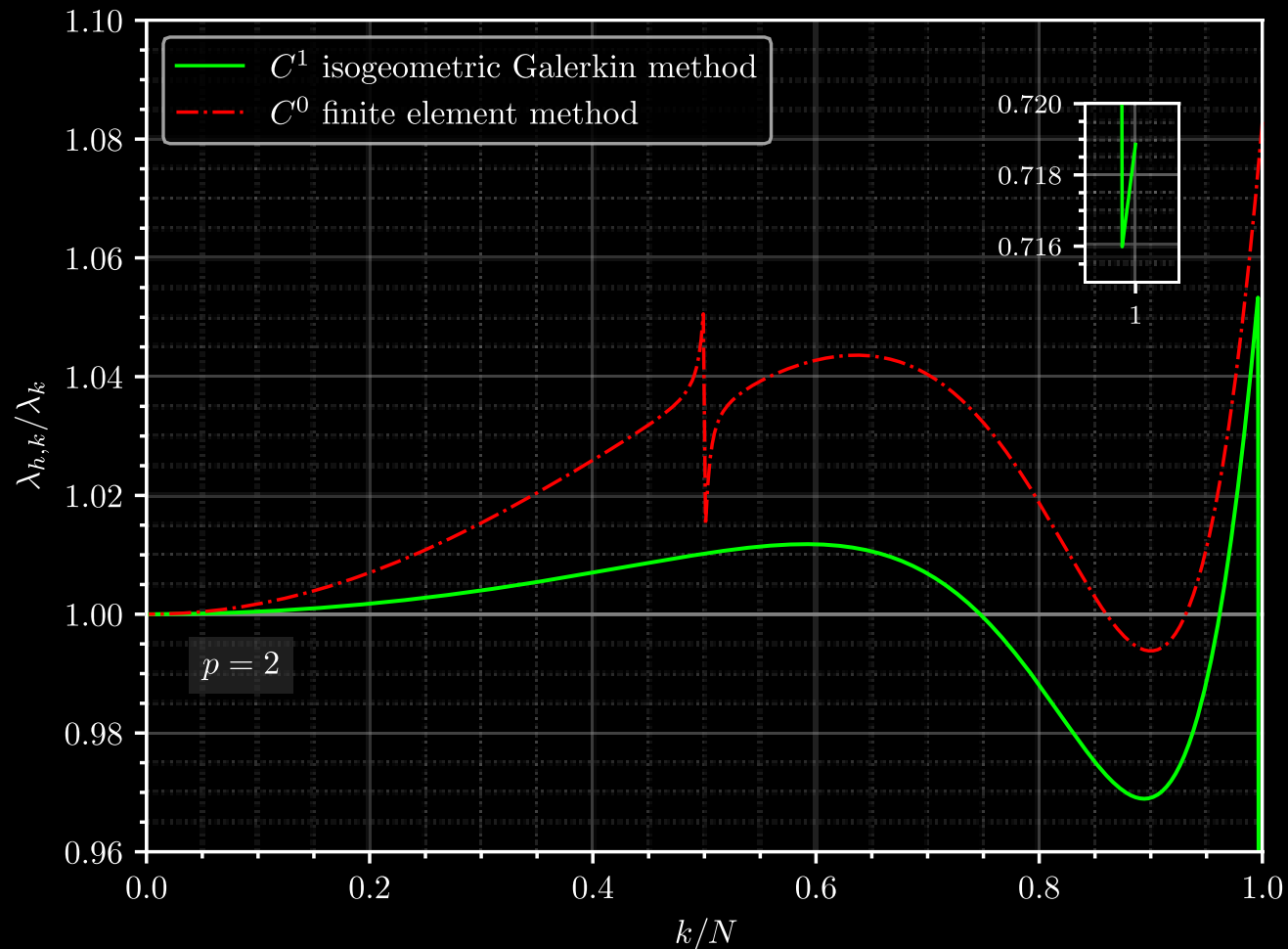
$$\int_{\mathcal{D}} \left( \int_{\mathcal{D}'} \Gamma(x, x') \phi_h(x') dx' - \lambda \phi_h(x) \right) \psi_h(x) dx = 0 \quad \forall \psi_h \in \mathcal{R}_h \subset L^2(\mathcal{D})$$

*Non-uniform rational B-splines*

<sup>1</sup> For an overview see the review paper by Betz et al. *Numerical methods for the discretization of random fields by means of the Karhunen–Loève expansion* (2014)

<sup>2</sup> Rahman, S., *A Galerkin isogeometric method for Karhunen–Loève approximation of random fields* (2018)

# Why an isogeometric Galerkin method?



Spectral properties of the method improve due to higher continuity the basis

Figure 2: Full spectrum of eigenvalues normalized with respect to a reference solution. Comparing quadratic  $C^1$  continuous B-splines and standard quadratic  $C^0$  continuous basis functions. One dimensional example with an exponential covariance function.



