IgANets: Physics-machine learning embedded into Isogeometric Analysis

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Joint work with Deepesh Toshniwal & Frank van Ruiten (TU Delft),
Casper van Leeuwen & Paul Melis (SURF), and Jaewook Lee (TU Vienna)

The future of engineering (?!)

Siemens blog: *Virtual Reality in Engineering - Are You Ready?* – 7 July 2021
https://blogs.sw.siemens.com/teamcenter/virtual-reality-in-engineering-are-you-ready/

Interactive Design-through-Analysis

Vision: unified computational framework for

- **rapid prototyping** (design exploration & optimization phase) and
- **thorough analysis** (design analysis & fine-tuning phase)

of engineering designs

Ingredients

- physics-informed machine learning for rapid prototyping
- isogeometric analysis for accurate analysis

A demo says more than 1,000 words...

The big picture

Front-ends

IgANet-frontend
by SURF

gustaf
by TU Vienna

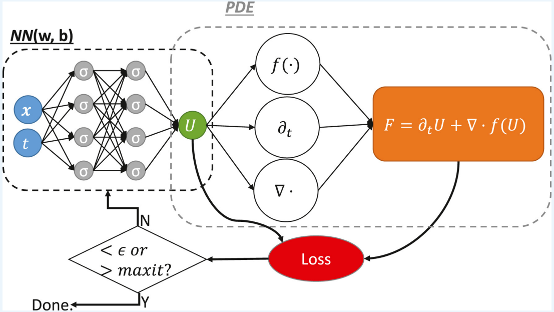
WebSockets protocol for interactive Design-through-Analysis

Back-ends

IgANet

Physics-informed machine learning

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



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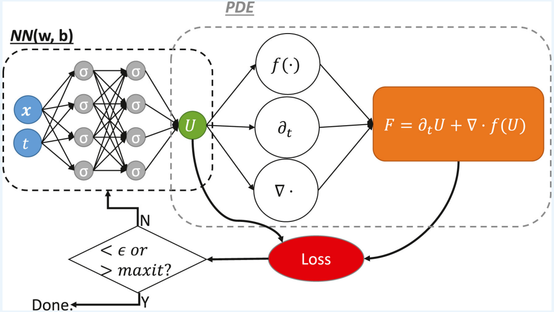

- easy to implement for 'any' PDE because AD magic does it for you
- combined un-/supervised learning
- poor extrapolation/generalization
- point-based approach requires re-evaluation of NN at every point
- rudimentary convergence theory

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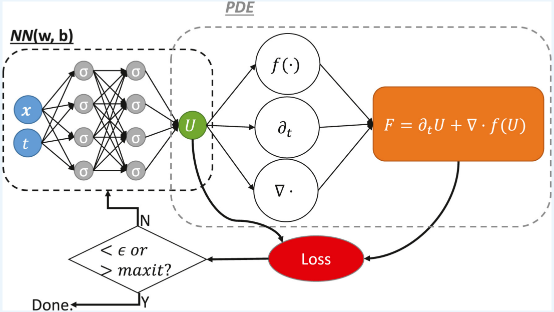

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$$G_\theta(u)(y) = \sum_{k=1}^{q} \underbrace{b_k(u(x_1), u(x_2), \ldots, u(x_m))}_{\text{branch}} \underbrace{t_k(y)}_{\text{trunk}}$$

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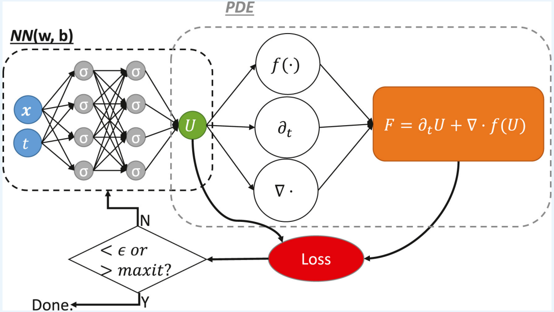

