IgANets: Physics-informed machine learning embedded into isogeometric analysis

Matthias Möller

Department of Applied Mathematics, TU Delft, The Netherlands

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Joint work with Deepesh Toshniwal, Frank van Ruiten (TU Delft), Ye Ji, Mengyun Wang (TU Delft, Dalian), Casper van Leeuwen, Paul Melis (SURF), and Jaewook Lee (TU Vienna)

Vision

Unified computational **design-through-analysis framework** for interactive rapid prototyping and thorough offline post-analysis of engineering designs

Ingredients

- physics-informed operator learning for prototyping
- isogeometric analysis for thorough post-analysis

Design principle: stay in the IGA paradigm [Hughes et al., 2005] to seamlessly blend between learning-based prototyping and compute-based post-analysis (even locally)

Tech preview

`https://visualization.surf.nl/iganet`

IGA in a nutshell

Integration of finite element analysis into NURBS-based computer-aided design

Benefits

- no tedious and time consuming meshing
- no geometric approximation error
- better accuracy per degree of freedom
- higher continuity of basis functions

IGA in a nutshell

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Challenges

- 'dirty' CAD geometries are not (directly) analysis suitable
- matrix assembly (in Galerkin-type IGA) is more costly than in FEA
- efficient h-, p- and k-robust iterative solvers are more involved
- continuity preserving multi-patch coupling is non-trivial

IGA variants

Galerkin-type IGA [Hughes et al., 2005]

- weak form w/ integration by parts $\rightarrow$ spline test/trial functions $\rightarrow$ $\mathbf{A}_h \mathbf{u}_h = \mathbf{f}_h$
- spline spaces: B-/HB-/THB-splines, T-/U-splines, LR-splines, ...
- multi-patch: Nitsche, D-Patch, Almost-C^1, Analysis-suitable G^1, Approximate C^1, ...

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Collocation-type IGA [Auricchio et al., 2010]

- weak form w/o integration by parts $\rightarrow$ δ test/spline trial functions $\rightarrow$ $\mathbf{A}_h \mathbf{u}_h = \mathbf{f}_h$
- collocation points: Demko, Greville, superconvergent [Anitescu et al., 2015], clustered SC points [Montardini et al., 2017], *least-squares collocation* [Lin et al., 2020]

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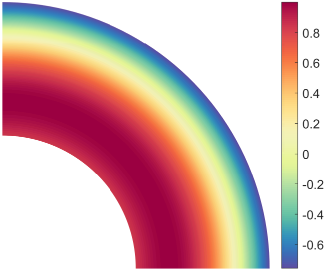
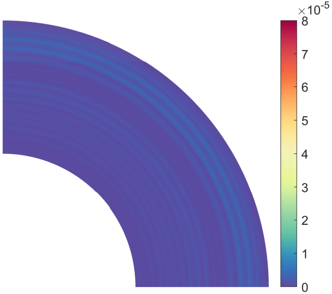
Variational collocation-type IGA [Gomez and Lorenzis, 2016]

- IGA-C at Cauchy-Galerkin points = IGA-G

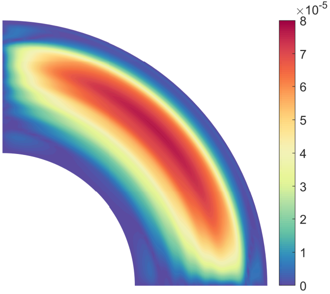
Comparison between Galerkin and collocation IGA



