Bridging the gap between isogeometric analysis and deep operator learning

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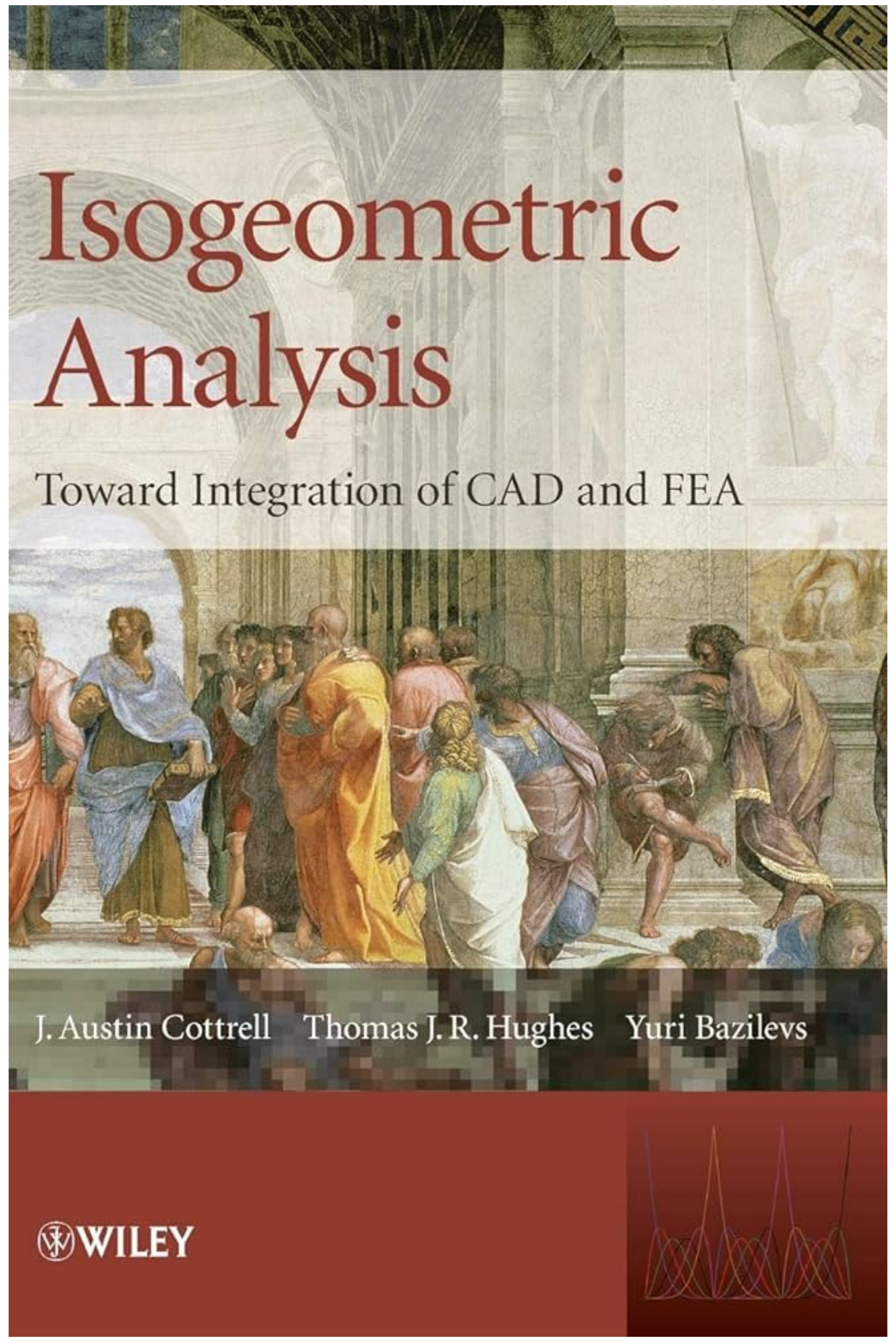
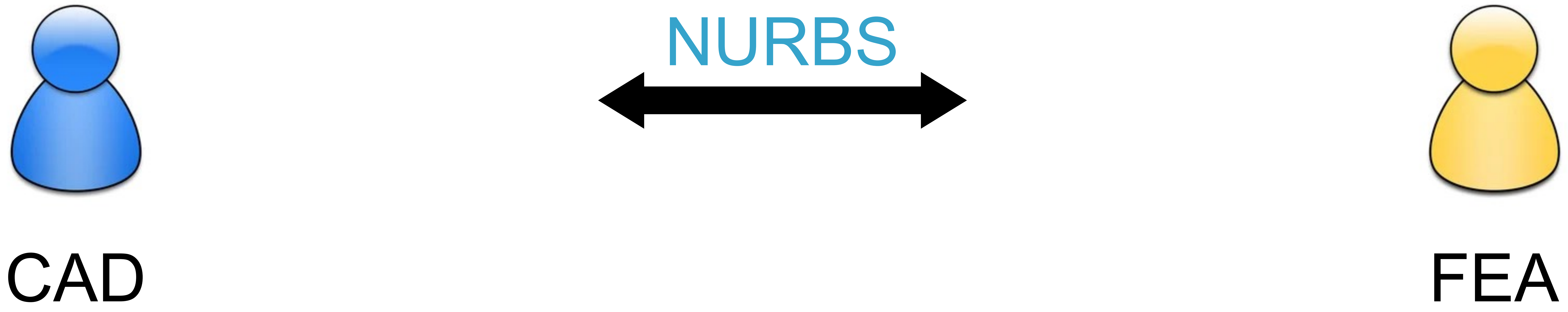
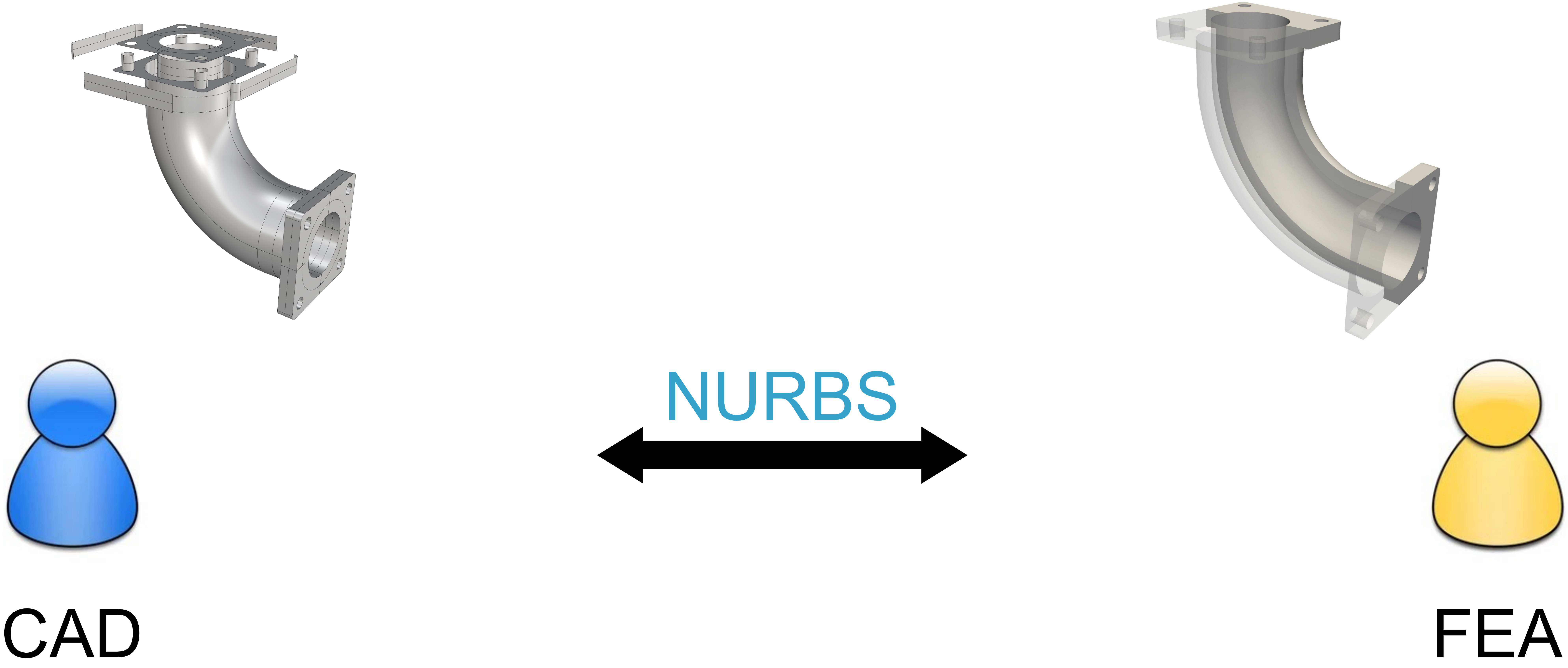
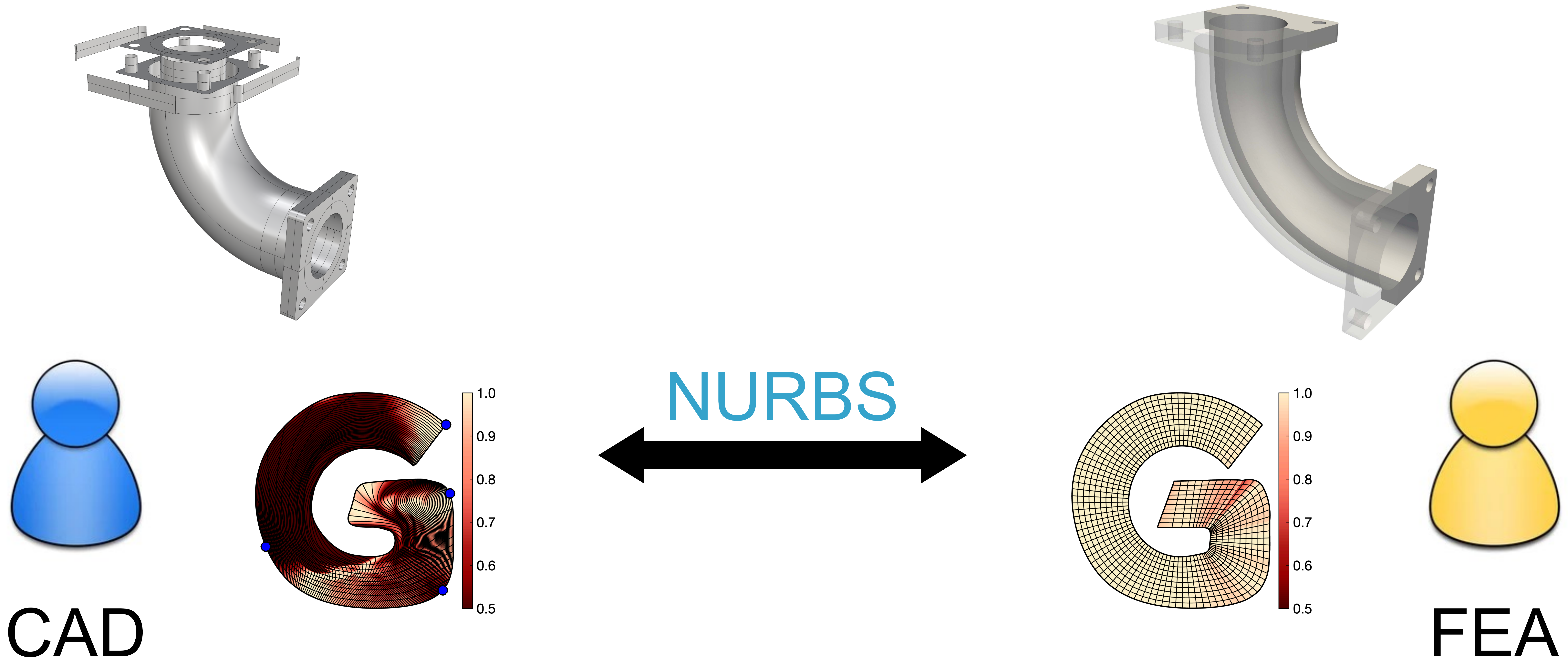
Acknowledgements: Ye Ji, Hugo Verhelst, Mengyun Wang (TU Delft), Jochen Hinz, Merle Backmeyer (ETH Zurich), Casper van Leeuwen (SURF), Jaewook Lee (TU Vienna), Veronika Trávníková (RWTH Aachen), …

Bridging the gap between CAD and FEA by using B-spline or NURBS basis functions for design <u>and</u> analysis . . .




NURBS
CAD
FEA


NURBS
CAD
FEA


NURBS
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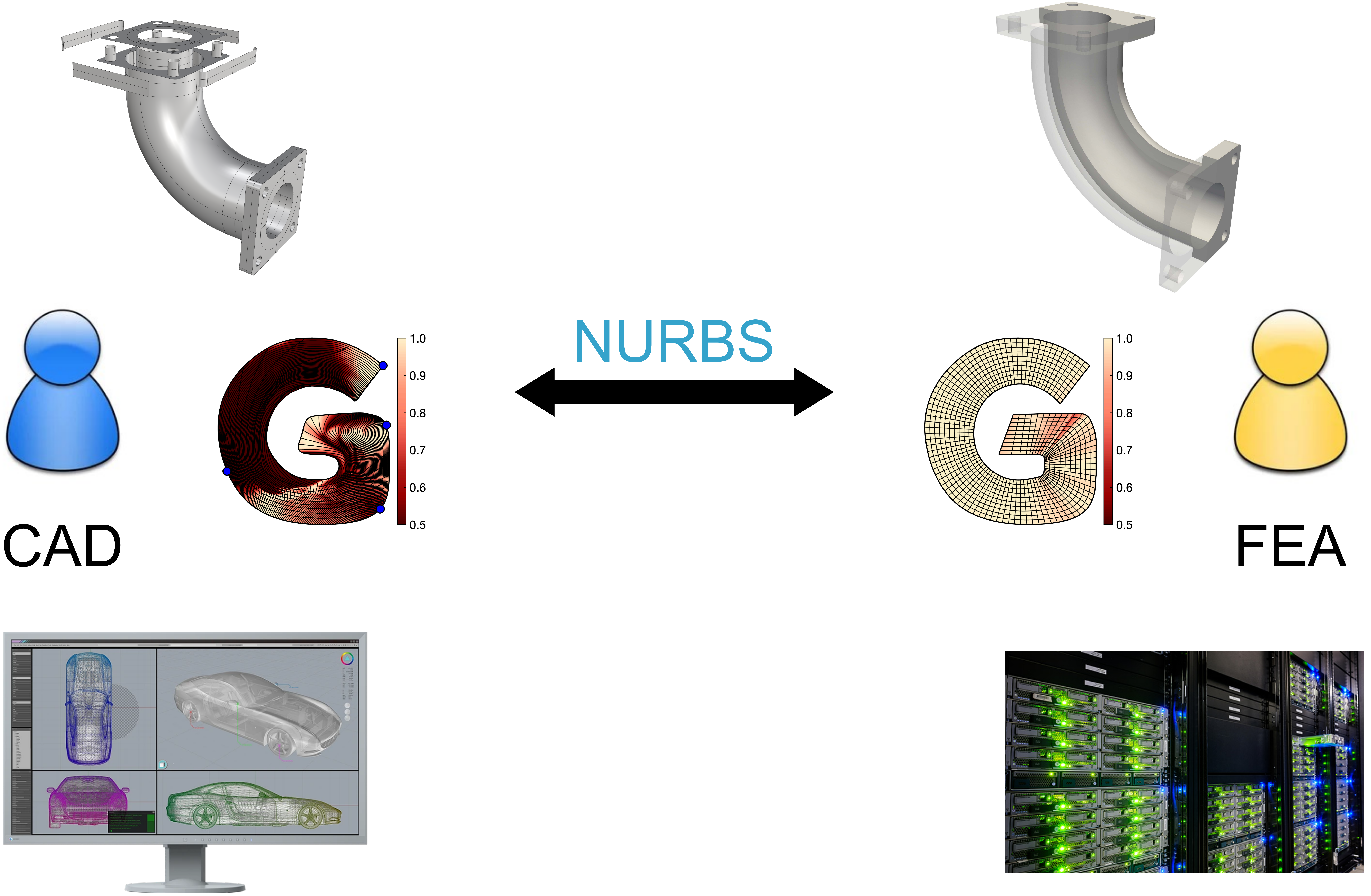