# Standard discretization

$$\mathbf{A} \in \mathbb{R}^{N \times N}, \mathbf{Z} \in \mathbb{R}^{N \times N}, \mathbf{v}_h \in \mathbb{R}^N, \lambda_h \in \mathbb{R}_0^+, (i, j) \in \mathcal{I}, N := \#\mathcal{I}$$

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

Generalized algebraic eigenvalue problem

$$\mathbf{A}_{ij} = \int_{\hat{\mathcal{D}}} \int_{\hat{\mathcal{D}}'} \hat{\Gamma}(\hat{x}, \hat{x}') N_i(\hat{x}) N_j(\hat{x}') \det \mathbf{D}F(\hat{x}) \det \mathbf{D}F(\hat{x}') d\hat{x} d\hat{x}'$$
$$\mathbf{Z}_{ij} = \int_{\hat{\mathcal{D}}} N_i(\hat{x}) N_j(\hat{x}) \det \mathbf{D}F(\hat{x}) d\hat{x}$$

Standard Galerkin methods for this class of integral eigenvalue problems are numerically challenging!

- i. Due to numerical integration over a  $2d$  dimensional domain the complexity of the assembly is  $O(N \rho^{3d})$
- ii. The main system matrix  $\mathbf{A}$  is a dense matrix, which requires  $8N^2$  bytes of memory in double precision arithmetic
- iii. The generalized algebraic eigenvalue problem (usually) requires a reformulation into a standard eigenvalue problem, i.e. using Cholesky decomposition of the right-hand-side mass matrix with complexity  $O(N^3)$

