IgaNets: Physics-Informed Machine Learning Embedded Into Isogeometric Analysis

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NMC Scientific Days

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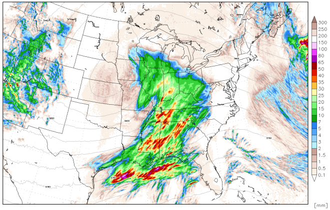
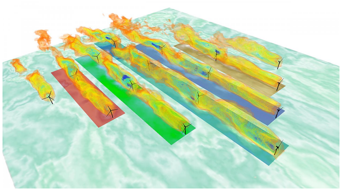
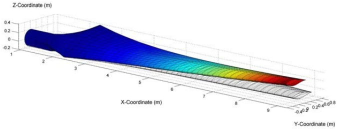
Numerics for PDE analysis







Many physical processes are modelled mathematically by (systems of) PDEs that require fast & accurate numerical methods to compute approximate solutions:

- 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), ...

Credit: `www.superzelle.de` – Janek Zimmer; University of Texas at Dallas (DOI: 10.1063/5.0036640); University of Minnesota – Eolos Wind Energy Research

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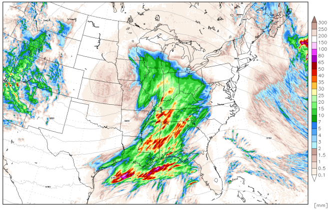

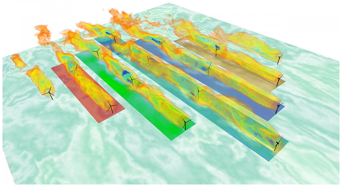

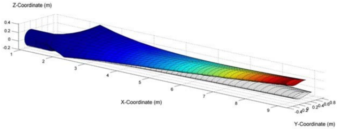

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How fast is fast? And is it just about analysis?

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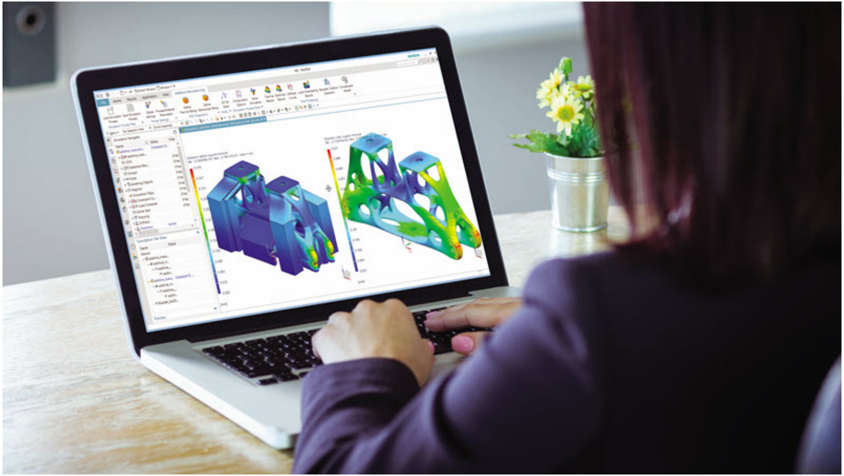
Design through Analysis

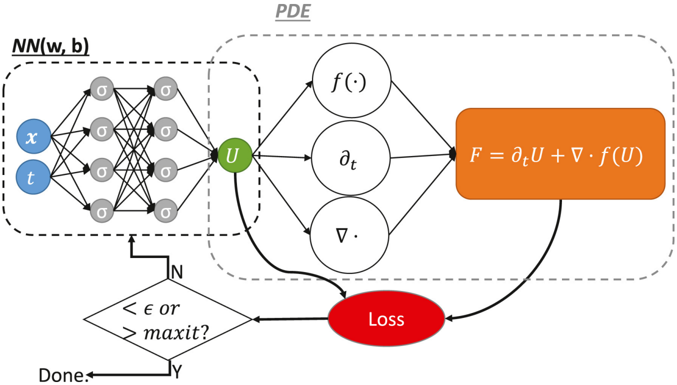


We want it all: from really fast & moderately accurate to moderately fast & highly accurate!

