IgANets: Physics-Informed Machine Learning Embedded Into Isogeometric Analysis

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SIAM CSE23

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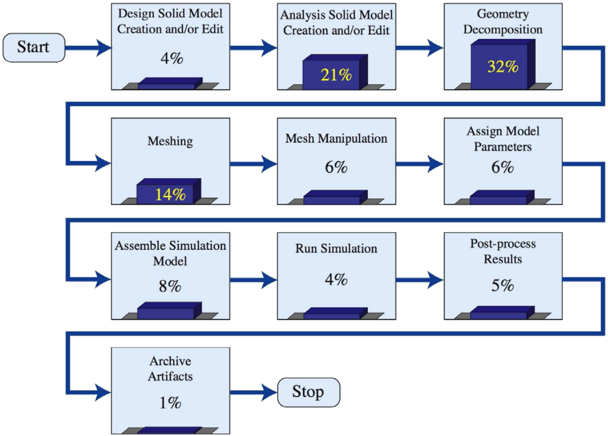
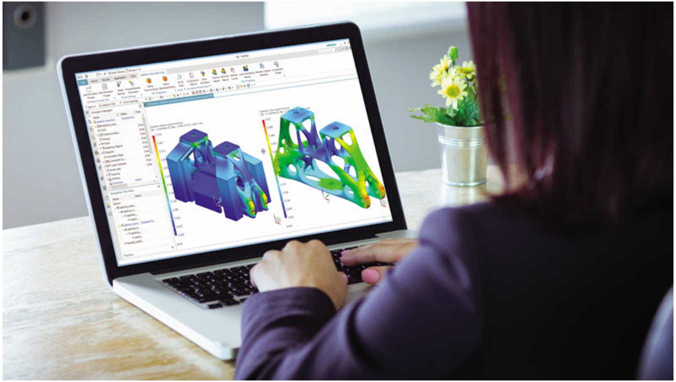
MS148: Bridging Numerical Analysis and Machine Learning I/II

Design-through-Analysis



Vision: seamless design and analysis workflows without time-consuming (often manual) geometry cleaning and meshing → **Isogeometric Analysis** (Hughes et al. '05)

Interactive Design-through-Analysis

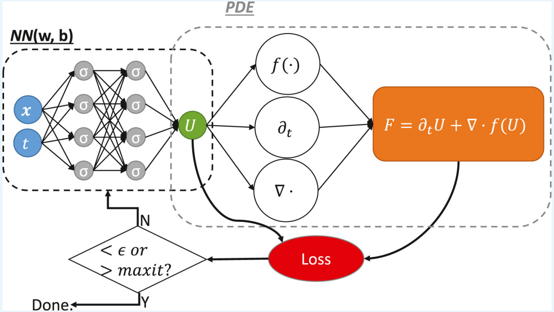


Vision: fast interactive qualitative analysis and accurate quantitative analysis within the same computational framework with seamless switching between both approaches

Photo: Siemens – Simulation for Design Engineers

Physics-informed machine learning

PINN (Raissi et al. 2018): *learns the (initial-)boundary-value problem*



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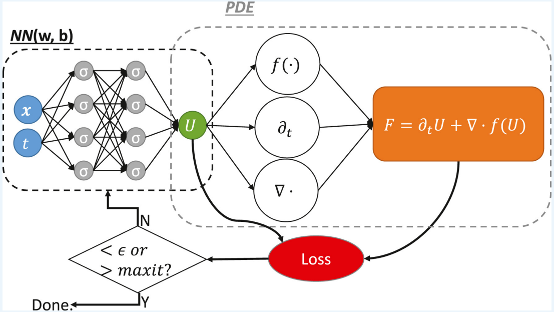

- easy to implement for ‘any‘ PDE because AD magic does it for you
- combined un-/supervised learning
- poor extrapolation/generalization
- point-based approach requires re-evaluation of NN at every point
- rudimentary convergence theory

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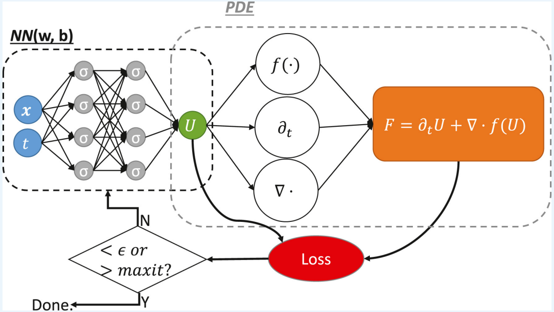

