Physics-Informed Machine Learning Embedded Into Isogeometric Analysis

Matthias Möller, Deepesh Toshniwal, Frank van Ruiten

Numerical Analysis, Department of Applied Mathematics
Delft University of Technology, NL

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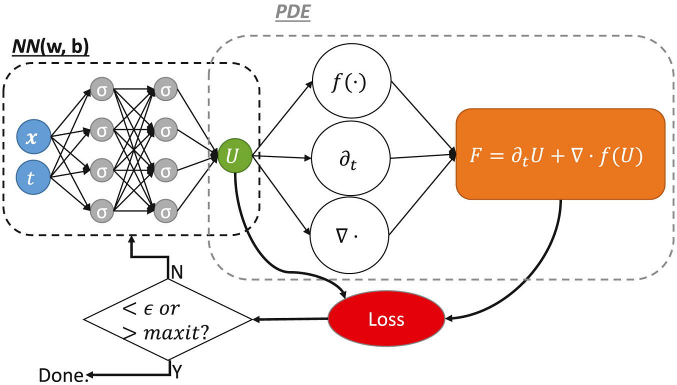
SciML for PDE analysis

- Physics-informed neural networks (PINNs) [Raissi, Perdikaris, Karniadakis, 2019]



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- Physics-informed neural networks (PINNs) [Raissi, Perdikaris, Karniadakis, 2019]

  + No pre-calculated data needed (unsupervised learning)
  + Applicable to arbitrary PDEs (extra effort might be needed to impose ‘physics’)
  + Can be augmented with data (faster conversion of loss function)

  – Convergence theory is in its infancy (different from FEM/IGA theory)
  – Poor extrapolation capabilities (different geometries, problem parameters)
  – Space-time treatment of time-dependent problems

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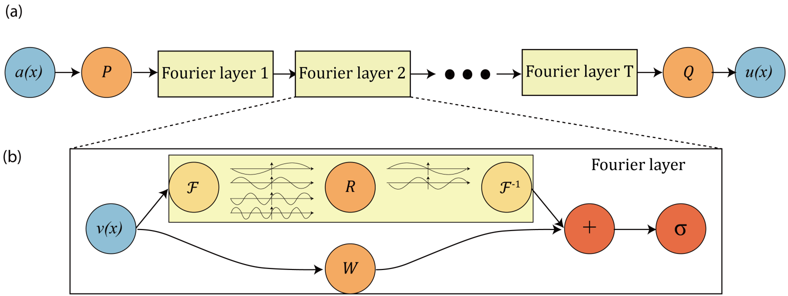

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  + Aims to learn the operator (not the PDE problem)

  - Pre-calculated training data is needed (supervised learning)
  - Assumes an efficient Fourier approximation of the solution
  - Designed for time-dependent PDEs

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  + Aims to learn the operator (not the PDE problem)
  + Claims to have excellent extrapolation capabilities

  – Pre-calculated training data is needed (supervised learning)
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The above approaches focus on PDE analysis only and do not pay much attention to linking it to computer-aided geometry modeling [seen before with CAD and FEA, right?].

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The idea of creating cost-efficient surrogate models for PDE analysis is not new, e.g., reduced-order models (ROM), proper orthogonal decomposition (POD) methods, etc.

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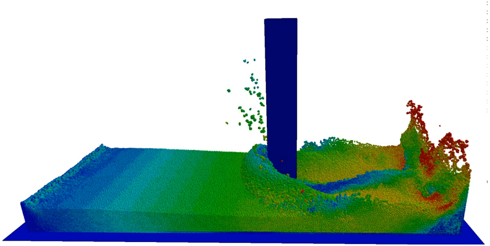
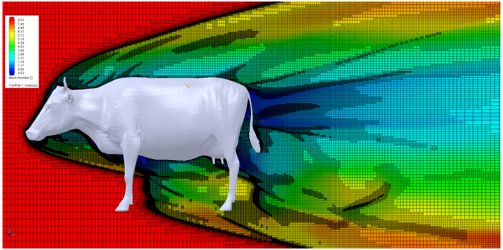
Life before PINNs

Simulation-based analysis of PDEs with numerical methods has a long tradition

- particle methods: PIC (1955), SPH (1977), DPD (1992), RKPM (1995), ...
- hybrid particle-mesh methods: MPM (1990s), ...
- mesh-based methods: FEM (1940s), FDM (1950s), FVM (1971), IGA (2005), ...