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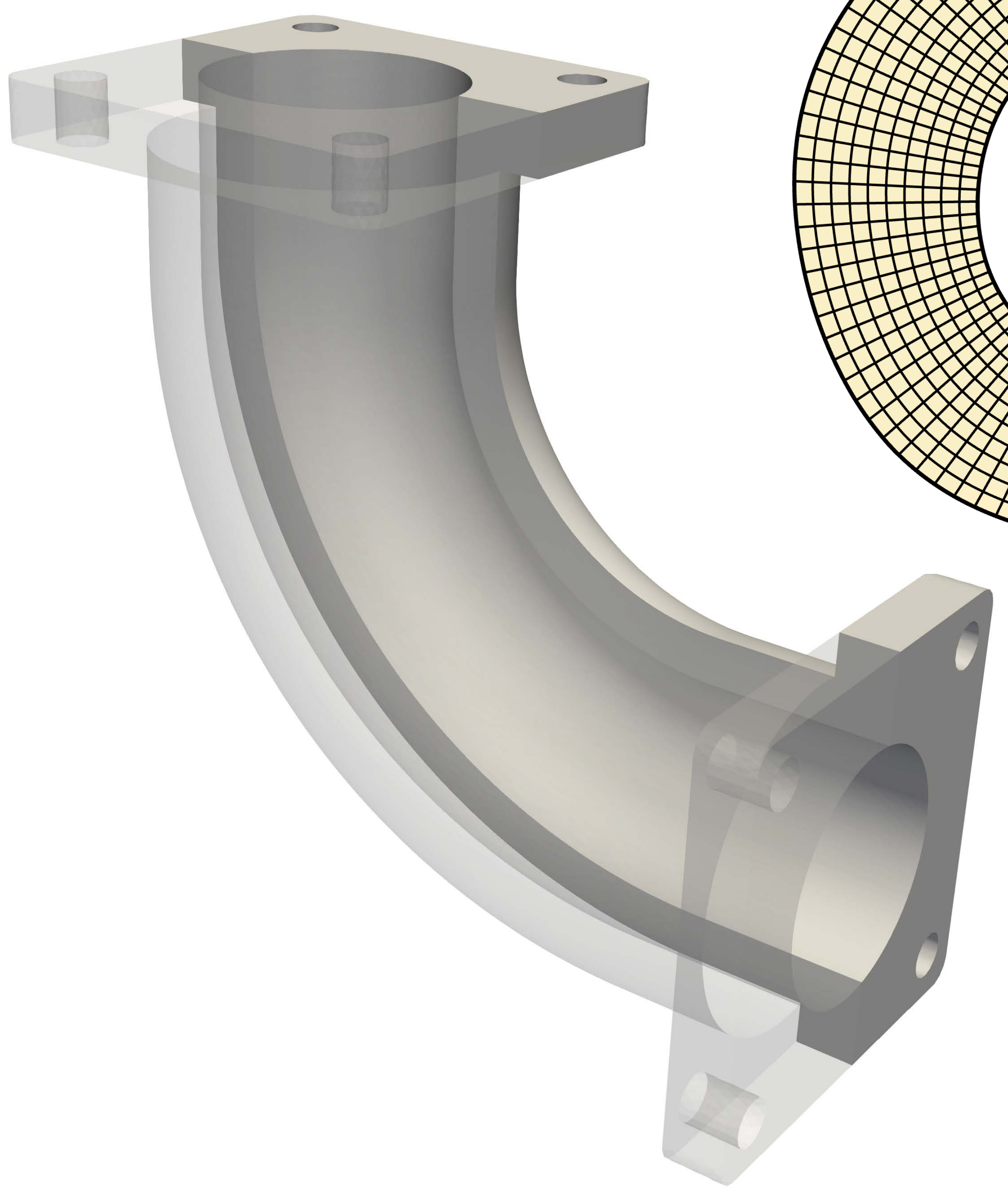
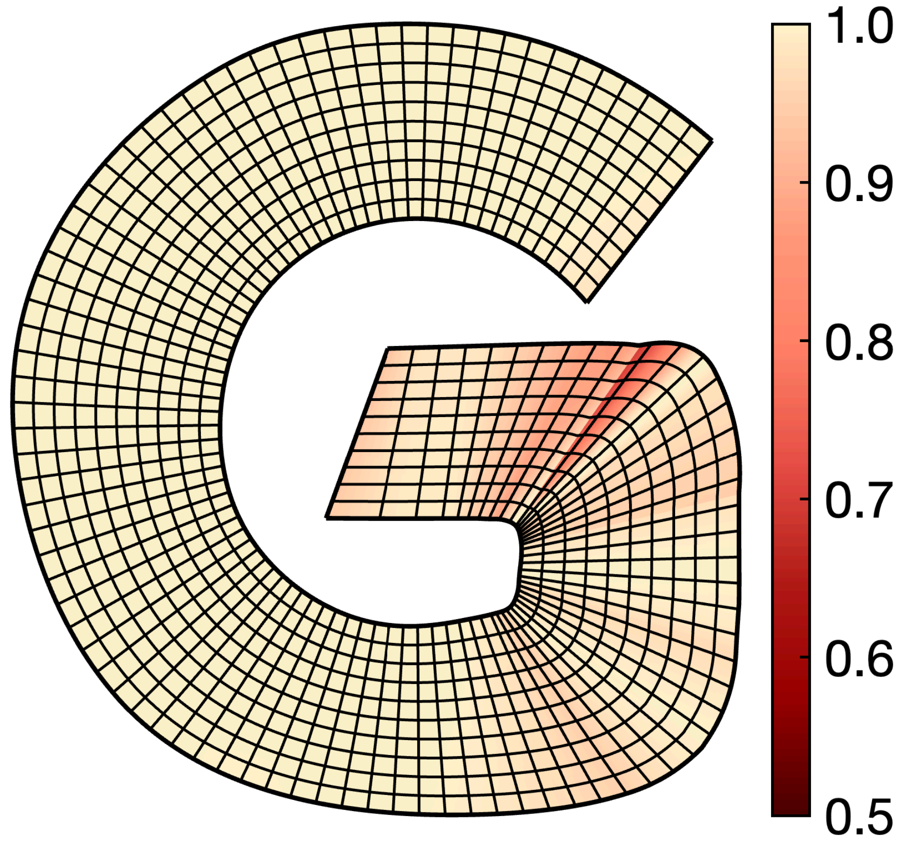
Vision





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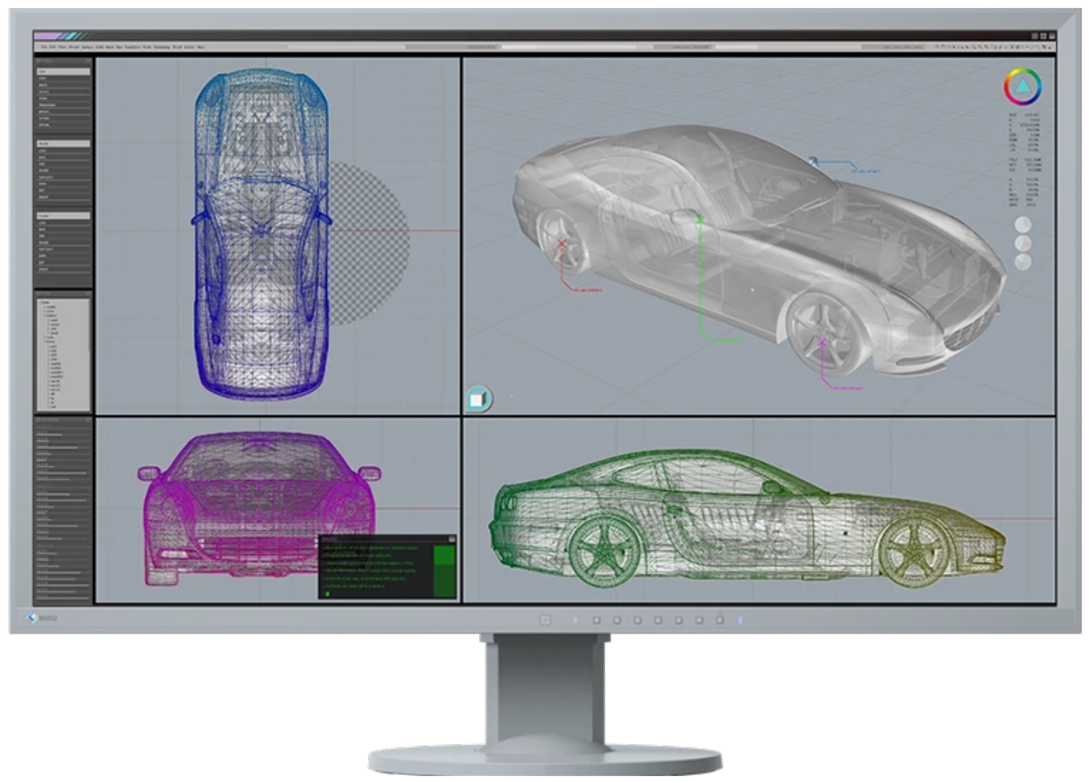

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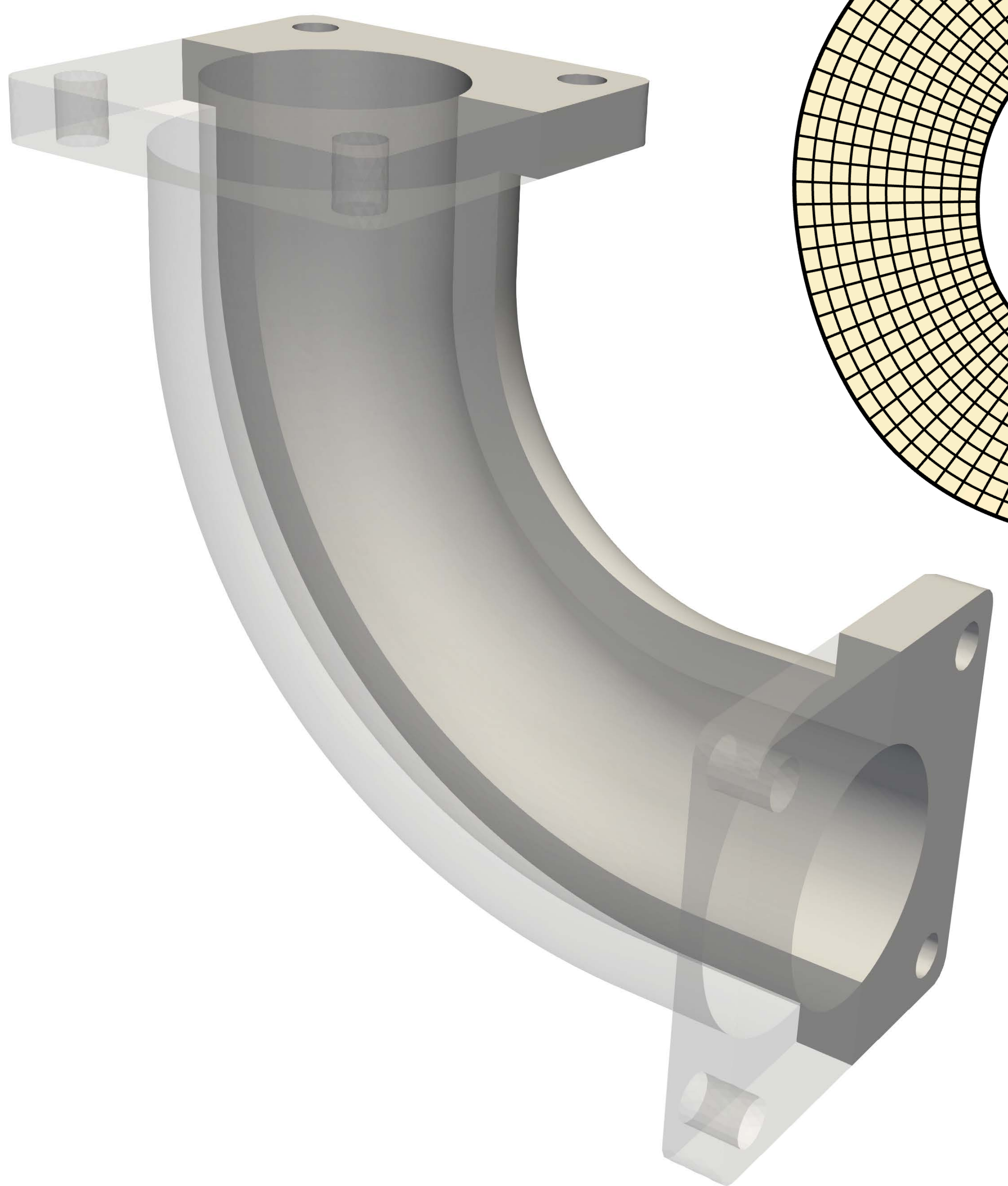
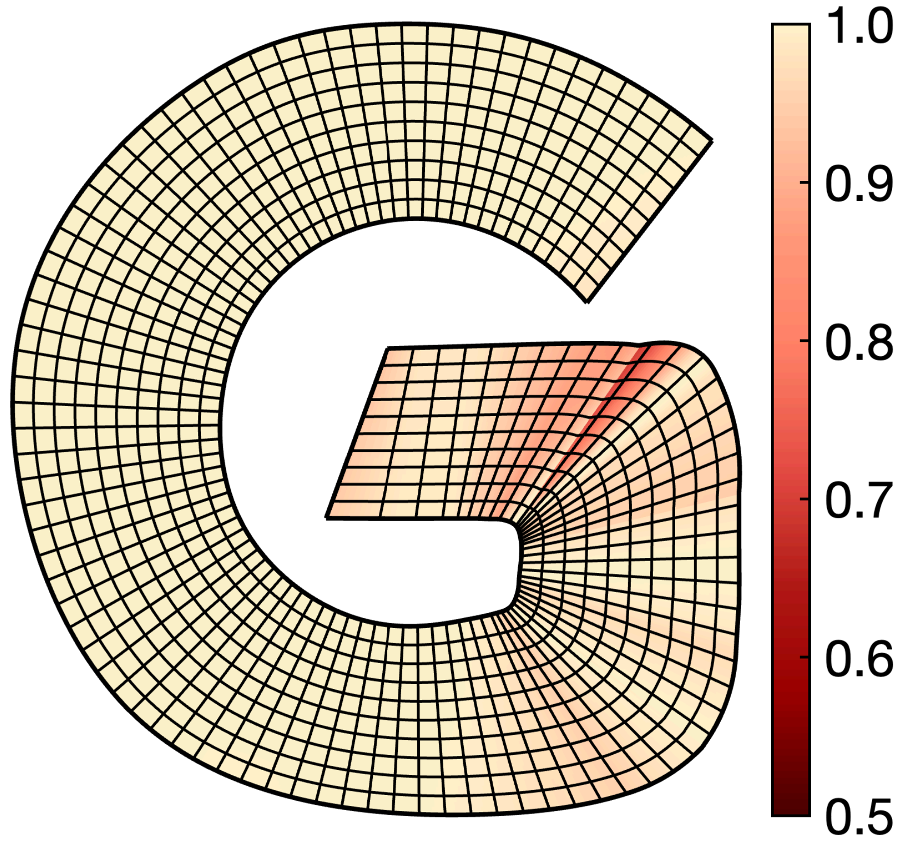
Vision