solution



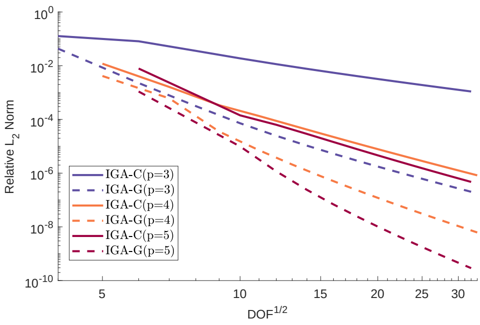
IGA-G abs. error



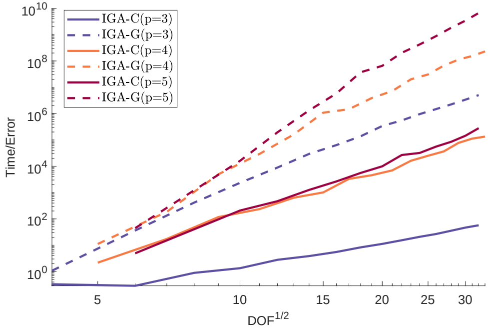
IGA-C abs. error

Results by Mengyun Wang

Comparison between Galerkin and collocation IGA



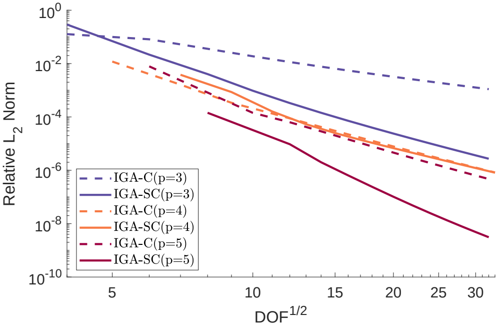
rel. L_2-error



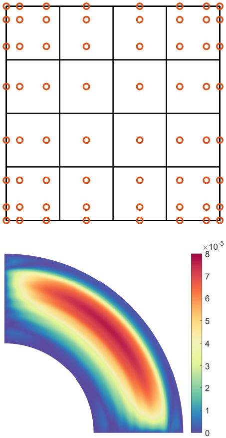
wallclock time/error

Results by Mengyun Wang

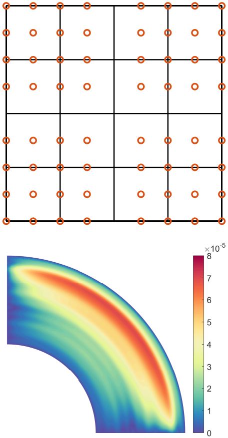
Comparison between Greville and clustered superconvergent points



rel. L_2-error



Greville



SC points

Results by Mengyun Wang

Collocation IGA

PDE problem

$$\mathcal{L}u = f \qquad \text{in } \Omega$$

$$\mathcal{B}u = g \qquad \text{on } \Gamma$$

Weighted residual form

$$\int_\Omega \phi_\Omega (\mathcal{L}u - f)\,\mathrm{d}\mathbf{x} + \int_\Gamma \phi_\Gamma (\mathcal{B}u - g)\,\mathrm{d}s = 0$$

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Let

$$\phi_\Omega = \sum_{i=1}^{k} c_i\,\delta_\Omega(\mathbf{x} - \mathbf{x}_i) \quad (\mathbf{x}_i \in \Omega) \qquad \text{and} \qquad \phi_\Gamma = \sum_{i=k+1}^{n} c_i\,\delta_\Gamma(\mathbf{x} - \mathbf{x}_i) \quad (\mathbf{x}_i \in \Gamma)$$

then

$$\sum_{i=1}^{k} c_i\,(\mathcal{L}u(\mathbf{x}_i) - f(\mathbf{x}_i)) + \sum_{i=1+k}^{n} c_i\,(\mathcal{B}u(\mathbf{x}_i) - g(\mathbf{x}_i)) = 0$$

Collocation IGA cont'd

As the coefficients c_i are arbitrary we obtain

$$\mathcal{L}u(\mathbf{x}_i) = f(\mathbf{x}_i) \qquad i = 1, \ldots, k$$

$$\mathcal{B}u(\mathbf{x}_i) = g(\mathbf{x}_i) \qquad i = k+1, \ldots, n$$

Collocation IGA cont'd

As the coefficients c_i are arbitrary and replacing $u \approx u_h = \sum_{j=1}^{n} b_j(\mathbf{x}) u_j$ we obtain

$$\begin{bmatrix} \mathcal{L}b_1(\mathbf{x}_1) & \dots & \mathcal{L}b_n(\mathbf{x}_1) \\ \vdots & \ddots & \vdots \\ \mathcal{L}b_1(\mathbf{x}_k) & \dots & \mathcal{L}b_n(\mathbf{x}_k) \\ \mathcal{B}b_1(\mathbf{x}_{k+1}) & \dots & \mathcal{B}b_n(\mathbf{x}_{k+1}) \\ \vdots & \ddots & \vdots \\ \mathcal{B}b_1(\mathbf{x}_n) & \dots & \mathcal{B}b_n(\mathbf{x}_n) \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_k \\ u_{k+1} \\ \vdots \\ u_n \end{bmatrix} = \begin{bmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_k) \\ g(\mathbf{x}_{k+1}) \\ \vdots \\ g(\mathbf{x}_n) \end{bmatrix}$$