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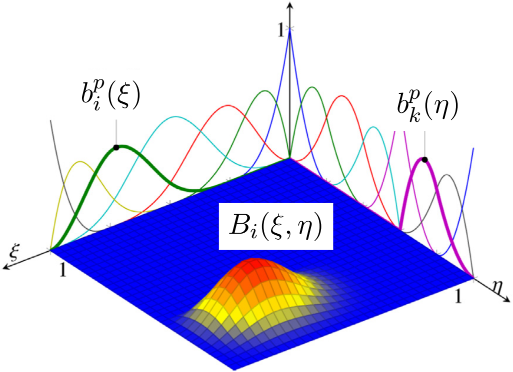
Don't we know good bases?

Tensor-product B-spline basis functions



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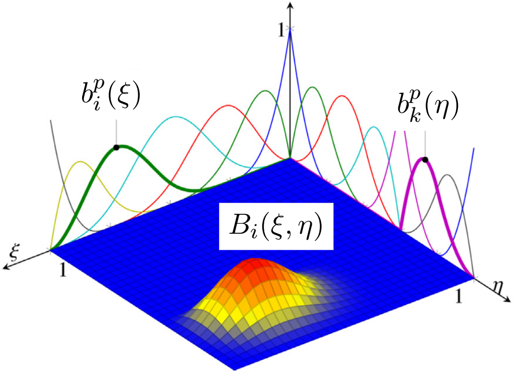
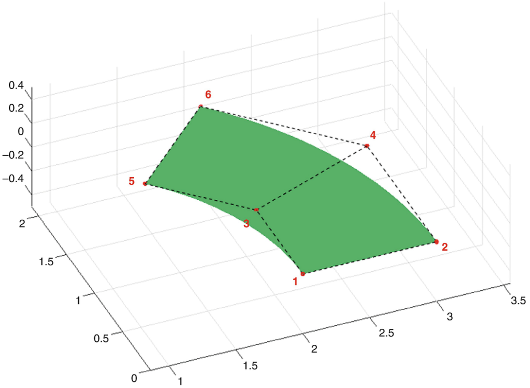


Properties: compact support, positive function values, partition of unity $\sum_{i=1}^{n} B_i(\xi,\eta) \equiv 1$, C^{p-1} continuity, derivatives of B-splines are combinations of lower-order B-splines, ...

Isogeometric Analysis

Geometry: bijective mapping from the unit square to the physical domain $\Omega_h \subset \mathbb{R}^d$

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



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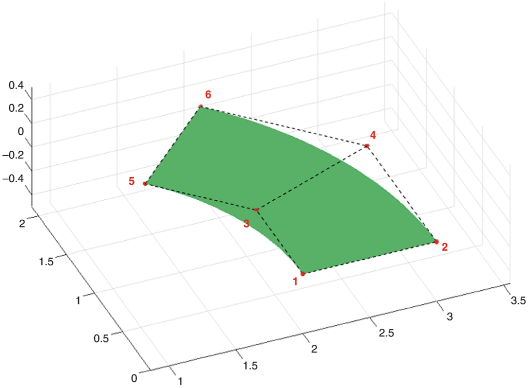

- the shape of Ω_h is fully specified by the set of **control points** $\mathbf{x}_i \in \mathbb{R}^d$
- interior control points must be chosen such that 'grid lines' do not fold as this violates the bijectivity of $\mathbf{x}_h : \hat{\Omega} \to \Omega_h$

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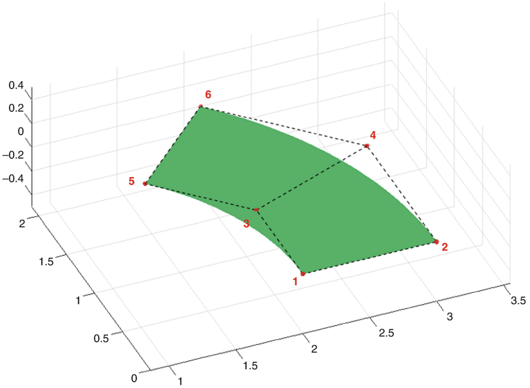

