# IgaNets: Physics-Informed Machine Learning Embedded Into Isogeometric Analysis 

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MS 12: Scientific Machine Learning in Computational Mechanics

## Motivation

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

PINNs, DeepONets, FourierNets, ...

VS.


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## Common misconceptions

- "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,

$B$ sound mathematical foundation
$B$ established engineering workflows
R no cost amortization over multiple runs, no real-time capability

## PINNs, DeepONets, FourierNets,

$\checkmark$ fast evaluation (costly training!)
$B$ inclusion of (measurement) data
$\beta$ lack of convergence theory
R lack of general acceptance

## Common misconceptions

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## Better questions to ask

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


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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



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

[^0]
## Physics-informed machine learning

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


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

DeepONet (Lu et al. 2019): learns the differential operator
$G_{\theta}(u)(y)=\sum_{k=1}^{q} \underbrace{b_{k}\left(u\left(x_{1}\right), u\left(x_{2}\right), \ldots, u\left(x_{m}\right)\right)}_{\text {branch }} \underbrace{t_{k}(y)}_{\text {trunk }}$

## Physics-informed machine learning

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## B-spline basis functions

## Cox de Boor recursion formula

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

## B-spline basis functions

## Cox de Boor recursion formula



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

## Isogeometric Analysis

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

$$
B_{i}(\xi, \eta):=b_{\ell}^{p}(\xi) \cdot b_{k}^{q}(\eta), \quad i:=(k-1) \cdot n_{\ell}+\ell, \quad 1 \leq \ell \leq n_{\ell}, \quad 1 \leq k \leq n_{k},
$$



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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, $\ldots$

## 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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- the shape of $\Omega_{h}$ is fully specified by the set of control points $\mathbf{x}_{i} \in \mathbb{R}^{d}$


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- interior control points must be chosen such that 'grid lines' do not fold as this violates the bijectivity of $\mathrm{x}_{h}: \hat{\Omega} \rightarrow \Omega_{h}$
- refinement in $h$ (knot insertion) and $p$ (order elevation) preserves the shape of $\Omega_{h}$ 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

$$
\begin{array}{rll}
\text { (r.h.s vector) } & f_{h} \circ \mathbf{x}_{h}(\xi, \eta)=\sum_{i=1}^{n} B_{i}(\xi, \eta) \cdot f_{i} & \forall(\xi, \eta) \in[0,1]^{2} \\
\text { (boundary conditions) } & g_{h} \circ \mathbf{x}_{h}(\xi, \eta)=\sum_{i=1}^{n} B_{i}(\xi, \eta) \cdot g_{i} & \forall(\xi, \eta) \in \partial[0,1]^{2} \\
\text { (solution) } & u_{h} \circ \mathbf{x}_{h}(\xi, \eta)=\sum_{i=1}^{n} B_{i}(\xi, \eta) \cdot u_{i} & \forall(\xi, \eta) \in[0,1]^{2}
\end{array}
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\end{array}
$$

Model problem: Poisson's equation

$$
-\Delta u_{h}=f_{h} \quad \text { in } \quad \Omega_{h}, \quad u_{h}=g_{h} \quad \text { on } \quad \partial \Omega_{h}
$$

## 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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- Galerkin-type IGA (Hughes et al. 2005 and many more)
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## Abstract representation

Given $\mathbf{x}_{i}$ (geometry), $f_{i}$ (r.h.s. vector), and $g_{i}$ (boundary conditions), compute

$$
\left[\begin{array}{c}
u_{1} \\
\vdots \\
u_{n}
\end{array}\right]=A^{-1}\left(\left[\begin{array}{c}
\mathbf{x}_{1} \\
\vdots \\
\mathbf{x}_{n}
\end{array}\right],\left[\begin{array}{c}
g_{1} \\
\vdots \\
g_{n}
\end{array}\right]\right) \cdot b\left(\left[\begin{array}{c}
\mathbf{x}_{1} \\
\vdots \\
\mathbf{x}_{n}
\end{array}\right],\left[\begin{array}{c}
f_{1} \\
\vdots \\
f_{n}
\end{array}\right],\left[\begin{array}{c}
g_{1} \\
\vdots \\
g_{n}
\end{array}\right]\right)
$$

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

$$
(\xi, \eta) \in[0,1]^{2} \quad \mapsto \quad u_{h} \circ \mathbf{x}_{h}(\xi, \eta)=\left[B_{1}(\xi, \eta), \ldots, B_{n}(\xi, \eta)\right] \cdot\left[\begin{array}{c}
u_{1} \\
\vdots \\
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u_{1} \\
\vdots \\
u_{n}
\end{array}\right]
$$

Let us interpret the sets of $\mathbf{B}$-spline coefficients $\left\{\mathbf{x}_{i}\right\},\left\{f_{i}\right\}$, and $\left\{g_{i}\right\}$ 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 $\left\{u_{i}\right\}$ of the solution.

