Physics-informed machine learning in design optimization

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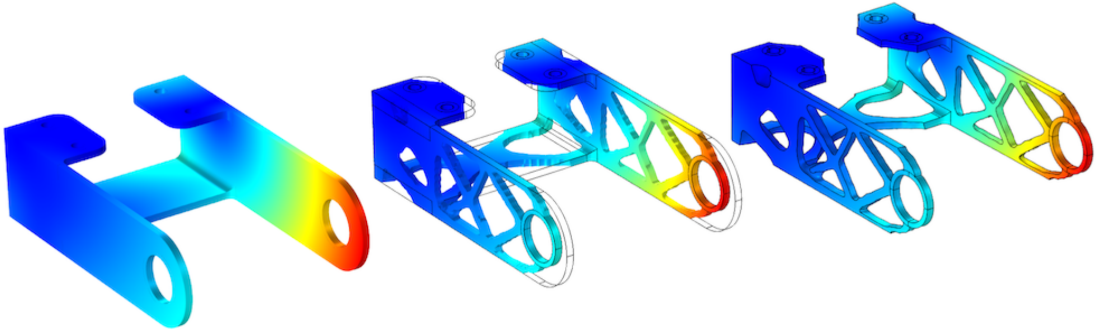
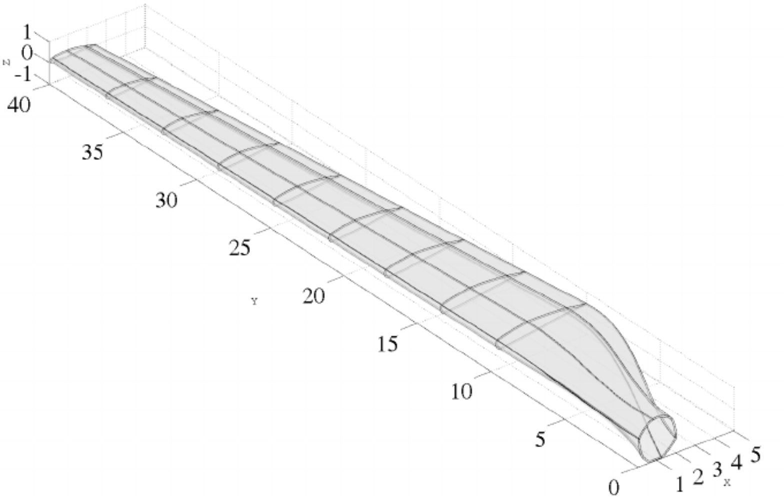
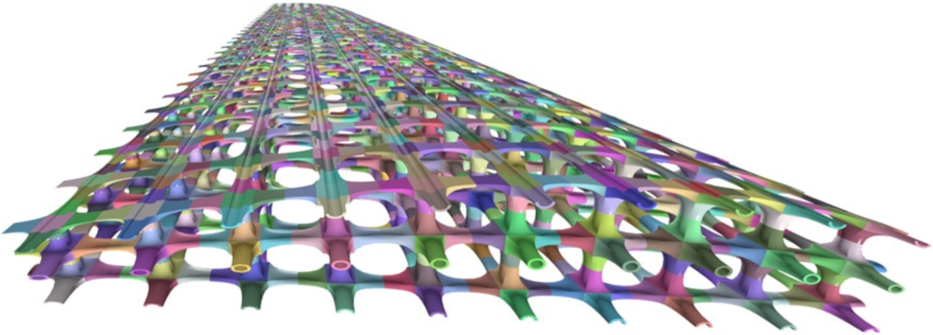
Design optimization: topology



Design optimization: shape



Design optimization: meso-/micro-structure and materials



How can SciML help?

- Create novel 'analysis-suitable' designs through generative AI

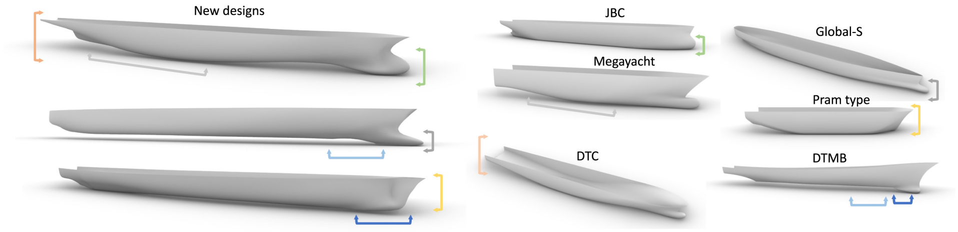


Figure from: *ShipHullGAN: A generic parametric modeller for ship hull design using deep convolutional generative model* [Khan et al., 2023]

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- Evaluate design's performance with physics-informed machine learning