CAD

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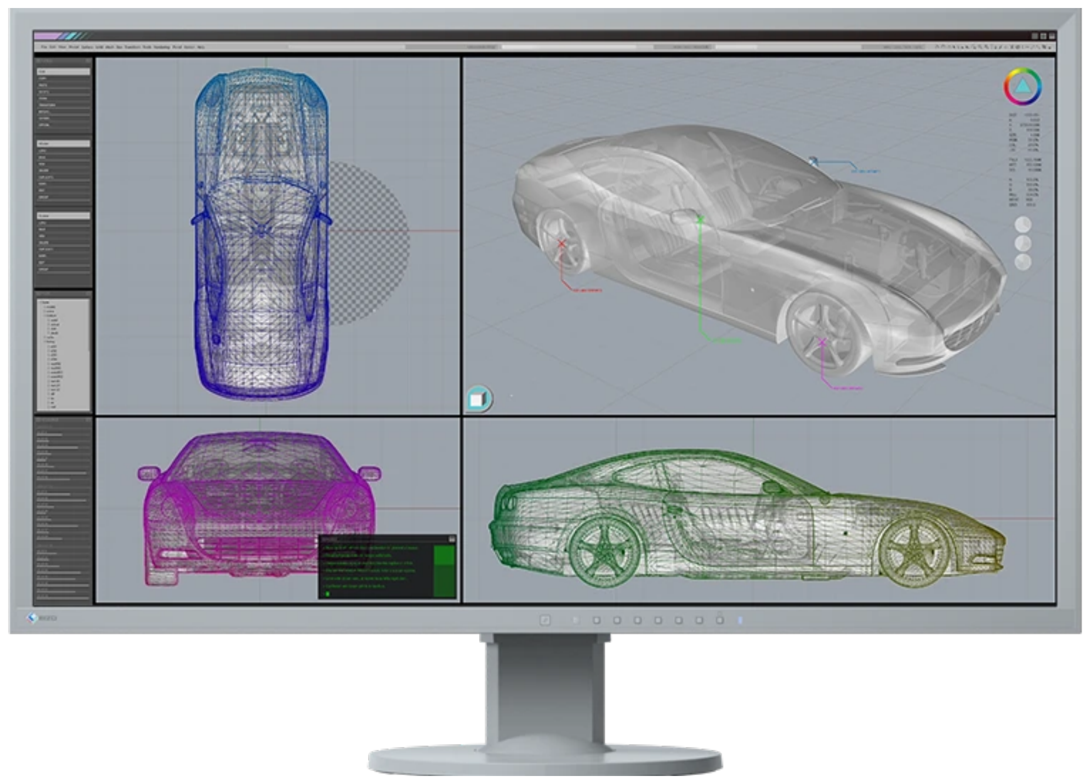

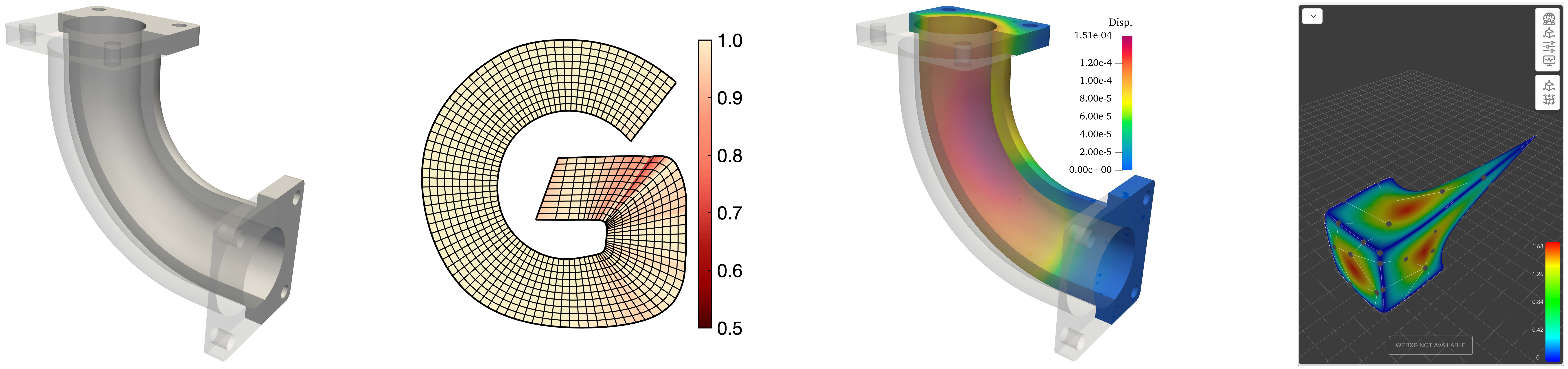
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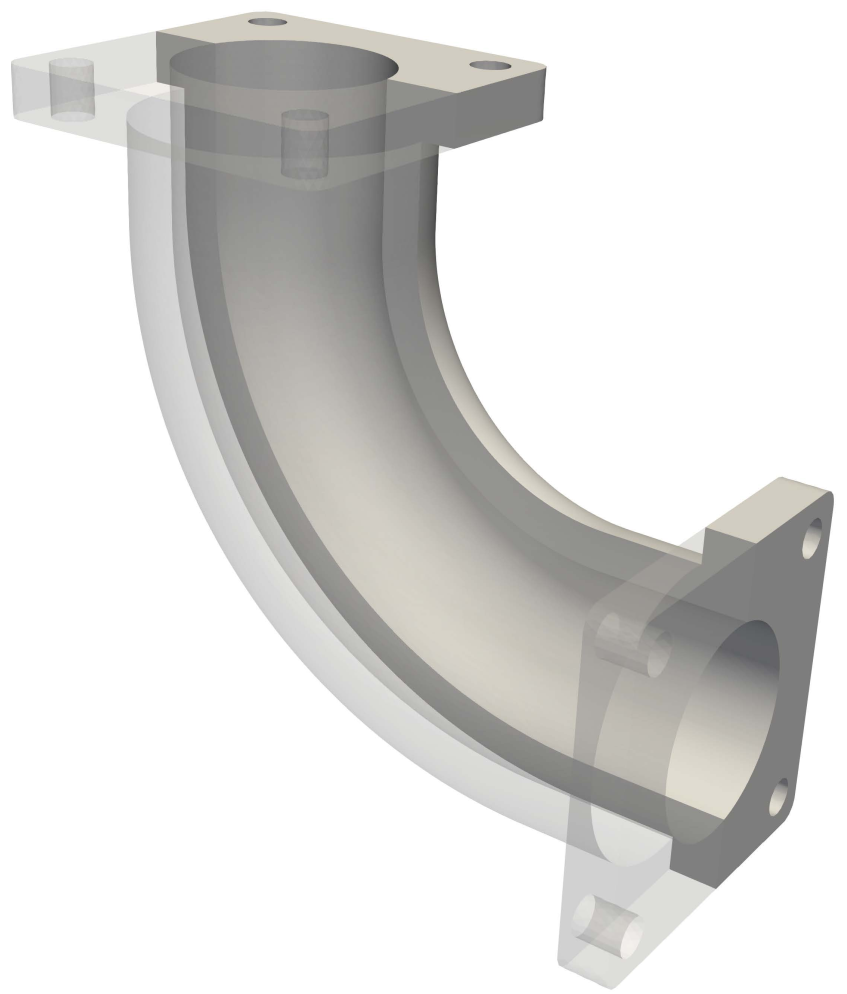
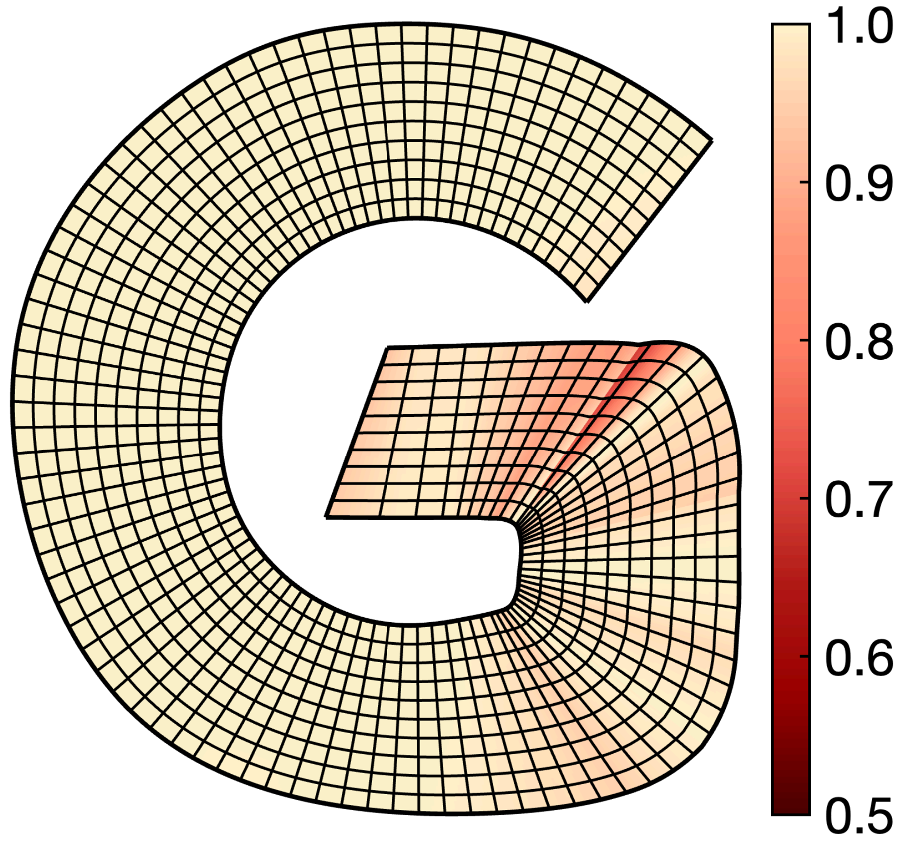
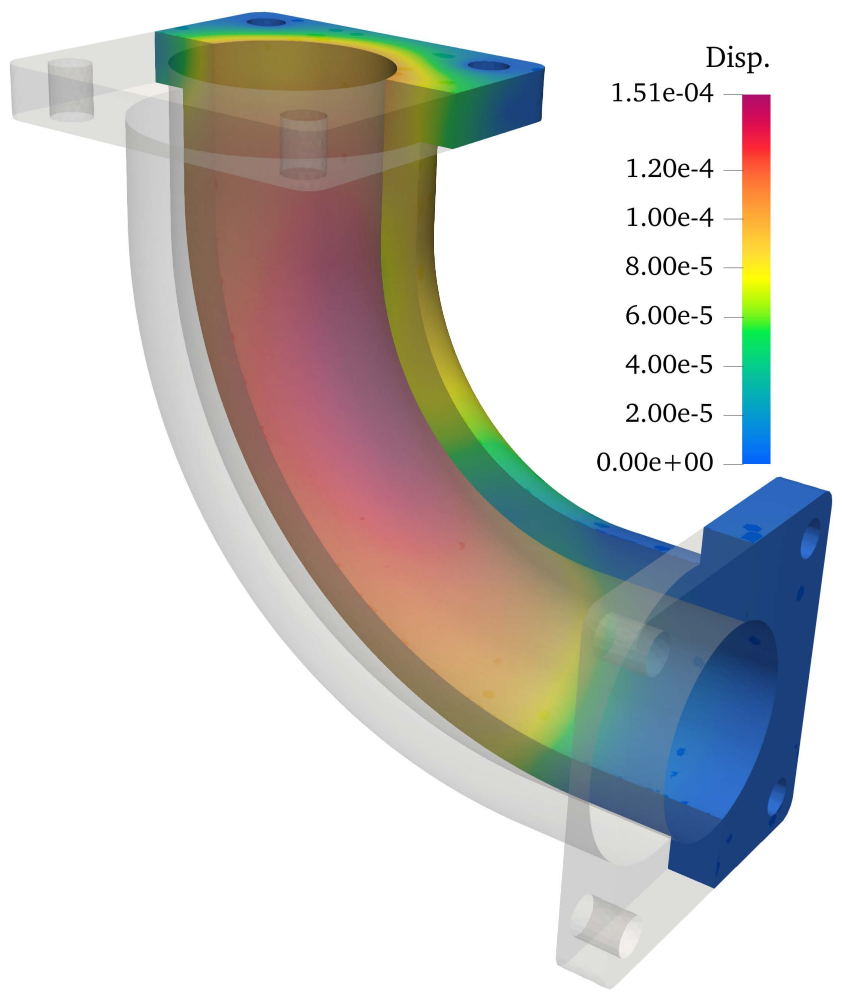


