

IgaNets: Physics-Informed Machine Learning Embedded Into Isogeometric Analysis

Matthias Möller

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KOLLOQUIUM ÜBER NEUERE ARBEITEN AUF DEM
GEBIETE DER MECHANIK UND STRÖMUNGSLEHRE
an der Technischen Universität Wien

Joint work with Deepesh Toshniwal and Frank van Ruiten

About

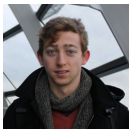
Associate Professor of Numerical Analysis

- Doctorate from TU Dortmund in 2008
- Started working at TU Delft in 2013

Research interests

- Finite element and isogeometric analysis
- Adaptive high-resolution schemes for flow problems
- Fast solution techniques for (non-)linear problems
- Quantum and high-performance computing
- Scientific machine learning

The IGA team (open position on IGA-FSI)



Hugo Verhelst
(TUD)



Ye Ji
(CSC)



Vijai Kumar
(TUD)



Roel Tielen
(ASML)



Jochen Hinz
(EPFL)



Andrzej Jaeschke
(Łódź)

The Quantum team (open positions to come)



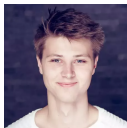
Merel Schalkers
(TUD)



Giorgio Tosti
(TUD)



Arne Wulff
(TUD)



Koen Mesman
(TUD)

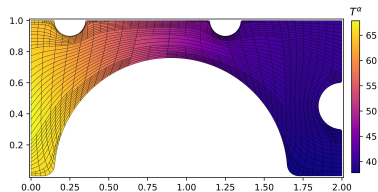
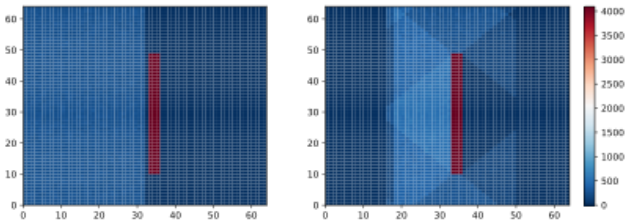
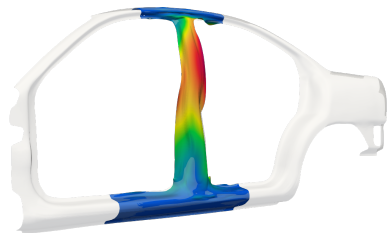
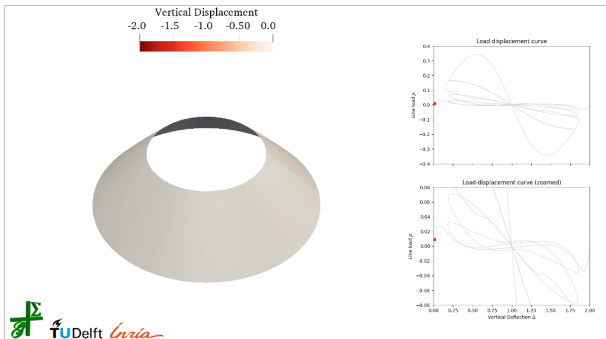


Swapan Venkata
(TUD)

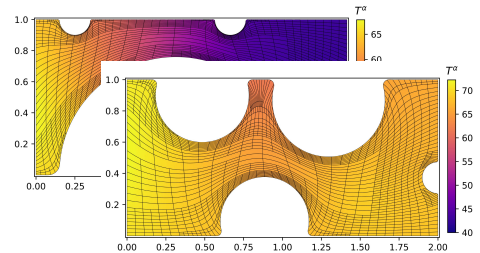
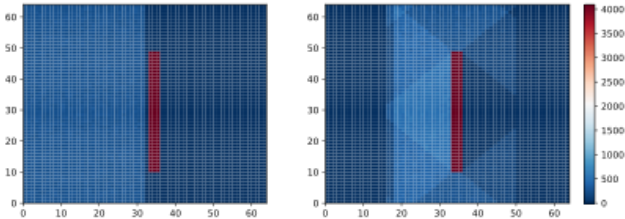
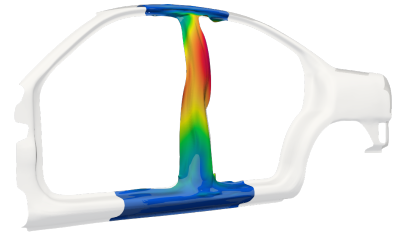
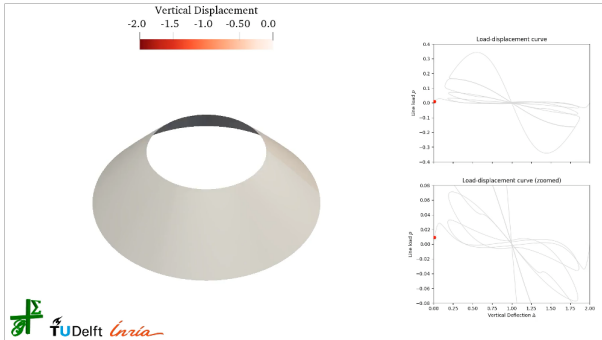


Philip Wurzner
(TUD)

Research results



Research results



Motivation

FDM, FVM, FEM, BEM, IGA, ...

vs.