Left: wave-structure interaction, LS-DYNA; right: supersonic flow around a cow, Siemens FloEFD

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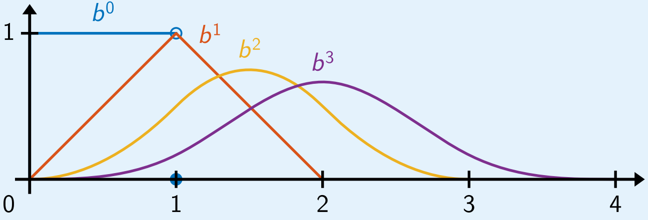
- mesh-based methods: FEM (1940s), FDM (1950s), FVM (1971), IGA (2005), ...
  - theoretical foundation: existence & uniqueness, convergence, ...
  - a priori/ a posteriori error estimates, practical error indicators
  - strategies for adaptive hp-mesh refinement
  - unified framework for computer-aided design and finite element analysis

Isogeometric Analysis

B-spline basis functions



knot vector $\Xi = [0, 1, 2, 3, 4]$

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

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

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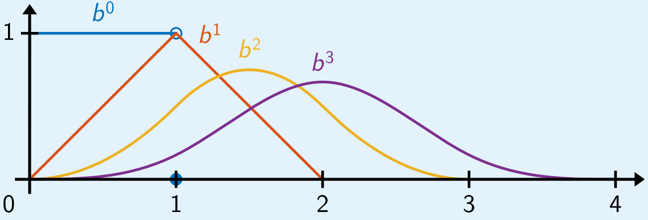

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Many good properties: compact support $[\xi_\ell, \xi_{\ell+p+1})$, positive function values over support interval, derivatives of B-splines are combinations of lower-order B-splines, ...

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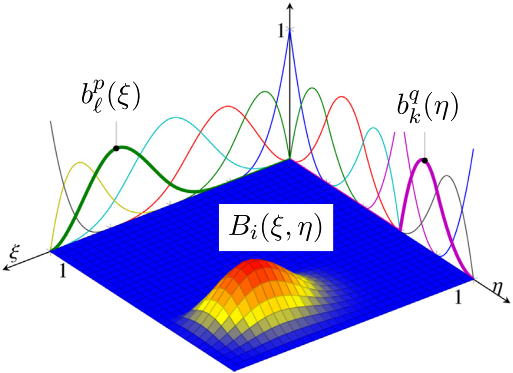
Isogeometric Analysis

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

$$B_i(\xi,\eta) := b^p_\ell(\xi) \cdot b^q_k(\eta), \qquad i := (k-1)\cdot n_\ell + \ell, \quad 1 \le \ell \le n_\ell, \quad 1 \le k \le n_k,$$



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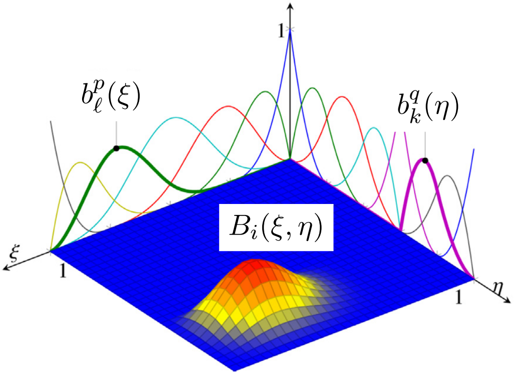
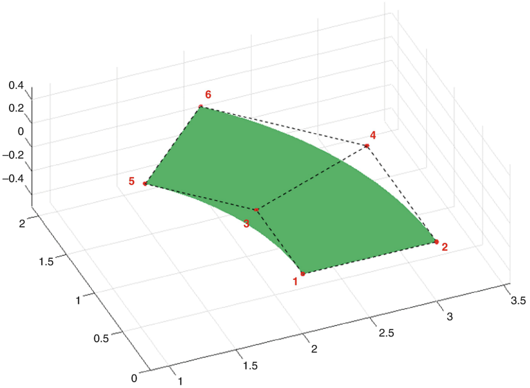


Many more good properties: partition of unity $\sum_{i=1}^{n} B_i(\xi,\eta) \equiv 1$, C^{p-1} continuity, ...