Figure 3: Complexity of assembly  $O(N p^{3d})$

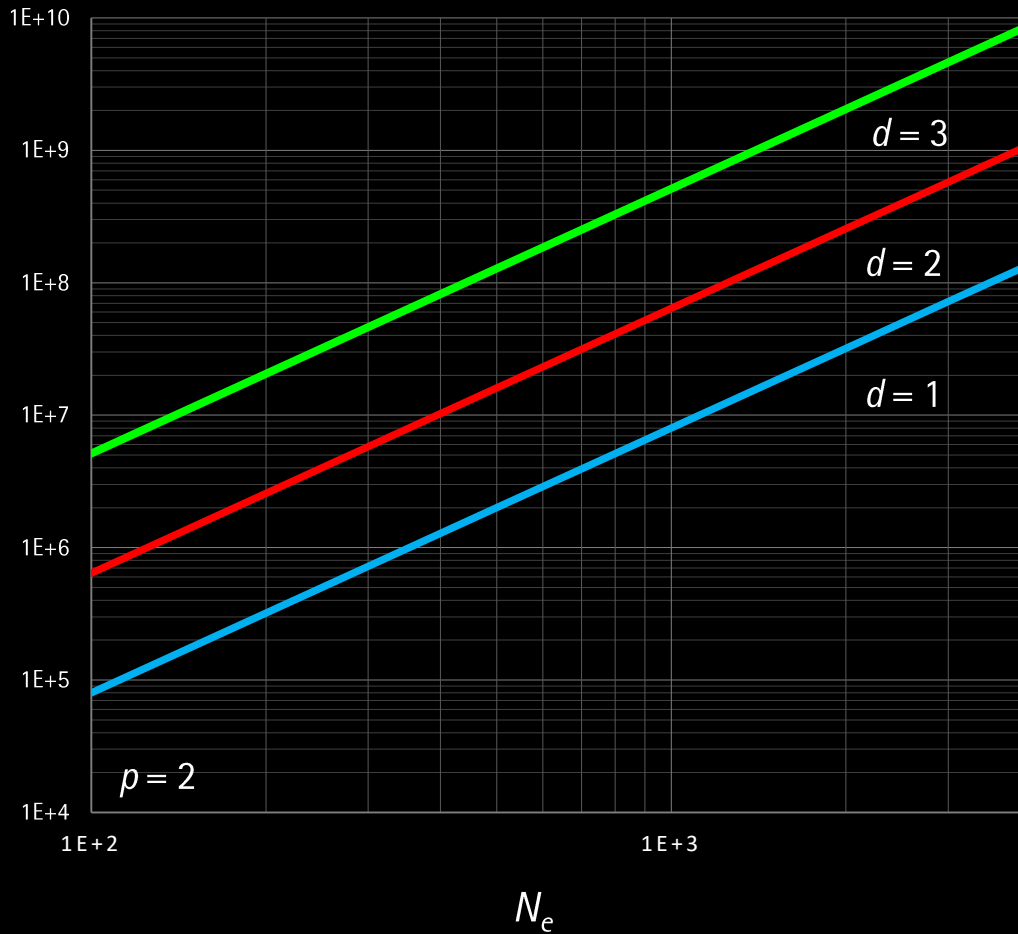


Figure 4: Complexity of Cholesky decomposition  $O(N^3)$

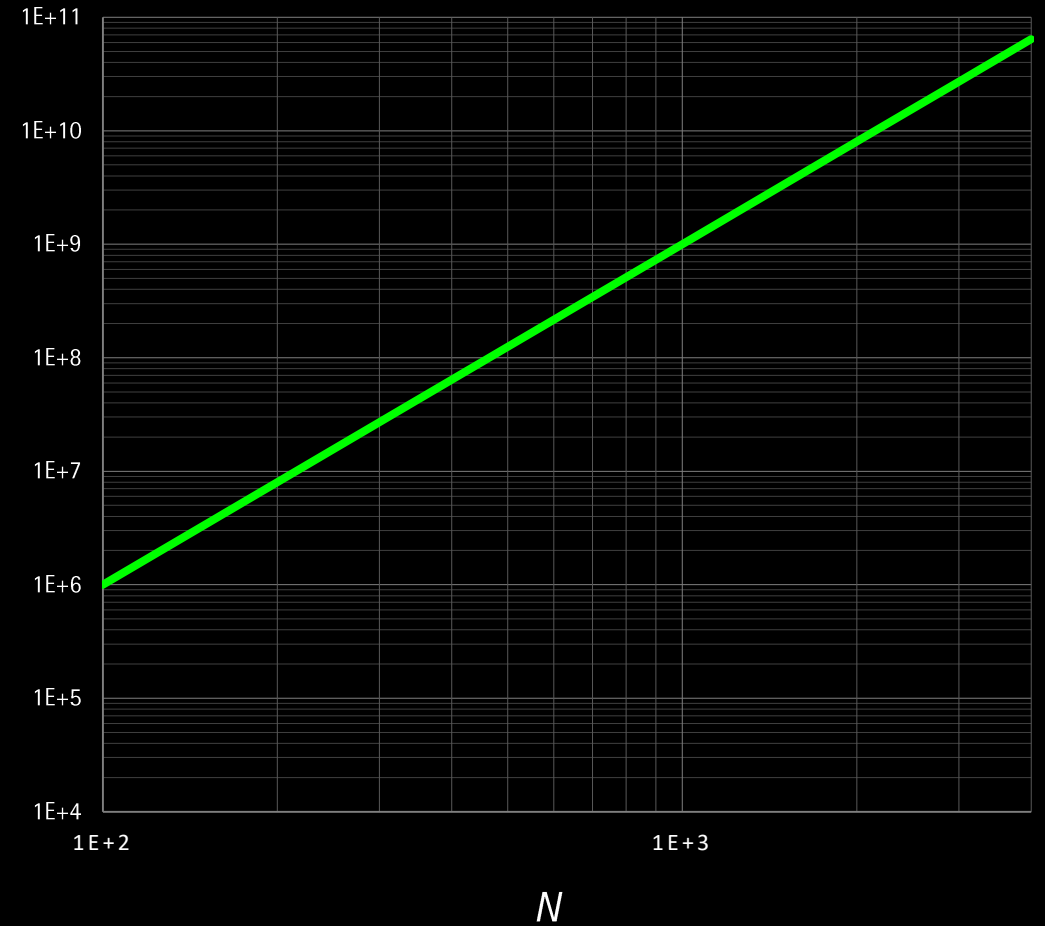


Table 1: Matrix-storage costs in double precision

Number of degrees of freedom	$10^3$	$10^4$	$10^5$	$10^6$
Matrix storage	8 MB	800 MB	80 GB	8 TB

# New trial space

Search in  $\mathcal{S}_h \subset L^2(\mathcal{D})$  where  $\mathcal{S}_h := \text{span} \left\{ \frac{B_i(\hat{x})}{\sqrt{\det DF(\hat{x})}} \right\}_{i \in \mathcal{I}}$

$$A_{ij} = \int_{\mathcal{D}} \int_{\mathcal{D}'} \hat{\Gamma}(\hat{x}, \hat{x}') \frac{B_i(\hat{x})}{\sqrt{\det DF(\hat{x})}} \frac{B_j(\hat{x}')}{\sqrt{\det DF(\hat{x}')}} \det DF(\hat{x}) \det DF(\hat{x}') d\hat{x} d\hat{x}'$$

$$Z_{ij} = \int_{\mathcal{D}} \frac{B_i(\hat{x})}{\sqrt{\det DF(\hat{x})}} \frac{B_j(\hat{x})}{\sqrt{\det DF(\hat{x})}} \det DF(\hat{x}) d\hat{x}$$

# New trial space

Search in  $\mathcal{S}_h \subset L^2(\mathcal{D})$  where  $\mathcal{S}_h := \text{span} \left\{ \frac{B_i(\hat{x})}{\sqrt{\det DF(\hat{x})}} \right\}_{i \in \mathcal{I}}$

$$A_{ij} = \int_{\mathcal{D}} \int_{\mathcal{D}'} \hat{\Gamma}(\hat{x}, \hat{x}') B_i(\hat{x}) B_j(\hat{x}') \sqrt{\det DF(\hat{x}) \det DF(\hat{x}')} d\hat{x} d\hat{x}'$$

$$Z_{ij} = \int_{\mathcal{D}} B_i(\hat{x}) B_j(\hat{x}) d\hat{x} = Z_d \otimes \cdots \otimes Z_1 \quad \text{where} \quad Z_k = \int_0^1 B_{i_k, p_k}(\hat{x}_k) B_{j_k, p_k}(\hat{x}_k) d\hat{x}_k$$

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

# Standard algebraic eigenvalue problem

$$A v_h = \lambda_h Z v_h \quad \Rightarrow \quad A' v_h = \lambda_h v_h$$

$$A' = L^{-1} A L^{-T} \quad \text{where} \quad L L^T = Z$$

Using the Kronecker structure of the matrix  $Z$  one can reduce the cost of a Cholesky decomposition from  $O(N)$  to  $O(n)$ , where  $n$  is the number of degrees of freedom in a single parametric direction

$$\begin{aligned} Z &= Z_d \otimes \cdots \otimes Z_1 \\ &= L_d L_d^T \otimes \cdots \otimes L_1 L_1^T \\ &= (L_d \otimes \cdots \otimes L_1) (L_d \otimes \cdots \otimes L_1)^T = L L^T \end{aligned}$$