PINNs, DeepONets, FourierNets, ...

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- “Method a is/is not as accurate as method b ”
- “Method a is x -times faster/slower than method b ”

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FDM, FVM, FEM, BEM, IGA, ...

- 👍 sound mathematical foundation
- 👍 established engineering workflows
- 👎 no cost amortization over multiple runs, no real-time capability

vs.

PINNs, DeepONets, FourierNets, ...

- 👍 fast evaluation (costly training!)
- 👍 inclusion of (measurement) data
- 👎 lack of convergence theory
- 👎 lack of general acceptance

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Better question to ask

- What are the specific **strengths/weaknesses** of the different approaches?

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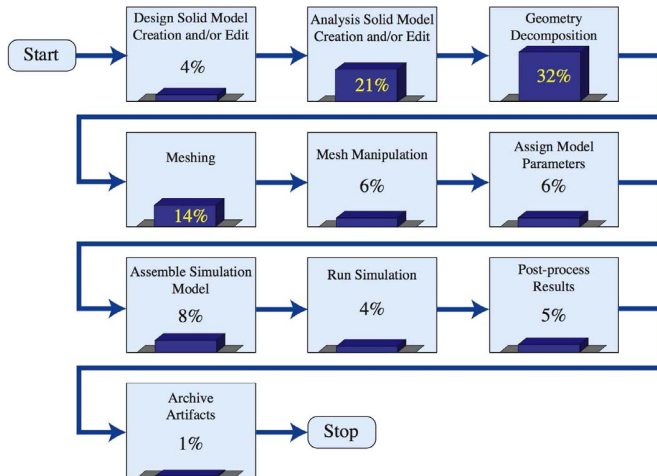
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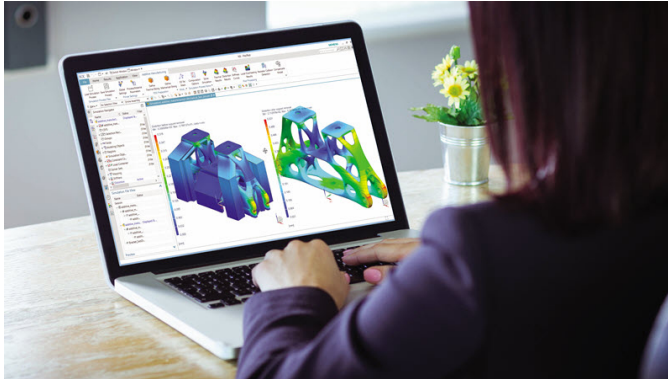
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- What are the specific **strengths/weaknesses** of the different approaches?
- How can we combine the **strengths** of both classes of methods?
- What is the envisaged purpose of the new approach?

Design-through-Analysis — IGA's ultimate goal from day one on



Design-through-Analysis — *IGA's ultimate goal from day one on*

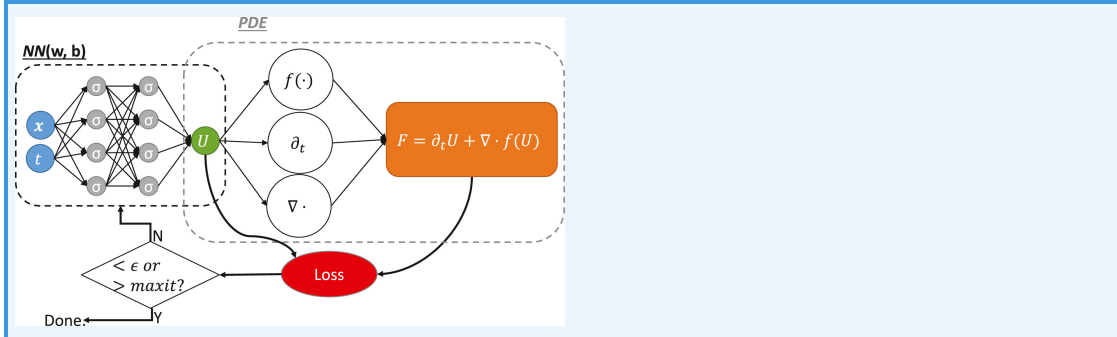


Vision: fast interactive qualitative analysis and accurate quantitative analysis within the same computational framework with seamless switching between both approaches

Photo: Siemens – Simulation for Design Engineers

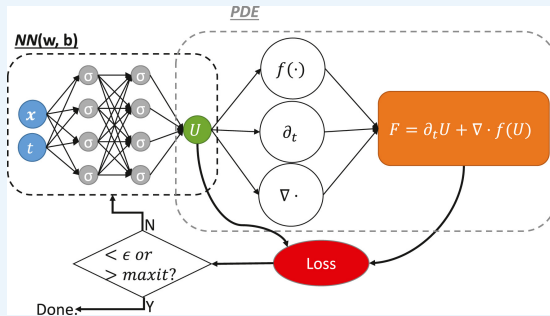
Physics-informed machine learning

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



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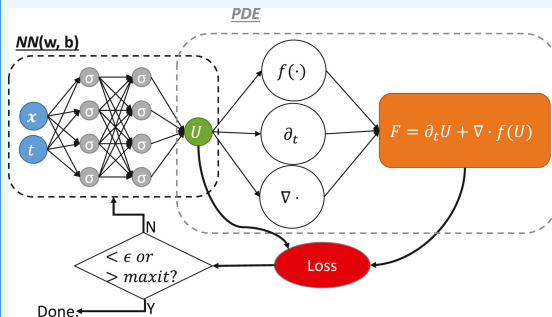
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- 👎 point-based approach requires re-evaluation of NN at every point
- 👎 rudimentary convergence theory