- the shape of Ω_h is fully specified by the set of **control points** $\mathbf{x}_i \in \mathbb{R}^d$
- interior control points must be chosen such that 'grid lines' do not fold as this violates the bijectivity of $\mathbf{x}_h : \hat{\Omega} \to \Omega_h$
- refinement in h (knot insertion) and p (order elevation) preserves the shape of Ω_h and can be used to generate finer computational 'grids' for the analysis

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

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

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

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

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

Isogeometric Analysis

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

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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.

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**

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

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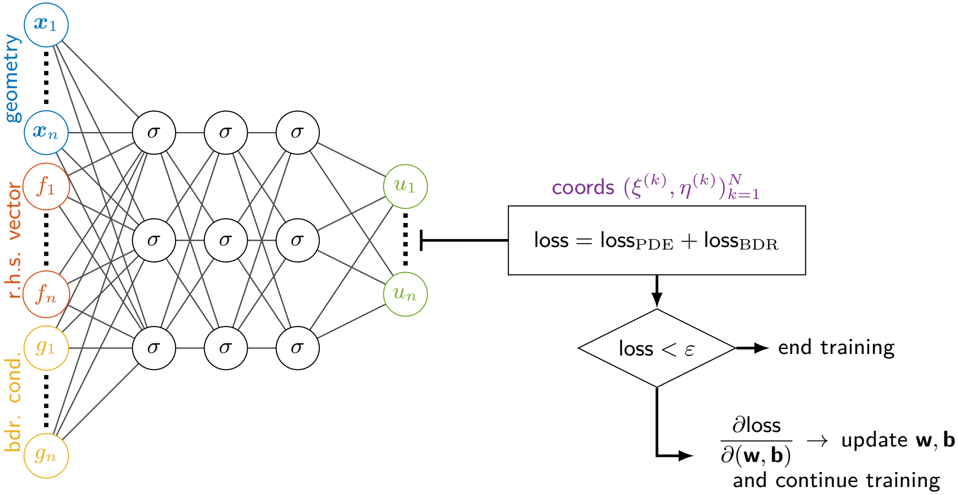
Compute the solution from the trained neural network as follows

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

IgANet architecture



Loss function

Model problem: Poisson's equation with Dirichlet boundary conditions

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

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

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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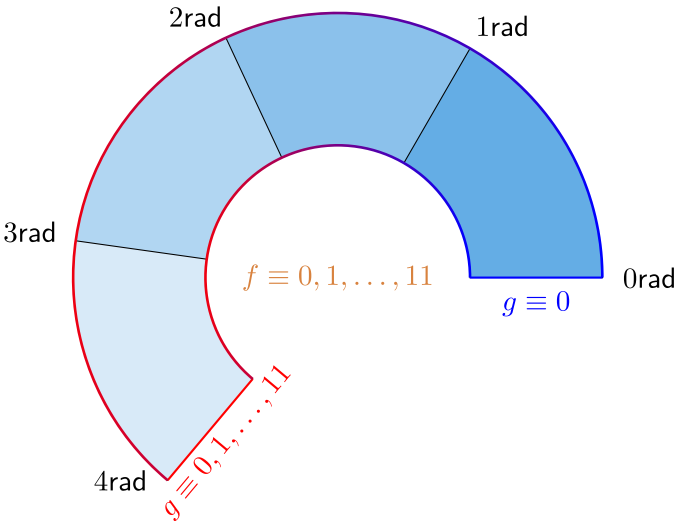
Test case: Poisson's equation on a variable annulus