Collocation IGA cont'd

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- basis functions b_i need to be at least C^ℓ such that $\mathcal{L}$ and $\mathcal{B}$ can be applied
- regular system matrix requires that #collocation points $=$ #basis functions and all collocation points must be pairwise distinct

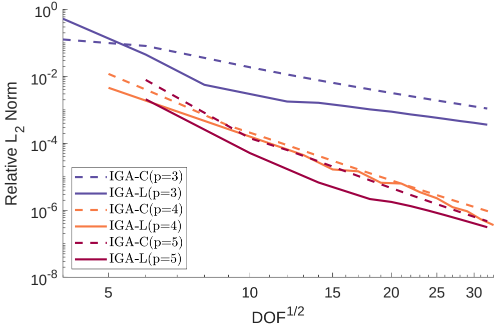
Least-squares collocation IGA

Idea: When #collocation points (m) $>$ #unknowns (n) then the system matrix is over-determined and the system can be solved in least-squares manner

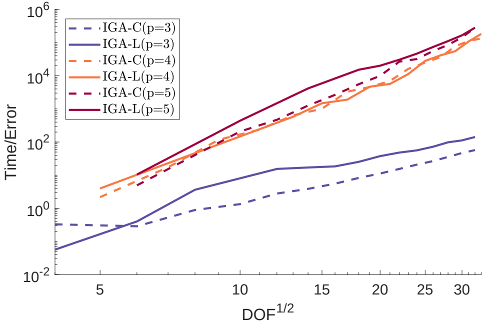
$$\min \sum_{i=1}^{k} \|\mathcal{L}u(\mathbf{x}_i) - f(\mathbf{x}_i)\|^2 + \sum_{i=k+1}^{m} \|\mathcal{B}u(\mathbf{x}_i) - g(\mathbf{x}_i)\|^2$$

[Lin et al., 2020] derives rigoros conditions under which least-squares collocation IGA (IGA-L) is consistent and convergent. In essence, there must be *at least one collocation point per element* (e.g., Greville points) but we can use more to increase the resolution.

Comparison between collocation and least-squares collocation IGA



rel. L_2-error



wallclock time/error

Results by Mengyun Wang

Least-squares collocation IGA revisited

Replacing u, f, and g by their approximations u_h, f_h, and g_h we obtain

$$\min \sum_{i=1}^{k} \| \sum_{j=1}^{n} \mathcal{L} b_j(\mathbf{x}_i) u_j - b_j(\mathbf{x}_i) f_j \|^2 + \sum_{i=k+1}^{m} \| \sum_{j=1}^{n} \mathcal{B} b_j(\mathbf{x}_i) u_j - b_j(\mathbf{x}_i) g_j \|^2$$

- B-spline basis functions $\hat{b}_j(\boldsymbol{\xi})$ are defined in the reference space $\hat{\Omega} = (0,1)^d$ and are mapped into physical space Ω through the **push-forward mapping**

$$\mathbf{x}_h(\boldsymbol{\xi}) = \sum_{i=1}^{n} \hat{b}_j(\boldsymbol{\xi}) \mathbf{x}_j,$$

Least-squares collocation IGA revisited

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$$\min \underbrace{\sum_{i=1}^{k} \| \sum_{j=1}^{n} \mathcal{L} b_j(\mathbf{x}_i) u_j - b_j(\mathbf{x}_i) f_j \|^2}_{\text{loss}_{\text{PDE}}(\{u_j\}_j, \{f_j\}_j; \{\mathbf{x}_i\}_i)} + \underbrace{\sum_{i=k+1}^{m} \| \sum_{j=1}^{n} \mathcal{B} b_j(\mathbf{x}_i) u_j - b_j(\mathbf{x}_i) g_j \|^2}_{\text{loss}_{\text{BC}}(\{u_j\}_j, \{g_j\}_j; \{\mathbf{x}_i\}_i)}$$