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DeepONet (Lu et al. 2019): *learns the differential operator*

$$G_\theta(u)(y) = \sum_{k=1}^{q} \underbrace{b_k(u(x_1), u(x_2), \ldots, u(x_m))}_{\text{branch}} \underbrace{t_k(y)}_{\text{trunk}}$$

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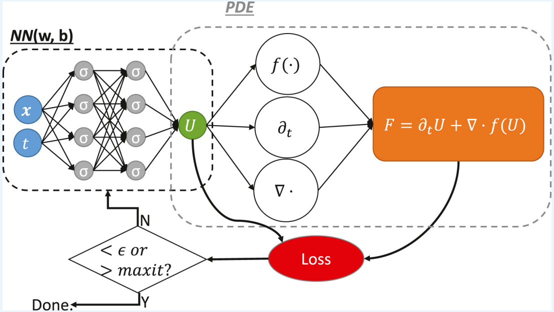

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Don't we know a good basis?

Isogeometric Analysis

Model problem: Poisson's equation

$$-\Delta u_h = f_h \quad \text{in} \quad \Omega_h, \qquad u_h = g_h \quad \text{on} \quad \partial\Omega_h$$

with

(geometry) $$\mathbf{x}_h(\xi,\eta) = \sum_{i=1}^{n} B_i(\xi,\eta) \cdot \mathbf{x}_i \qquad \forall(\xi,\eta) \in [0,1]^2$$

(solution) $$u_h \circ \mathbf{x}_h(\xi,\eta) = \sum_{i=1}^{n} B_i(\xi,\eta) \cdot u_i \qquad \forall(\xi,\eta) \in [0,1]^2$$

(r.h.s vector) $$f_h \circ \mathbf{x}_h(\xi,\eta) = \sum_{i=1}^{n} B_i(\xi,\eta) \cdot f_i \qquad \forall(\xi,\eta) \in [0,1]^2$$

(boundary conditions) $$g_h \circ \mathbf{x}_h(\xi,\eta) = \sum_{i=1}^{n} B_i(\xi,\eta) \cdot g_i \qquad \forall(\xi,\eta) \in \partial[0,1]^2$$

Abstract representation

Given $\mathbf{x}_i$ (geometry), f_i (r.h.s. vector), and g_i (boundary conditions), **compute**

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = A^{-1}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}\right) \cdot b\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}\right)$$

Any point of the solution can afterwards be obtained by a simple **function evaluation**

$$(\xi,\eta) \in [0,1]^2 \quad \mapsto \quad u_h \circ \mathbf{x}_h(\xi,\eta) = [B_1(\xi,\eta), \dots, B_n(\xi,\eta)] \cdot \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}$$

Isogeometric Analysis

Abstract representation

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$$(\xi,\eta) \in [0,1]^2 \quad \mapsto \quad u_h \circ \mathbf{x}_h(\xi,\eta) = [B_1(\xi,\eta),\dots,B_n(\xi,\eta)] \cdot \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}$$

Let us interpret the sets of B-spline coefficients $\{\mathbf{x}_i\}$, $\{f_i\}$, and $\{g_i\}$ as an efficient encoding of our PDE problem that is fed into our IgA machinery as **input**.

The **output** of our IgA machinery are the B-spline coefficients $\{u_i\}$ of the solution.

Isogeometric Analysis + Physics-Informed Machine Learning

IgANet: replace **computation**

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = A^{-1}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}\right) \cdot b\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}\right)$$

Isogeometric Analysis + Physics-Informed Machine Learning

IgANet: replace **computation** by **physics-informed machine learning**

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = \text{IgANet}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}; (\xi^{(k)}, \eta^{(k)})_{k=1}^{N_\text{samples}} \right)$$