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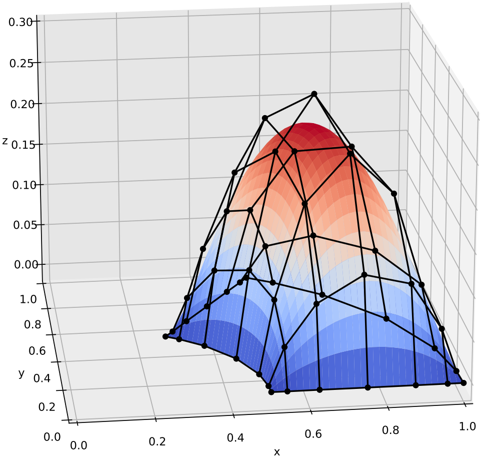
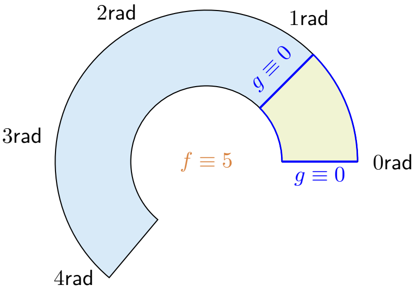
Preliminary results





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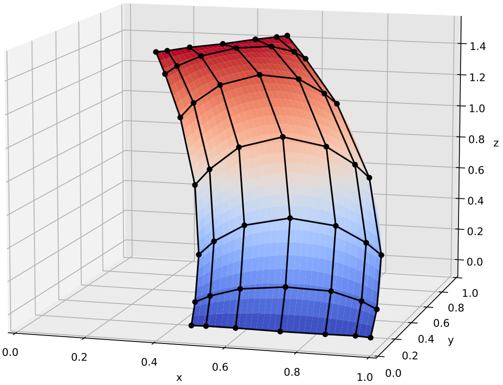

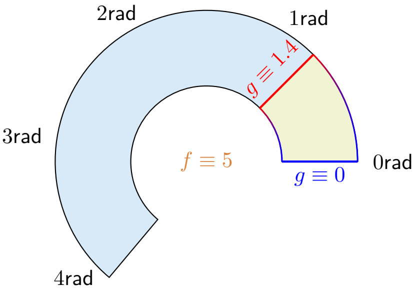

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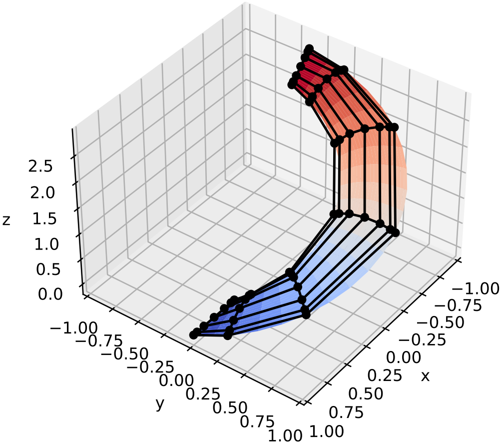

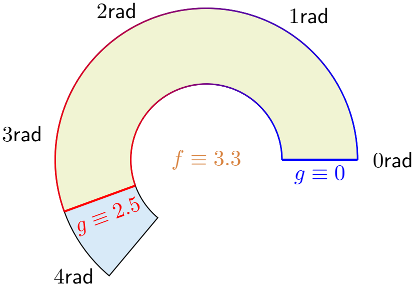

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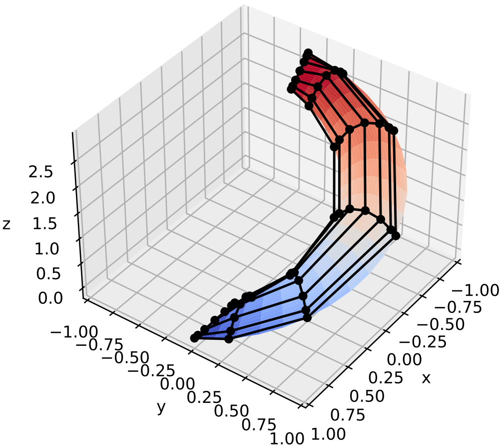