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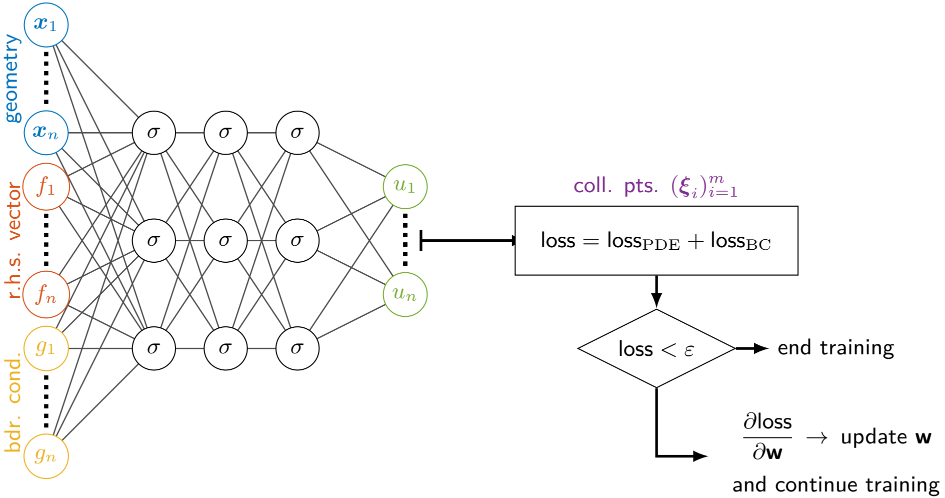
- problem is fully parameterized through f_j's, g_j's, and $\mathbf{x}_j$'s relative to a fixed basis $\hat{b}_j$

IgANet architecture



Training and evaluation

Training

For $[f_1, \ldots, f_n] \in \mathcal{S}_{\text{rhs}}$, $[g_1, \ldots, g_n] \in \mathcal{S}_{\text{bcond}}$, $[\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathcal{S}_{\text{geo}}$ **do**

For a batch of collocation points $\boldsymbol{\xi}_i \in [0,1]^2$ (e.g., Greville points + more) **do**

Train IgANet $([f_1, \ldots, f_n], [g_1, \ldots, g_n], [\mathbf{x}_1, \ldots, \mathbf{x}_n]) \mapsto [u_1, \ldots, u_n]$

EndFor

EndFor

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EndFor

EndFor

Evaluation

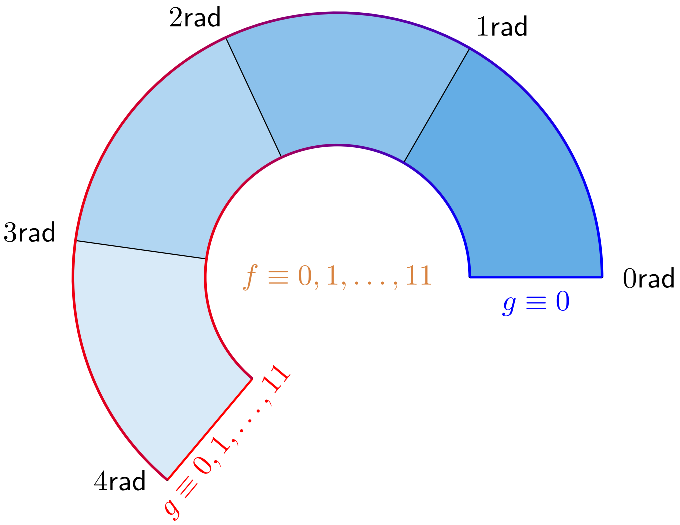
For $[f_1, \dots, f_n] \in \mathcal{S}_{\text{rhs}}$, $[g_1, \dots, g_n] \in \mathcal{S}_{\text{bcond}}$, $[\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathcal{S}_{\text{geo}}$ **do**

Evaluate IgANet $([f_1, \dots, f_n], [g_1, \dots, g_n], [\mathbf{x}_1, \dots, \mathbf{x}_n]) \mapsto [u_1, \dots, u_n]$

Use basis representation $u_h(\mathbf{x}) = \sum_{j=1}^{n} b_j(\mathbf{x}) u_j$ for all further purposes