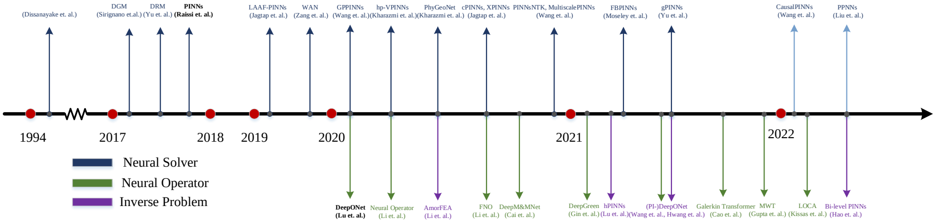

Figure from: *Physics-informed machine learning: A survey on problems, methods and applications* [Hao et al., 2022]

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- Speed up classical numerical methods with SciML technologies

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Questions

1. How can we input 'analysis-suitable' designs into SciML?
2. How can we design a PIML framework that can be blended with classical methods?
   Aka: SciML for the quick pre-design analysis, <ABC> for in-depth analysis

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Questions

1. How can we input 'analysis-suitable' designs into SciML?

   Our designs are described by B-spline/NURBS parametrizations

2. How can we design a PIML framework that can be blended with classical methods?
   Aka: SciML for the quick pre-design analysis, <ABC> for in-depth analysis

   *Our <ABC> is **Isogeometric Analysis** (IGA) [Hughes et al., 2005]*
   Aka: 'finite elements' based on B-spline/NURBS basis functions

Univariate B-splines

Knot vector

$$\Xi = \{\xi_1, \xi_2, \ldots, \xi_{n+d+1}\}, \qquad \xi_i \leq \xi_{i+1}, \quad \forall i = 1, \ldots, n+d$$

with ξ_i being a *knot*, n the *number* and d the *degree* of the B-spline basis functions

Recurrence formula [de Boor, 1971]

$$b_{i;\Xi}^{0}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

$$b_{i;\Xi}^{d}(\xi) = \frac{\xi - \xi_i}{\xi_{i+d} - \xi_i} b_{i;\Xi}^{d-1}(\xi) + \frac{\xi_{i+d+1} - \xi}{\xi_{i+d+1} - \xi_{i+1}} b_{i+1;\Xi}^{d-1}(\xi) \qquad „\frac{0}{0}" := 0$$

Univariate B-spline properties

Local support and non-negativity

$$b_{i;\Xi}^{d}(\xi)\begin{cases} >0 & \forall\xi\in\text{supp}\left(b_{i;\Xi}^{d}\right):=[\xi_i,\xi_{i+d+1}),\\ =0 & \text{otherwise}\end{cases}$$

Partition of unity

$$\sum_{i=1}^{n} b_{i;\Xi}^{d}(\xi)\equiv 1,\quad \forall\xi\in\hat{I}_{\Xi}:=[\xi_1,\ldots\xi_{n+d+1})$$

Knot vectors

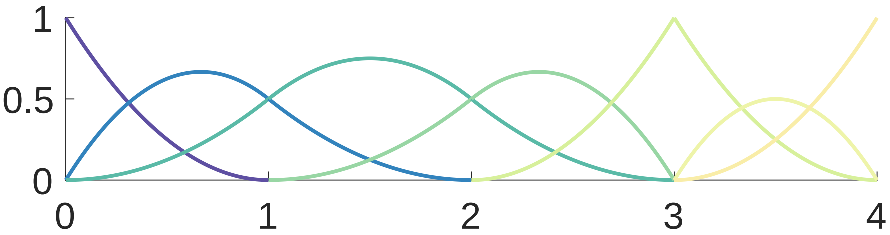
Open knot vector (i.e. $d+1$ repetition of the first and last knot)

$$\Xi = [\xi_1 = \cdots = \xi_{d+1}, \quad \xi_{d+2}, \ldots, \quad \xi_n = \cdots = \xi_{n+d+1}]$$

First and last basis functions are *interpolatory* at the left and right endpoint, respectively.

Repeated knots reduce the continuity of the basis functions that are non-zero at the respective knot from C^{d-1} to C^{d-m_i} *locally* with m_i being the multiplicity of the i-th knot.

The power of knot repetition



$$\Xi = \{0,0,0,1,2,3,3,4,4,4\}, \quad \hat{I}_\Xi = (0,4), \quad n = 7, \quad d = 2$$

The spline space $\mathbb{S}_{\Xi}^{d,s}$

$$\begin{aligned}\mathbb{S}_{\Xi}^{d,s} &= \text{span}\left\{b_{1;\Xi}^{d}, \dots, b_{n;\Xi}^{d}\right\} \\ &= \left\{\sum_{i=1}^{n} b_{i;\Xi}^{d}(\xi)\, c_i \;:\; c_i \in \mathbb{R}^s, \text{ for } 1 \le i \le n,\ \xi \in \hat{I}_{\Xi}\right\}\end{aligned}$$