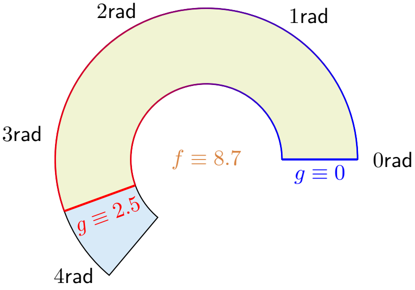

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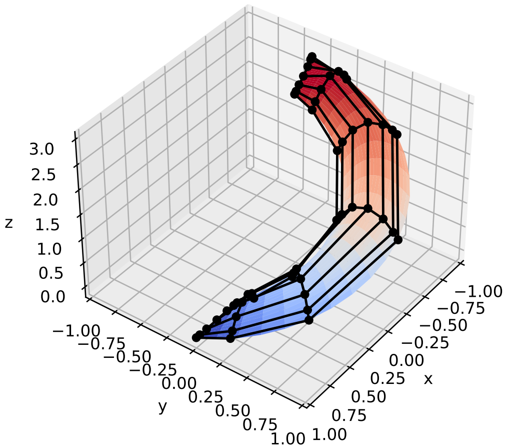

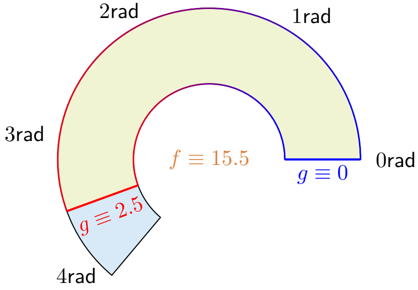

Let's have a look under the hood

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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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)

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

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 $r \geq 0$

$$D^r u(\xi) = \left[D^r b^p_{i-p}(\xi), \ldots, D^r b^p_i(\xi) \right] \cdot \underbrace{[u_{i-p}, \ldots, u_i]}_{\text{network's output}}$$

Textbook derivatives

$$D^r b^p_i(\xi) = p \left(\frac{D^{r-1} b^{p-1}_i(\xi)}{\xi_{i+p} - \xi_i} - \frac{D^{r-1} b^{p-1}_{i+1}(\xi)}{\xi_{i+p-1} - \xi_{i+1}} \right)$$

with (cf. Cox-de-Boor recursion formula)

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

Towards an ML-friendly B-spline evaluation

Matrix representation of B-splines (Lyche and Mørken 2018)

$$\left[D^r b^p_{i-p}(\xi), \ldots, D^r b^p_i(\xi)\right] = \frac{p!}{(p-r)!}\mathbf{R}_1(\xi)\cdots\mathbf{R}_{p-r}(\xi)D\mathbf{R}_{p-r+1}\cdots D\mathbf{R}_p$$

with $k \times k+1$ matrices $\mathbf{R}_k(\xi)$

$$\mathbf{R}_1(\xi) = \begin{bmatrix} \frac{\xi_{i+1}-\xi}{\xi_{i+1}-\xi_i} & \frac{\xi-\xi_i}{\xi_{i+1}-\xi_i} \end{bmatrix}, \quad \mathbf{R}_2(\xi) = \begin{bmatrix} \frac{\xi_{i+1}-\xi}{\xi_{i+1}-\xi_{i-1}} & \frac{\xi-\xi_{i-1}}{\xi_{i+1}-\xi_{i-1}} & 0 \\ 0 & \frac{\xi_{i+2}-\xi}{\xi_{i+2}-\xi_i} & \frac{\xi-\xi_i}{\xi_{i+2}-\xi_i} \end{bmatrix}, \quad \ldots$$

and

$$D\mathbf{R}_1(\xi) = \begin{bmatrix} \frac{-1}{\xi_{i+1}-\xi_i} & \frac{1}{\xi_{i+1}-\xi_i} \end{bmatrix}, \quad D\mathbf{R}_2(\xi) = \begin{bmatrix} \frac{-1}{\xi_{i+1}-\xi_{i-1}} & \frac{1}{\xi_{i+1}-\xi_{i-1}} & 0 \\ 0 & \frac{-1}{\xi_{i+2}-\xi_i} & \frac{1}{\xi_{i+2}-\xi_i} \end{bmatrix}, \quad \ldots$$