# Novel interpolation based quadrature method<sup>1,2</sup>

To reduce assembly costs of the main system matrix, we propose a novel method that

- i. is **optimal** with regard to the **number of integration points**
- ii. has **complexity independent** of **polynomial degree**, which enables **higher order methods**

Computational complexity in comparison

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

*Standard FEM*

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

*Sum factorization*

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

*Interpolation based quadrature*

<sup>1</sup> Arthur, D.W., *The Solution of Fredholm Integral Equations Using Spline Functions* (1973)

<sup>2</sup> Mantzaflaris, A., Jüttler, B., *Integration by interpolation and look-up for Galerkin-based isogeometric analysis* (2015)

# Interpolation based quadrature

$$A_{ij} = \int_{\mathcal{D}} \int_{\mathcal{D}'} \hat{\Gamma}(\hat{x}, \hat{x}') \sqrt{\det DF(\hat{x}) \det DF(\hat{x}')} B_i(\hat{x}) B_j(\hat{x}') d\hat{x} d\hat{x}'$$

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



Interpolation i.e. at Greville abscissae

$$\tilde{G}(\hat{x}_m, \hat{x}'_n) := \sum_{k,l \in \tilde{\mathcal{I}}} \tilde{G}_{kl} \tilde{B}_k(\hat{x}_m) \tilde{B}_l(\hat{x}'_n) = \tilde{B}^T \tilde{G} \tilde{B}$$

$$\tilde{A}_{ij} = \int_{\mathcal{D}} \int_{\mathcal{D}'} \tilde{G}(\hat{x}, \hat{x}') B_i(\hat{x}) B_j(\hat{x}') d\hat{x} d\hat{x}'$$

$$\tilde{A}_{ij} = \sum_{k,l \in \tilde{\mathcal{I}}} \tilde{G}_{kl} \int_{\mathcal{D}} \tilde{B}_k(\hat{x}) B_i(\hat{x}) d\hat{x} \int_{\mathcal{D}'} \tilde{B}_l(\hat{x}') B_j(\hat{x}') d\hat{x}'$$