Define spline function $f \in \mathbb{S}_{\Xi}^{d,s}$, i.e. mapping from $\hat{I}_{\Xi}$ to $\mathbb{R}^s$ through

$$f(\xi) = \begin{bmatrix} b_{1;\Xi}^{d}(\xi) & \dots & b_{n;\Xi}^{d}(\xi) \end{bmatrix} \cdot \begin{bmatrix} c_1 & \dots & c_n \end{bmatrix} = \mathbf{b} \cdot \mathbf{c}$$

and fix the B-spline coefficients $c_i \in \mathbb{R}^s$ relative to the given B-spline basis

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Extension to multiple dimensions via tensor-product construction $\rightarrow$ live demo

An efficient algorithm for evaluating univariate B-splines

Algorithm 2.22 from [Lyche and Mørken, 2018] with modifications

1. $\mathbf{b} = 1$
2. For $k = 1, \ldots, d-r$
   1. $\mathbf{t}_1 = (\xi_{i-k+1}, \ldots, \xi_i)$
   2. $\mathbf{t}_{21} = (\xi_{i+1}, \ldots, \xi_{i+k}) - \mathbf{t}_1$
   3. $\textsf{mask} = (\mathbf{t}_{21} < \textsf{tol})$
   4. $\mathbf{w} = (\xi - \mathbf{t}_1 - \textsf{mask}) \div (\mathbf{t}_{21} - \textsf{mask})$
   5. $\mathbf{b} = [(1-\mathbf{w}) \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$
3. For $k = d-r+1, \ldots, d$
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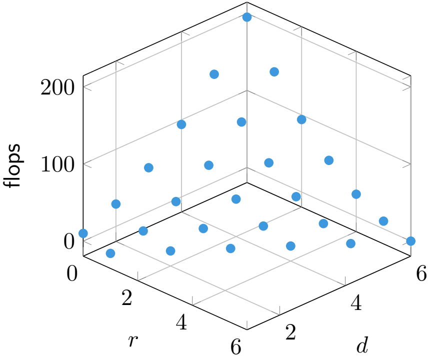
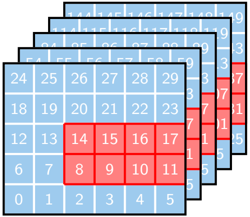
   4. $\mathbf{w} = (1 - \textsf{mask}) \div (\mathbf{t}_{21} - \textsf{mask})$
   5. $\mathbf{b} = [-\mathbf{w} \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$



where $\div$ and $\odot$ denote the element-wise division and multiplication of vectors, respectively.

Memory layout of tensors

Example: $n_1 = 6, n_2 = 5, n_3 = 5$ and $d_1 = 3, d_2 = 1, d_3 = 4$



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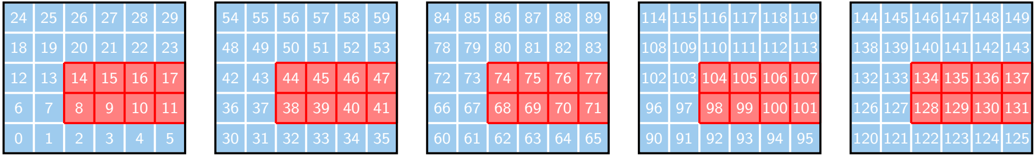

$$\mathbf{c} = [8 \quad 9 \quad 10 \quad 11 \quad 14 \quad 15 \quad 16 \quad 17 \quad 38 \quad 39 \quad \ldots \quad 136 \quad 137]$$

A brief recap of the Kronecker product

Definition

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} \mathbf{A}_{11}\mathbf{B} & \mathbf{A}_{12}\mathbf{B} \\ \mathbf{A}_{21}\mathbf{B} & \mathbf{A}_{22}\mathbf{B} \end{bmatrix} \qquad (n_A \cdot m_A \cdot n_B \cdot m_B \text{ flops})$$

Mixed-product property (if matrices are so that $\mathbf{AC}$ and $\mathbf{BD}$ exists)

$$(\mathbf{A} \otimes \mathbf{B})\,(\mathbf{C} \otimes \mathbf{D}) = (\mathbf{AC}) \otimes (\mathbf{BD})$$

Multiplicative decomposition (extendable to arbitrary number of matrices)

$$(\mathbf{A}_1 \otimes \mathbf{I}_2)\,(\mathbf{I}_1 \otimes \mathbf{A}_2) = (\mathbf{A}_1\mathbf{I}_1) \otimes (\mathbf{A}_2\mathbf{I}_2) = \mathbf{A}_1 \otimes \mathbf{A}_2$$

Efficient evaluation of multi-variate B-splines

It follows form the multiplicative decomposition of the Kronecker product that

$$f(\xi,\eta,\zeta) = \left(\mathbf{b}^{d_1} \otimes \mathbf{b}^{d_2} \otimes \mathbf{b}^{d_3}\right) \cdot \mathbf{c} = \left(\mathbf{I}_1 \otimes \mathbf{I}_2 \otimes \mathbf{b}^{d_3}\right) \cdot \left(\mathbf{I}_1 \otimes \mathbf{b}^{d_2} \otimes \mathbf{I}_3\right) \cdot \left(\mathbf{b}^{d_1} \otimes \mathbf{I}_2 \otimes \mathbf{I}_3\right) \cdot \mathbf{c}$$