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Costs of matrix assembly (arithmetic operations)

$$3p^2 - 3p - r^2 + r \text{ (leading } D\mathbf{R}'s) \quad \text{vs.} \quad 2p^2 - 2p + r^2 - r \text{ (trailing } D\mathbf{R}'s)$$

Costs of matrix-matrix products ($p \geq 3$)

$$(4p^3 - 3p^2 - 7p - 6)/6 \text{ (L2R)} \quad \text{vs.} \quad (4p^4 - 15p^3 + 17p^2 - 6p)/6 \text{ (R2L)}$$

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Can we do better?

An ML-friendly B-spline evaluation

Algorithm 2.22 from (Lyche and Mørken 2018) with 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. $\mathbf{b} = [(1 - \mathbf{w}) \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$
3. For $k = p - r + 1, \ldots, p$
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   2. $\mathbf{t}_{21} = (\xi_{i+1}, \ldots, \xi_{i+k}) - \mathbf{t}_1$
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   4. $\mathbf{w} = (1 - \textbf{mask}) \div (\mathbf{t}_{21} - \textbf{mask})$
   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.

An ML-friendly B-spline evaluation

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

Costs: $5(p^2 + p)$ arithmetic operations $+ \ 2p - 1$ for $\mathbf{b} \cdot \mathbf{u}$

An ML-friendly *multi-variate* B-spline evaluation

Task: Given pre-evaluated vectors of univariate B-spline basis functions $\mathbf{b}^d$ compute

$$u(\xi, \eta, \zeta) = [\mathbf{b}_1(\xi) \otimes \mathbf{b}_2(\eta) \otimes \mathbf{b}_3(\zeta)] \cdot \mathbf{u}$$

but sub-matrix of coefficients $\mathbf{u} := u[\mathbf{i} - \mathbf{p} : \mathbf{i}]$ is not contiguous in memory

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Since $(\mathbf{b}_1 \otimes \mathbf{b}_2 \otimes \mathbf{b}_3) \cdot \mathbf{u} = (\mathbf{I} \otimes \mathbf{I} \otimes \mathbf{b}_3) \cdot (\mathbf{I} \otimes \mathbf{b}_2 \otimes \mathbf{I}) \cdot (\mathbf{b}_1 \otimes \mathbf{I} \otimes \mathbf{I}) \cdot \mathbf{u}$ we can use

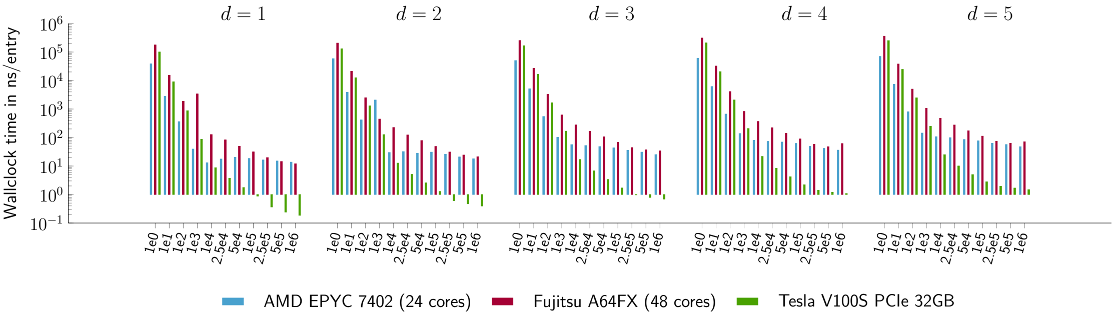
Algorithm 993 from (Fackler 2019) with modifications