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

$$M_{ki} = M_d \otimes \cdots \otimes M_1 \quad \text{where}$$

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

*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

# Interpolation error analysis

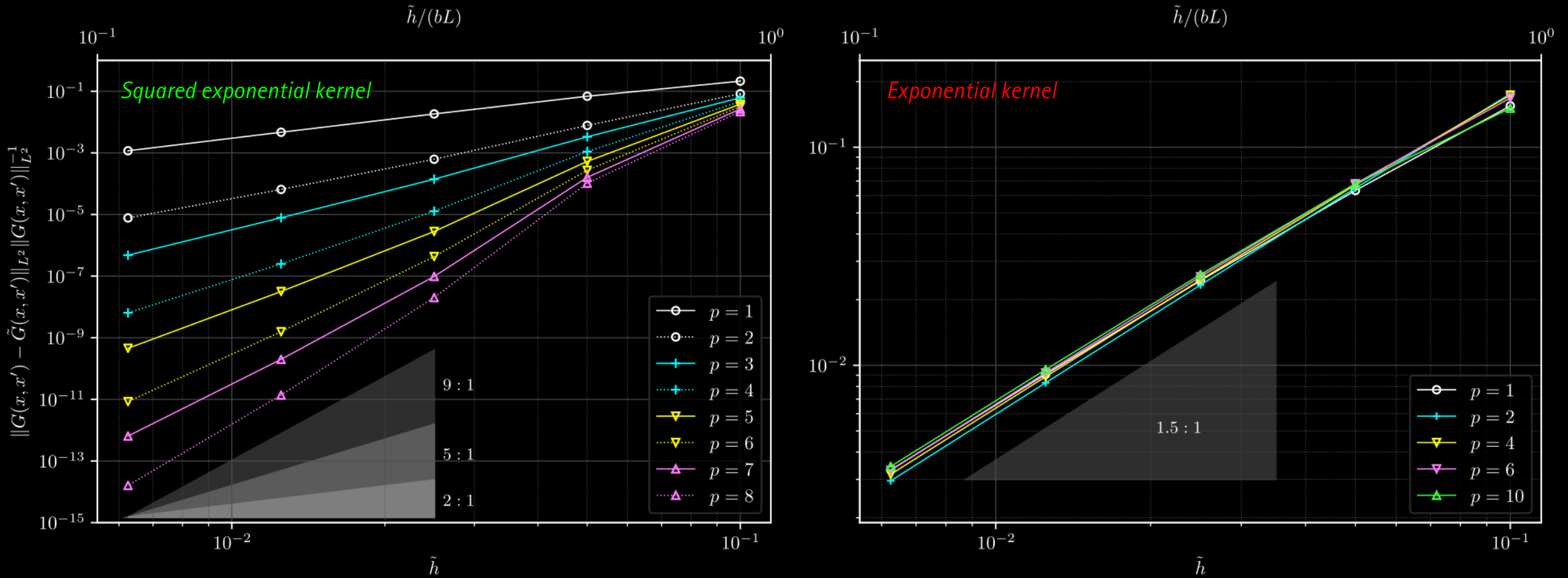
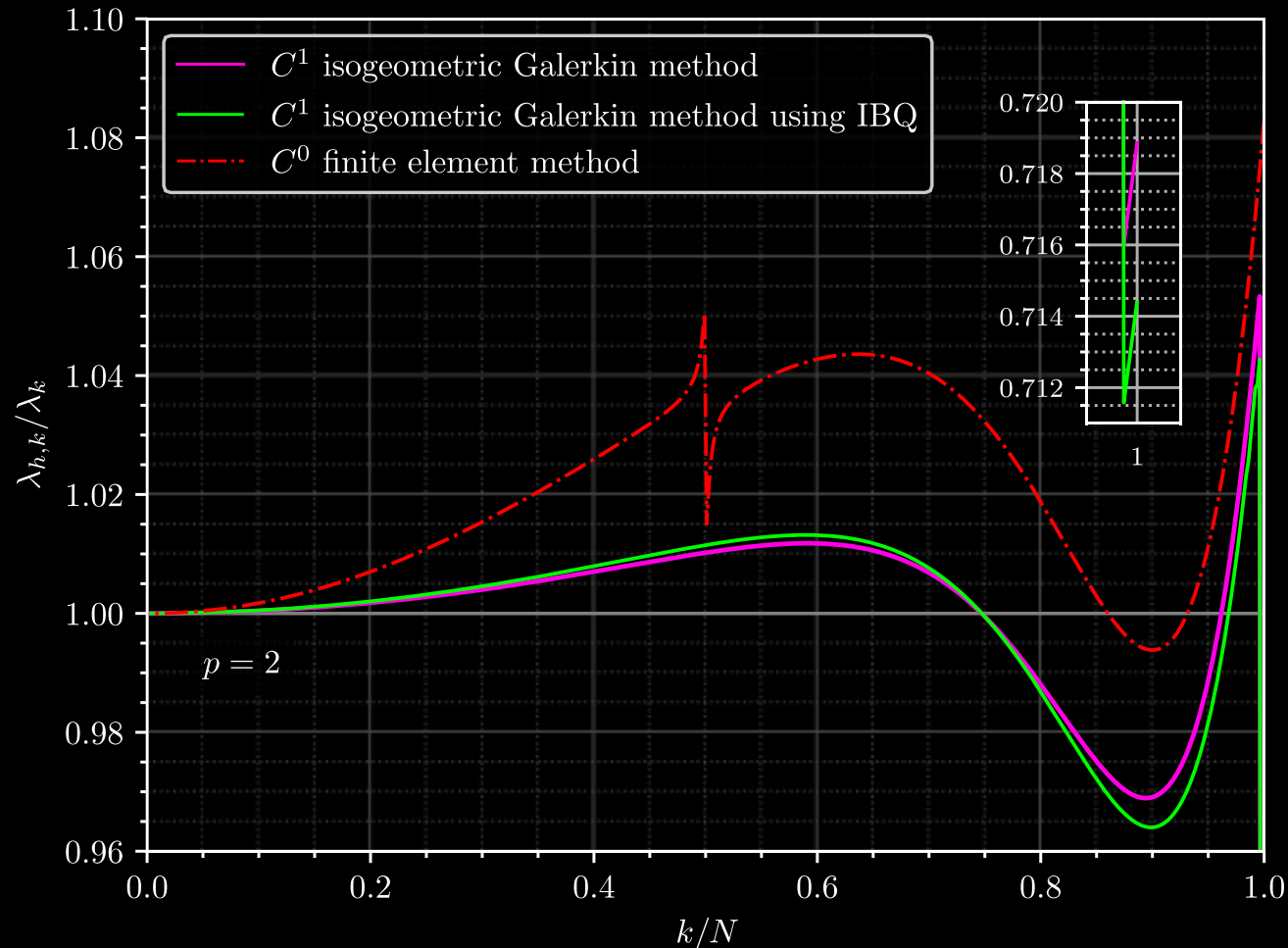


Figure 5: Normalized  $L^2$  interpolation error in a one-dimensional study case for the **squared exponential kernel** (left) and the **exponential kernel** (right) with convergence rates  $O(\tilde{h}^{p+1})$  and  $O(\tilde{h}^{3/2})$ , respectively.



# Reproduction of spectral properties



Spectral properties of the standard isogeometric Galerkin method remain preserved while applying the interpolation based quadrature

Figure 6: Full spectrum of eigenvalues normalized with respect to a reference solution. Comparing quadratic  $C^1$  continuous B-splines,  $C^1$  continuous B-splines using interpolation based quadrature (IBQ) and standard quadratic  $C^0$  continuous basis functions. One dimensional example with an exponential covariance function.

