IgaNets: Physics-Informed Machine Learning Embedded Into Isogeometric Analysis

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MS 12: Scientific Machine Learning in Computational Mechanics



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

VS.

PINNs, DeepONets, FourierNets, ...





Common misconceptions

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

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

- m theta established engineering workflows
- no cost amortization over multiple runs, no real-time capability

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Better questions to ask

• What are the specific strengths/weaknesses of the different approaches?

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- fast evaluation (costly training!)
- 🖒 inclusion of (measurement) data
 - $\boldsymbol{\nabla}$ lack of convergence theory
 - $\mathbf{\nabla}$ lack of general acceptance

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

 ${oldsymbol{\mathcal{O}}}$ sound mathematical foundation

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- 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



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







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



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

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TUDelft

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B-spline basis functions



B-spline basis functions



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, ...



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, ...

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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- 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

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

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

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

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



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Model problem: Poisson's equation

$$-\Delta u_h = f_h$$
 in Ω_h , $u_h = g_h$ on $\partial \Omega_h$



Different solution approaches

- Galerkin-type IGA (Hughes et al. 2005 and many more)
- Isogeometric collocation methods (Reali, Hughes, 2015)
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Abstract representation

Given 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

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



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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

$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = A^{-1} \left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix} \right) \cdot b \left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix} \right)$$
$$\begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = \mathsf{PINN} \left(\begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}; (\boldsymbol{\xi}^{(k)}, \boldsymbol{\eta}^{(k)})_{k=1}^{N_{\mathsf{samples}}} \right)$$

Compute the solution by evaluating the trained neural network

$$u_{h}(\boldsymbol{\xi},\boldsymbol{\eta}) \approx \left[B_{1}(\boldsymbol{\xi},\boldsymbol{\eta}),\ldots,B_{n}(\boldsymbol{\xi},\boldsymbol{\eta})\right] \cdot \begin{bmatrix} u_{1} \\ \vdots \\ u_{n} \end{bmatrix} = \mathsf{PINN}\left(\begin{bmatrix} \mathbf{x}_{1} \\ \vdots \\ \mathbf{x}_{n} \end{bmatrix}, \begin{bmatrix} f_{1} \\ \vdots \\ f_{n} \end{bmatrix}, \begin{bmatrix} g_{1} \\ \vdots \\ g_{n} \end{bmatrix}; (\boldsymbol{\xi},\boldsymbol{\eta})\right)$$



IgaNet architecture



IgaNet architecture





Loss function

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

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

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

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

Ongoing master thesis work of Frank van Ruiten, TU Delft

Test case: Poisson's equation on a variable annulus



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Common computational task

Given sampling point $\xi \in [\xi_\ell,\xi_{\ell+1})$ compute for $r \geq 0$

$$\frac{\mathrm{d}^r}{\mathrm{d}\xi}\chi(\xi) = \left[\frac{\mathrm{d}^r}{\mathrm{d}\xi}b_{\ell-p}^p(\xi), \dots, \frac{\mathrm{d}^r}{\mathrm{d}\xi}b_{\ell}^p(\xi)\right] \cdot \underbrace{[\chi_{\ell-p}, \dots, \chi_{\ell}]}_{\text{network's output}}$$



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• The above needs to be performed for all sampling points $\xi^{(k)}$ in the batch

 $\operatorname{sum}(\operatorname{d}^{r}\mathcal{B}^{p}\odot\mathcal{X},2)$



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• The above needs to be differentiated by the AD engine during backpropagation

$$\frac{\partial \left(\mathrm{d}^{r} b_{\ell}^{p} \chi_{\ell}\right)}{\partial w} = \mathrm{d}^{r+1} b_{\ell}^{p} \frac{\partial \xi}{\partial w} \chi + \mathrm{d}^{r} b_{\ell}^{p} \frac{\partial \chi}{\partial \xi}$$



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Textbook derivatives

$$\frac{\mathrm{d}^r}{\mathrm{d}\xi}b_{\ell}^p(\xi) = (p-1)\left(\frac{1}{\xi_{\ell+p} - \xi_{\ell+1}} \frac{-\mathrm{d}^{r-1}}{\mathrm{d}\xi}b_{\ell+1}^{p-1}(\xi) + \frac{1}{\xi_{\ell+p-1} - \xi_{\ell}} \frac{\mathrm{d}^{r-1}}{\mathrm{d}\xi}b_{\ell}^{p-1}(\xi)\right)$$

with

$$b_{\ell}^{p}(\xi) = \frac{\xi - \xi_{\ell}}{\xi_{\ell+p} - \xi_{\ell}} b_{\ell}^{p-1}(\xi) + \frac{\xi_{\ell+p+1} - \xi}{\xi_{\ell+p+1} - \xi_{\ell+1}} b_{\ell+1}^{p-1}(\xi), \quad b_{\ell}^{0}(\xi) = \begin{cases} 1 & \text{if } \xi_{\ell} \le \xi < \xi_{\ell+1} \\ 0 & \text{otherwise} \end{cases}$$

Matrix representation of B-splines (Lyche and Morken 2011)

$$\left[\frac{\mathrm{d}^r}{\mathrm{d}\xi}b^p_{\ell-p}(\xi),\ldots,\frac{\mathrm{d}^r}{\mathrm{d}\xi}b^p_{\ell}(\xi)\right] = \frac{p!}{(p-r)!}R_1(\xi)\cdots R_{p-r}(\xi)\mathrm{d}R_{p-r+1}\cdots\mathrm{d}R_p$$

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

$$R_{1}(\xi) = \begin{bmatrix} \frac{\xi_{\ell+1} - \xi}{\xi_{\ell+1} - \xi_{\ell}} & \frac{x - \xi_{\ell}}{\xi_{\ell+1} - \xi_{\ell}} \end{bmatrix}$$
$$R_{2}(\xi) = \begin{bmatrix} \frac{\xi_{\ell+1} - \xi}{\xi_{\ell+1} - \xi_{\ell-1}} & \frac{x - \xi_{\ell-1}}{\xi_{\ell+1} - \xi_{\ell-1}} & 0\\ 0 & \frac{\xi_{\ell+2} - \xi}{\xi_{\ell+2} - \xi_{\ell}} & \frac{x - \xi_{\ell}}{\xi_{\ell+2} - \xi_{\ell}} \end{bmatrix}$$
$$R_{3}(\xi) = \dots$$

There exists an efficient algorithm based on elementwise operations on vectors.



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.



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