Isogeometric Analysis

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

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



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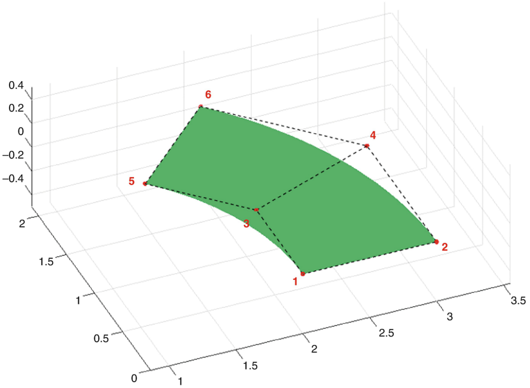

- the shape of Ω_h is fully specified by the set of **control points** $\mathbf{x}_i \in \mathbb{R}^d$
- interior control points must be chosen such that 'grid lines' do not fold as this violates the bijectivity of $\mathbf{x}_h : \hat{\Omega} \to \Omega_h$

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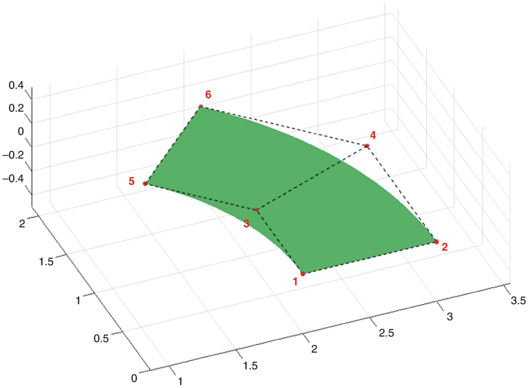

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- interior control points must be chosen such that 'grid lines' do not fold as this violates the bijectivity of $\mathbf{x}_h : \hat{\Omega} \to \Omega_h$
- refinement in h (knot insertion) and p (order elevation) preserves the shape of Ω_h and can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

Isogeometric Analysis

Data, boundary conditions, and solution: forward mappings from the unit square

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

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

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

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Model problem: Poisson's equation

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

Isogeometric Analysis

Different solution approaches

- Galerkin-type IGA (Hughes *et al.* 2005 and many more)
- Isogeometric collocation methods (Reali, Hughes, 2015)
- Variational collocation method (Gomez, De Lorenzis, 2016)

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Abstract representation

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

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

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

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

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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 expected **output** of our IGA machinery are the B-spline coefficients u_i of the solution.

Isogeometric Analysis + PINNs

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

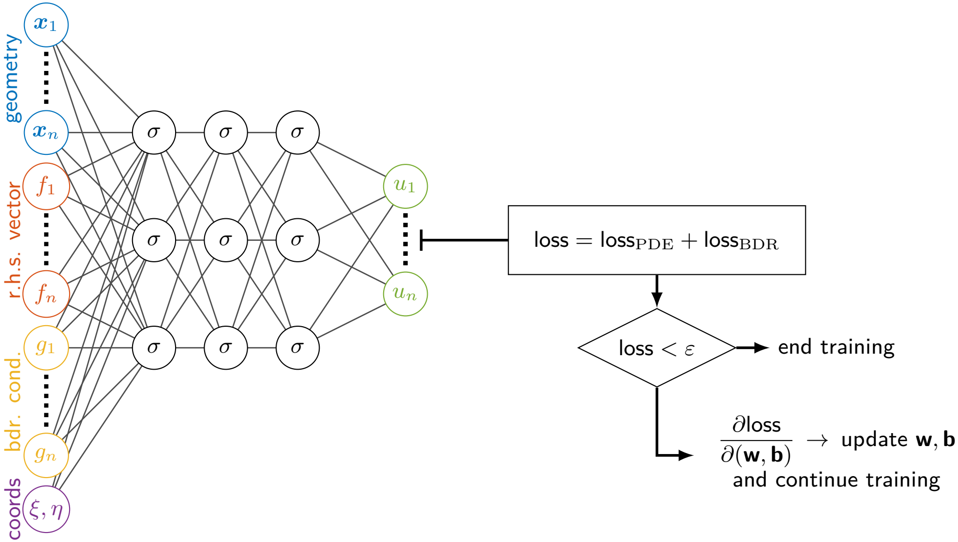
$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = A^{-1}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}\right) \cdot b\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\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