# Proposed matrix-free matrix-vector product $\tilde{\mathbf{A}}' \mathbf{v} = \mathbf{v}'$

$$\tilde{\mathbf{A}}' = \mathbf{L}^{-1} \mathbf{M}^T \tilde{\mathbf{B}}^{-1} \mathbf{J} \mathbf{\Gamma} \mathbf{J} \tilde{\mathbf{B}}^{-T} \mathbf{M} \mathbf{L}^{-T}$$

$\mathbf{\Gamma} := \hat{\Gamma}(\hat{x}_k, \hat{x}_l)$   
 $\mathbf{J} := \text{diag} \sqrt{\det DF(\hat{x}_k)}$   
 $\mathbf{G} = \mathbf{J} \mathbf{\Gamma} \mathbf{J}$  Kernel evaluation at Greville abscissae  
 $\tilde{\mathbf{G}} = \tilde{\mathbf{B}}^{-1} \mathbf{G} \tilde{\mathbf{B}}^{-T}$  Kernel interpolation  
 $\tilde{\mathbf{A}} = \mathbf{M}^T \tilde{\mathbf{G}} \mathbf{M}$  Evaluation of the system equation  
 $\tilde{\mathbf{A}}' = \mathbf{L}^{-1} \tilde{\mathbf{A}} \mathbf{L}^{-T}$  Reformulation into a standard eigenvalue problem

**Input:**  $v_{i_1 \dots i_d} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ ,  $J_{l_1 \dots l_d} \in \mathbb{R}^{\tilde{n}_1 \times \dots \times \tilde{n}_d}$ ,  
 $B_{i_k j_k} \in \mathbb{R}^{\tilde{n}_k \times \tilde{n}_k}$  and  $M_{l_k j_k} \in \mathbb{R}^{\tilde{n}_k \times n_k}$   
**Output:**  $v'_{i_1 \dots i_d} \in \mathbb{R}^{n_1 \times \dots \times n_d}$

- 1:  $V_{j_1 \dots j_d} \leftarrow L_{i_1 j_1}^{-1} \dots L_{i_d j_d}^{-1} v_{i_1 \dots i_d}$
- 2:  $X_{k_1 \dots k_d} \leftarrow M_{k_1 j_1} \dots M_{k_d j_d} V_{j_1 \dots j_d}$
- 3:  $Y_{l_1 \dots l_d} \leftarrow B_{k_1 l_1}^{-1} \dots B_{k_d l_d}^{-1} X_{k_1 \dots k_d}$
- 4:  $Y'_{l_1 \dots l_d} \leftarrow J_{l_1 \dots l_d} \odot Y_{l_1 \dots l_d}$
- 5:  $Z'_{k_1 \dots k_d} \leftarrow \hat{\Gamma}_{k_1 \dots k_d l_1 \dots l_d} Y'_{l_1 \dots l_d} \Leftarrow \mathcal{O}(\tilde{N}^2 N_{\text{iter}} / N_{\text{threads}})$
- 6:  $Z_{k_1 \dots k_d} \leftarrow J_{k_1 \dots k_d} \odot Z'_{k_1 \dots k_d}$
- 7:  $Y_{j_1 \dots j_d} \leftarrow B_{j_1 k_1}^{-1} \dots B_{j_d k_d}^{-1} Z_{k_1 \dots k_d}$
- 8:  $V_{l_1 \dots l_d} \leftarrow M_{j_1 l_1} \dots M_{j_d l_d} Y_{j_1 \dots j_d}$
- 9:  $v'_{i_1 \dots i_d} \leftarrow L_{i_1 l_1}^{-1} \dots L_{i_d l_d}^{-1} V_{l_1 \dots l_d}$

Algorithm 1: Matrix-free matrix-vector product using the Kronecker structure and tensor contraction<sup>1</sup> for efficient evaluation

Besides the kernel evaluation, all matrices have a **Kronecker product structure** – we can utilize it to efficiently implement the matrix-vector product for iterative eigenvalue solvers!

<sup>1</sup> Bressan, A., Takacs, S., *Sum factorization techniques in Isogeometric Analysis* (2019)

# Benchmark case

In this benchmark we compare the performance of a solution obtained by Rahman (2018) using the standard isogeometric Galerkin method and our own fast IBO method, while keeping the estimated eigenvalues comparable