Credit: Siemens – Simulation for Design Engineers

SciML for PDE analysis

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



SciML for PDE analysis

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

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

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

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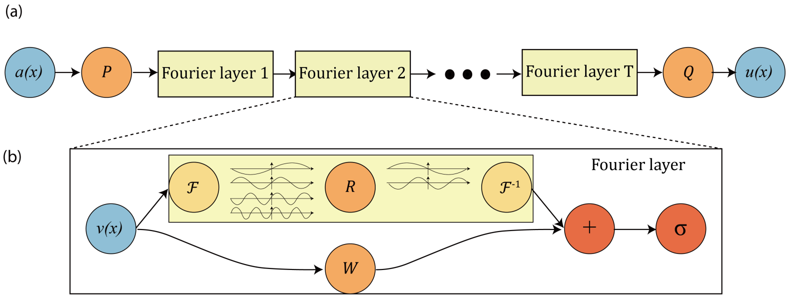

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  + Aims to learn the operator (not the PDE problem)

  – 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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- Learning nonlinear operators (DeepONets) [Lu, Jin, Pang, Zhang, Karniadakis, 2021]

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

\+ Aims to learn the operator (not the PDE problem)
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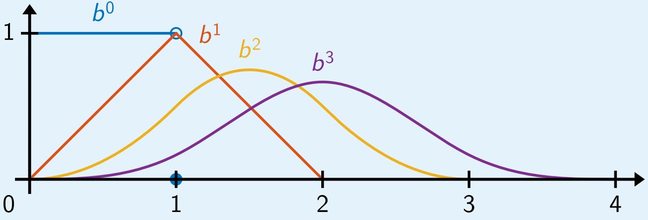
Combine mesh-based numerics with SciML for PDE analysis

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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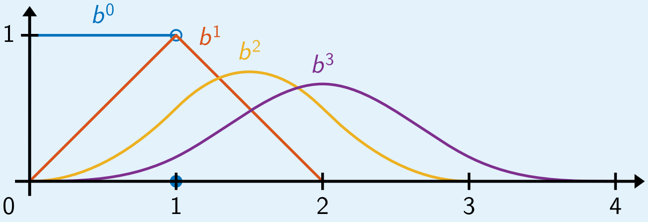

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Many good properties: compact support $[\xi_\ell, \xi_{\ell+p+1})$, positive function values over support interval, derivatives of B-splines are combinations of lower-order B-splines, ...

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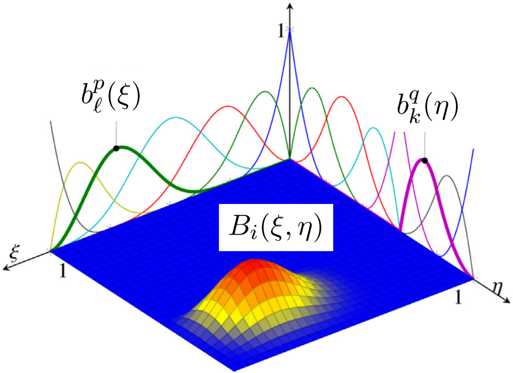
Isogeometric Analysis

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

$$B_i(\xi,\eta) := b_\ell^p(\xi)\cdot b_k^q(\eta), \qquad i := (k-1)\cdot n_\ell + \ell, \quad 1\le \ell \le n_\ell, \quad 1 \le k \le n_k,$$



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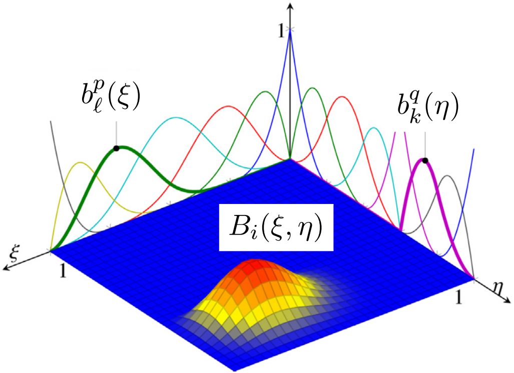
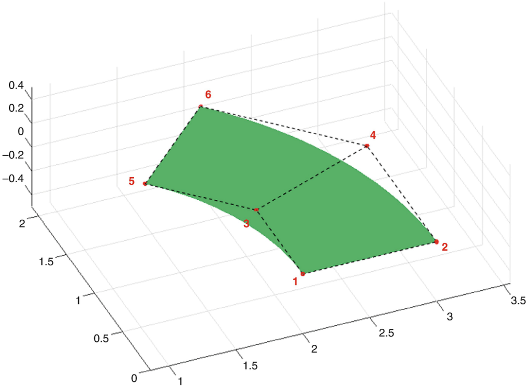


Many more good properties: partition of unity $\sum_{i=1}^{n} B_i(\xi,\eta) \equiv 1$, C^{p-1} continuity, ...