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

Compute the solution by evaluating the trained neural network

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

IGA-PINN



geometry
$\boldsymbol{x}_1$
$\boldsymbol{x}_n$
r.h.s. vector
f_1
f_n
bdr. cond.
g_1
g_n
coords
ξ, η
σ
u_1
u_n
loss $=$ loss$_{\mathrm{PDE}}$ $+$ loss$_{\mathrm{BDR}}$
loss $< \varepsilon$
end training
$\frac{\partial \text{loss}}{\partial(\mathbf{w}, \mathbf{b})} \rightarrow$ update $\mathbf{w}, \mathbf{b}$
and continue training

Loss function

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

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

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 $(\xi_k, \eta_k) \in [0,1]^2$ **do**

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

EndFor

EndFor

IGA details: 7×7 bi-cubic tensor-product B-splines for $\mathbf{x}_h$ and u_h, C^2-continuous

PINN details: 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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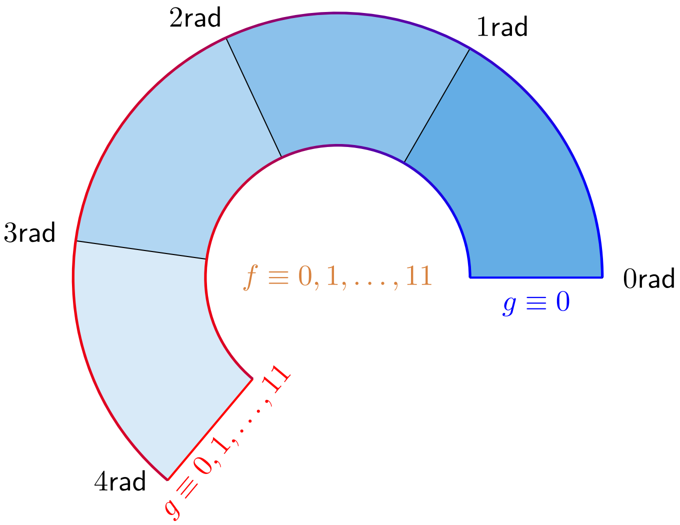
Test case: Poisson's equation on a variable annulus



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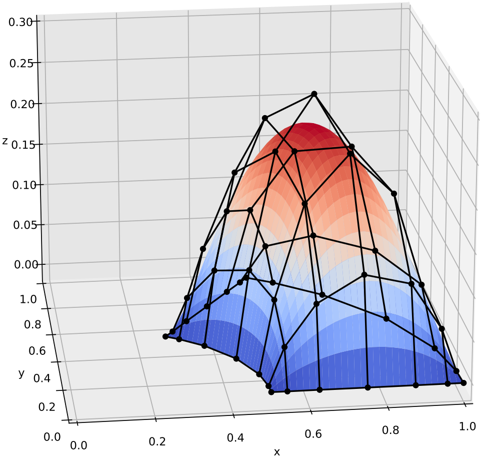
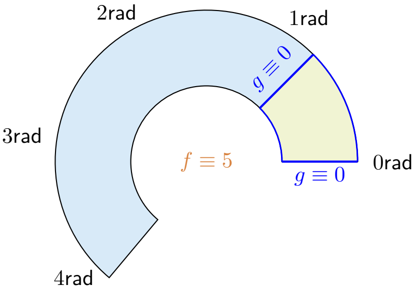
Preliminary results





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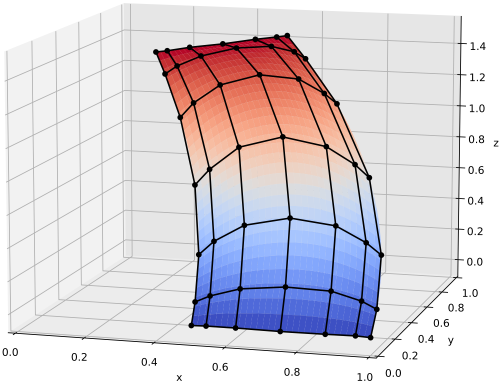