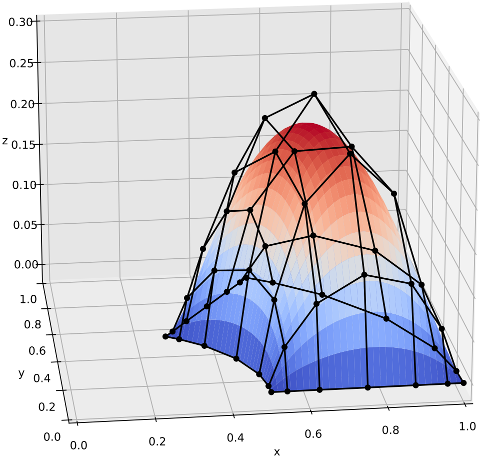
EndFor

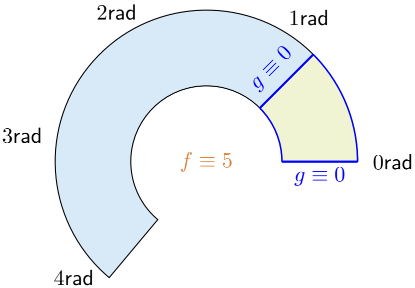
Test case: Poisson's equation on a variable annulus



Master thesis work by Frank van Ruiten, TU Delft

Validation results





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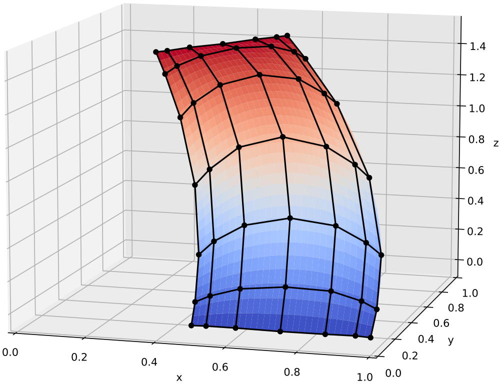

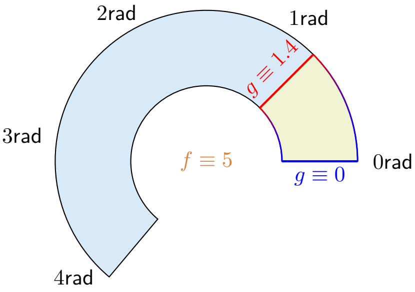

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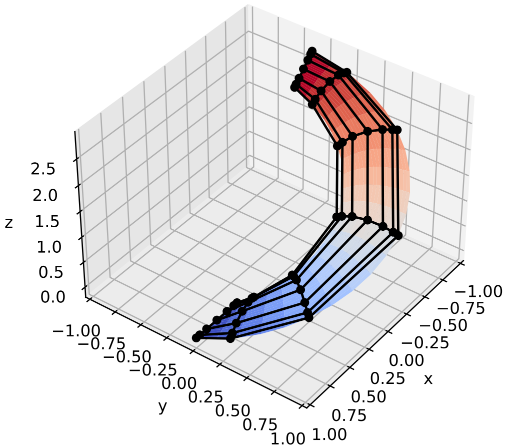

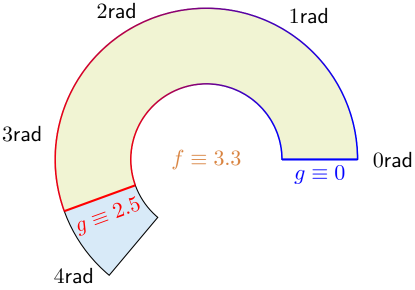

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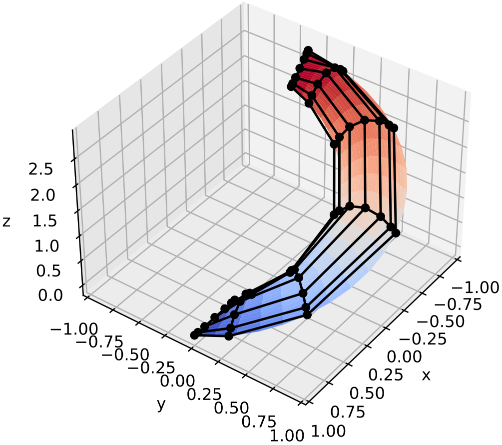

