IgANets: Physics-machine learning embedded into Isogeometric Analysis

Matthias Möller

Department of Applied Mathematics, TU Delft

IGA 2023 – 18-21 June 2023, Lyon (France)

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

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 thorough analysis

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 thorough analysis

Design principle: stay in the IGA paradigm

The big picture

Front-ends

IgANet-frontend
by SURF

gustaf
by TU Vienna

WebSockets protocol for interactive Design-through-Analysis

Back-ends

IgANet

Outline

Isogeometric collocation method

Model problem: Poisson's equation

$$-\Delta u = f \quad \text{in} \quad \Omega, \qquad u = g \quad \text{on} \quad \partial\Omega$$

Petrov-Galerkin formulation

$$\int_\Omega \delta(\Delta u + f)\mathrm{d}\mathbf{x} = 0 \quad \xrightarrow{\delta \text{ Dirac delta}} \quad \Delta u(\mathbf{x}_i) + f(\mathbf{x}_i) = 0 \quad \forall \mathbf{x}_i$$

with collocation points $\mathbf{x}_i$, e.g., the images of the Greville abscissae

$$\bar{\xi}_i = \frac{\xi_{i+1} + \cdots + \xi_{i+p}}{p}$$

Isogeometric collocation method

Model problem: Poisson's equation

$$-\Delta u = f \quad \text{in} \quad \Omega, \qquad u = g \quad \text{on} \quad \partial\Omega$$

Petrov-Galerkin formulation

$$\int_\Omega \delta(\Delta u + f)\mathrm{d}\mathbf{x} = 0 \quad \xrightarrow{\delta \text{ Dirac delta}} \quad \Delta u(\mathbf{x}_i) + f(\mathbf{x}_i) = 0 \quad \forall \mathbf{x}_i$$

with collocation points $\mathbf{x}_i$, e.g., the images of the Greville abscissae

$$\bar{\xi}_i = \frac{\xi_{i+1} + \cdots + \xi_{i+p}}{p}$$

Next: discretization

Discretization $Au = b$

(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**

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

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**

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

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.

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

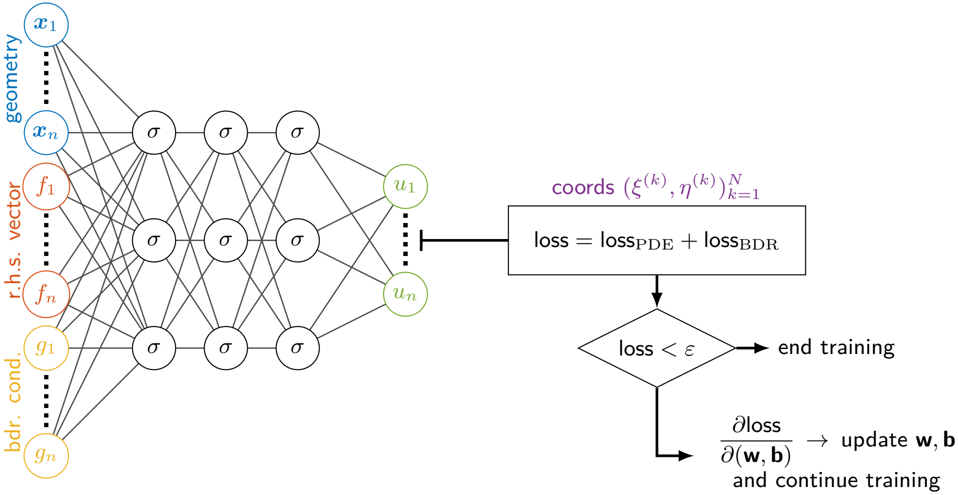
IgANet: replace **computation** by **physics-informed machine learning**