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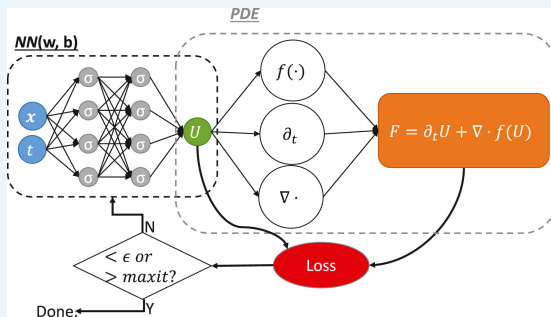
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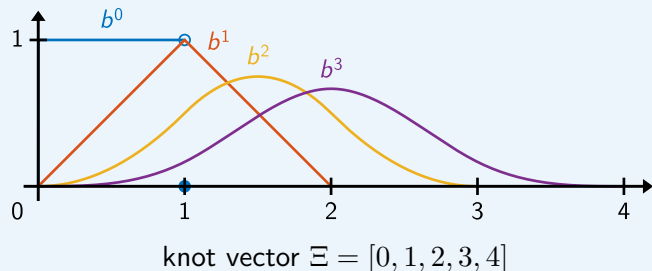
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Don't we know a good **basis**?

B-spline basis functions

Cox de Boor recursion formula

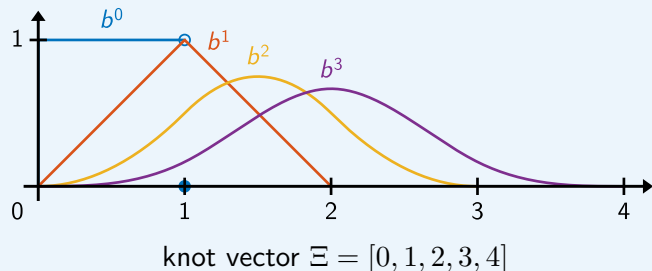


$$b_i^0(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

$$b_i^p(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} b_i^{p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} b_{i+1}^{p-1}(\xi)$$

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Many good properties: compact support $[\xi_i, \xi_{i+p+1})$, positive function values over support interval, derivatives of B-splines are combinations of lower-order B-splines, ...

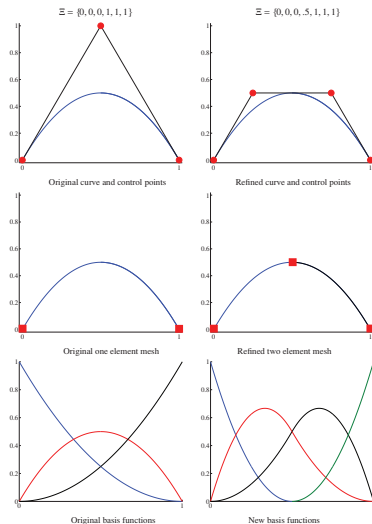
Refinement techniques

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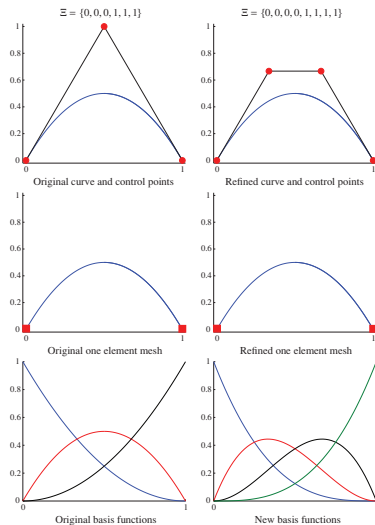
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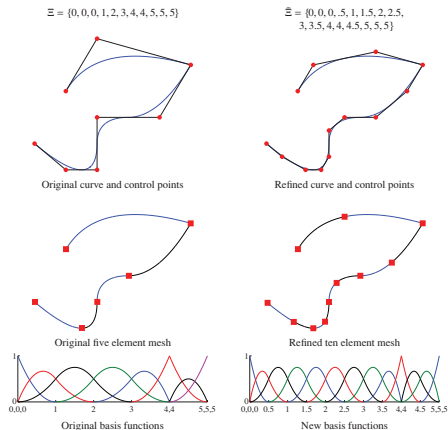


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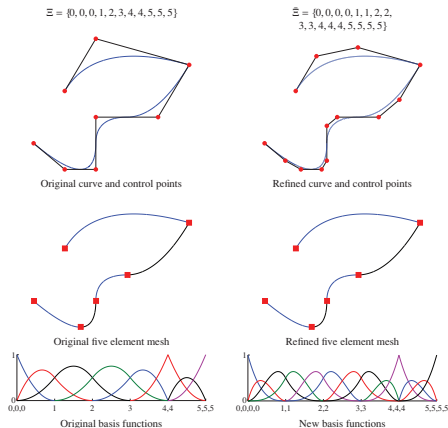