Isogeometric Analysis + Physics-Informed Machine Learning

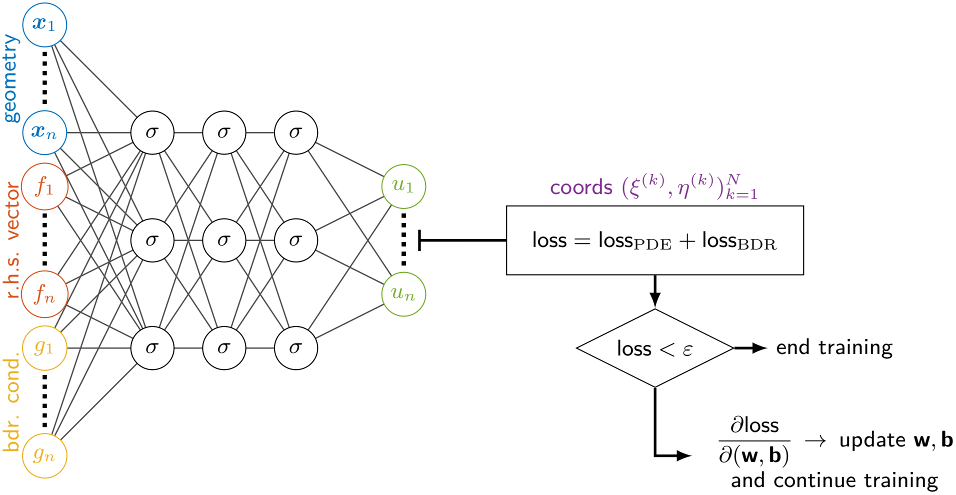
IgANet: replace **computation** by **physics-informed machine learning**

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = \text{IgANet}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}; (\xi^{(k)}, \eta^{(k)})_{k=1}^{N_{\text{samples}}} \right)$$

Compute the solution from the trained neural network as follows

$$u_h(\xi,\eta) = [B_1(\xi,\eta), \dots, B_n(\xi,\eta)] \cdot \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}, \qquad \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = \text{IgANet}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix} \right)$$

IgANet architecture



Loss function

$$\text{loss}_{\mathrm{PDE}} = \frac{\alpha}{N_\Omega} \sum_{k=1}^{N_\Omega} \left| \Delta \left[u_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) \right] - f_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) \right|^2$$

$$\text{loss}_{\mathrm{BDR}} = \frac{\beta}{N_\Gamma} \sum_{k=1}^{N_\Gamma} \left| u_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) - g_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) \right|^2$$

Express derivatives with respect to physical space variables using the Jacobian J, the Hessian H and the matrix of squared first derivatives Q (Schillinger *et al.* 2013):

$$\begin{bmatrix} \frac{\partial^2 B}{\partial x^2} \\ \frac{\partial^2 B}{\partial x \partial y} \\ \frac{\partial^2 B}{\partial y^2} \end{bmatrix} = Q^{-\top} \left(\begin{bmatrix} \frac{\partial^2 B}{\partial \xi^2} \\ \frac{\partial^2 B}{\partial \xi \partial \eta} \\ \frac{\partial^2 B}{\partial \eta^2} \end{bmatrix} - H^\top J^{-\top} \begin{bmatrix} \frac{\partial B}{\partial \xi} \\ \frac{\partial B}{\partial \eta} \end{bmatrix} \right)$$

Two-level training strategy

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

For a batch of randomly sampled $(\xi_k, \eta_k) \in [0,1]^2$ (or the Greville abscissae) **do**

$$\text{Train IgANet}\left(\begin{bmatrix}\mathbf{x}_1\\ \vdots \\ \mathbf{x}_n\end{bmatrix}, \begin{bmatrix}f_1\\ \vdots \\ f_n\end{bmatrix}, \begin{bmatrix}g_1\\ \vdots \\ g_n\end{bmatrix}; (\xi_k, \eta_k)_{k=1}^{N_{\text{samples}}}\right) \mapsto \begin{bmatrix}u_1\\ \vdots \\ u_n\end{bmatrix}$$

EndFor

EndFor

Details:

- 7×7 bi-cubic tensor-product B-splines for $\mathbf{x}_h$ and u_h, C^2-continuous
- TensorFlow 2.6, 7-layer neural network with 50 neurons per layer and ReLU activation function (except for output layer), Adam optimizer, 30.000 epochs, training is stopped after 3.000 epochs w/o improvement of the loss value

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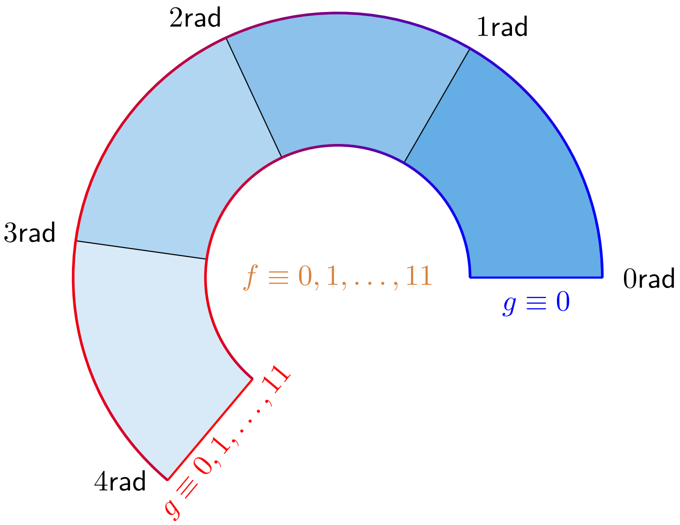
Test case: Poisson's equation on a variable annulus