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Algorithm 993 from [Fackler, 2019] with modifications

Set $\mathbf{f} := \mathbf{c}$

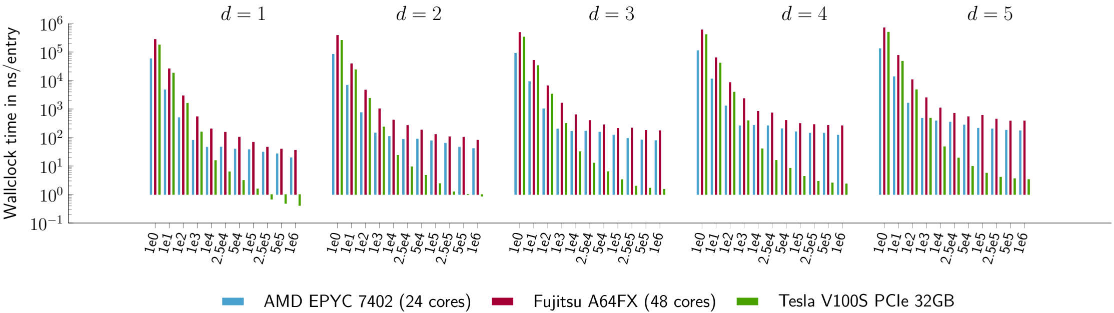
For $\ell = 1, 2, 3$

1. $\mathbf{f} :=$ reshape$(\mathbf{f}, [\cdot], d_\ell + 1)$
2. $\mathbf{f} := \mathbf{b}^{d_\ell} \cdot \mathbf{f}^\top$

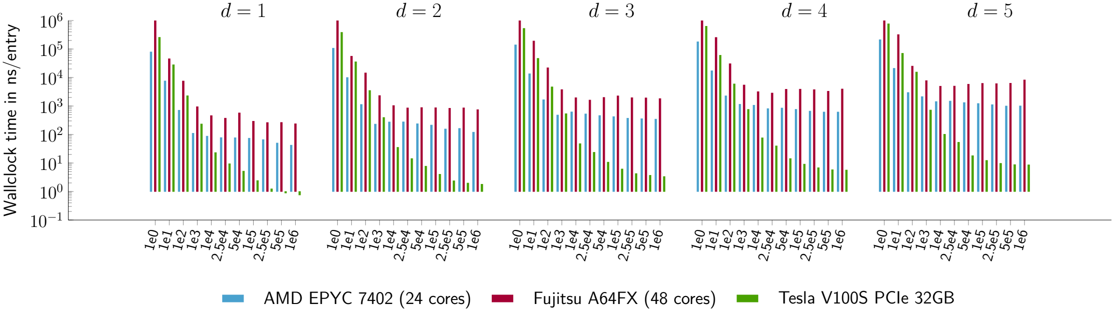
Output: $\mathbf{f} = f(\xi,\eta,\zeta)$

$$\mathbf{c} = \underbrace{\begin{bmatrix} 8 & 9 & 10 & 11 \\ 14 & 15 & 16 & 17 \\ 38 & 39 & 40 & 41 \\ \vdots & \vdots & \vdots & \vdots \\ 134 & 135 & 136 & 137 \end{bmatrix}}_{d_1+1 \text{ columns}} \begin{array}{c} (d_2+1)(d_3+1) \\ \text{rows} \end{array}$$

Performance evaluation - bivariate B-splines



Performance evaluation - trivariate B-splines



Collocation IGA

PDE problem

$$\mathcal{L}u = f \qquad \text{in } \Omega$$

$$\mathcal{B}u = g \qquad \text{on } \Gamma$$

Weighted residual form

$$\int_{\Omega} \phi_{\Omega}(\mathcal{L}u - f)\,\mathrm{d}\mathbf{x} + \int_{\Gamma} \phi_{\Gamma}(\mathcal{B}u - g)\,\mathrm{d}s = 0$$

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Let

$$\phi_\Omega = \sum_{i=1}^{k} \delta_\Omega(\mathbf{x} - \mathbf{x}_i)\,c_i \quad (\mathbf{x}_i \in \Omega) \qquad \text{and} \qquad \phi_\Gamma = \sum_{i=k+1}^{n} \delta_\Gamma(\mathbf{x} - \mathbf{x}_i)\,c_i \quad (\mathbf{x}_i \in \Gamma)$$

then

$$\sum_{i=1}^{k} \left(\mathcal{L}u(\mathbf{x}_i) - f(\mathbf{x}_i)\right)\,c_i + \sum_{i=1+k}^{n} \left(\mathcal{B}u(\mathbf{x}_i) - g(\mathbf{x}_i)\right)\,c_i = 0$$