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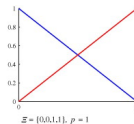
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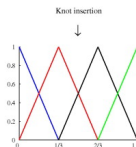
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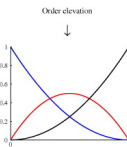
- **k -refinement** is a unique IGA feature to achieve higher order *and* higher continuity at the same time



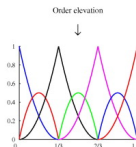
(a)



$$\Xi = \{0, 0, \frac{1}{3}, \frac{2}{3}, 1, 1\}, p = 1$$

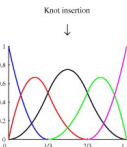


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(b)



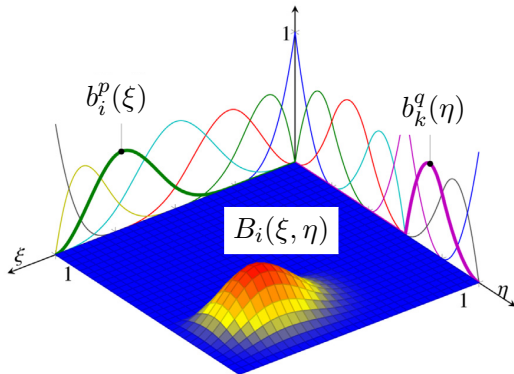
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(c)

Isogeometric Analysis

Paradigm: represent 'everything' in terms of tensor products of B-spline basis functions

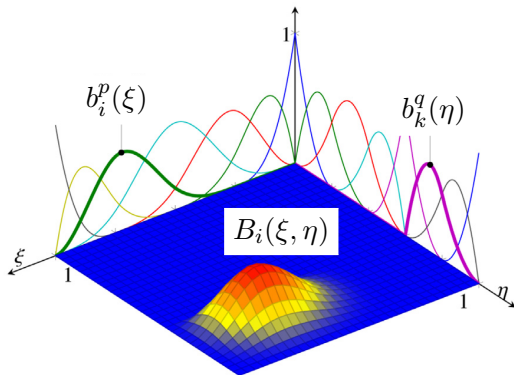
$$B_i(\xi, \eta) := b_i^p(\xi) \cdot b_k^q(\eta), \quad i := (k-1) \cdot n_i + i, \quad 1 \leq i \leq n_i, \quad 1 \leq k \leq n_k,$$



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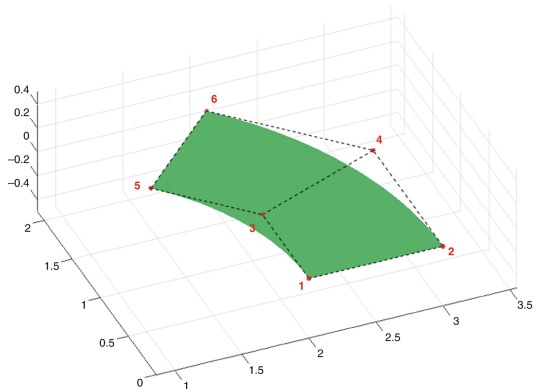
Many more good properties: partition of unity $\sum_{i=1}^n B_i(\xi, \eta) \equiv 1$, C^{p-1} continuity, ...

Isogeometric Analysis

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

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

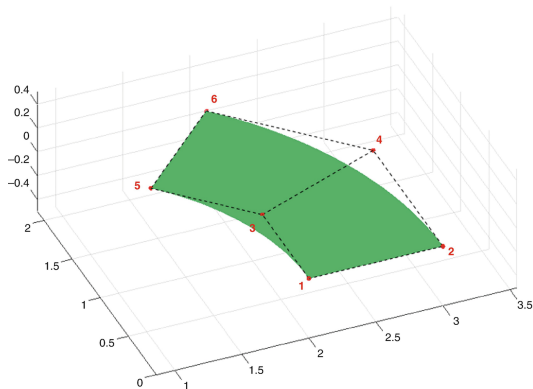
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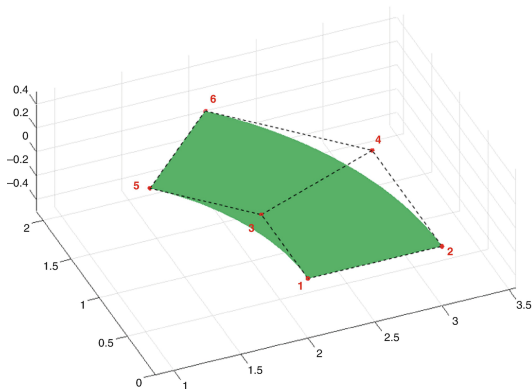


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- refinement in h (knot insertion) and p (order elevation) preserves the shape of Ω_h and can be used to generate finer computational 'grids' for the analysis

Isogeometric Analysis

Model problem: Poisson's equation

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

with

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

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

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

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

Solution approaches

- Galerkin-type IGA (Hughes *et al.* 2005 and many more)

$$\int_{\Omega} \nabla w_h(\mathbf{x}) \cdot \nabla u_h(\mathbf{x}) \, d\mathbf{x} = \int_{\Omega} w_h(\mathbf{x}) f_h(\mathbf{x}) \, d\mathbf{x} \quad \rightarrow \quad Au = b$$