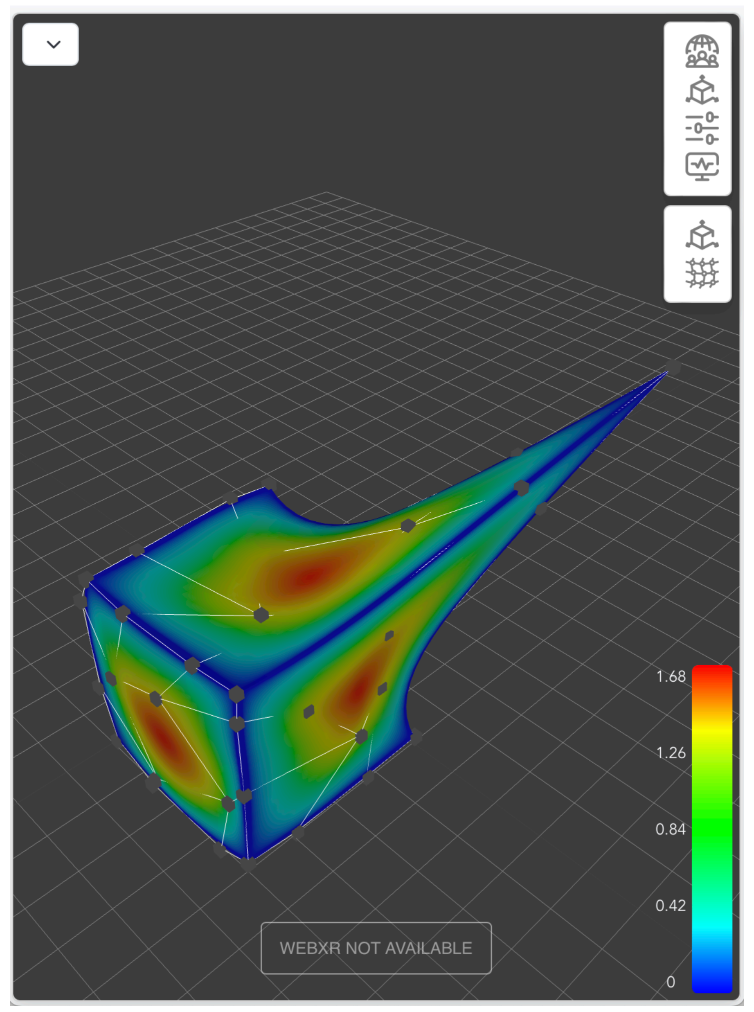
1. Creation of VReps from BReps



2. Reparameterization techniques

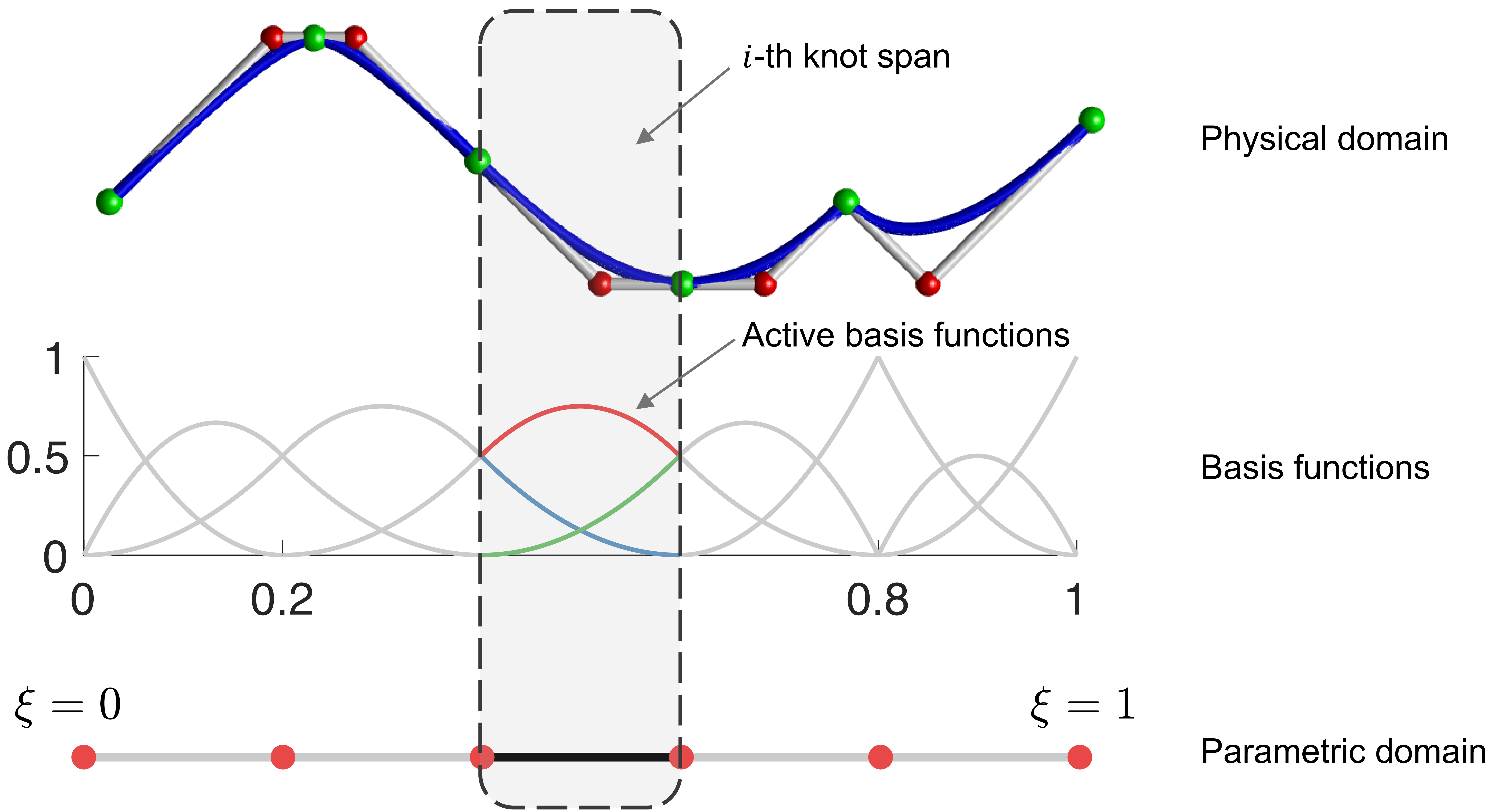


3. Isogeometric Analysis and IgANets

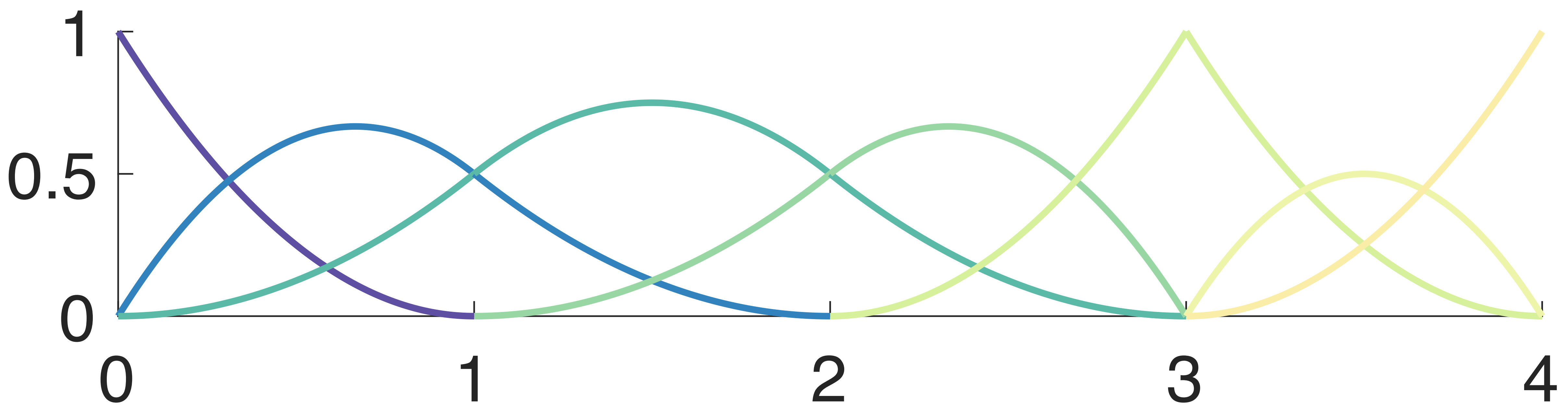


4. Interactive Design-through-Analysis

Spline curves



Univariate B-splines



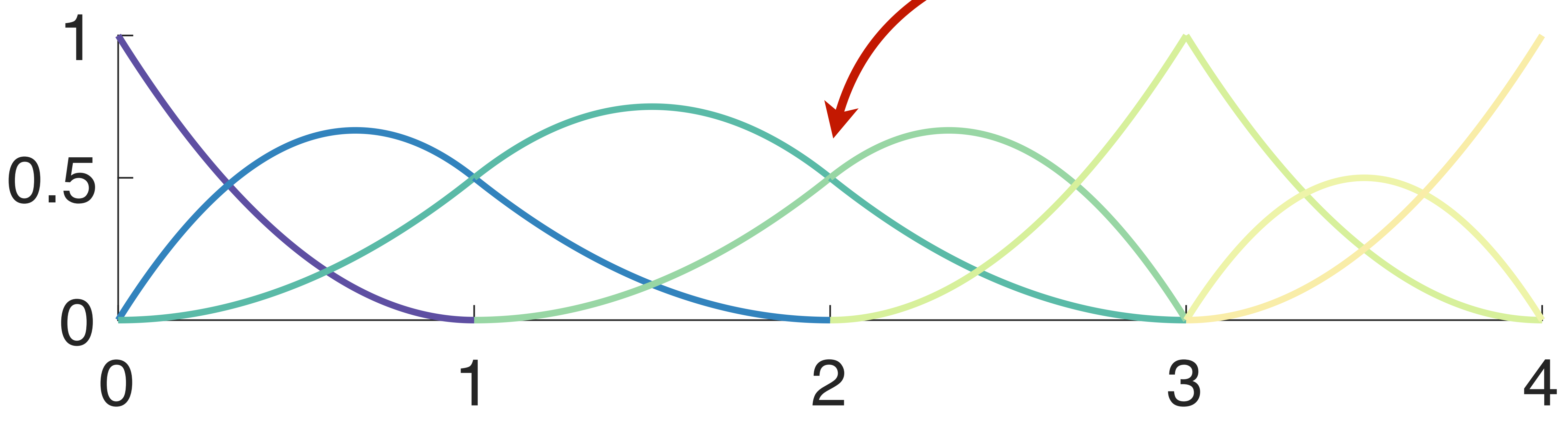
$$\Xi = \{0,0,0,1,2,3,3,4,4,4\}, \quad n = 7, \quad d = 2$$

B-spline basis functions [de Boor, 1971]

$$b^0_{i;\Xi}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

$$b^d_{i;\Xi}(\xi) = \frac{\xi - \xi_i}{\xi_{i+d} - \xi_i} b^{d-1}_{i;\Xi}(\xi) + \frac{\xi_{i+d+1} - \xi}{\xi_{i+d+1} - \xi_{i+1}} b^{d-1}_{i+1;\Xi}(\xi) \qquad ''\frac{0}{0}'' := 0$$

Univariate B-splines



C^{d-1}

$$\Xi = \{0,0,0,1,\boxed{2},3,3,4,4,4\}, \quad n = 7, \quad d = 2$$

B-spline basis functions [de Boor, 1971]

$$b^0_{i;\Xi}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

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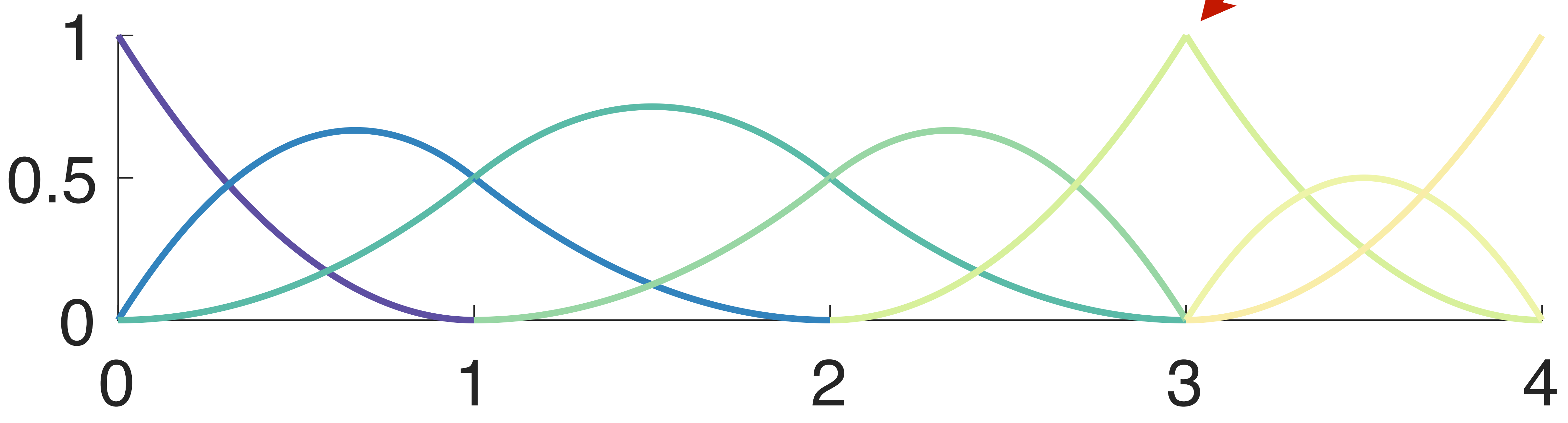
Univariate B-splines



C^{d-2}

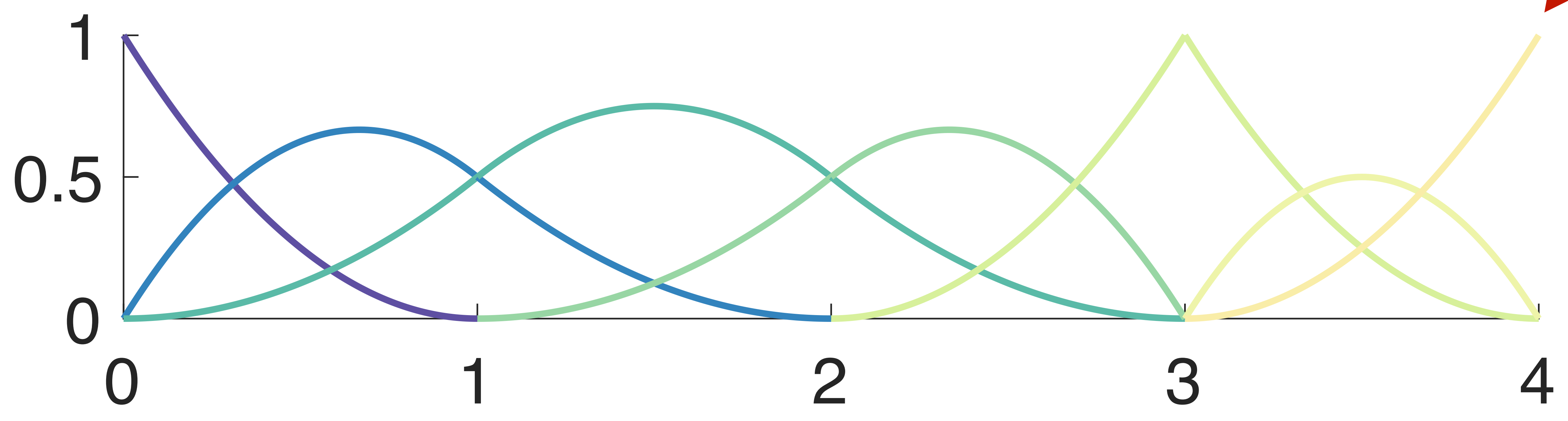
$$\Xi = \{0,0,0,1,2,\boxed{3,3},4,4,4\}, \quad n = 7, \quad d = 2$$