Collocation IGA cont'd

As the coefficients c_i are arbitrary we obtain

$$\mathcal{L}u(\mathbf{x}_i) = f(\mathbf{x}_i) \qquad i = 1, \ldots, k$$

$$\mathcal{B}u(\mathbf{x}_i) = g(\mathbf{x}_i) \qquad i = k+1, \ldots, n$$

Collocation IGA cont'd

As the coefficients c_i are arbitrary and replacing $u \approx u_h = \sum_{j=1}^{n} b_j(\mathbf{x})u_j$ we obtain

$$\begin{bmatrix} \mathcal{L}b_1(\mathbf{x}_1) & \dots & \mathcal{L}b_n(\mathbf{x}_1) \\ \vdots & \ddots & \vdots \\ \mathcal{L}b_1(\mathbf{x}_k) & \dots & \mathcal{L}b_n(\mathbf{x}_k) \\ \mathcal{B}b_1(\mathbf{x}_{k+1}) & \dots & \mathcal{B}b_n(\mathbf{x}_{k+1}) \\ \vdots & \ddots & \vdots \\ \mathcal{B}b_1(\mathbf{x}_n) & \dots & \mathcal{B}b_n(\mathbf{x}_n) \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_k \\ u_{k+1} \\ \vdots \\ u_n \end{bmatrix} = \begin{bmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_k) \\ g(\mathbf{x}_{k+1}) \\ \vdots \\ g(\mathbf{x}_n) \end{bmatrix}$$

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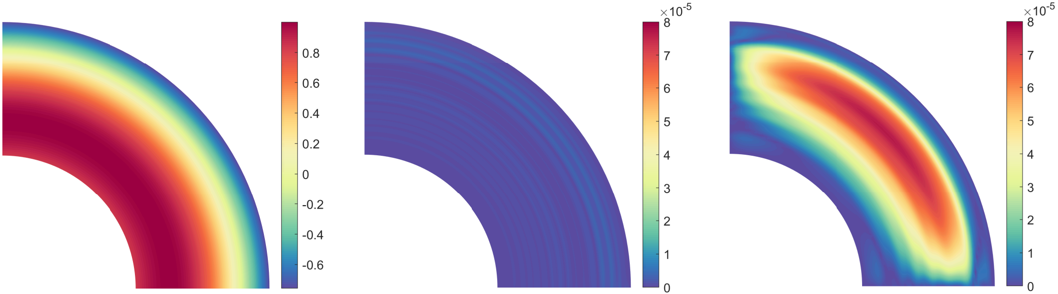
- basis functions b_i need to be at least C^ℓ such that $\mathcal{L}$ and $\mathcal{B}$ can be applied
- regular system matrix requires that #collocation points = #basis functions and all collocation points must be pairwise distinct

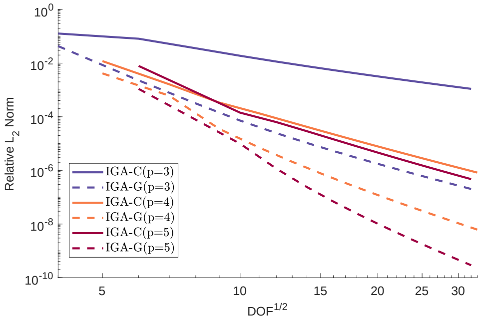
Comparison between Galerkin and collocation IGA



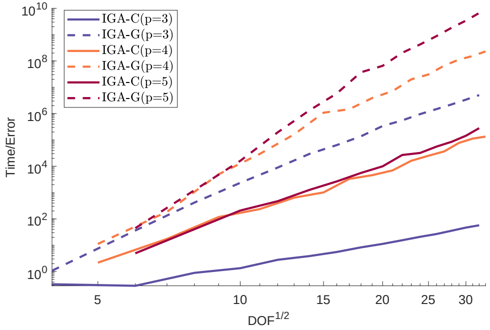
solution IGA-G abs. error IGA-C abs. error

Results by Mengyun Wang

Comparison between Galerkin and collocation IGA



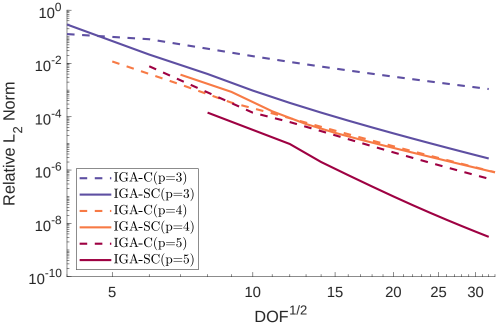
rel. L_2-error



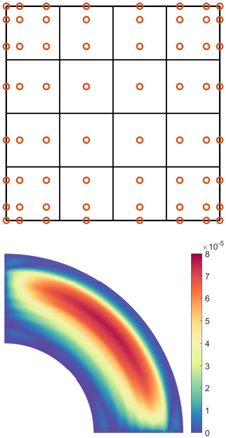
wallclock time/error

Results by Mengyun Wang

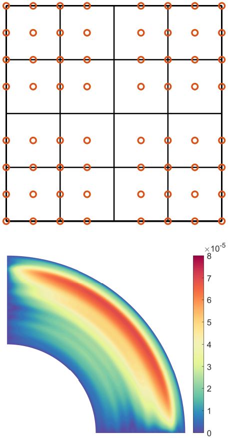
Comparison between Greville and clustered superconvergent points