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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**

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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**

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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

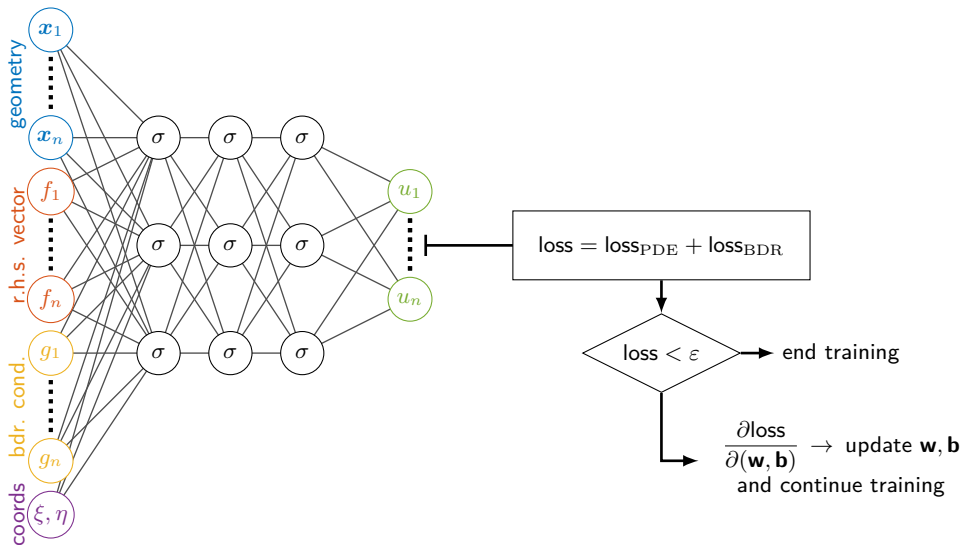
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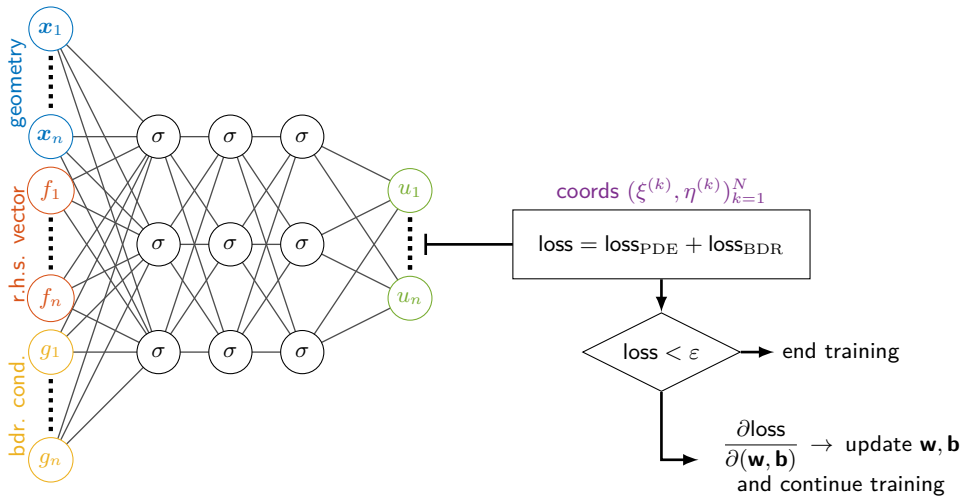
Compute the solution from the trained neural network as follows

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

IgaNet architecture (close to it but not yet)



IgaNet architecture



Loss function

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

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**

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

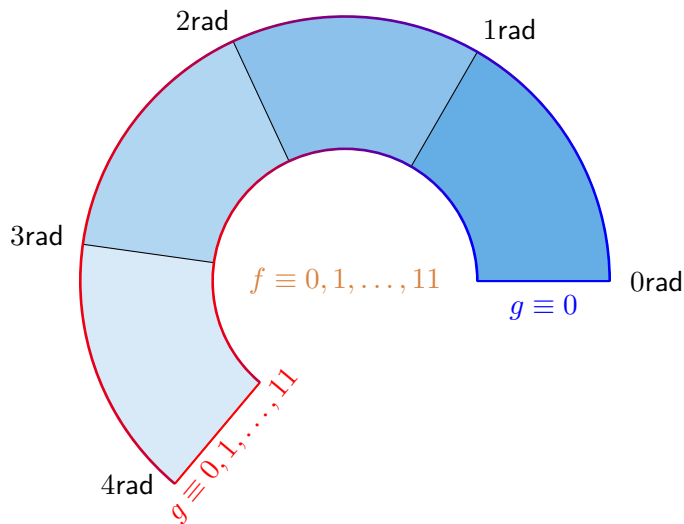
EndFor

EndFor

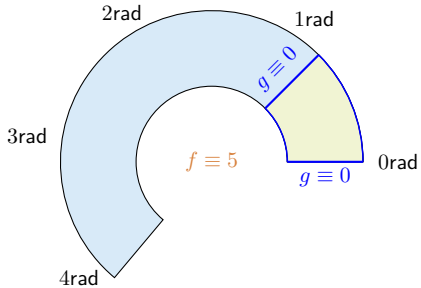
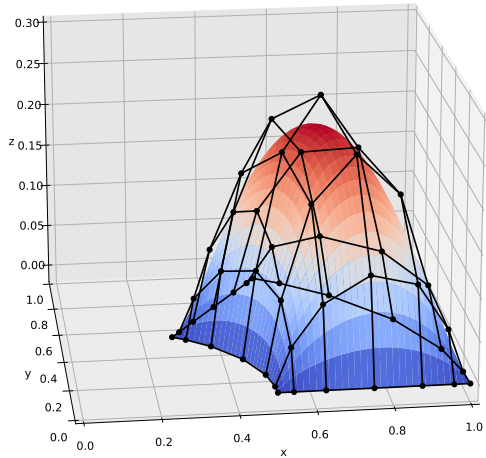
Details:

