IgaNets: Physics-Informed Machine Learning Embedded Into Isogeometric Analysis

Matthias Möller, Deepesh Toshniwal, Frank van Ruiten

Department of Applied Mathematics
Delft University of Technology, The Netherlands

USACM Thematic Conference on Isogeometric Analysis 2022
7–9 November 2022, Banff, Canada

New Frontiers in IGA - II
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New Frontiers in IGA - II
# Motivation

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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”

Better question to ask
- 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?
Motivation

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vs.

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<td>✓ fast evaluation <em>(costly training!)</em></td>
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<td>✓ established engineering workflows</td>
<td>✓ inclusion of (measurement) data</td>
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<td>❌ no cost amortization over multiple runs, no real-time capability</td>
<td>❌ lack of convergence theory</td>
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Better questions to ask

- 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?
Vision: fast interactive qualitative analysis and accurate quantitative analysis within the same computational framework with seamless switching between both approaches
Physics-informed machine learning

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

\[
F = \partial_t U + \nabla \cdot f(U)
\]
Physics-informed machine learning

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

- easy to implement for ‘any’ PDE because AD magic does it for you
- combined un-/supervised learning
- poor extrapolation/generalization
- point-based approach requires re-evaluation of NN at every point
- rudimentary convergence theory
Physics-informed machine learning

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**DeepONet** (Lu et al. 2019): *learns the differential operator*

$$G_\theta(u)(y) = \sum_{k=1}^{q} b_k(u(x_1), u(x_2), \ldots, u(x_m)) t_k(y)$$
Physics-informed machine learning

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

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\[ G_\theta(u)(y) = \sum_{k=1}^{q} b_k(u(x_1), u(x_2), \ldots, u(x_m)) t_k(y) \]

Don’t we know a good basis?
Isogeometric Analysis

**Model problem:** Poisson’s equation

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

with

(geometric) \quad x_h(\xi, \eta) = \sum_{i=1}^{n} B_i(\xi, \eta) \cdot x_i \quad \forall (\xi, \eta) \in [0, 1]^2

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

(right-hand side vector) \quad f_h \circ x_h(\xi, \eta) = \sum_{i=1}^{n} B_i(\xi, \eta) \cdot f_i \quad \forall (\xi, \eta) \in [0, 1]^2

(boundary conditions) \quad g_h \circ x_h(\xi, \eta) = \sum_{i=1}^{n} B_i(\xi, \eta) \cdot g_i \quad \forall (\xi, \eta) \in \partial[0, 1]^2
Isogeometric Analysis

Abstract representation
Given $x_i$ (geometry), $f_i$ (r.h.s. vector), and $g_i$ (boundary conditions), compute

$$
\begin{bmatrix}
u_1 \\
\vdots \\
u_n
\end{bmatrix} = A^{-1} \left( \begin{bmatrix} x_1 \\
\vdots \\
x_n \end{bmatrix}, \begin{bmatrix} g_1 \\
\vdots \\
g_n \end{bmatrix} \right) \cdot b \left( \begin{bmatrix} x_1 \\
\vdots \\
x_n \end{bmatrix}, \begin{bmatrix} f_1 \\
\vdots \\
f_n \end{bmatrix}, \begin{bmatrix} g_1 \\
\vdots \\
g_n \end{bmatrix} \right)
$$

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

$$(\xi, \eta) \in [0, 1]^2 \quad \rightarrow \quad u_h \circ x_h(\xi, \eta) = [B_1(\xi, \eta), \ldots, B_n(\xi, \eta)] \cdot \begin{bmatrix}
u_1 \\
\vdots \\
u_n
\end{bmatrix}$$
Isogeometric Analysis

Abstract representation
Given $x_i$ (geometry), $f_i$ (r.h.s. vector), and $g_i$ (boundary conditions), compute

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  x_1 \\
  \vdots \\
  x_n
\end{bmatrix}, \begin{bmatrix}
  g_1 \\
  \vdots \\
  g_n
\end{bmatrix} \right) \cdot b \left( \begin{bmatrix}
  x_1 \\
  \vdots \\
  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

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

Let us interpret the sets of B-spline coefficients $\{x_i\}$, $\{f_i\}$, 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 + Physics-Informed Machine Learning