rel. L_2-error



Greville



SC points

Results by Mengyun Wang

Least-squares collocation IGA

Idea: When #collocation points (m) $>$ #unknowns (n) then the system matrix is over-determined and the system can be solved in least-squares manner

$$\min_{u_h} \sum_{i=1}^{k} \|\mathcal{L}u_h(\mathbf{x}_i) - f(\mathbf{x}_i)\|^2 + \sum_{i=k+1}^{m} \|\mathcal{B}u_h(\mathbf{x}_i) - g(\mathbf{x}_i)\|^2$$

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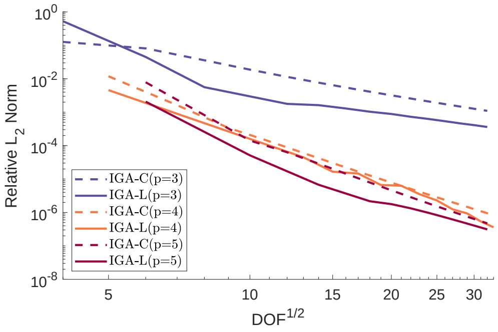
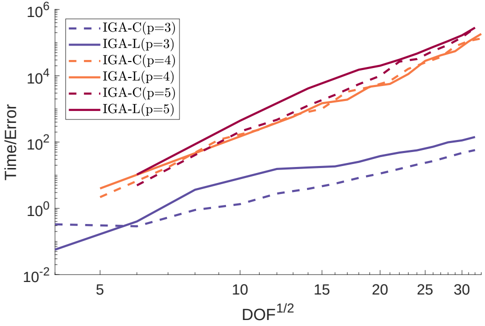
[Lin et al., 2020] derives rigorous conditions under which least-squares collocation IGA (IGA-L) is consistent and convergent. In essence, there must be *at least one collocation point per element* (e.g., Greville points) but we can use more to increase the resolution.

Comparison between collocation and least-squares collocation IGA



rel. L_2-error



wallclock time/error

Results by Mengyun Wang

Least-squares collocation IGA revisited

Replacing f, and g by their approximations f_h, and g_h we obtain

$$\min_{\{u_j\}_j} \sum_{i=1}^{k} \| \sum_{j=1}^{n} \mathcal{L} b_j(\mathbf{x}_i) u_j - b_j(\mathbf{x}_i) f_j \|^2 + \sum_{i=k+1}^{m} \| \sum_{j=1}^{n} \mathcal{B} b_j(\mathbf{x}_i) u_j - b_j(\mathbf{x}_i) g_j \|^2$$

- B-spline basis functions $\hat{b}_j(\boldsymbol{\xi})$ are defined in the reference space $\hat{\Omega} = (0,1)^d$ and are mapped into physical space Ω through the **push-forward mapping**

$$\mathbf{x}_h(\boldsymbol{\xi}) = \sum_{i=1}^{n} \hat{b}_j(\boldsymbol{\xi}) \mathbf{x}_j,$$

Least-squares collocation IGA revisited

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$$\min_{\{u_j\}_j} \underbrace{\sum_{i=1}^{k} \| \sum_{j=1}^{n} \mathcal{L} b_j(\mathbf{x}_i) u_j - b_j(\mathbf{x}_i) f_j \|^2}_{\mathsf{loss}_{\mathsf{PDE}}(\{u_j\}_j, \{f_j\}_j; \{\mathbf{x}_i\}_i)} + \underbrace{\sum_{i=k+1}^{m} \| \sum_{j=1}^{n} \mathcal{B} b_j(\mathbf{x}_i) u_j - b_j(\mathbf{x}_i) g_j \|^2}_{\mathsf{loss}_{\mathsf{BC}}(\{u_j\}_j, \{g_j\}_j; \{\mathbf{x}_i\}_i)}$$

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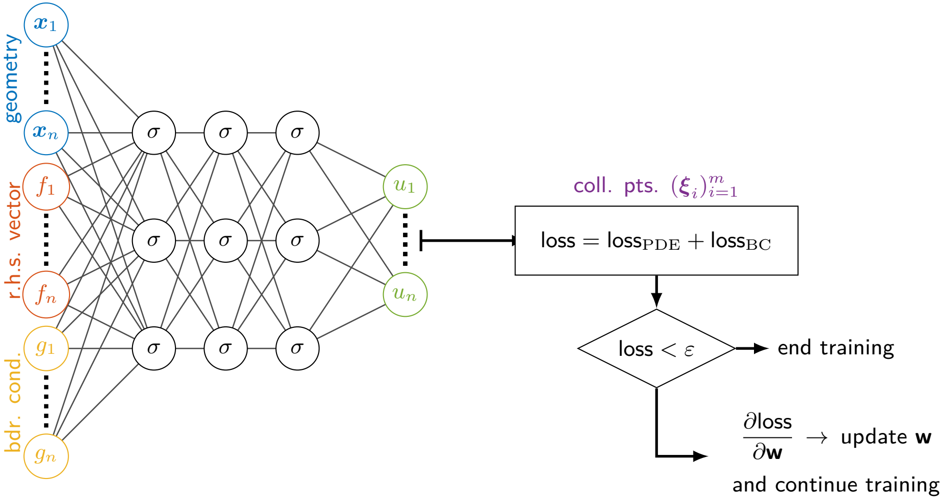
$$\mathbf{x}_h(\boldsymbol{\xi}) = \sum_{i=1}^{n} \hat{b}_j(\boldsymbol{\xi}) \mathbf{x}_j,$$