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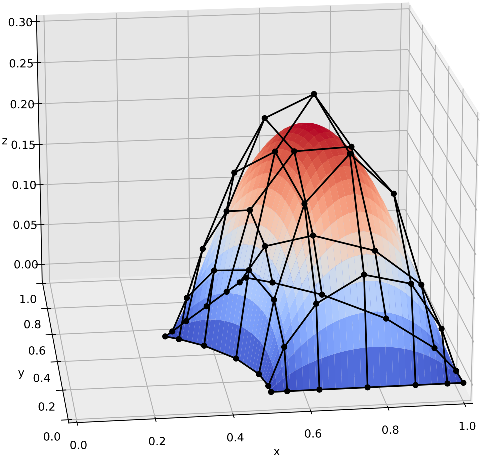
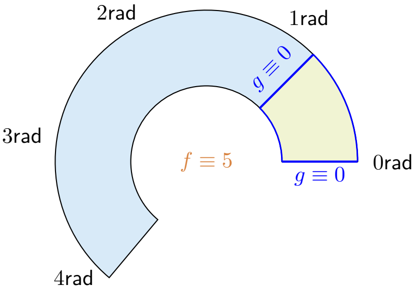
Preliminary results





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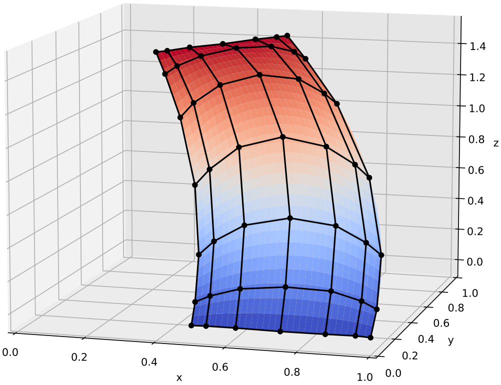

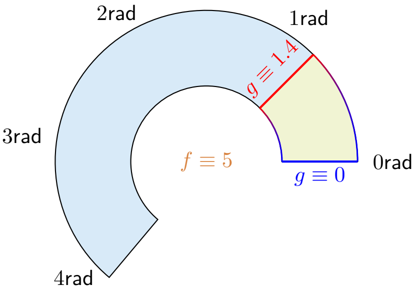

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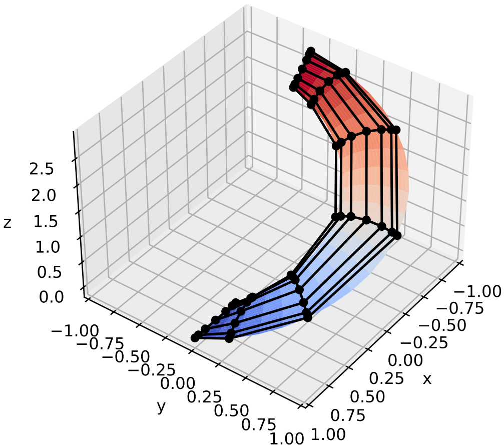

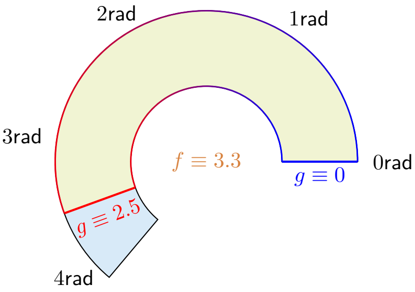

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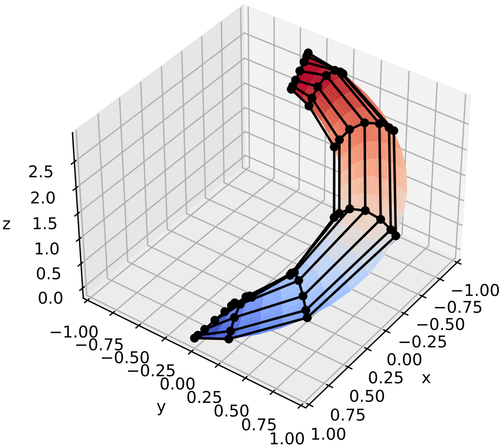