- 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

Test case: Poisson's equation on a variable annulus

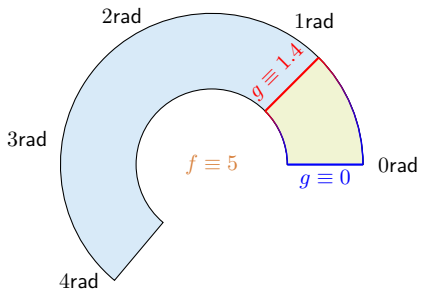
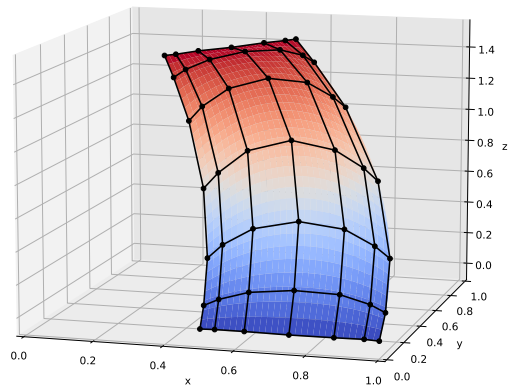


Preliminary results



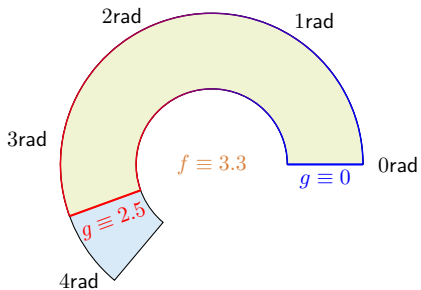
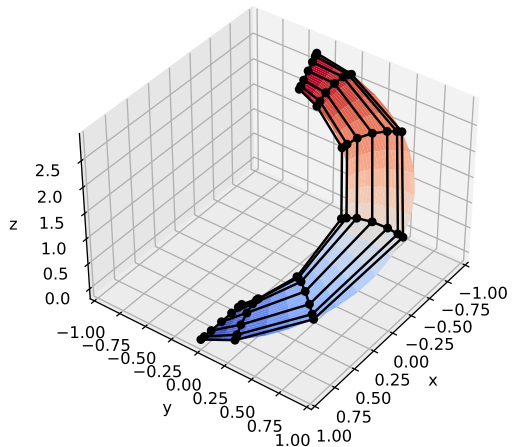
Ongoing master thesis work of Frank van Ruiten, TU Delft

Preliminary results

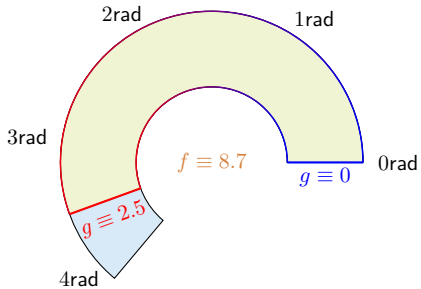
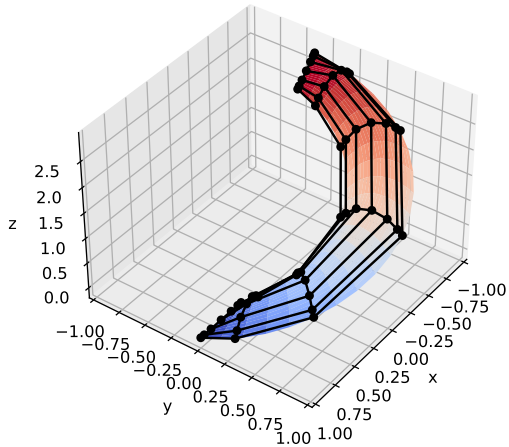


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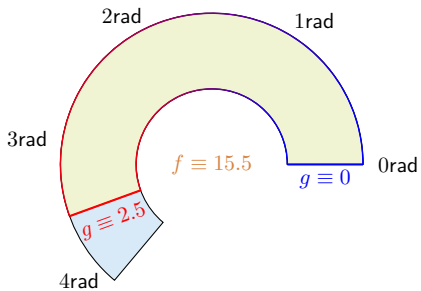
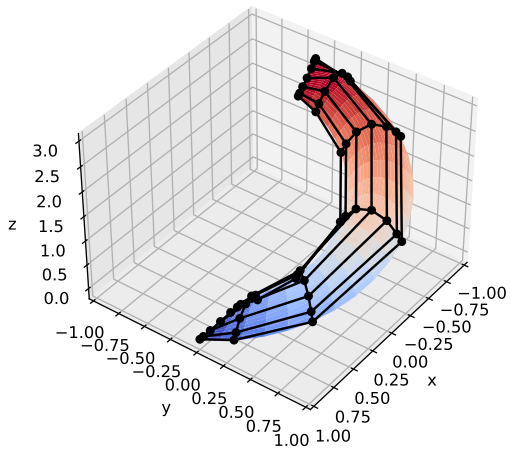