**IgaNet:** replace *computation*

\[
\begin{bmatrix}
u_1 \\
\vdots \\
u_n
\end{bmatrix} = A^{-1} \begin{pmatrix}
x_1 & \vdots & g_1 \\
\vdots & \ddots & \vdots \\
x_n & \vdots & g_n
\end{pmatrix} \cdot b \begin{pmatrix}
x_1 & \vdots & f_1 \\
\vdots & \ddots & \vdots \\
x_n & \vdots & f_n
\end{pmatrix}
\]
Isogeometric Analysis + Physics-Informed Machine Learning

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

\[
\begin{pmatrix}
  u_1 \\
  \vdots \\
  u_n
\end{pmatrix} = \text{IgaNet} \left( \begin{pmatrix}
  x_1 \\
  \vdots \\
  x_n
\end{pmatrix}, \begin{pmatrix}
  f_1 \\
  \vdots \\
  f_n
\end{pmatrix}, \begin{pmatrix}
  g_1 \\
  \vdots \\
  g_n
\end{pmatrix}; \left( \xi^{(k)}, \eta^{(k)} \right)_{k=1}^{N_{\text{samples}}} \right)
\]
Isogeometric Analysis + Physics-Informed Machine Learning

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

\[
\begin{bmatrix}
u_1 \\
\vdots \\
u_n
\end{bmatrix} = \text{IgaNet} \left( \begin{bmatrix}
x_1 \\
\vdots \\
x_n
\end{bmatrix}, \begin{bmatrix}
f_1 \\
\vdots \\
f_n
\end{bmatrix}, \begin{bmatrix}
g_1 \\
\vdots \\
g_n
\end{bmatrix}; \left( \xi^{(k)}, \eta^{(k)} \right)_{k=1}^{N_{\text{samples}}} \right)
\]

Compute the solution from the trained neural network as follows

\[
u_h(\xi, \eta) = [B_1(\xi, \eta), \ldots, B_n(\xi, \eta)] \cdot \begin{bmatrix}
u_1 \\
\vdots \\
u_n
\end{bmatrix}, \quad \begin{bmatrix}
u_1 \\
\vdots \\
u_n
\end{bmatrix} = \text{IgaNet} \left( \begin{bmatrix}
x_1 \\
\vdots \\
x_n
\end{bmatrix}, \begin{bmatrix}
f_1 \\
\vdots \\
f_n
\end{bmatrix}, \begin{bmatrix}
g_1 \\
\vdots \\
g_n
\end{bmatrix} \right)
\]
IgaNet architecture

\[ \text{loss} = \text{loss}_{\text{PDE}} + \text{loss}_{\text{BDR}} \]

\[ \frac{\partial \text{loss}}{\partial (w, b)} \rightarrow \text{update } w, b \text{ and continue training} \]

end training

\[ \text{coords } (\xi^{(k)}, \eta^{(k)})_{k=1}^{N} \]
Loss function

\[
\text{loss}_{\text{PDE}} = \frac{\alpha}{N_\Omega} \sum_{k=1}^{N_\Omega} \left| \Delta \left[ u_h \circ x_h \left( \xi^{(k)}, \eta^{(k)} \right) \right] - f_h \circ x_h \left( \xi^{(k)}, \eta^{(k)} \right) \right|^2
\]

\[
\text{loss}_{\text{BDR}} = \frac{\beta}{N_\Gamma} \sum_{k=1}^{N_\Gamma} \left| u_h \circ x_h \left( \xi^{(k)}, \eta^{(k)} \right) - g_h \circ x_h \left( \xi^{(k)}, \eta^{(k)} \right) \right|^2
\]

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

\begin{align*}
\text{For } [x_1, \ldots, x_n] \in S_{\text{geo}}, [f_1, \ldots, f_n] \in S_{\text{rhs}}, [g_1, \ldots, g_n] \in S_{\text{bcond}} \text{ do} \\
\quad \text{For a batch of randomly sampled } (\xi_k, \eta_k) \in [0, 1]^2 \text{ (or the Greville abscissae) do} \\
\quad \quad \text{Train IgaNet} \\
\quad \quad \quad \left( \begin{array}{ccc}
    x_1 & f_1 & g_1 \\
    \vdots & \vdots & \vdots \\
    x_n & f_n & g_n
\end{array} \right) ; (\xi_k, \eta_k)^{N_{\text{samples}}}_{k=1} \implies \\
\quad \quad \quad \left( \begin{array}{c}
    u_1 \\
    \vdots \\
    u_n
\end{array} \right)
\quad \text{EndFor}
\quad \text{EndFor}
\end{align*}

Details:

- $7 \times 7$ bi-cubic tensor-product B-splines for $x_h$ 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