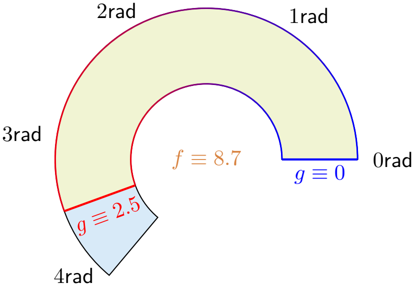

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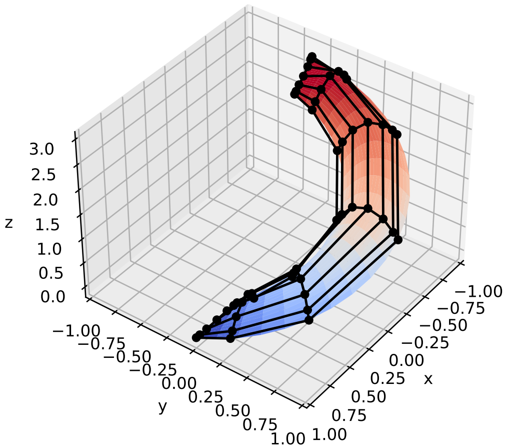

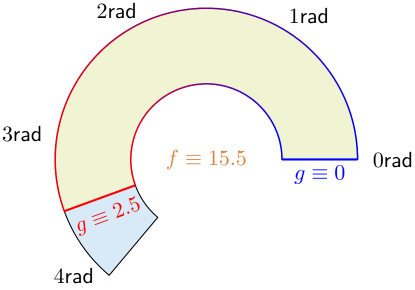

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Automatic placement of interior control points

Harmonic mapping: $\mathbf{x} : \hat{\Omega} \to \Omega$ by solving

$$\begin{aligned} \nabla \cdot \nabla \xi(x,y) &= 0 \\ \nabla \cdot \nabla \eta(x,y) &= 0 \end{aligned} \qquad \text{such that } \mathbf{x}^{-1}|_{\Gamma} = \hat{\Gamma}$$

- $\mathbf{x}^{-1}$ exists and is unique if the curvature of $\hat{\Omega}$ is non-positive and the boundary $\hat{\Gamma}$ when considered with respect to the metric on Ω is convex [Eells and Lemaire, 1978]
- $\mathbf{x}^{-1}$ is one-to-one by the Radó-Kneser-Choquet theorem [Duren and Hengartner, 1997]

Automatic placement of interior control points cont'd

Weak form in H^2 [Hinz et al., 2020]

$$\int_{\hat{\Omega}} \mathbf{b}\tilde{\mathcal{L}}x \,\mathrm{d}\hat{\Omega} = \mathbf{0} \qquad \int_{\hat{\Omega}} \mathbf{b}\tilde{\mathcal{L}}y \,\mathrm{d}\hat{\Omega} = \mathbf{0} \qquad \text{such that } \mathbf{x}^{-1}|_{\Gamma} = \hat{\Gamma}$$

where

$$\tilde{\mathcal{L}} = \left(g_{22}\frac{\partial^2}{\partial \xi^2} - 2g_{12}\frac{\partial^2}{\partial \xi \partial \eta} + g_{11}\frac{\partial^2}{\partial \eta^2} \right) / \left(g_{11} + g_{22} \right)$$

Automatic placement of interior control points cont'd

Weak form in H^2 [Hinz et al., 2020]

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such that $\mathbf{x}^{-1}|_\Gamma = \hat{\Gamma}$

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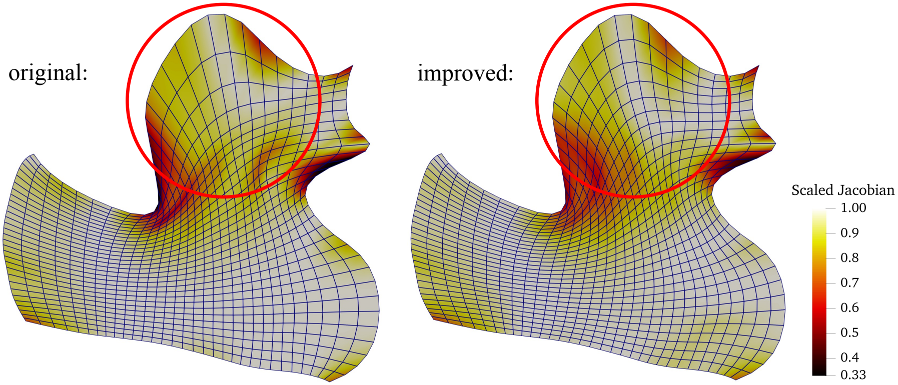
New **weak form** in H^1 [Ji et al., 2023]

$$\int_{\hat{\Omega}} \nabla_{\mathbf{x}}\mathbf{b} \cdot \nabla_{\mathbf{x}}\xi \,\mathrm{d}\hat{\Omega} = \mathbf{0} \qquad \int_{\hat{\Omega}} \nabla_{\mathbf{x}}\mathbf{b} \cdot \nabla_{\mathbf{x}}\eta \,\mathrm{d}\hat{\Omega} = \mathbf{0}$$