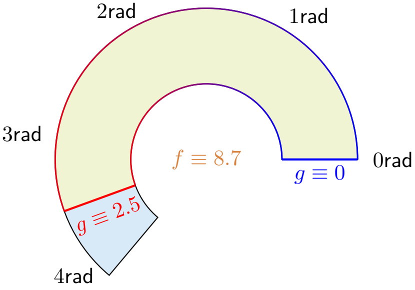

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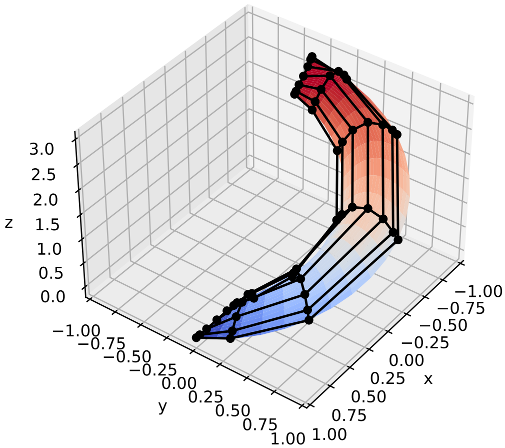

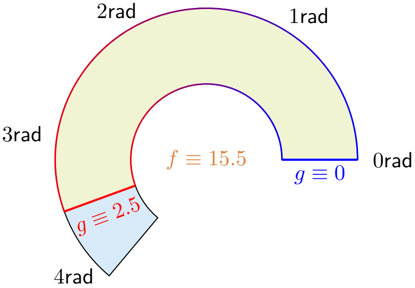

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Let's have a look under the hood

Computational costs of PINN vs. IgANets, implementation aspects, ...

Computational costs

Working principle of PINNs

$$\mathbf{x} \mapsto u(\mathbf{x}) := \mathsf{NN}(\mathbf{x}; f, g, G) = \sigma_L(\mathbf{W}_L \sigma(\ldots(\sigma_1(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1))) + \mathbf{b}_L)$$

- use AD engine (automated chain rule) to compute derivatives, e.g., $u_x = \mathsf{NN}_x$
- use AD engine on top of AD tree (!!!) to compute gradients w.r.t. weights for training

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- use AD engine (automated chain rule) to compute derivatives, e.g., $u_x = \mathsf{NN}_x$
- use AD engine on top of AD tree (!!!) to compute gradients w.r.t. weights for training

Working principle of IgANets

$$[\mathbf{x}_i, f_i, g_i]_{i=1,\dots,n} \mapsto [u_i]_{i=1,\dots,n} := \mathsf{NN}(\mathbf{x}_i, f_i, g_i, i = 1, \dots, n)$$

- use mathematics to compute derivatives, e.g., $\nabla_{\mathbf{x}} u = \left(\sum_{i=1}^n \nabla_{\boldsymbol{\xi}} B_i(\boldsymbol{\xi}) u_i\right) J_G^{-t}$
- use AD to compute gradients w.r.t. weights for training, i.e. (illustrated in 1D)

$$\frac{\partial(\mathrm{d}_\xi^r u(\xi))}{\partial w_k} = \sum_{i=1}^n \frac{\partial(\mathrm{d}_\xi^r b_i^p u_i)}{\partial w_k} = \cancel{\sum_{i=1}^n \mathrm{d}_\xi^{r+1} b_i^p \frac{\partial \xi}{\partial w_k} u_i} + \sum_{i=1}^n \mathrm{d}_\xi^r b_i^p \frac{\partial u_i}{\partial w_k}$$

Towards an ML-friendly B-spline evaluation

Major computational task (illustrated in 1D)

Given sampling point $\xi \in [\xi_i, \xi_{i+1})$ compute for $r \geq 0$

$$\mathrm{d}_\xi^r u(\xi) = \left[\mathrm{d}_\xi^r b_{i-p}^p(\xi), \ldots, \mathrm{d}_\xi^r b_i^p(\xi)\right] \cdot \underbrace{[u_{i-p}, \ldots, u_i]}_{\text{network's output}}$$