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

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

Model problem: Poisson's equation with Dirichlet boundary conditions

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

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

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

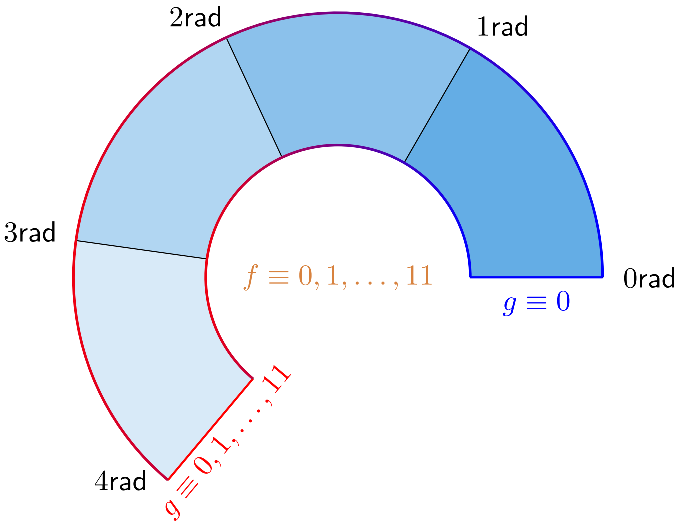
EndFor

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

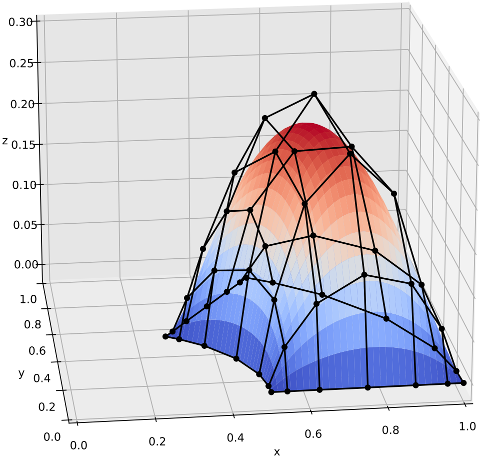
Master thesis work by Frank van Ruiten, TU Delft

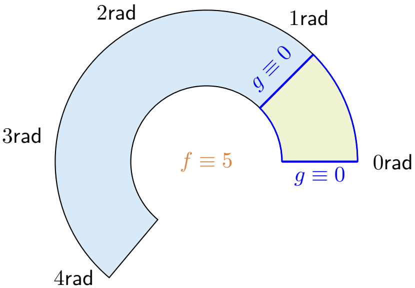
Test case: Poisson's equation on a variable annulus