Ongoing master thesis work of Frank van Ruiten, TU Delft
Test case: Poisson’s equation on a variable annulus

\[ g \equiv 0, 1, \ldots, 11 \]

\[ f \equiv 0, 1, \ldots, 11 \]

Ongoing master thesis work of Frank van Ruiten, TU Delft
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

\[ x \mapsto u(x) := \text{NN}(x; f, g, G) = \sigma_L(W_L\sigma(\ldots(\sigma_1(W_1x + b_1))) + b_L) \]

- 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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\[ x \mapsto u(x) := \text{NN}(x; f, g, G) = \sigma_L(W_L\sigma(\ldots(\sigma_1(W_1x + b_1)))) + b_L \]

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- use AD engine on top of AD tree (!!!) to compute gradients w.r.t. weights for training

Working principle of IgaNets

\[ [x_i, f_i, g_i]_{i=1,...,n} \mapsto [u_i]_{i=1,...,n} := \text{NN}(x_i, f_i, g_i, i = 1, \ldots, n) \]

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

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

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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 $r \geq 0$

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

**Textbook derivatives**

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

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)

\[
\begin{bmatrix}
  d^r_{\xi} b^p_{i-p}(\xi), \ldots, d^r_{\xi} b^p_i(\xi)
\end{bmatrix} = \frac{p!}{(p - r)!} R_1(\xi) \cdots R_{p-r}(\xi) d_\xi R_{p-r+1} \cdots d_\xi R_{p}
\]

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

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

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

\[
R_3(\xi) = \ldots
\]
Algorithm 2.22 from (Lyche and Morken 2011)

1. $b = 1$
2. For $k = 1, \ldots, p - r$
   1. $t_1 = (\xi_{i-k+1}, \ldots, \xi_i)$
   2. $t_2 = (\xi_{i+1}, \ldots, \xi_{i+k})$
   3. $w = (\xi - t_1) \div (t_2 - t_1)$
   4. $b = [(1 - w) \odot b, 0] + [0, w \odot b]$
3. For $k = p - r + 1, \ldots, p$
   1. $t_1 = (\xi_{i-k+1}, \ldots, \xi_i)$
   2. $t_2 = (\xi_{i+1}, \ldots, \xi_{i+k})$
   3. $w = 1 \div (t_2 - t_1)$
   4. $b = [-w \odot b, 0] + [0, w \odot b]$

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

1. \( b = 1 \)
2. For \( k = 1, \ldots, p - r \)
   1. \( t_1 = (\xi_{i-k+1}, \ldots, \xi_i) \)
   2. \( t_{21} = (\xi_{i+1}, \ldots, \xi_{i+k}) - t_1 \)
   3. \( \text{mask} = (t_{21} < \text{tol}) \)
   4. \( w = (\xi - t_1 \text{ - mask}) \div (t_{21} - \text{mask}) \)
   5. \( b = [(1 - w) \odot b, 0] + [0, w \odot b] \)
3. For \( k = p - r + 1, \ldots, p \)
   1. \( t_1 = (\xi_{i-k+1}, \ldots, \xi_i) \)
   2. \( t_{21} = (\xi_{i+1}, \ldots, \xi_{i+k}) - t_1 \)
   3. \( \text{mask} = (t_{21} < \text{tol}) \)
   4. \( w = (1 - \text{mask}) \div (t_{21} - \text{mask}) \)
   5. \( b = [-w \odot b, 0] + [0, w \odot b] \)

where \( \div \) and \( \odot \) denote the element-wise division and multiplication of vectors, respectively.
Performance evaluation - univariate B-splines

Wallclock time in ns/entry

$p = 1$  $p = 2$  $p = 3$  $p = 4$  $p = 5$

Tesla V100S PCIe 32G  AMD EPYC 7402 24-Core Processor  reference
Performance evaluation - bivariate B-splines

Wallclock time in ns/entry

$p = 1$  $p = 2$  $p = 3$  $p = 4$  $p = 5$

Tesla V100S PCIe 32G  AMD EPYC 7402 24-Core Processor  reference
Performance evaluation - trivariate B-splines

Wallclock time in ns/entry

$\begin{align*}
p = 1 & \quad p = 2 & \quad p = 3 & \quad p = 4 & \quad p = 5
\end{align*}$

- $p = 1$
- $p = 2$
- $p = 3$
- $p = 4$
- $p = 5$

- Tesla V100S PCIe 32G
- AMD EPYC 7402 24-Core Processor
- reference
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
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