Preliminary results



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Preliminary results



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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

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

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

Computational costs

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

Working principle of IgaNets

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

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

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

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 $r \geq 0$

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

Textbook derivatives

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

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)

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

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

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

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

$$R_3(\xi) = \dots$$

An ML-friendly B-spline evaluation

Algorithm 2.22 from (Lyche and Morken 2011)

- 1 $\mathbf{b} = 1$
- 2 For $k = 1, \dots, p - r$
 - 1 $\mathbf{t}_1 = (\xi_{i-k+1}, \dots, \xi_i)$
 - 2 $\mathbf{t}_2 = (\xi_{i+1}, \dots, \xi_{i+k})$
 - 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 $k = p - r + 1, \dots, p$
 - 1 $\mathbf{t}_1 = (\xi_{i-k+1}, \dots, \xi_i)$
 - 2 $\mathbf{t}_2 = (\xi_{i+1}, \dots, \xi_{i+k})$
 - 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.

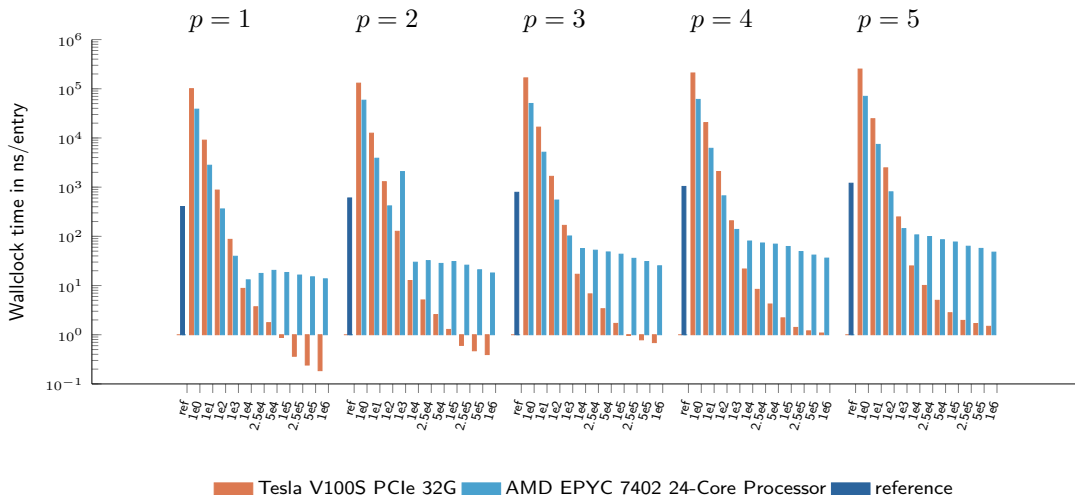
An ML-friendly B-spline evaluation

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

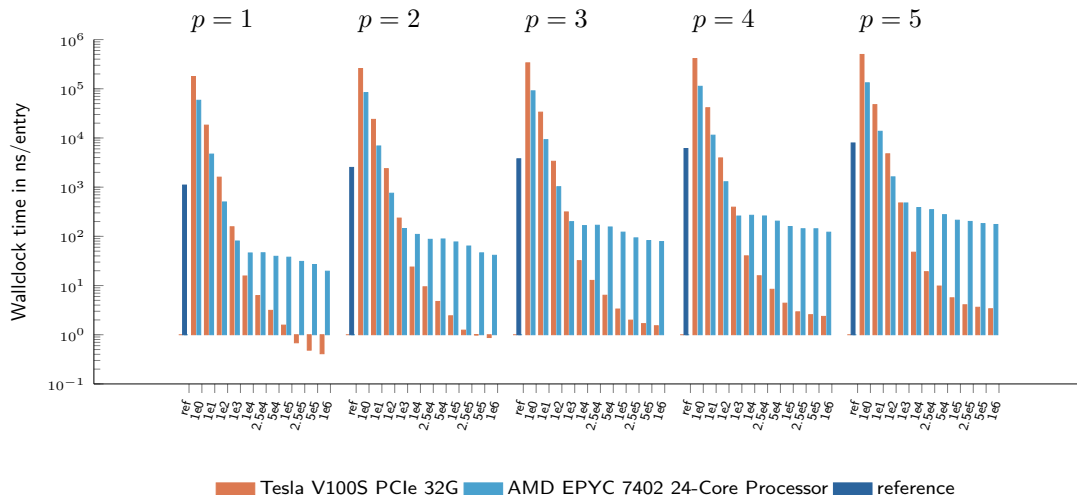