Master thesis work by Frank van Ruiten, TU Delft

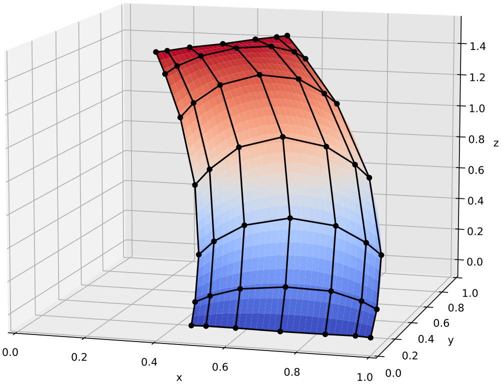
Preliminary results

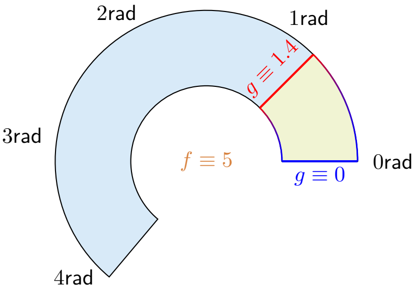




Master thesis work by Frank van Ruiten, TU Delft

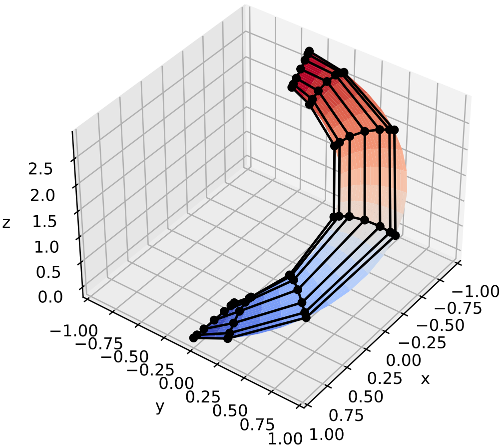
Preliminary results

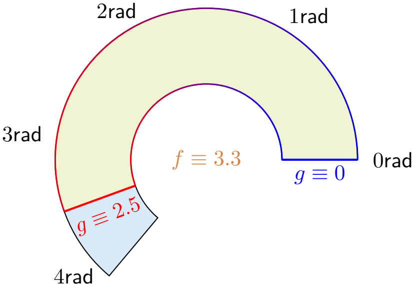




Master thesis work by Frank van Ruiten, TU Delft

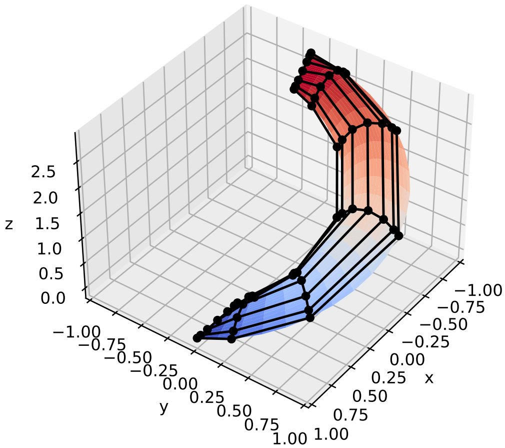
Preliminary results

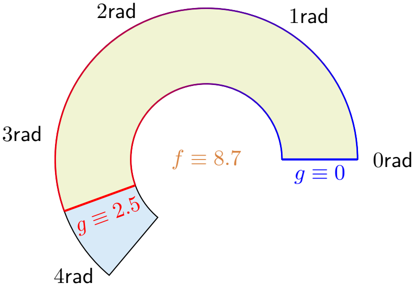




Master thesis work by Frank van Ruiten, TU Delft

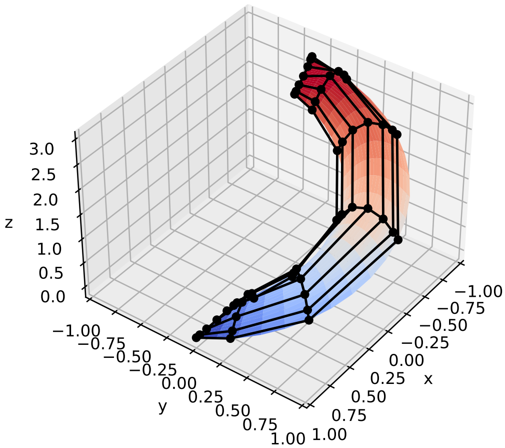
Preliminary results

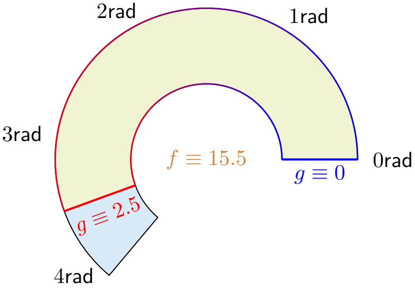




Master thesis work by Frank van Ruiten, TU Delft

Preliminary results





Master thesis work by Frank van Ruiten, TU Delft


MANUAL FOR
SPEED
SPEED
SPEED

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

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

Working principle of IgANets

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

- 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

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

Towards an ML-friendly B-spline evaluation

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

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

Costs of matrix assembly (arithmetic operations)

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

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

$(4p^3 - 3p^2 - 7p - 6)/6$ (L2R) vs. $(4p^4 - 15p^3 + 17p^2 - 6p)/6$ (R2L)

Towards an ML-friendly B-spline evaluation

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

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

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 ($p \geq 3$)

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

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 $k = p - r + 1, \ldots, p$
   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. $\mathbf{w} = (1 - \textbf{mask}) \div (\mathbf{t}_{21} - \textbf{mask})$
   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

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 $k = p - r + 1, \ldots, p$
   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. $\mathbf{w} = (1 - \textbf{mask}) \div (\mathbf{t}_{21} - \textbf{mask})$
   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.