B-spline basis functions [de Boor, 1971]

$$b^0_{i;\Xi}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

$$b^d_{i;\Xi}(\xi) = \frac{\xi - \xi_i}{\xi_{i+d} - \xi_i} b^{d-1}_{i;\Xi}(\xi) + \frac{\xi_{i+d+1} - \xi}{\xi_{i+d+1} - \xi_{i+1}} b^{d-1}_{i+1;\Xi}(\xi) \qquad ''\frac{0}{0}'' := 0$$

Univariate B-splines



C^{d-3}

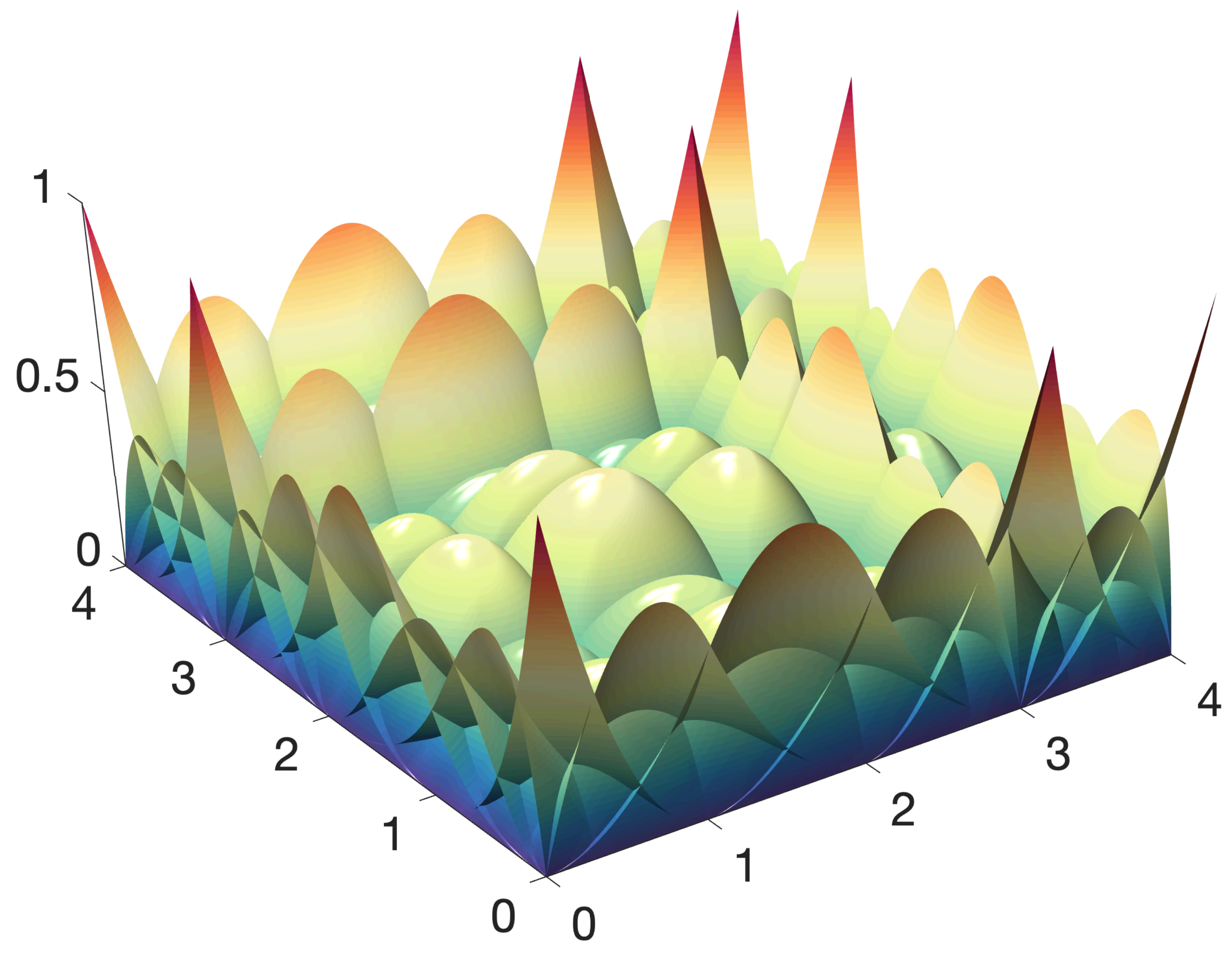
$$\Xi = \{0,0,0,1,2,3,3,\boxed{4,4,4}\}, \quad n = 7, \quad d = 2$$

B-spline basis functions [de Boor, 1971]

$$b^0_{i;\Xi}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

$$b^d_{i;\Xi}(\xi) = \frac{\xi - \xi_i}{\xi_{i+d} - \xi_i} b^{d-1}_{i;\Xi}(\xi) + \frac{\xi_{i+d+1} - \xi}{\xi_{i+d+1} - \xi_{i+1}} b^{d-1}_{i+1;\Xi}(\xi) \qquad ``\frac{0}{0}" := 0$$

Multivariate B-splines



Tensor-product basis functions

$$b^{\mathbf{d}}_{\mathbf{i};\boldsymbol{\Xi}}(\boldsymbol{\xi}) = \prod_{k=1}^{p} b^{d_k}_{i_k;\Xi_k}(\xi_k)$$

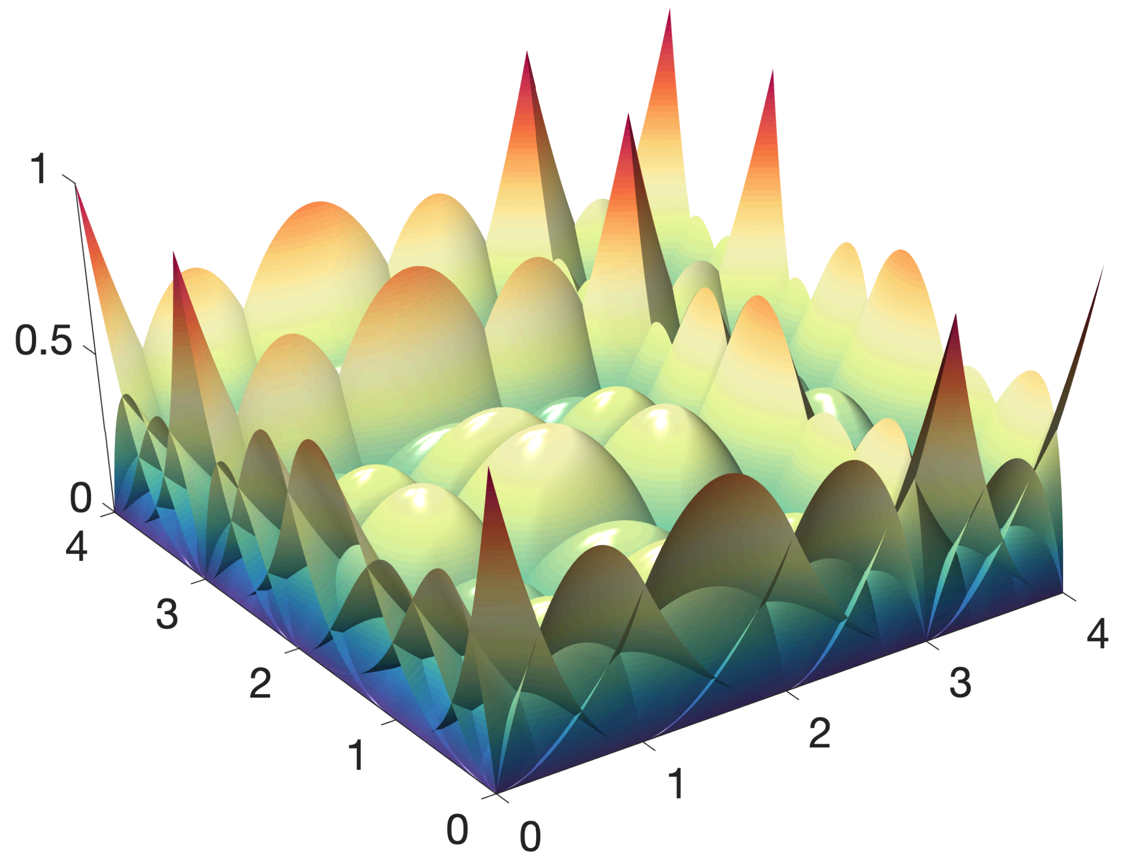
with multi-indices $\mathbf{i}$ and $\mathbf{d}$, $\boldsymbol{\Xi} = \left(\Xi_1, \ldots, \Xi_p\right)$ and parametric domain

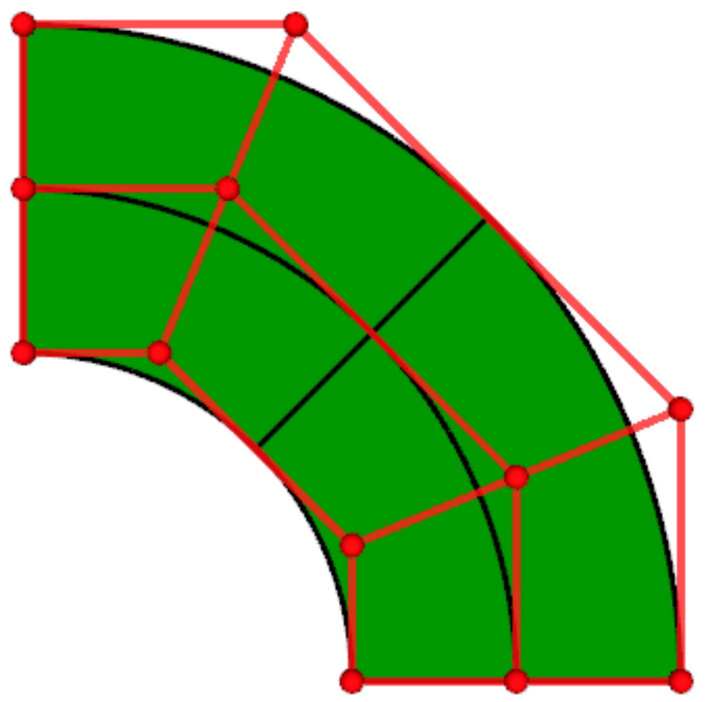
$$\hat{\Omega}_{\boldsymbol{\Xi}} = \bigotimes_{k=1}^{p} [\xi_{k,d_k+1}, \xi_{k,n_k})$$

Spline space

$$\mathbb{S}^{\mathbf{d},s}_{\boldsymbol{\Xi}} = \text{span}\left\{b^{\mathbf{d}}_{\mathbf{1};\boldsymbol{\Xi}}, \ldots, b^{\mathbf{d}}_{\mathbf{n};\boldsymbol{\Xi}}\right\} = \left\{\sum_{\mathbf{i}=\mathbf{1}}^{\mathbf{n}} c_{\mathbf{i}}\, b^{\mathbf{d}}_{\mathbf{i};\boldsymbol{\Xi}}(\boldsymbol{\xi}) \ : \ c_{\mathbf{i}} \in \mathbb{R}^s, \text{for } \mathbf{1} \leq \mathbf{i} \leq \mathbf{n}, \boldsymbol{\xi} \in \hat{\Omega}_{\boldsymbol{\Xi}}\right\}$$