## Isogeometric Analysis + PINNs

IgaNet: replace computation by physics-informed machine learning

$$
\begin{aligned}
& {\left[\begin{array}{c}
u_{1} \\
\vdots \\
u_{n}
\end{array}\right]=A^{-1}\left(\left[\begin{array}{c}
\mathbf{x}_{1} \\
\vdots \\
\mathbf{x}_{n}
\end{array}\right],\left[\begin{array}{c}
g_{1} \\
\vdots \\
g_{n}
\end{array}\right]\right) \cdot b\left(\left[\begin{array}{c}
\mathbf{x}_{1} \\
\vdots \\
\mathbf{x}_{n}
\end{array}\right],\left[\begin{array}{c}
f_{1} \\
\vdots \\
f_{n}
\end{array}\right],\left[\begin{array}{c}
g_{1} \\
\vdots \\
g_{n}
\end{array}\right]\right)} \\
& {\left[\begin{array}{c}
u_{1} \\
\vdots \\
u_{n}
\end{array}\right]=\operatorname{PINN}\left(\left[\begin{array}{c}
\mathbf{x}_{1} \\
\vdots \\
\mathbf{x}_{n}
\end{array}\right],\left[\begin{array}{c}
f_{1} \\
\vdots \\
f_{n}
\end{array}\right],\left[\begin{array}{c}
g_{1} \\
\vdots \\
g_{n}
\end{array}\right] ;\left(\xi^{(k)}, \eta^{(k)}\right)_{k=1}^{N_{\text {samples }}}\right)}
\end{aligned}
$$

Compute the solution by evaluating the trained neural network

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

## IgaNet architecture



## IgaNet architecture



## Loss function

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

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):

$$
\left[\begin{array}{l}
\frac{\partial^{2} B}{\partial x^{2}} \\
\frac{\partial^{2} B}{\partial x \partial y} \\
\frac{\partial^{2} B}{\partial y^{2}}
\end{array}\right]=Q^{-\top}\left(\left[\begin{array}{c}
\frac{\partial^{2} B}{\partial \xi^{2}} \\
\frac{\partial^{2} B}{\partial \xi \partial \eta} \\
\frac{\partial^{2} B}{\partial \eta^{2}}
\end{array}\right]-H^{\top} J^{-\top}\left[\begin{array}{c}
\frac{\partial B}{\partial \xi} \\
\frac{\partial B}{\partial \eta}
\end{array}\right]\right)
$$

## Two-level training strategy

For $\left[\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right] \in \mathcal{S}_{\text {geo }},\left[f_{1}, \ldots, f_{n}\right] \in \mathcal{S}_{\text {rhs }},\left[g_{1}, \ldots, g_{n}\right] \in \mathcal{S}_{\text {bcond }} \mathbf{d o}$
For a batch of randomly sampled $\left(\xi_{k}, \eta_{k}\right) \in[0,1]^{2}$ do

$$
\text { Train PINN }\left(\left[\begin{array}{c}
\mathbf{x}_{1} \\
\vdots \\
\mathbf{x}_{n}
\end{array}\right],\left[\begin{array}{c}
f_{1} \\
\vdots \\
f_{n}
\end{array}\right],\left[\begin{array}{c}
g_{1} \\
\vdots \\
g_{n}
\end{array}\right] ;\left(\xi_{k}, \eta_{k}\right)_{k=1}^{N_{\text {samples }}}\right) \mapsto\left[\begin{array}{c}
u_{1} \\
\vdots \\
u_{n}
\end{array}\right]
$$

## EndFor

## EndFor

IGA details: $7 \times 7$ 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

[^1]
## Test case: Poisson's equation on a variable annulus



Ongoing master thesis work of Frank van Ruiten, TU Delft

## Preliminary results




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## Towards an ML-friendly B-spline formulation

## Common computational task

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

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

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

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

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

- 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

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

## Towards an ML-friendly B-spline formulation

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

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

with $k \times k+1$ matrices $R_{k}(\xi)$, e.g.

$$
\begin{aligned}
R_{1}(\xi) & =\left[\begin{array}{lll}
\frac{\xi_{\ell+1}-\xi}{\xi_{\ell+1}-\xi_{\ell}} & \frac{x-\xi_{\ell}}{\xi_{\ell+1}-\xi_{\ell}}
\end{array}\right] \\
R_{2}(\xi) & =\left[\begin{array}{ccc}
\frac{\xi_{\ell+1}-\xi}{\xi_{\ell+1}-\xi_{\ell-1}} & \frac{x-\xi_{\ell-1}}{\xi_{\ell+1}-\xi_{\ell-1}} & 0 \\
0 & \frac{\xi_{\ell+2}-\xi}{\xi_{\ell+2}-\xi_{\ell}} & \frac{x-\xi_{\ell}}{\xi_{\ell+2}-\xi_{\ell}}
\end{array}\right] \\
R_{3}(\xi) & =\ldots
\end{aligned}
$$

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. 鲯


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## Thank you for your attention!


[^0]:    Photo: Siemens - Simulation for Design Engineers

[^1]:    Ongoing master thesis work of Frank van Ruiten, TU Delft