- problem is fully parameterized through f_j's, g_j's, and $\mathbf{x}_j$'s relative to a fixed basis $\hat{b}_j$

IgANet architecture



Training and evaluation

Training

For $[f_1, \dots, f_n] \in \mathcal{S}_{\text{rhs}}$, $[g_1, \dots, g_n] \in \mathcal{S}_{\text{bcond}}$, $[\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathcal{S}_{\text{geo}}$ **do**

For a batch of collocation points $\boldsymbol{\xi}_i \in [0, 1]^2$ (e.g., Greville points + more) **do**

Train IgANet $([f_1, \dots, f_n], [g_1, \dots, g_n], [\mathbf{x}_1, \dots, \mathbf{x}_n]) \mapsto [u_1, \dots, u_n]$

EndFor

EndFor

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EndFor

EndFor

Evaluation

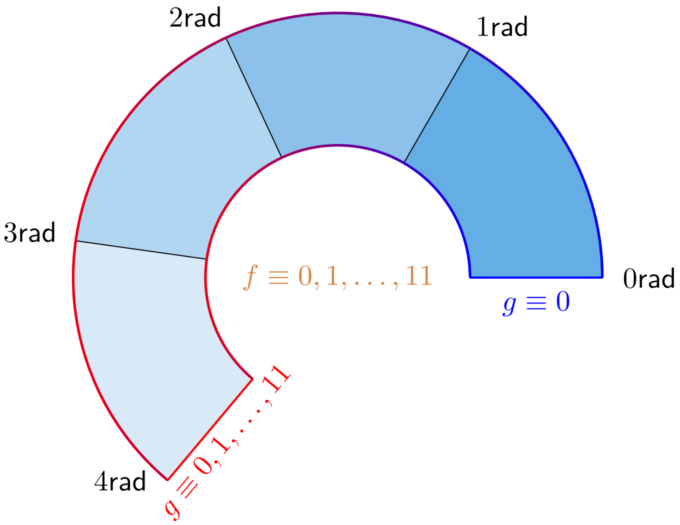
For $[f_1, \dots, f_n] \in \mathcal{S}_{\text{rhs}}$, $[g_1, \dots, g_n] \in \mathcal{S}_{\text{bcond}}$, $[\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathcal{S}_{\text{geo}}$ **do**

Evaluate IgANet $([f_1, \dots, f_n], [g_1, \dots, g_n], [\mathbf{x}_1, \dots, \mathbf{x}_n]) \mapsto [u_1, \dots, u_n]$

Use basis representation $u_h(\mathbf{x}) = \sum_{j=1}^{n} b_j(\mathbf{x}) u_j$ for all further purposes

EndFor

Test case: Poisson's equation on a variable annulus



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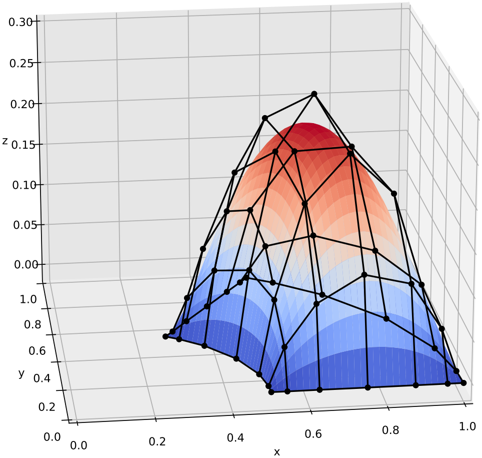
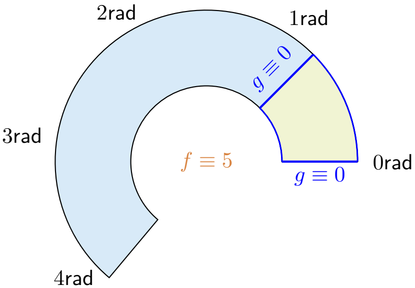
Validation results