Isogeometric analysis in a nutshell

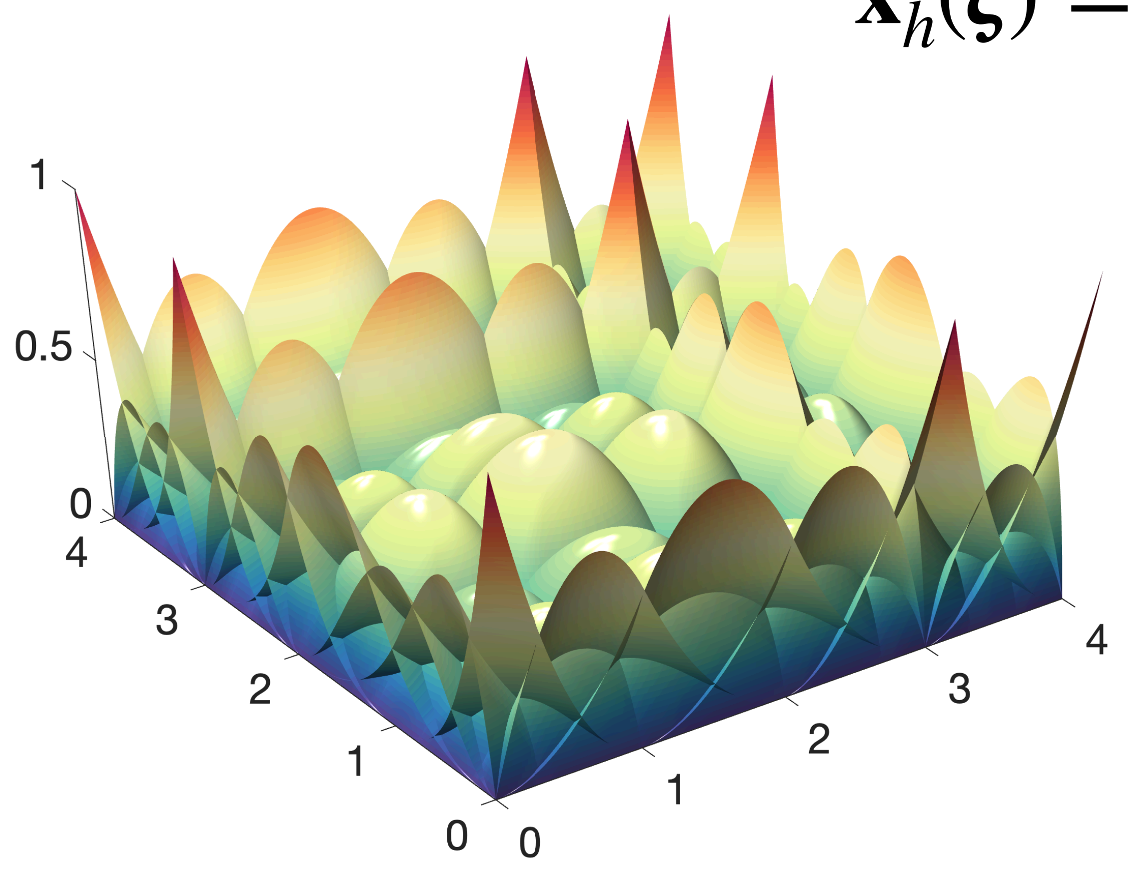


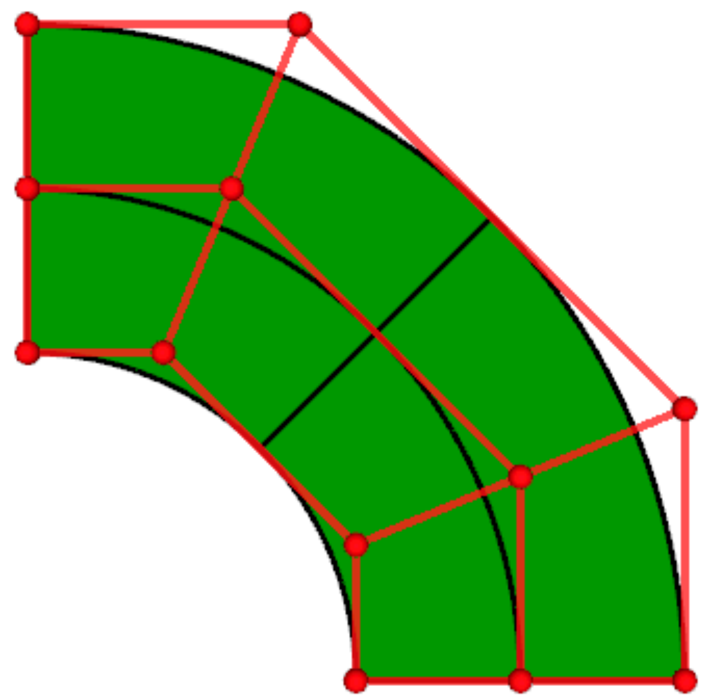


Isogeometric analysis in a nutshell

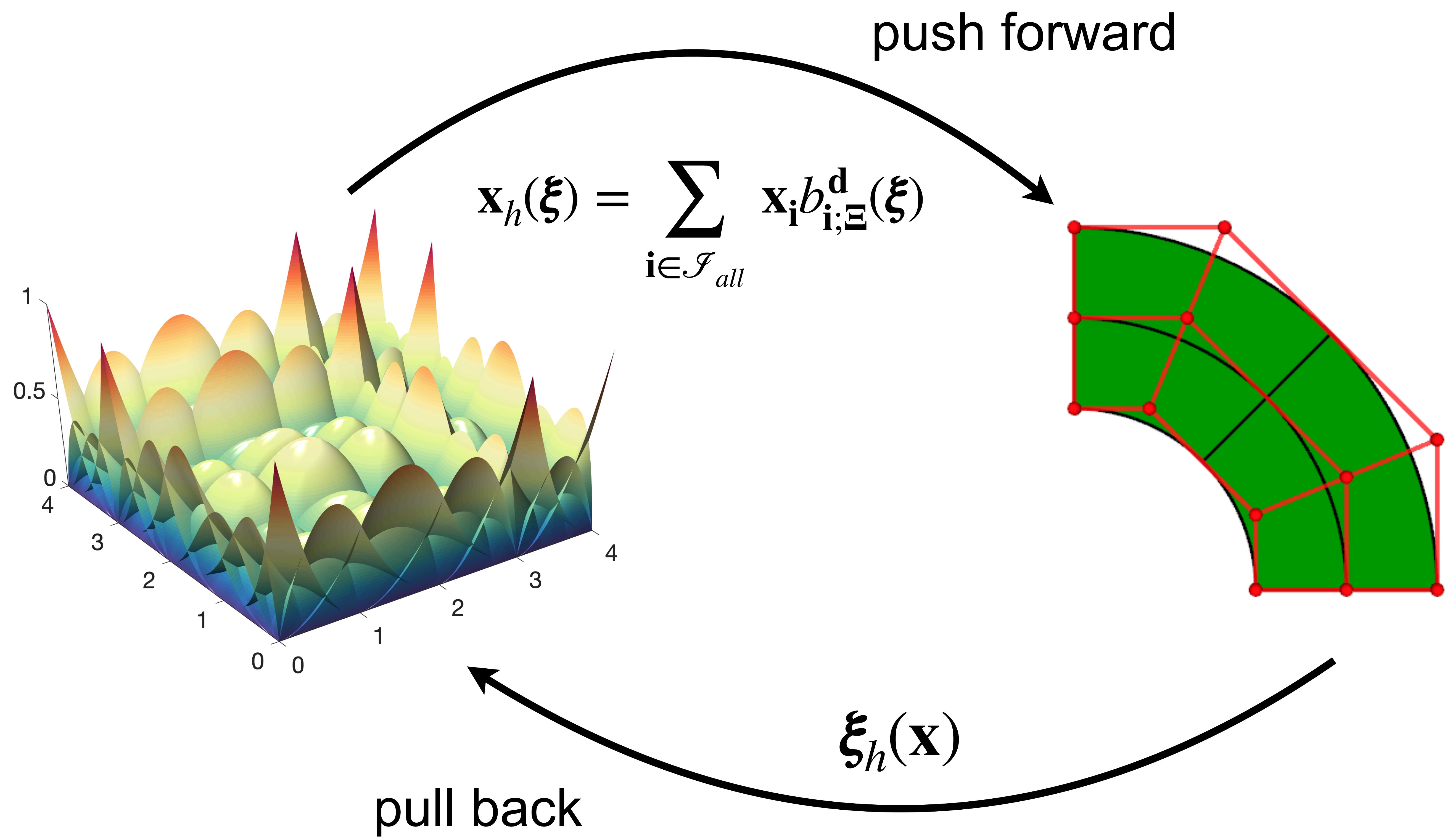
push forward

$$\mathbf{x}_h(\boldsymbol{\xi}) = \sum_{\mathbf{i}\in\mathscr{I}_{all}} \mathbf{x}_{\mathbf{i}} b^{\mathbf{d}}_{\mathbf{i};\Xi}(\boldsymbol{\xi})$$