Isogeometric Analysis

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

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



- the shape of Ω_h is fully specified by the set of **control points** $\mathbf{x}_i \in \mathbb{R}^d$

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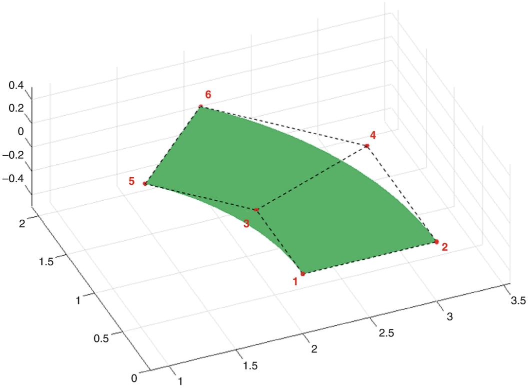

- the shape of Ω_h is fully specified by the set of **control points** $\mathbf{x}_i \in \mathbb{R}^d$
- interior control points must be chosen such that 'grid lines' do not fold as this violates the bijectivity of $\mathbf{x}_h : \hat{\Omega} \to \Omega_h$

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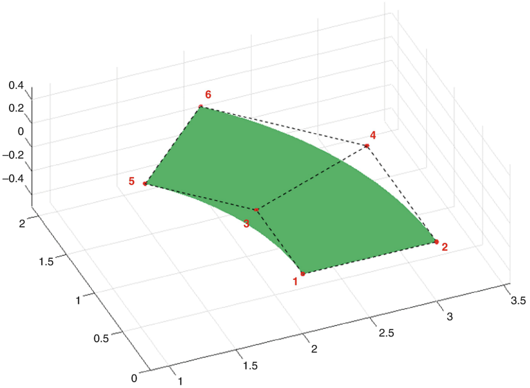

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- interior control points must be chosen such that 'grid lines' do not fold as this violates the bijectivity of $\mathbf{x}_h : \hat{\Omega} \to \Omega_h$
- refinement in h (knot insertion) and p (order elevation) preserves the shape of Ω_h and can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

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

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

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

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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.

Isogeometric Analysis + PINNs

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

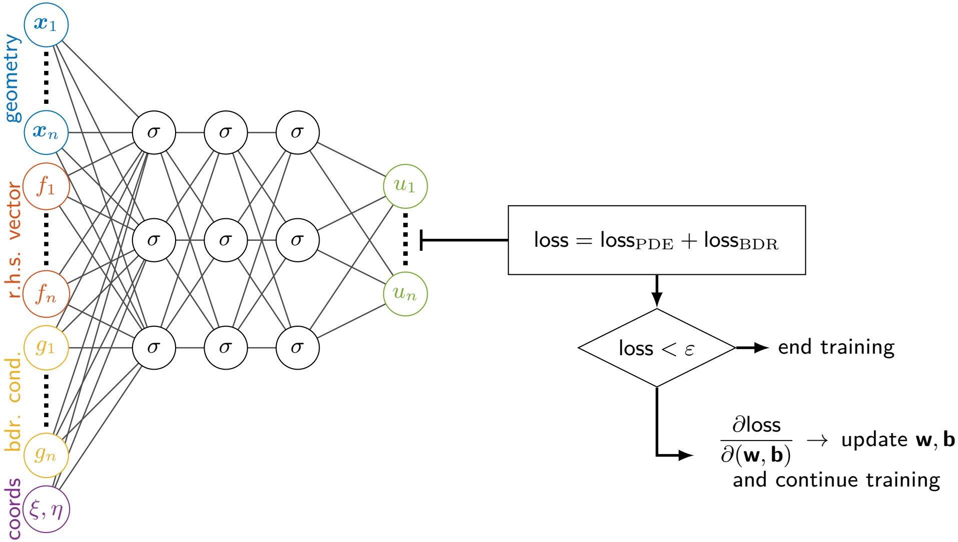
$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = A^{-1}\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}\right) \cdot b\left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\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