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- 2 For $k = 1, \dots, p - r$
 - 1 $\mathbf{t}_1 = (\xi_{i-k+1}, \dots, \xi_i)$
 - 2 $\mathbf{t}_{21} = (\xi_{i+1}, \dots, \xi_{i+k}) - \mathbf{t}_1$
 - 3 **mask** = $(\mathbf{t}_{21} < \text{tol})$
 - 4 $\mathbf{w} = (\xi - \mathbf{t}_1 - \mathbf{mask}) \div (\mathbf{t}_{21} - \mathbf{mask})$
 - 5 $\mathbf{b} = [(1 - \mathbf{w}) \odot \mathbf{b}, 0] + [0, \mathbf{w} \odot \mathbf{b}]$
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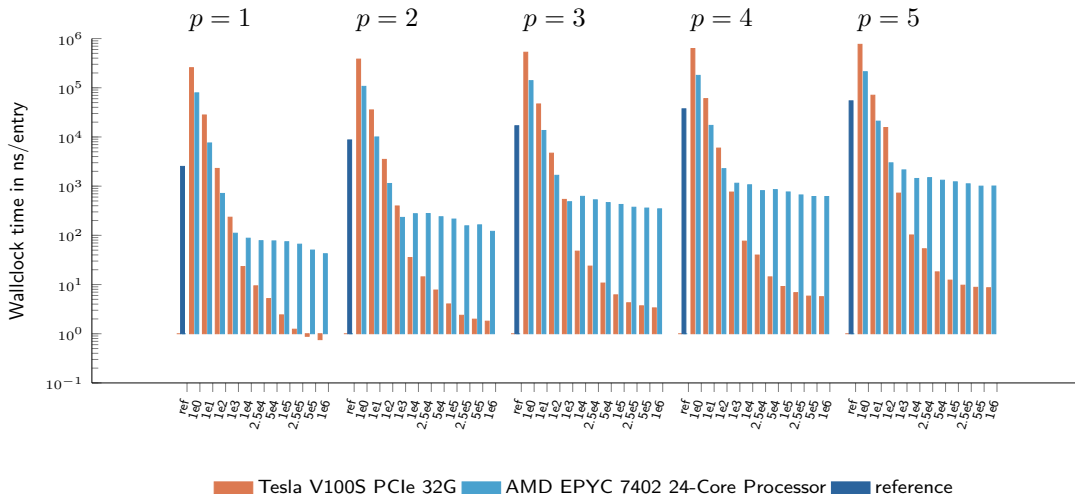
Performance evaluation — univariate B-splines



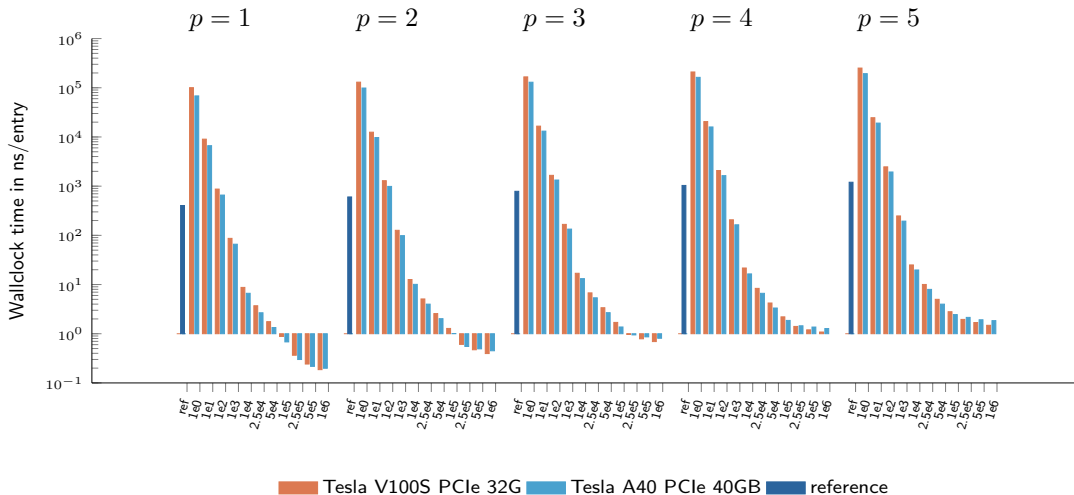
Performance evaluation — bivariate B-splines



Performance evaluation — trivariate B-splines



Performance evaluation — univariate B-splines



Conclusion and outlook

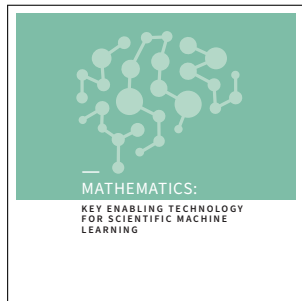
IgaNets combine classical numerics with physics-informed machine learning and may finally enable **integrated and interactive design-through-analysis** workflows

WIP/What's next

- interactive modelling & visualization
- extension to multi-patch topologies
- use of IGA and IgaNets in concert
- transfer learning upon basis refinement
- theoretical foundation & error analysis

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

Journal paper and code release in preparation



IgaNets: Physics-Informed Machine Learning Embedded Into Isogeometric Analysis

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Delft University of Technology, The Netherlands

KOLLOQUIUM ÜBER NEUERE ARBEITEN AUF DEM
GEBIETE DER MECHANIK UND STRÖMUNGSLEHRE

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Joint work with Deepesh Toshniwal and Frank van Ruiten

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Thank you very much!