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

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

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 $d = 1, 2, 3$

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

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

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

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

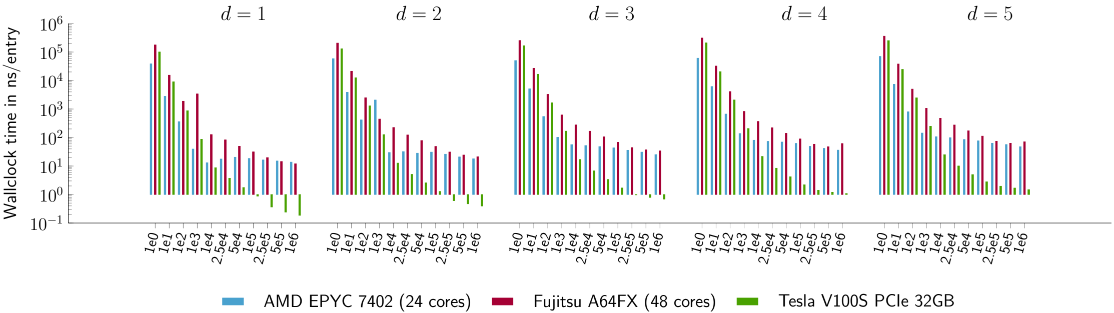
For $d = 1, 2, 3$

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

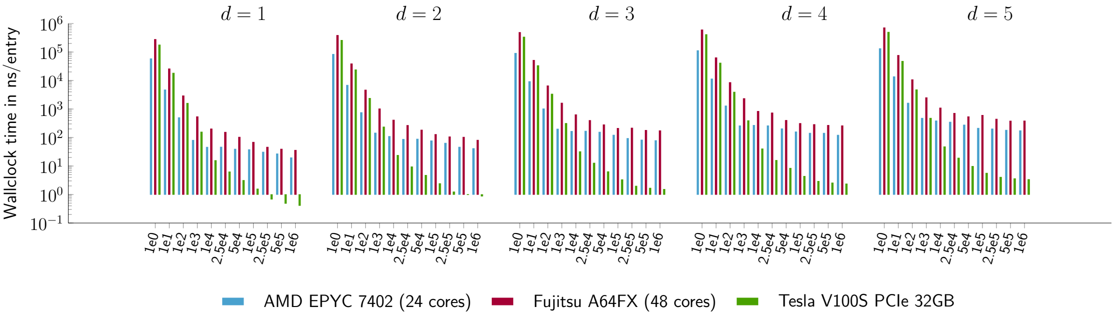
Output: $\mathbf{u} = u(\xi, \eta, \zeta)$

Tensorized version to evaluate multiple (ξ, η, ζ) points simultaneously

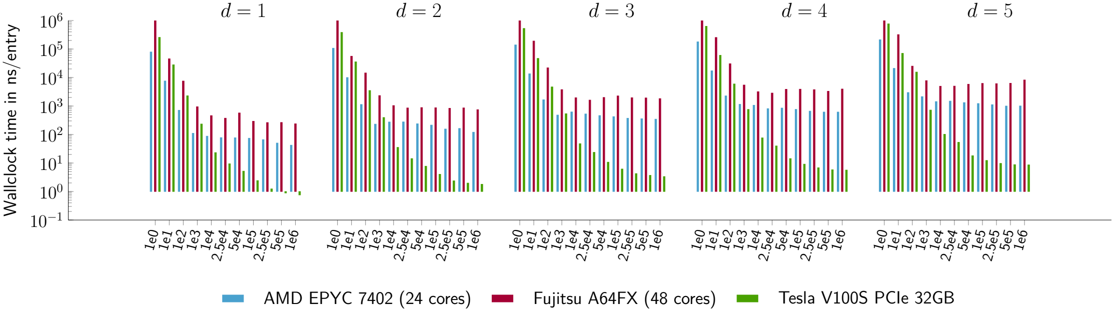
Performance evaluation - univariate B-splines



Performance evaluation - bivariate B-splines



Performance evaluation - trivariate B-splines



Conclusions and outlook

IgANets: in-paradigm combination of IGA and physics-informed machine learning

- for interactive design-through-analysis workflows
- as initial guess generator for iterative solvers
- maybe as a preconditioner

What's next

- Journal paper and code release (including Python API) in preparation
- 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

IGA 2023 – 18-21 June 2023, Lyon (France)

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!