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

Compute the solution by evaluating the trained neural network

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

IgaNet architecture



Loss function

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

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

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**

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

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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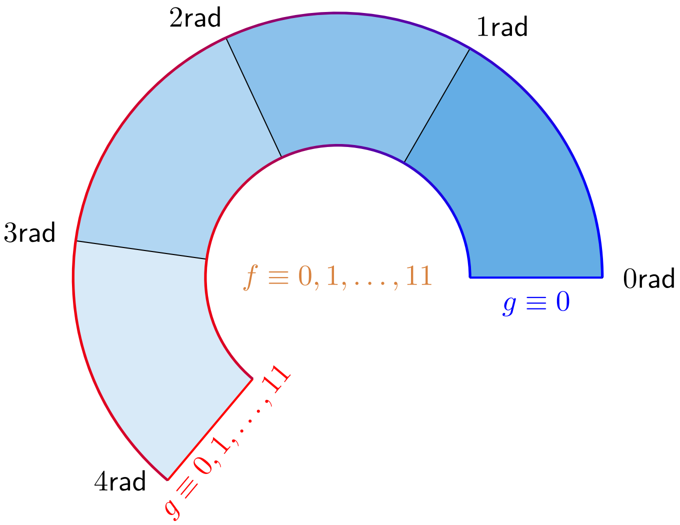
Test case: Poisson's equation on a variable annulus



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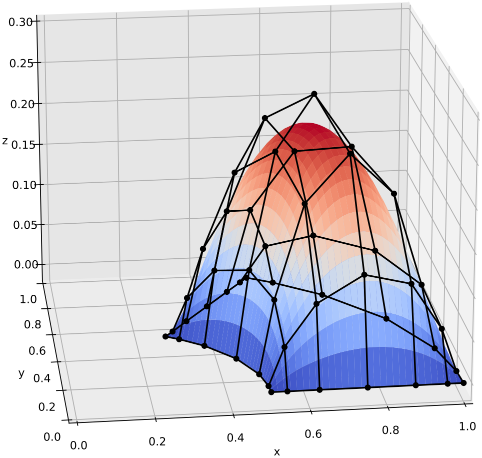
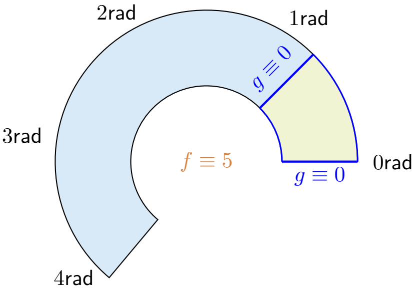
Preliminary results





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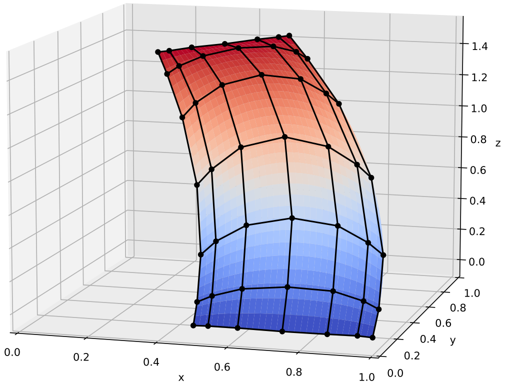

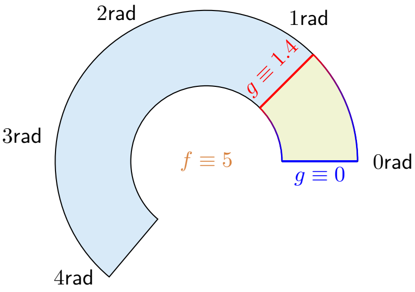

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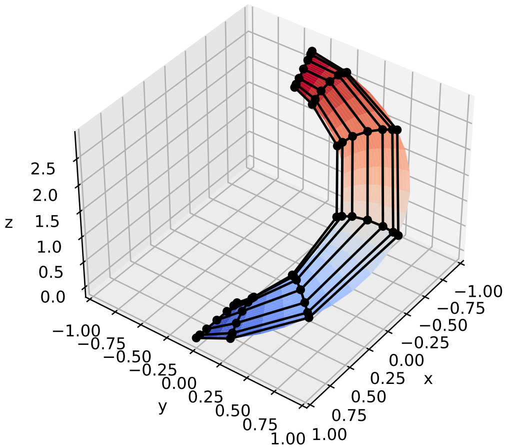