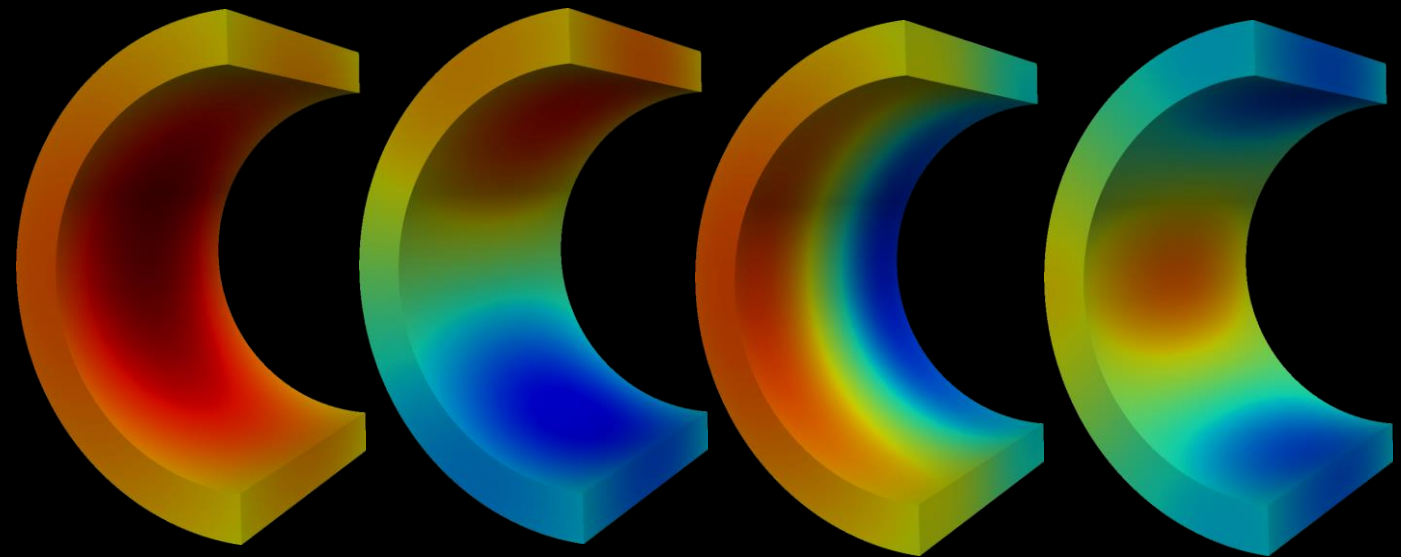
Kernel under consideration is the **exponential kernel**

Mode #	IBO	Benchmark
1	162.7993245	162.7993688
2	91.43092739	91.43079317
3	57.56741771	57.56765769
4	51.09028325	51.09029418
5	38.79796382	38.79808752
6	27.90416545	27.90392169
7	25.05648777	25.05681566

Table 2: Comparison of eigenvalues with the analogous test case presented by Rahman (2018)

	IBO	Benchmark
Solution time	12.91 s	> 24 h
NDOF Solution space	59940	1050
NDOF Interpolation	8525	–
Memory	0.587 GB	–
Number of iterations	63	–

Table 3: Performance comparison between IBO and the standard isogeometric Galerkin method presented by Rahman (2018)



$$p = \{2, 1, 1\}$$

# High-order test case

In this benchmark we use a high-order interpolation and solution space and compare performance and eigenvalues for two computations under  $h$ -refinement of the solution space

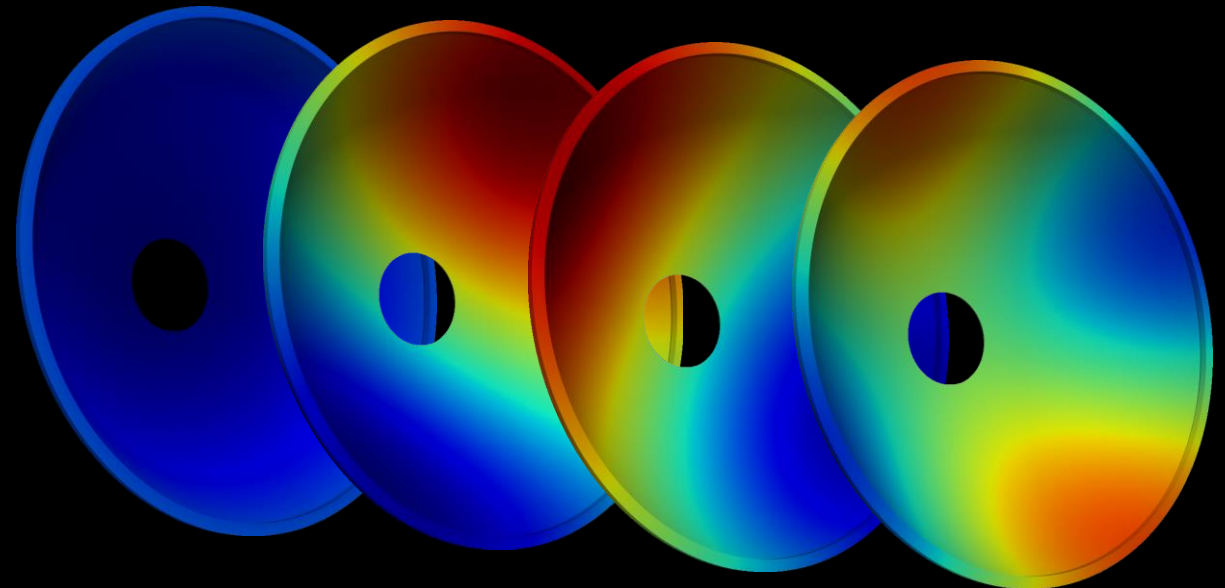
Kernel under consideration is the **squared exponential kernel**

Mode #	Case 1	Case 2
1	14476.27783	14476.27783
2	6531.770729	6531.770729
3	6531.77072 <u>8</u>	6531.77072 <u>5</u>
4	2091.87701 <u>2</u>	2091.87701 <u>5</u>
5	2091.87700 <u>3</u>	2091.87701 <u>2</u>
6	1971.74713 <u>5</u>	1971.74713 <u>6</u>
7	552.708626 <u>9</u>	552.708626 <u>2</u>