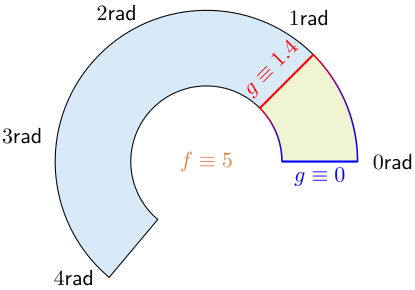

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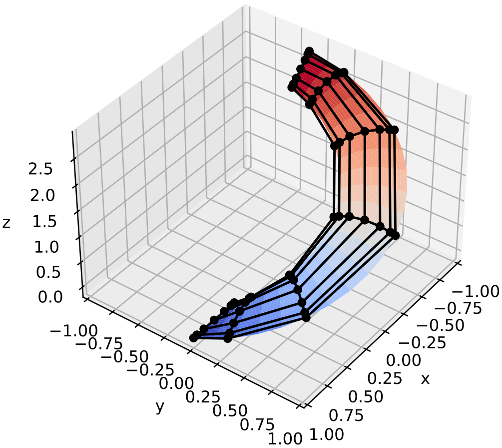

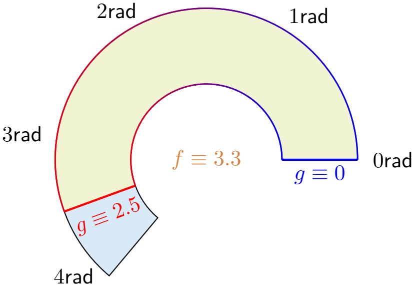

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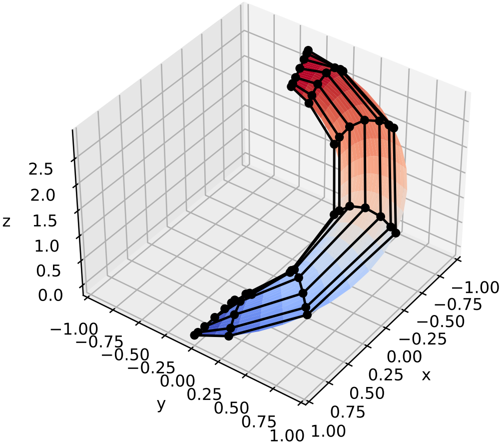

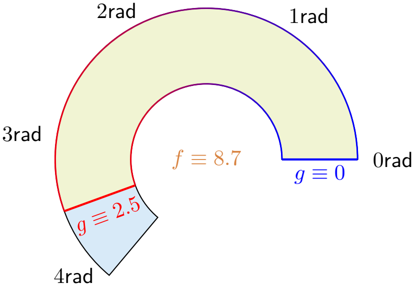

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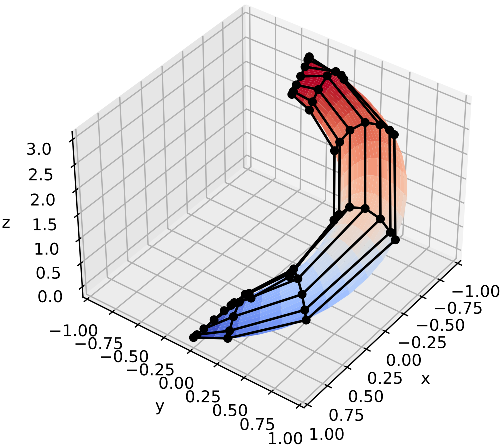

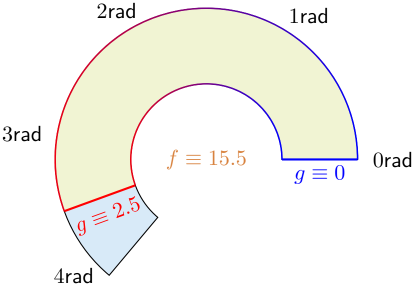

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Conclusion and outlook

IgaNets combine the best of both worlds and may finally enable
integrated and interactive computer-aided design-and-analysis workflows

Todo

- performance and hyper-parameter tuning
- extension to multi-patch topologies
- use of IGA and IgaNets in concert
- transfer learning upon refinement of basis functions

Short paper: Möller, Toshniwal, van Ruiten. Physics-informed machine learning embedded into isogeometric analysis. In Mathematics: Key enabling technology for scientific machine learning. Platform Wiskunde, 2021

WIP: G+Smo-compatible implementation of IgaNets in C++ using libtorch.

Thank you for your attention!