For $d = 1, 2$

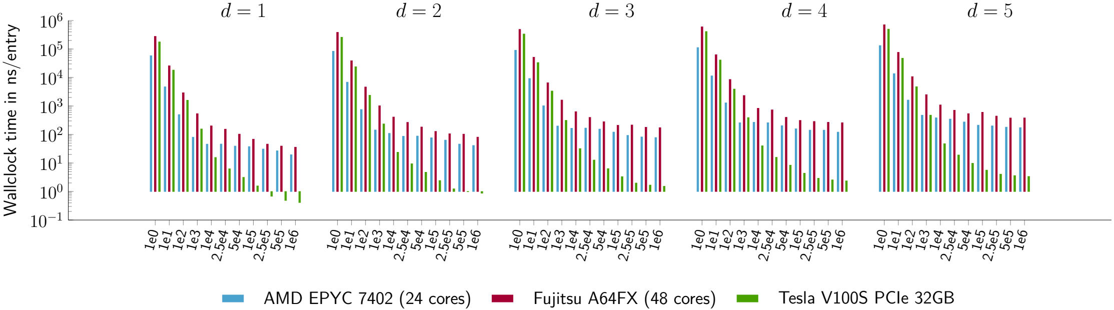
1. $\mathbf{u} = \text{reshape}(\mathbf{u}, [\cdot], n_d)$
2. $\mathbf{u} = \mathbf{b}_d \cdot \mathbf{u}^\top$

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

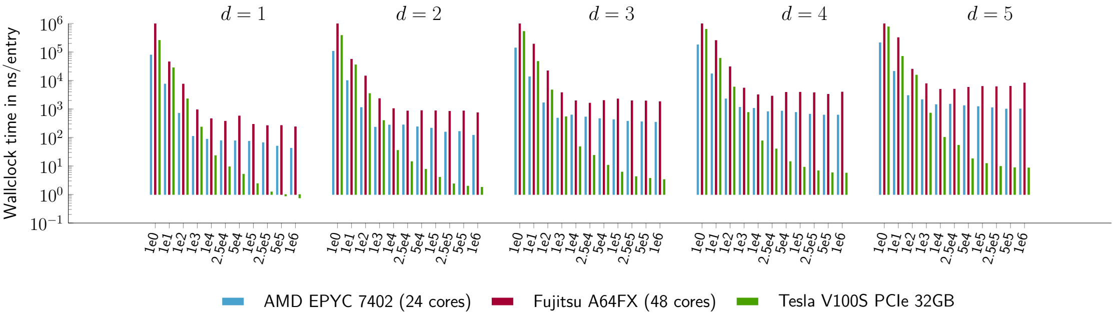
Performance evaluation - univariate B-splines



Performance evaluation - bivariate B-splines



Performance evaluation - trivariate B-splines

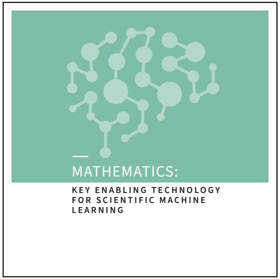


Conclusion and outlook

IgANets combine isogeometric analysis with physics-informed machine learning to enable **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. CISM-ECCOMAS Summer School *Scientific Machine Learning in Design Optimization*

IgANets: Physics-machine learning embedded into Isogeometric Analysis

Matthias Möller

Department of Applied Mathematics, TU Delft

HOFEIM 2023

Joint work with Deepesh Toshniwal & Frank van Ruiten (TU Delft),
Casper van Leeuwen & Paul Melis (SURF), and Jaewook Lee (TU Vienna)

Thank you very much!