Textbook derivatives

$$\mathrm{d}_\xi^r b_i^p(\xi) = (p-1)\left(\frac{-\mathrm{d}_\xi^{r-1} b_{i+1}^{p-1}(\xi)}{\xi_{i+p} - \xi_{i+1}} + \frac{\mathrm{d}_\xi^{r-1} b_i^{p-1}(\xi)}{\xi_{i+p-1} - \xi_i}\right)$$

with

$$b_i^p(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} b_i^{p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} b_{i+1}^{p-1}(\xi), \quad b_i^0(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

Towards an ML-friendly B-spline evaluation

Matrix representation of B-splines (Lyche and Morken 2011)

$$\left[\mathrm{d}_\xi^r b_{i-p}^p(\xi), \ldots, \mathrm{d}_\xi^r b_i^p(\xi)\right] = \frac{p!}{(p-r)!} R_1(\xi) \cdots R_{p-r}(\xi) \mathrm{d}_\xi R_{p-r+1} \cdots \mathrm{d}_\xi R_p$$

with $k \times k+1$ matrices $R_k(\xi)$, e.g.

$$R_1(\xi) = \begin{bmatrix} \frac{\xi_{i+1}-\xi}{\xi_{i+1}-\xi_i} & \frac{\xi-\xi_i}{\xi_{i+1}-\xi_i} \end{bmatrix}$$

$$R_2(\xi) = \begin{bmatrix} \frac{\xi_{i+1}-\xi}{\xi_{i+1}-\xi_{i-1}} & \frac{\xi-\xi_{i-1}}{\xi_{i+1}-\xi_{i-1}} & 0 \\ 0 & \frac{\xi_{i+2}-\xi}{\xi_{i+2}-\xi_i} & \frac{\xi-\xi_i}{\xi_{i+2}-\xi_i} \end{bmatrix}$$

$$R_3(\xi) = \ldots$$

An ML-friendly B-spline evaluation

Algorithm 2.22 from (Lyche and Morken 2011)

1. $\mathbf{b} = 1$
2. For $k = 1, \ldots, p - r$
   1. $\mathbf{t}_1 = (\xi_{i-k+1}, \ldots, \xi_i)$
   2. $\mathbf{t}_2 = (\xi_{i+1}, \ldots, \xi_{i+k})$
   3. $\mathbf{w} = (\xi - \mathbf{t}_1) \div (\mathbf{t}_2 - \mathbf{t}_1)$
   4. $\mathbf{b} = [(1 - \mathbf{w}) \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$
3. For $k = p - r + 1, \ldots, p$
   1. $\mathbf{t}_1 = (\xi_{i-k+1}, \ldots, \xi_i)$
   2. $\mathbf{t}_2 = (\xi_{i+1}, \ldots, \xi_{i+k})$
   3. $\mathbf{w} = 1 \div (\mathbf{t}_2 - \mathbf{t}_1)$
   4. $\mathbf{b} = [-\mathbf{w} \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$