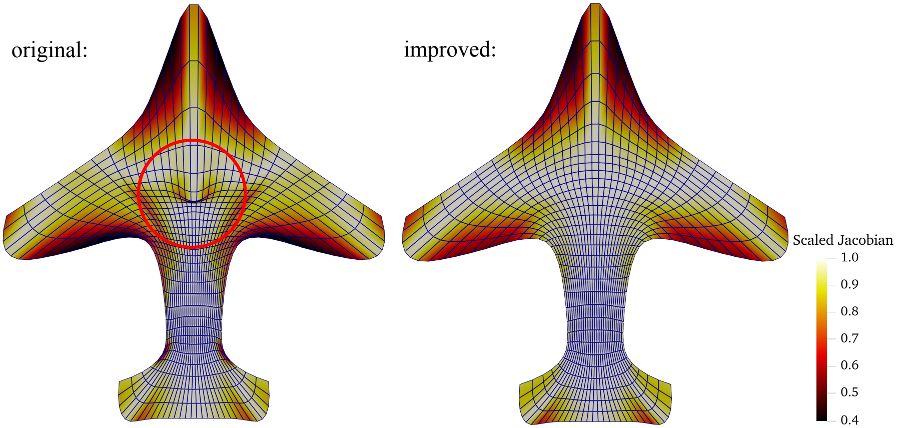
such that $\mathbf{x}^{-1}|_\Gamma = \hat{\Gamma}$