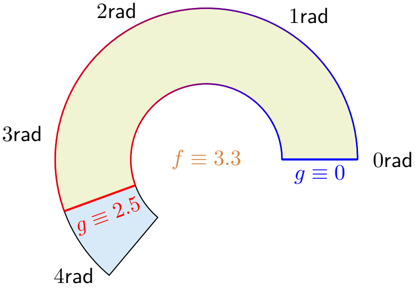

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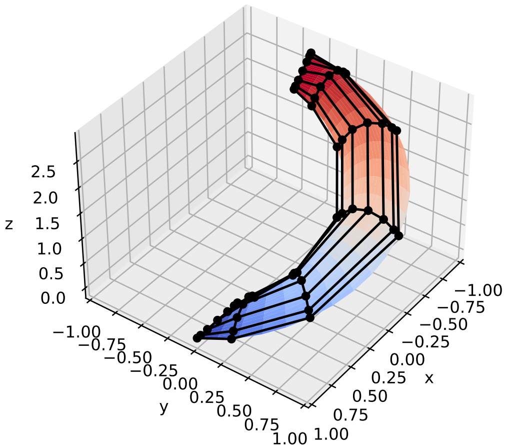

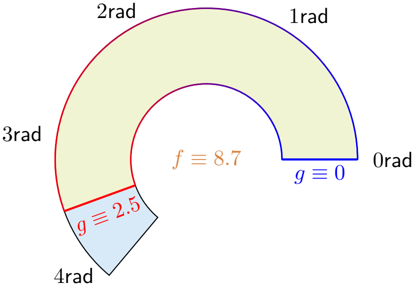

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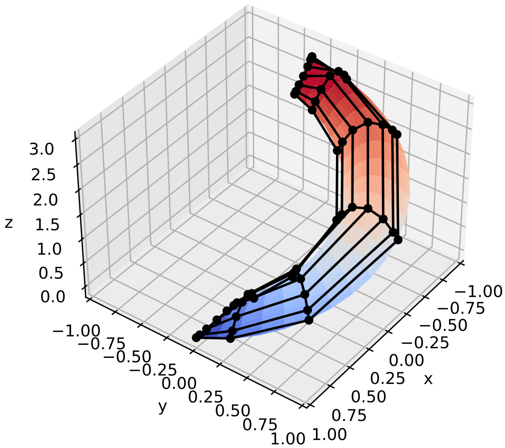

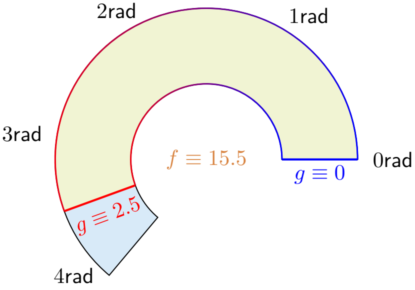

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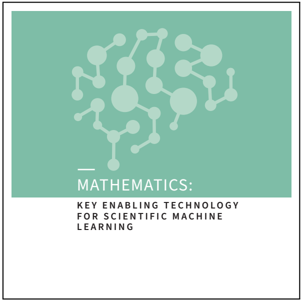
Conclusion and outlook

IgaNets combine classical numerics with scientific machine learning and may finally enable integrated and interactive computer-aided **design-through-analysis** workflows

Todo

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



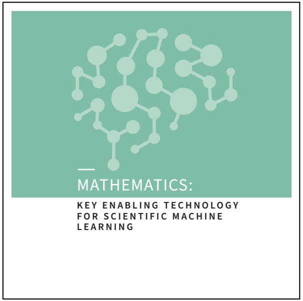
Short paper: Möller, Toshniwal, van Ruiten: *Physics-informed machine learning embedded into isogeometric analysis*, 2021.

Conclusion and outlook

IgaNets combine classical numerics with scientific machine learning and may finally enable integrated and interactive computer-aided **design-through-analysis** workflows

Todo

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



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We are hiring! AIO position will open soon! Thank you for your attention!