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

An ML-friendly B-spline evaluation

Algorithm 2.22 from (Lyche and Morken 2011) with slight modifications

1. $\mathbf{b} = 1$
2. For $k = 1, \ldots, p - r$
   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. $\textbf{mask} = (\mathbf{t}_{21} < \text{tol})$
   4. $\mathbf{w} = (\xi - \mathbf{t}_1 - \textbf{mask}) \div (\mathbf{t}_{21} - \textbf{mask})$
   5. $\mathbf{b} = [(1 - \mathbf{w}) \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$
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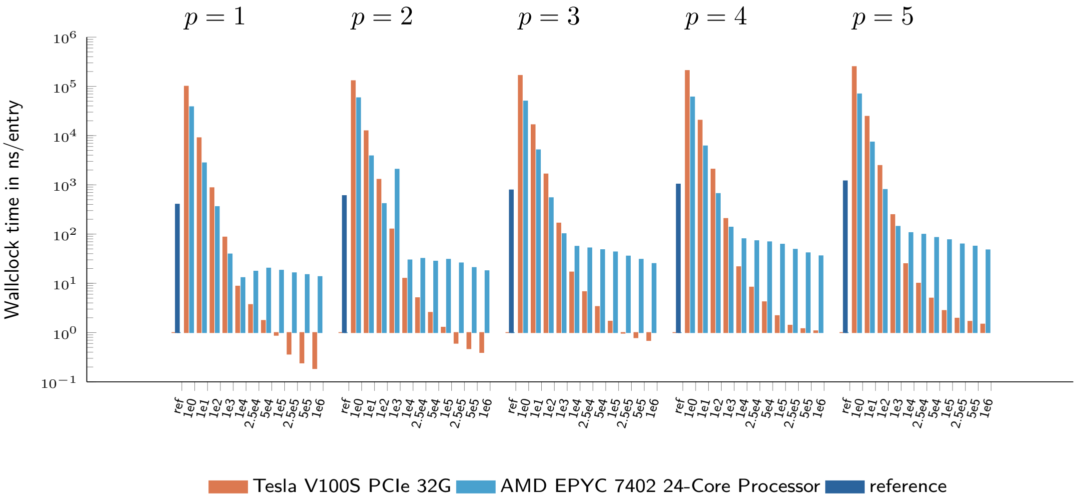
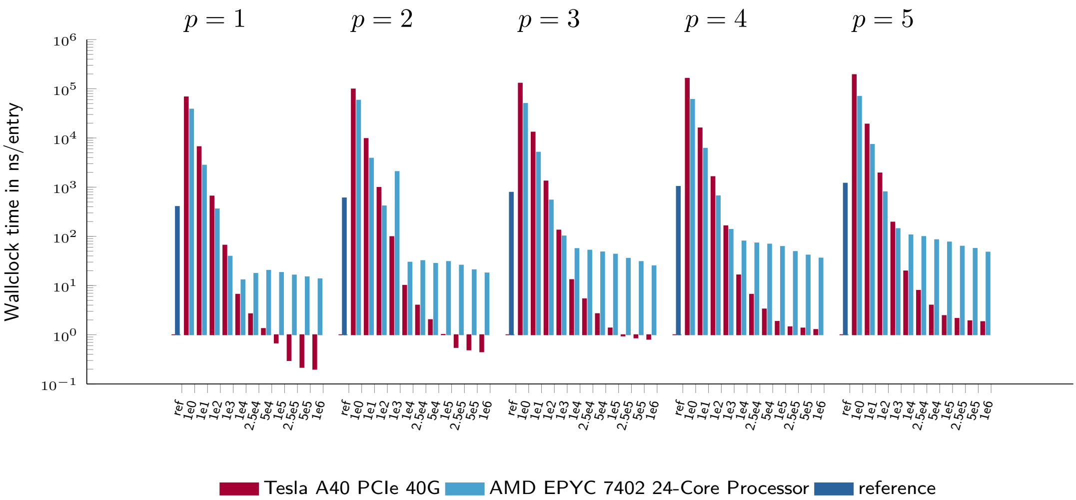
where $\div$ and $\odot$ denote the element-wise division and multiplication of vectors, respectively.

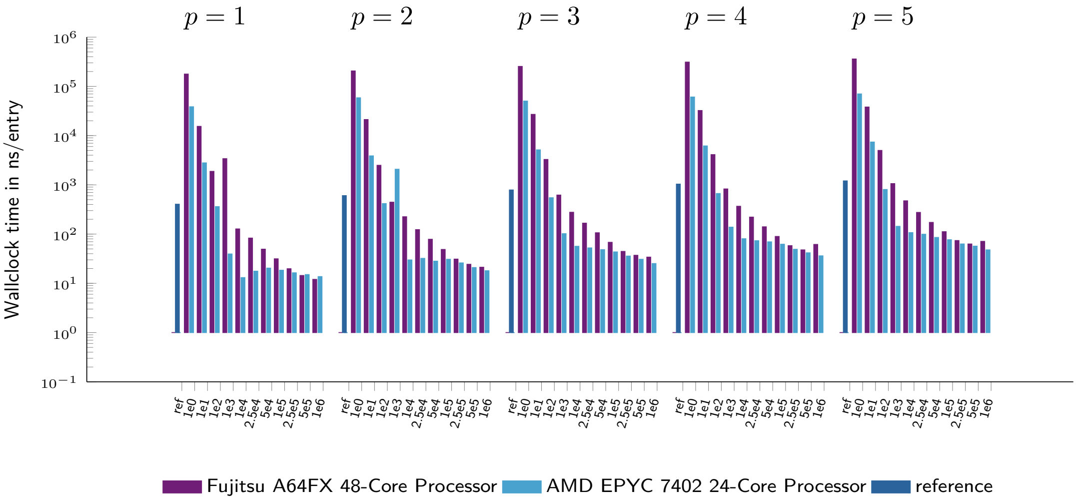
Performance evaluation - univariate B-splines