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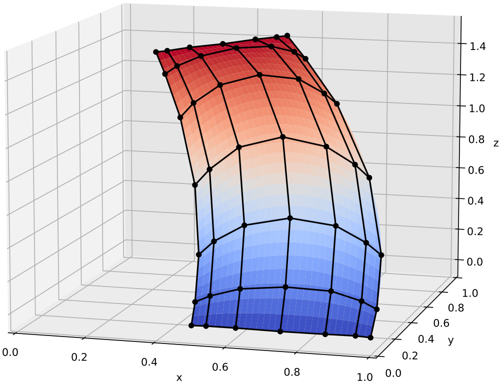
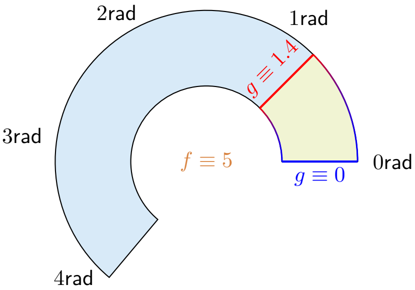
Validation results





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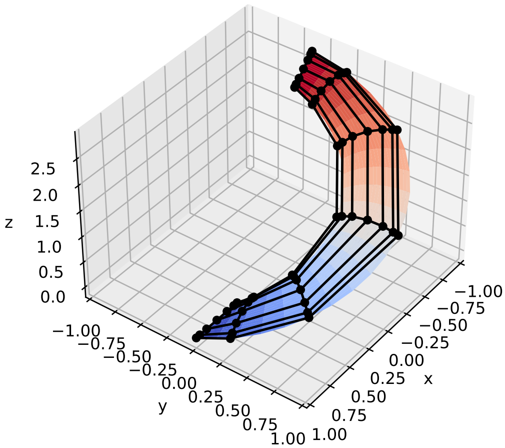
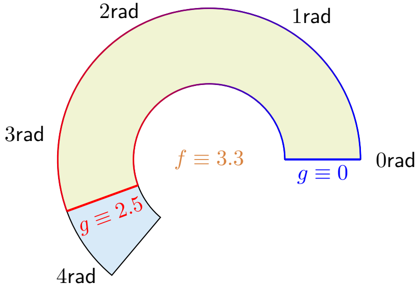
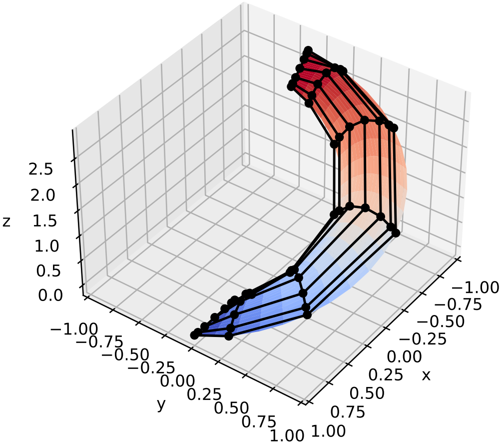
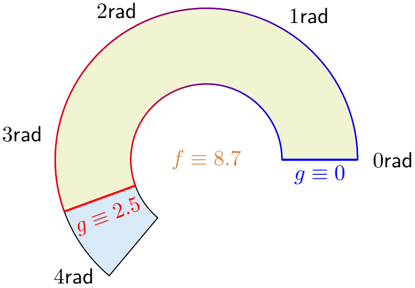
Validation results





Validation results





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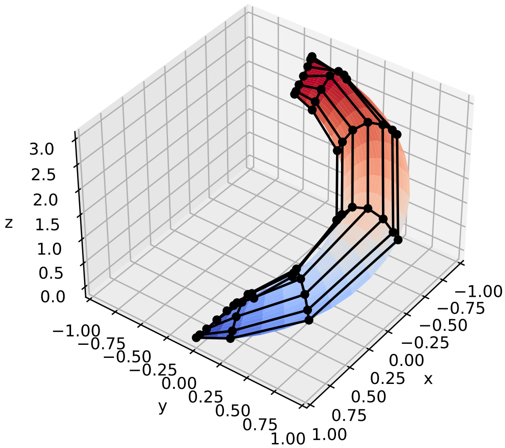
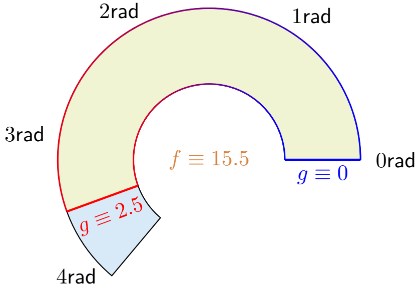
Validation results





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Summary and outlook

- Least-squares collocation IGA enables seamless in-paradigm blending between fast learning-based pre-analysis and in-depth simulation-based (post-)analysis
- Theory from IGA-L carries over to NN (e.g., interpretation of loss function)
- Iterative refinement of NN's output by 'classical' IGA-L is possible

What's next?

- Interactive collaborative design modelling and optimization workflow

`https://visualization.surf.nl/iganet/`

Physics-informed machine learning in design optimization

Matthias Möller

Department of Applied Mathematics, TU Delft, The Netherlands

Scientific machine learning workshop @ CWI, December 6-8, 2023

Thank you very much!

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