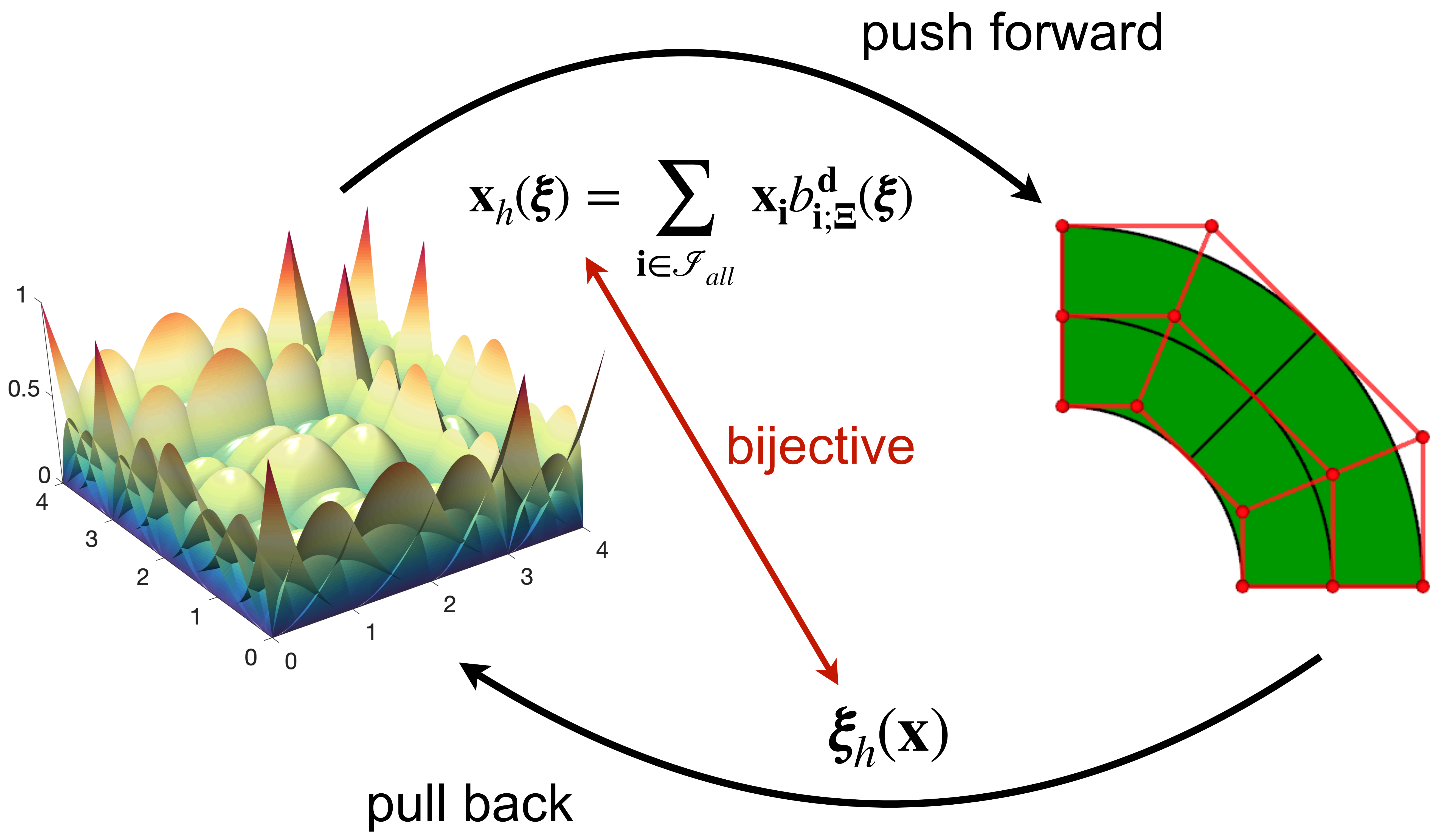




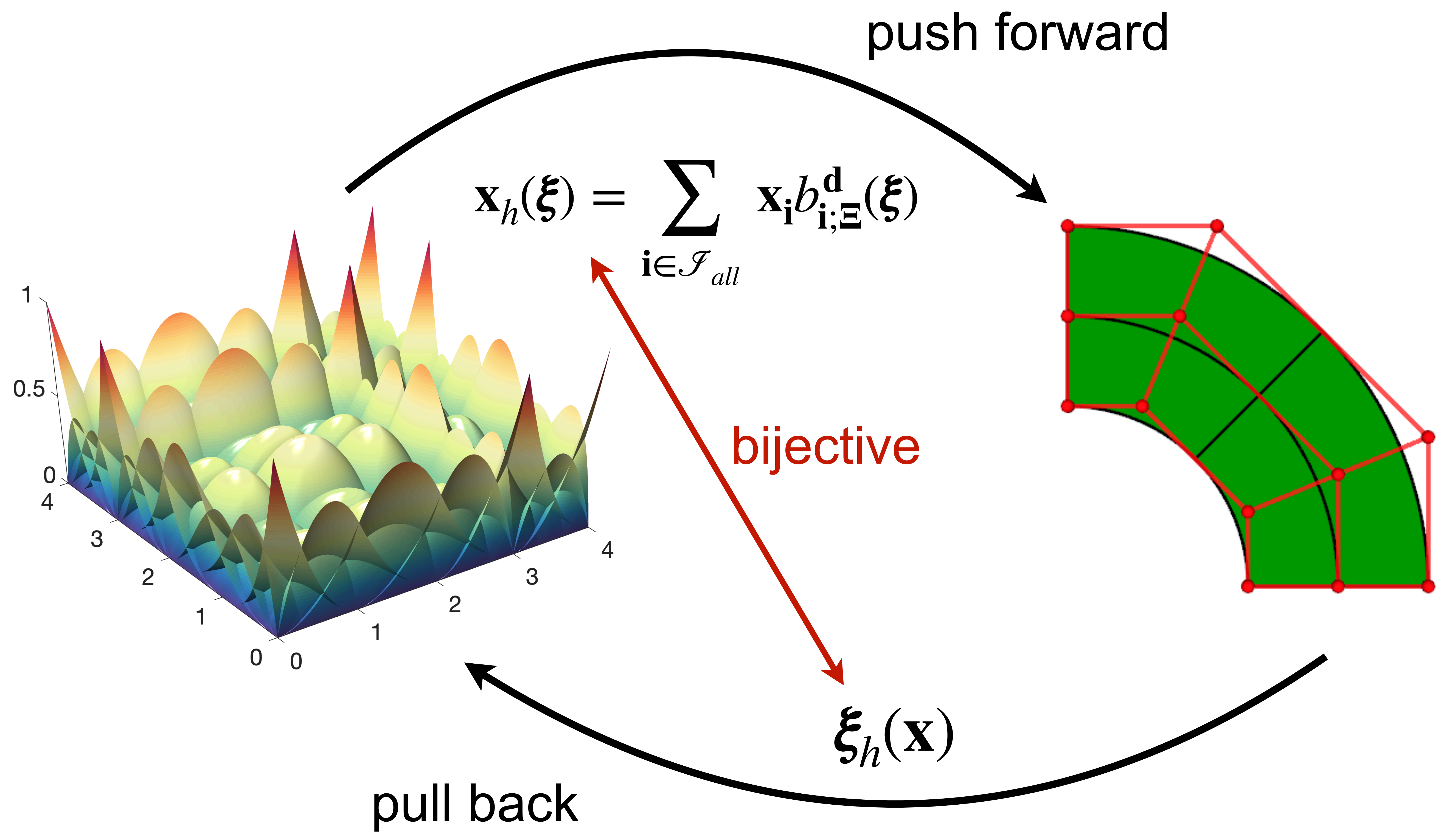
Isogeometric analysis in a nutshell

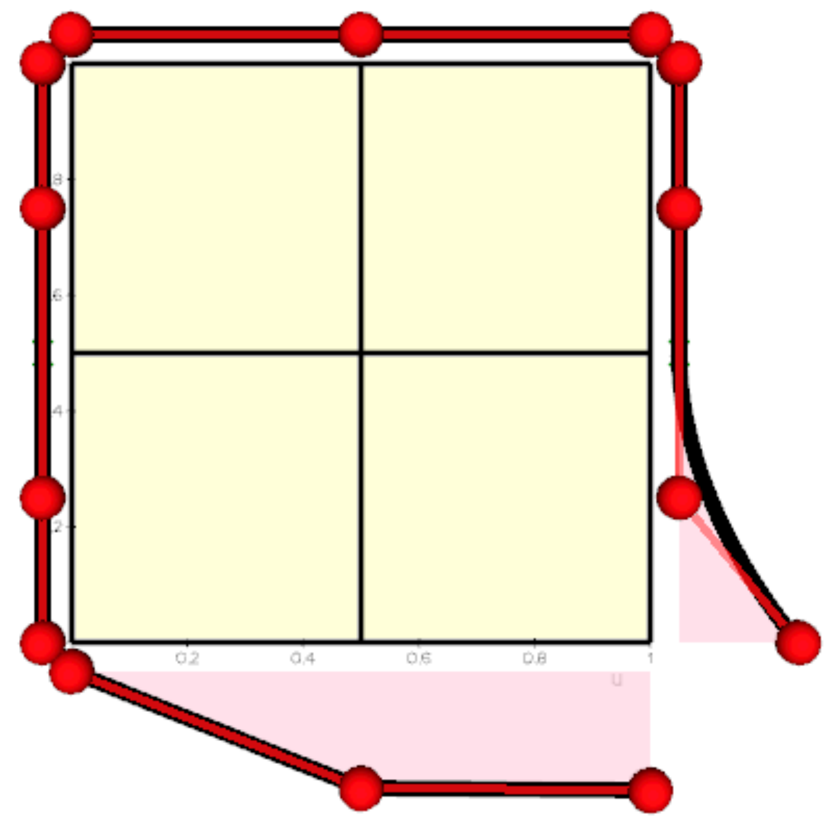


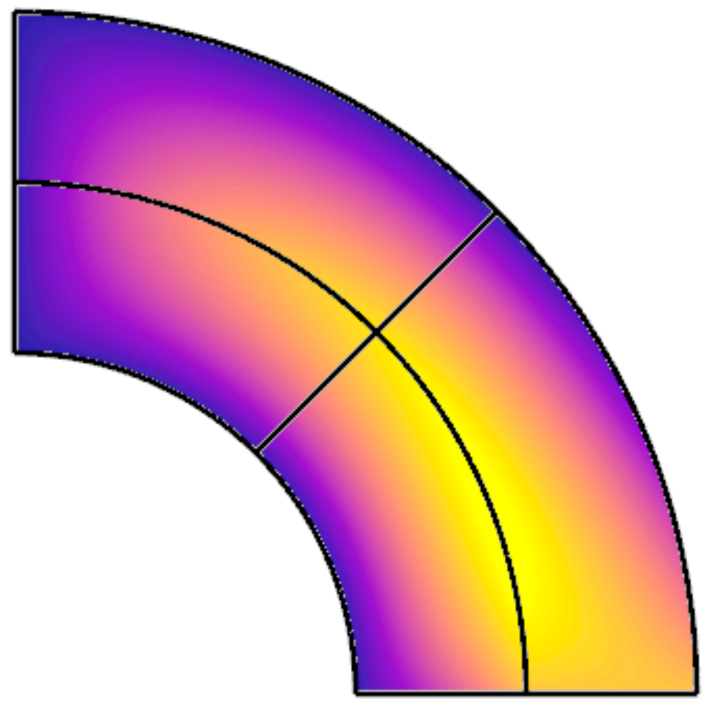
Isogeometric analysis in a nutshell



Isogeometric analysis in a nutshell

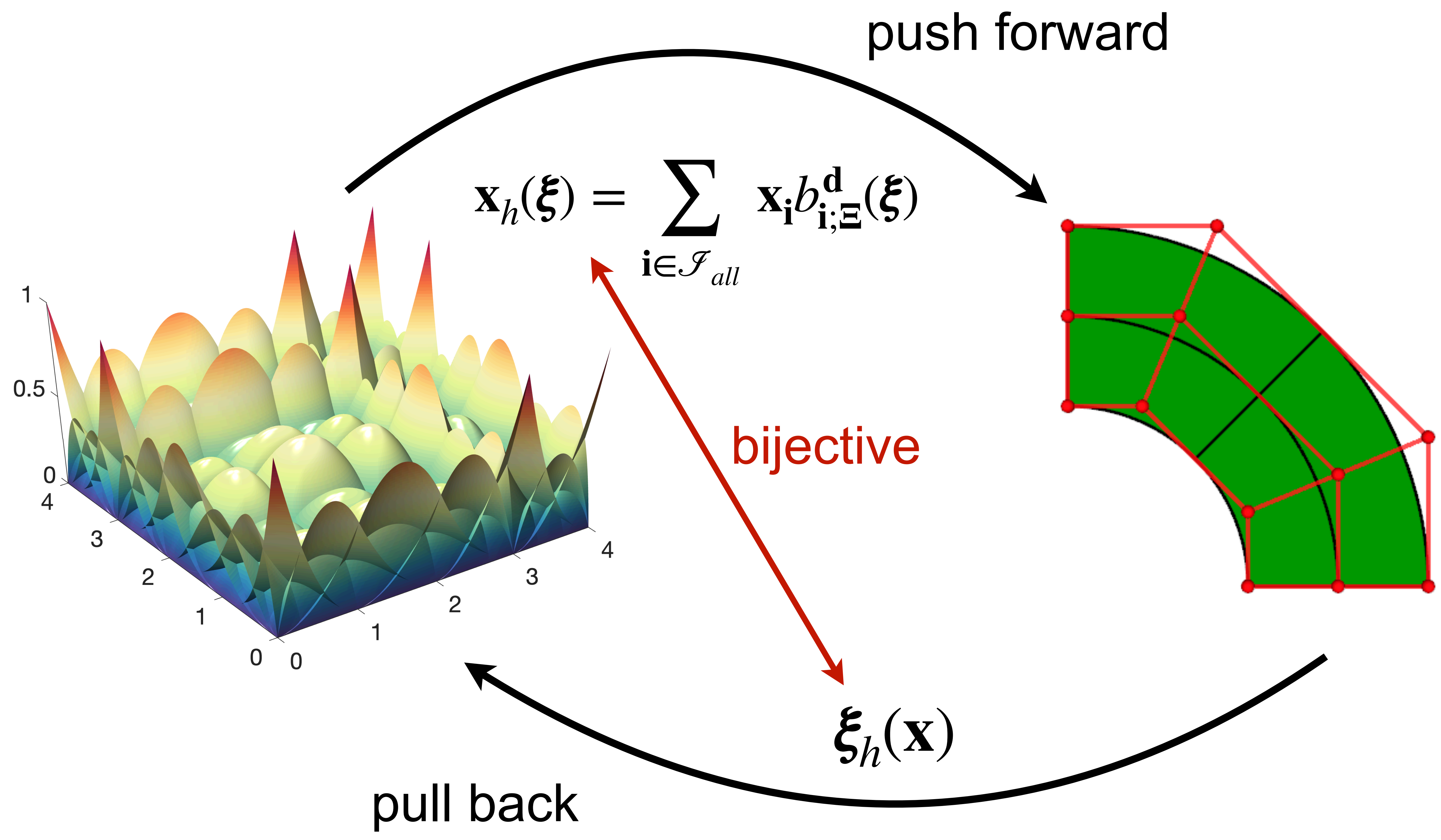


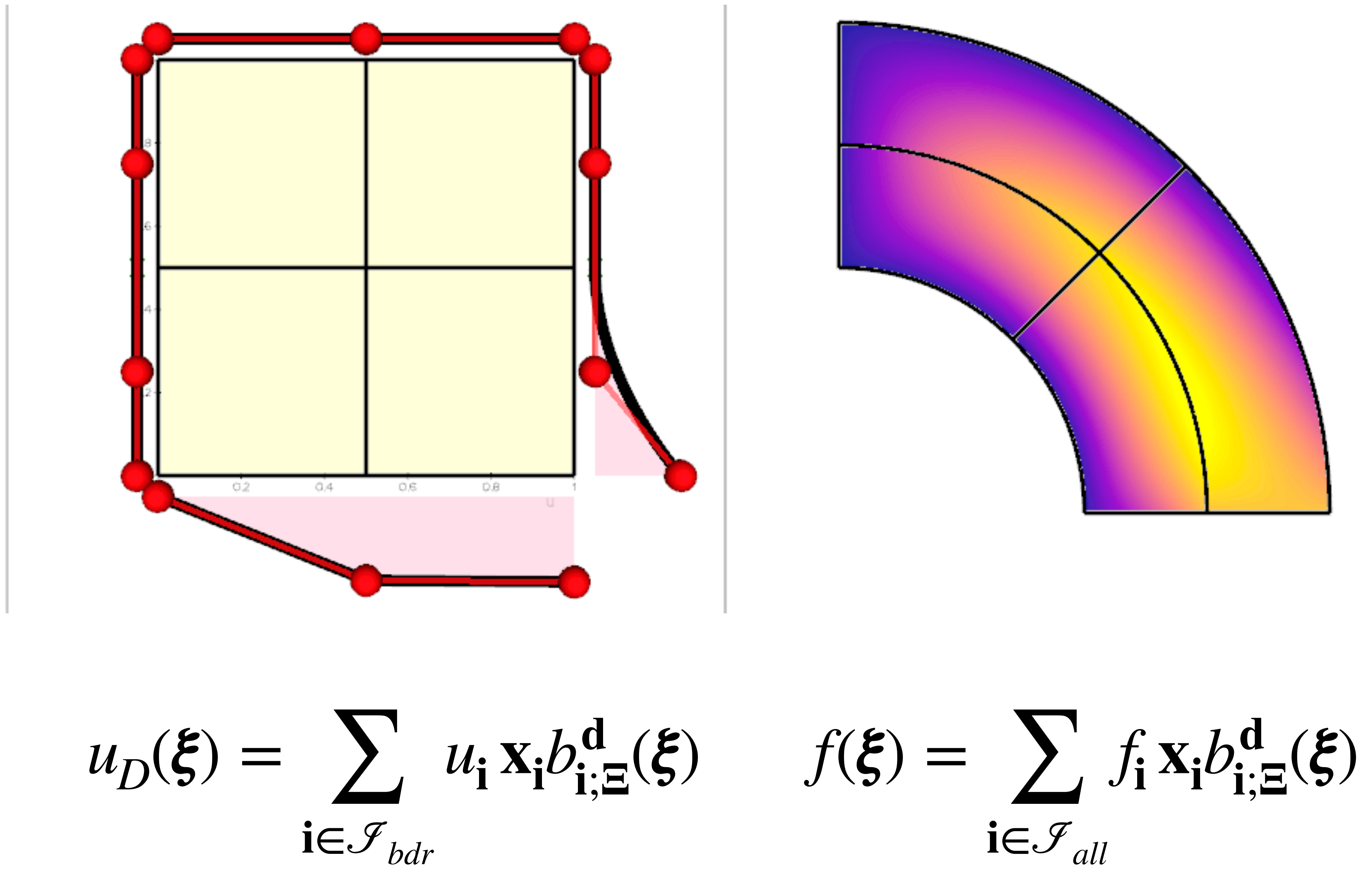




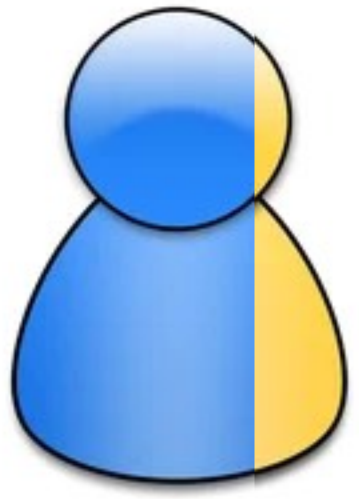
$$u_D(\boldsymbol{\xi}) = \sum_{\mathbf{i}\in\mathcal{I}_{bdr}} u_{\mathbf{i}}\, \mathbf{x}_{\mathbf{i}} b^{\mathbf{d}}_{\mathbf{i};\Xi}(\boldsymbol{\xi}) \qquad f(\boldsymbol{\xi}) = \sum_{\mathbf{i}\in\mathcal{I}_{all}} f_{\mathbf{i}}\, \mathbf{x}_{\mathbf{i}} b^{\mathbf{d}}_{\mathbf{i};\Xi}(\boldsymbol{\xi})$$

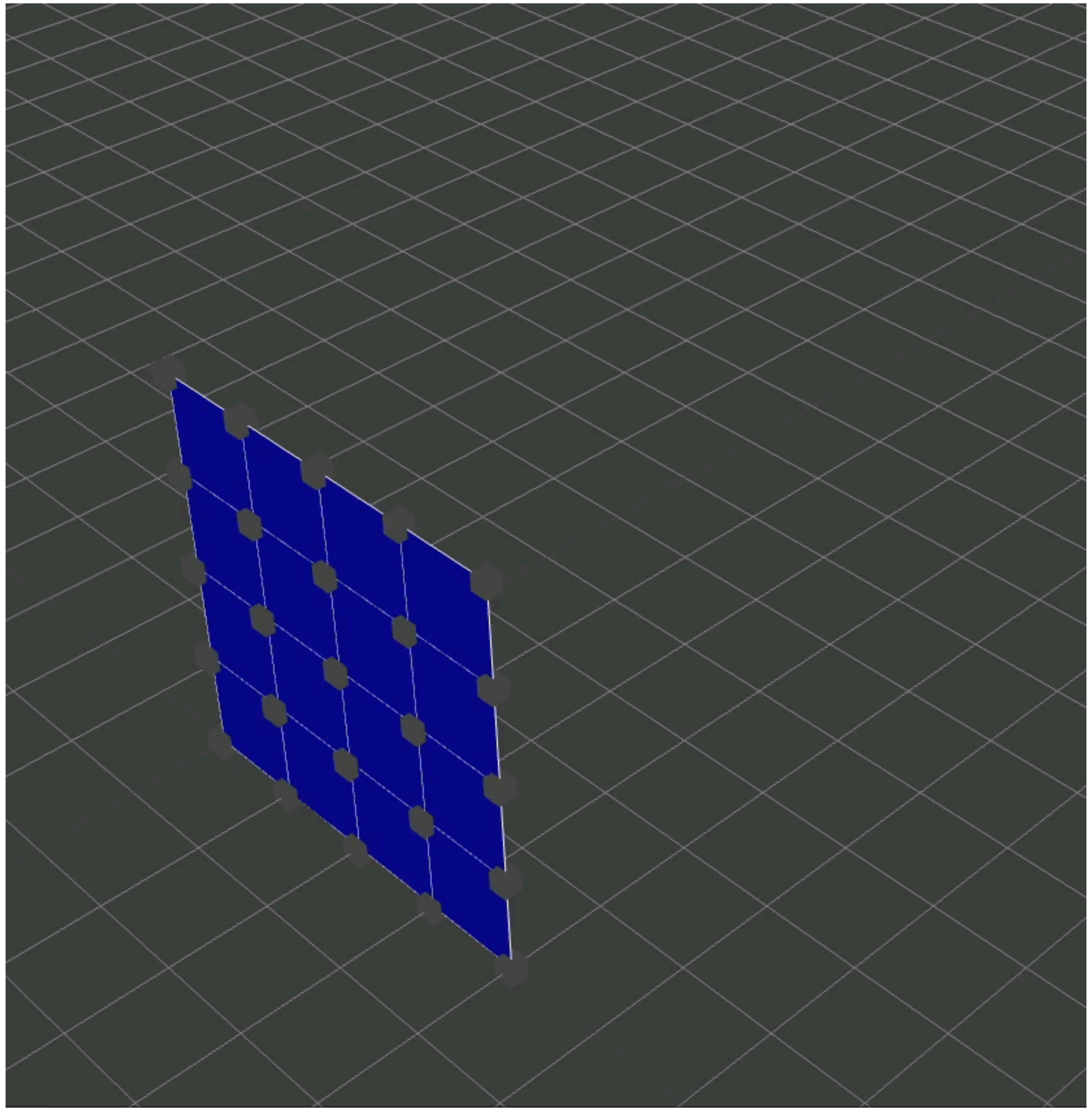
Isogeometric analysis in a nutshell

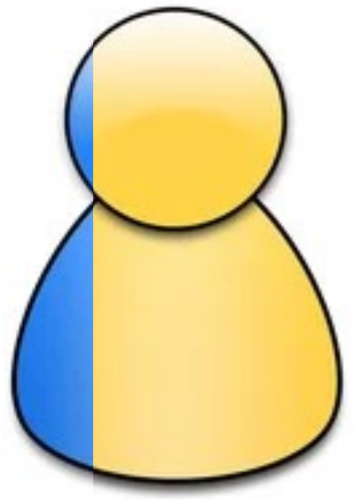




Compute solution $u(\boldsymbol{\xi}) = u_D(\boldsymbol{\xi}) + \sum_{\mathbf{i}\in\mathcal{I}_{int}} u_{\mathbf{i}}\, \mathbf{x}_{\mathbf{i}} b^{\mathbf{d}}_{\mathbf{i};\Xi}(\boldsymbol{\xi})$ using Galerkin or collocation IGA