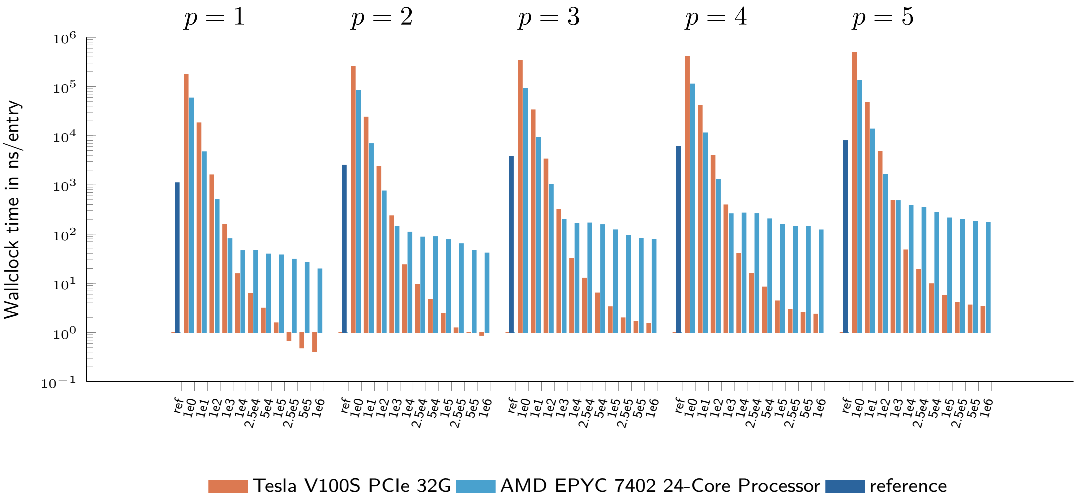
Performance evaluation - univariate B-splines



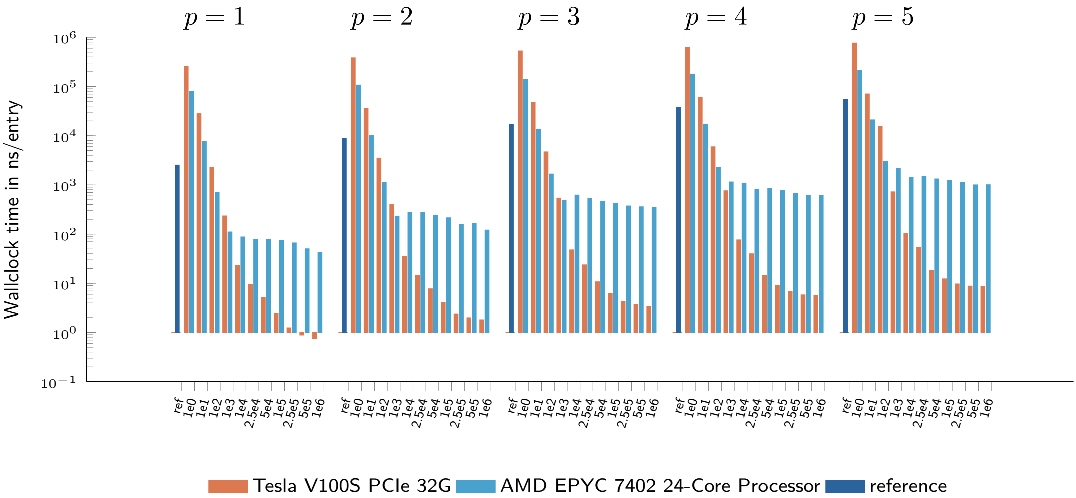
Performance evaluation - univariate B-splines



Performance evaluation - bivariate B-splines



Performance evaluation - trivariate B-splines

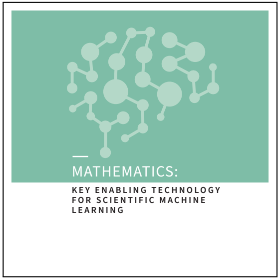


Conclusion and outlook

IgANets combine classical numerics with physics-informed machine learning and may finally enable **integrated and interactive design-through-analysis** workflows

WIP

- interactive DTA workflow (/w SURF)
- use of IgA and IgANets in concert
- transfer learning upon basis refinement



Short paper: Möller, Toshniwal, van Ruiten: *Physics-informed machine learning embedded into isogeometric analysis*, 2021. ☞

What's next

1. Journal paper and code release (including Python API) in preparation
2. Open PhD position on design optimization of very flexible floating structure with IgA
3. CISM-ECCOMAS Summer School *Scientific Machine Learning in Design Optimization*

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Delft University of Technology, The Netherlands

SIAM CSE23
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Thank you very much!