Comparison between H^1 and H^2 approaches



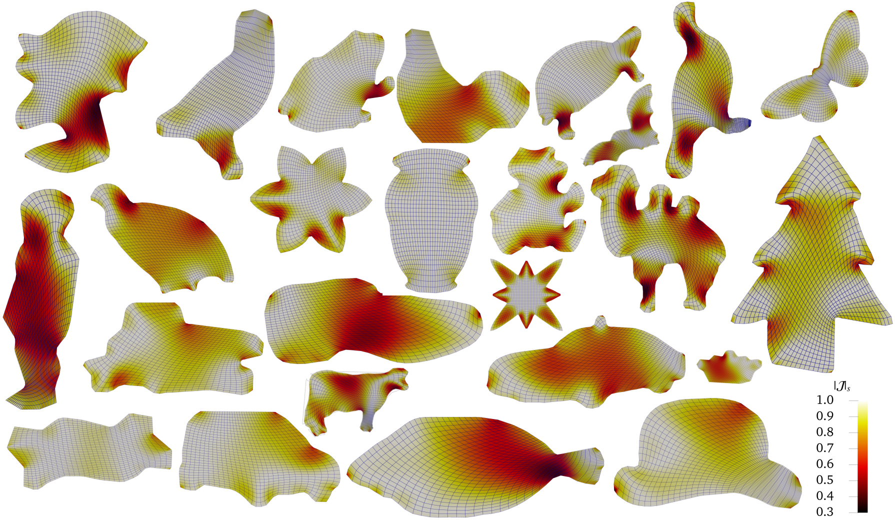
Results by Ye Ji

Comparison between H^1 and H^2 approaches



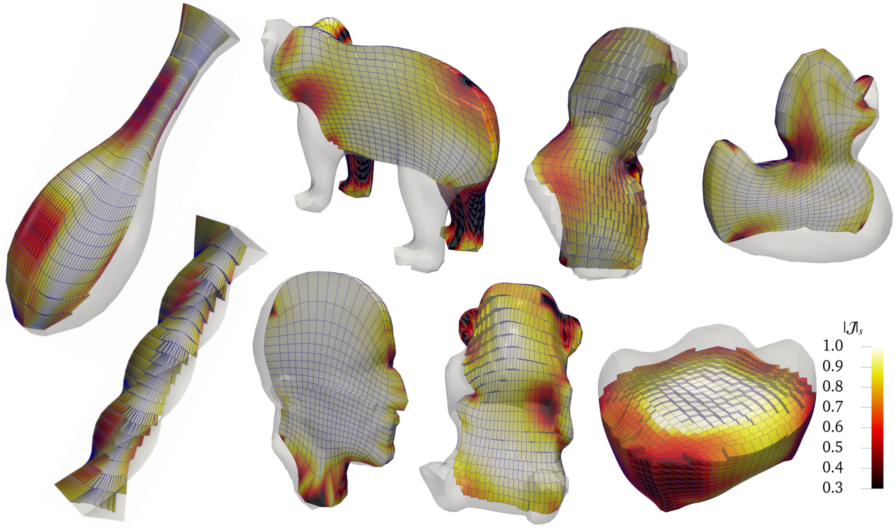
Results by Ye Ji

Planar results



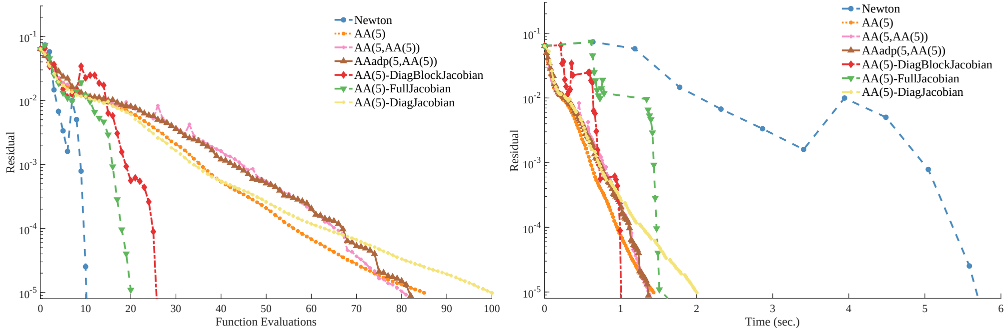
Results by Ye Ji

Volumetric results



Results by Ye Ji

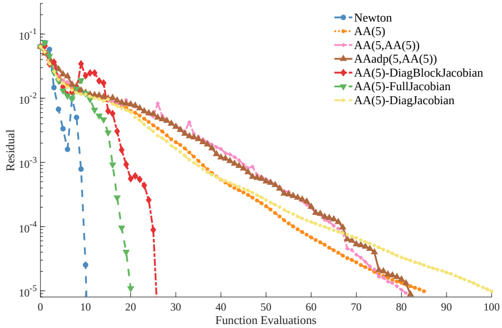
Solution of nonlinear systems by preconditioned Anderson acceleration



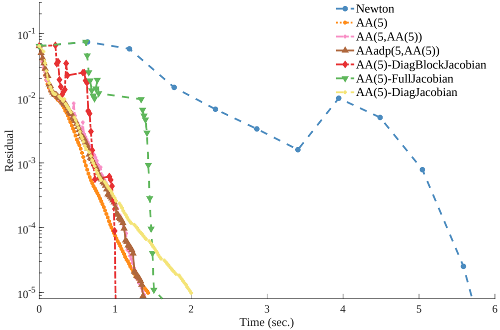
function evaluations

wallclock time

Solution of nonlinear systems by preconditioned Anderson acceleration



function evaluations



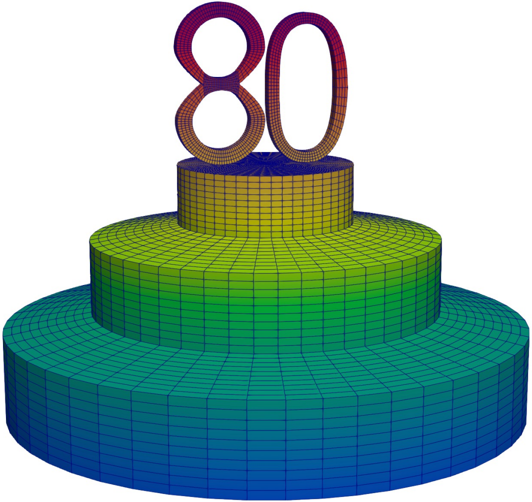
wallclock time

But: 1sec is not interactive anymore! Maybe IGA-L + operator learning will help?

Happy

birthday

Tom!



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Department of Applied Mathematics, TU Delft, The Netherlands

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Joint work with Deepesh Toshniwal, Frank van Ruiten (TU Delft), Ye Ji, Mengyun Wang (TU Delft, Dalian), Casper van Leeuwen, Paul Melis (SURF), and Jaewook Lee (TU Vienna)

Thank you very much!

References I

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