Table 4: Comparison of eigenvalues in both test cases

	Case 1	Case 2
Polynomial order	16	16
Solution time	1.65 h	1.63 h
NDOF Solution space	1.80E5	4.21E5
NDOF Interpolation	1.80E5	1.80E5
Memory	1.34 GB	7.48 GB
Number of iterations	41	41

Table 5: Performance comparison between both test cases



# In conclusion

- Novel **projection based quadrature** of the weak form is used for **efficient** formation of high-dimensional integrands of **high polynomial order**
- Inexpensive **reformulation** of the generalized eigenvalue problem into a **standard eigenvalue problem** using Kronecker product of univariate mass matrices
- Reduced memory usage by implementing a fast **multithreaded matrix-free matrix-vector product** for iterative eigenvalue solvers by using tensor contraction of Kronecker structured matrices

Further research effort is required towards analysis of the error, as well as the spectral properties of the method

# Discussion

### Nondeterminism of (physical) systems

$\mathcal{L}(x)u(x) = f(x)$  deterministic

method:  $\mathcal{L}(x, \theta)u(x, \theta) = f(x, \theta)$

Most physical systems exhibit randomness, which, because of its lack of patterns or regularity, can not be explicitly captured by deterministic mathematical models

### Karhunen-Loève expansion

$T\phi_k = \lambda_k \phi_k, \quad (T\phi)(x) = \int_D \Gamma(x, x')\phi(x') dx'$

$f_i(x) = \sqrt{\lambda_i} \phi_i(x) \Rightarrow \tilde{u}_M(x, \theta) = \mu(x) + \sum_{i=1}^M \sqrt{\lambda_i} \phi_i(x) \xi_i(\theta)$

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

### Novel interpolation based quadrature method<sup>1,2</sup>

To reduce assembly costs of the main system matrix, we propose a novel method that

- is optimal with regard to the number of integration points
- has complexity independent of polynomial degree, which enables higher order methods

Computational complexity in computation:

- $\mathcal{O}(N_x^2(p+1)^M)$  (Standard FEM)
- $\mathcal{O}(2dN_x^2(p+1)^{M+1})$  (Sum factorization)
- $\mathcal{O}(N_x^2 N_{\text{inter}}/N_{\text{iknnd}})$  (Interpolation based quadrature)

### Interpolation based quadrature

$A_0 = \int_D \int_{D'} f(x, x') \sqrt{\det DF(x)} \sqrt{\det DF(x')} B(x) B(x') dx dx'$

$G(x, x') := f(x, x') \sqrt{\det DF(x)} \sqrt{\det DF(x')}$

$\tilde{G}(x_{\text{int}}, x'_{\text{int}}) := \sum_{k, l=2}^p \tilde{G}_{kl}(x_{\text{int}}, x'_{\text{int}}) \tilde{B}_k(x) \tilde{B}_l(x') = \tilde{B}^T \tilde{G} \tilde{B}$

$\tilde{A}_0 = \int_D \int_{D'} \tilde{G}(x, x') \tilde{B}_k(x) \tilde{B}_l(x') dx dx'$

$\tilde{A}_0 = \sum_{k, l=2}^p \tilde{G}_{kl} \int_D \tilde{B}_k(x) \tilde{B}_l(x) dx \int_{D'} \tilde{B}_l(x') \tilde{B}_k(x') dx'$

The approximation error strictly obeys Strassen's rule

### Reproduction of spectral properties

Spectral properties of the standard isogeometric Galerkin method remain preserved when applying the interpolation based quadrature

Figure 6: Full spectra of eigenvalues normalized with respect to a reference solution. Comparing isogeometric Galerkin method (IGK) and standard quadrature (C) continuous basis functions. One dimensional example with an exponential covariance function.

### Proposed matrix-free matrix-vector product $\tilde{A}v = v'$

Requires the kernel evaluation, all matrices have a Kronecker product structure:  $\tilde{A} = \tilde{B} \tilde{C} \tilde{B}^T$  decomposition

Figure 7: Matrix-free matrix-vector product using the Kronecker structure and tensor contraction<sup>1</sup> by efficient evaluation

### Benchmark case

In this benchmark we compare the performance of a relative reference by Reference (REF) using the standard isogeometric Galerkin method and our own by (IGK) method, while keeping the minimum eigenvalues invariant

Method	IGK	Reference
Solution time	1.171 s	1.000 s
IGK Solution time	1.000 s	1.000 s
IGK Interpolation	0.55 s	-
Memory	0.181 GB	-
Number of iterations	43	-

Figure 8: The benchmark comparison between REF and the standard isogeometric Galerkin method proposed by Rubin [30, 31]

Table 2: Comparison of eigenvalues with the analogous test case presented by Rubin [30, 31]

### High-order test case

In this benchmark we use a high-order isogeometric and compare its performance and operation for the interpolation based quadrature method

Method	Case 1	Case 2
Polynomial order	12	12
Solution time	1.02 s	1.02 s
IGK Solution time	1.000 s	1.000 s
IGK Interpolation	1.000 s	1.000 s
Memory	1.04 GB	1.04 GB
Number of iterations	41	41

Figure 9: Performance comparison between both test cases

Table 3: Comparison of eigenvalues in both test cases

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