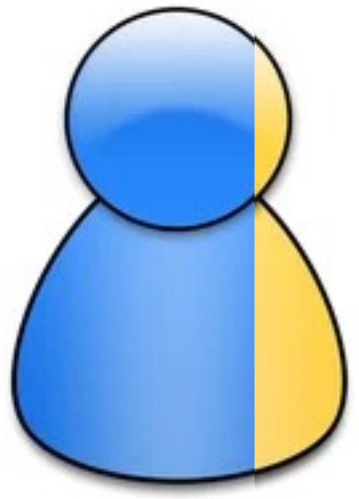






CAD

FEA



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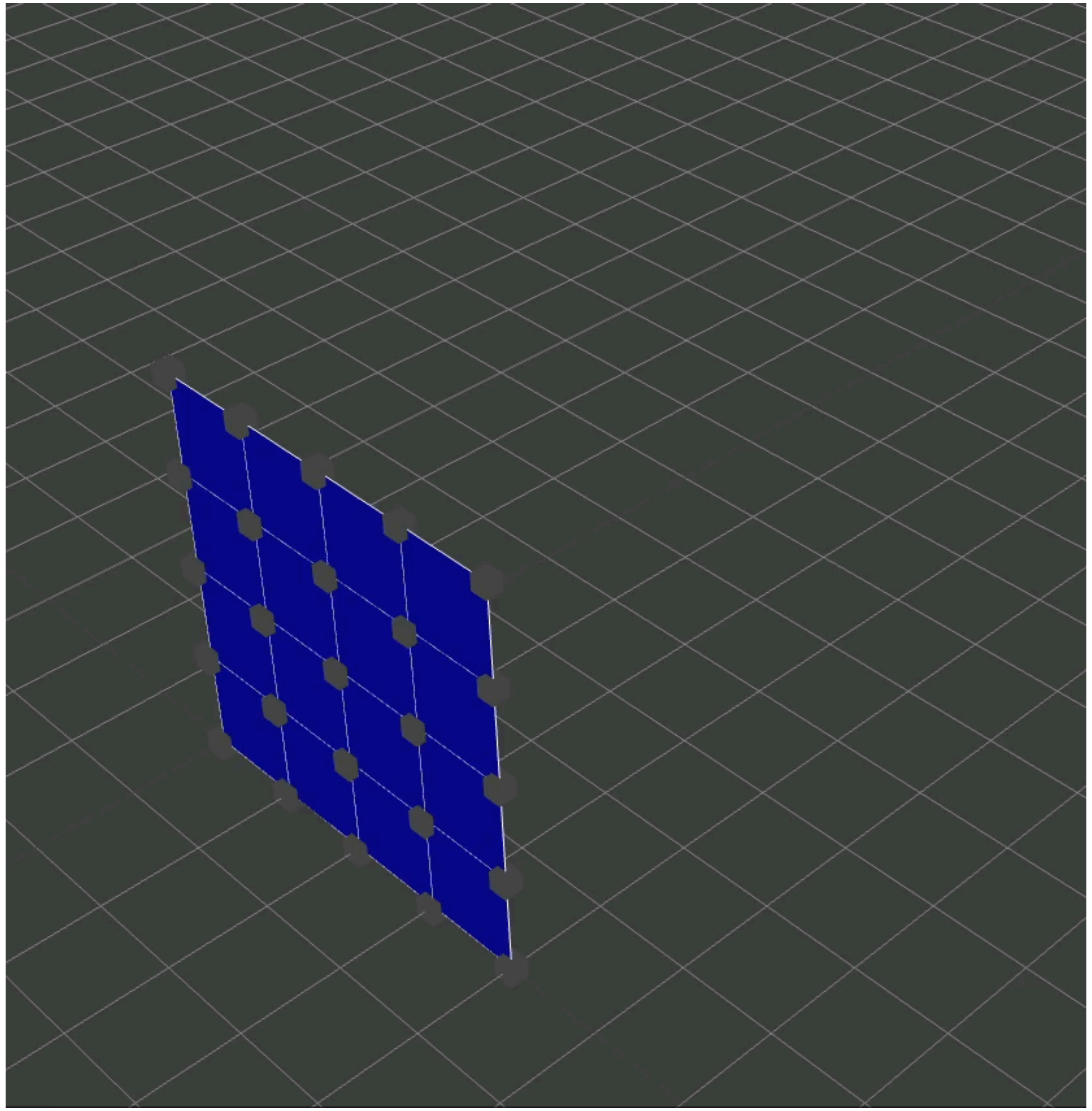

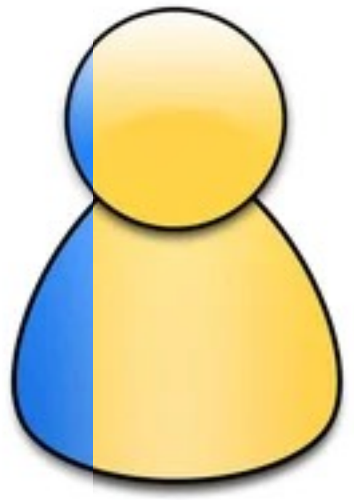

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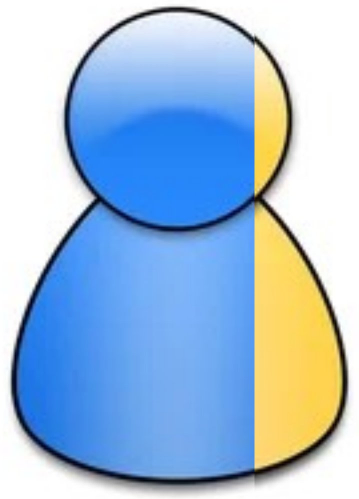

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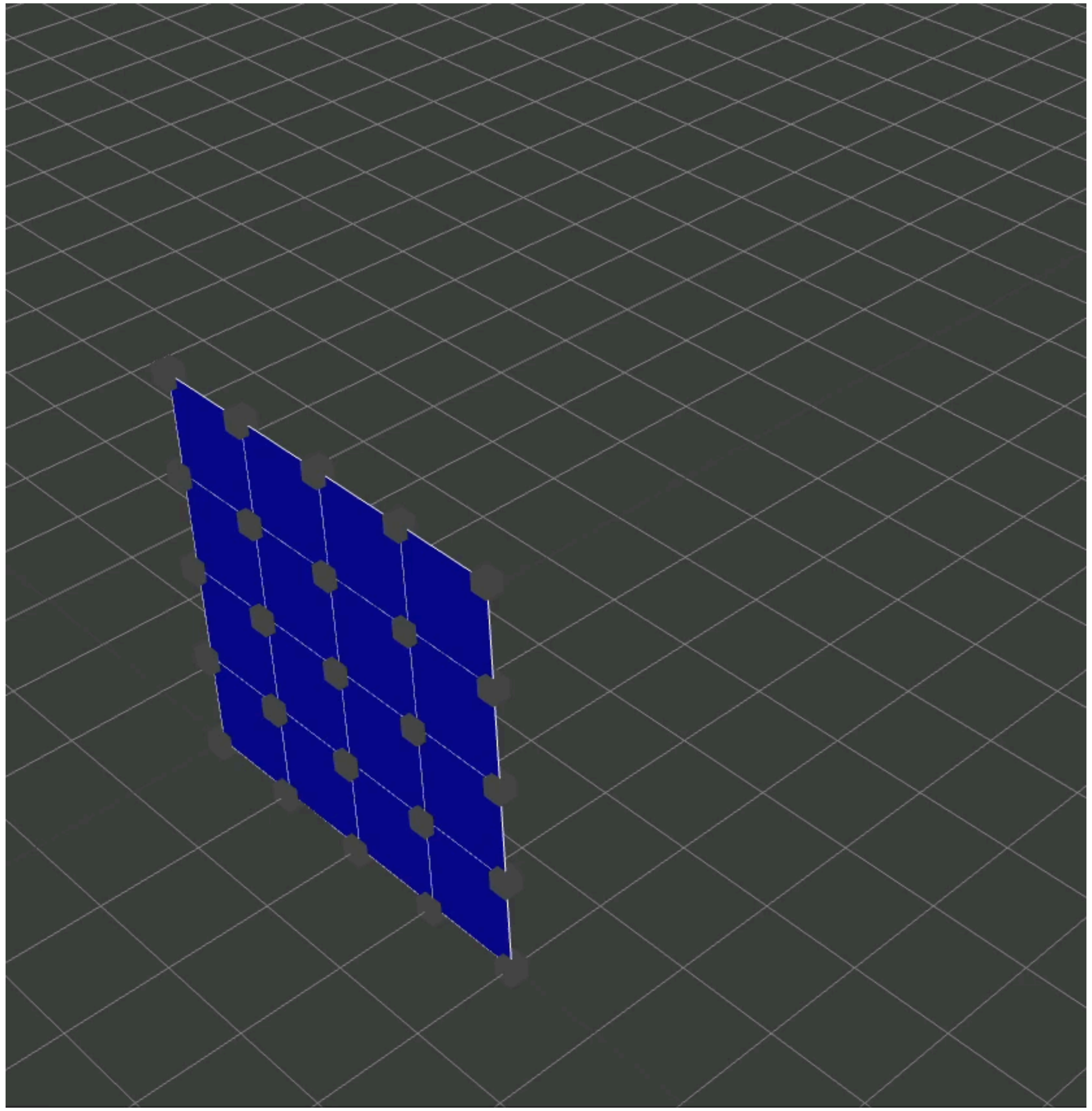
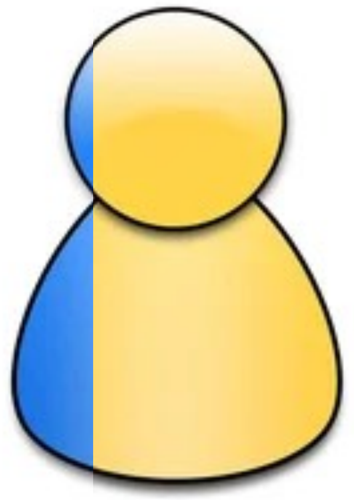


Automatic reparameterization of surfaces!



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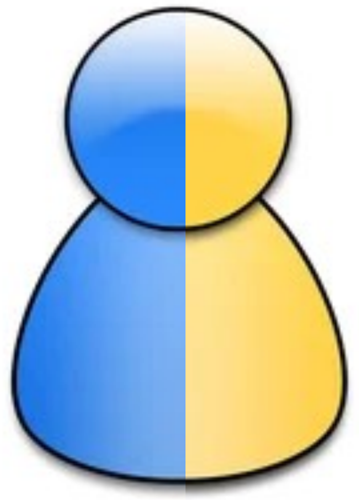

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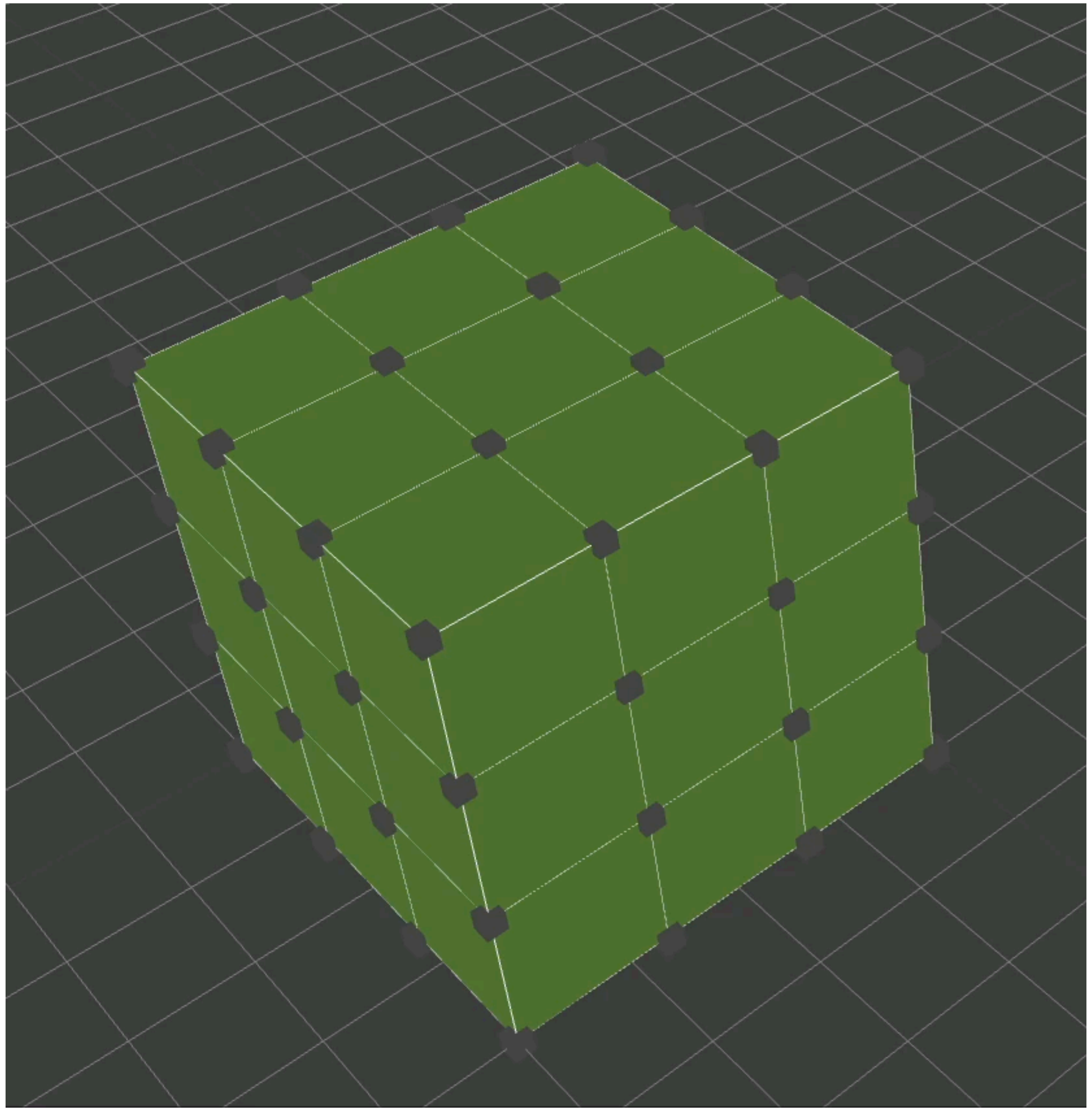

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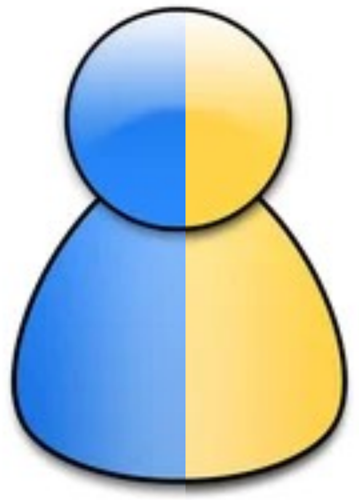
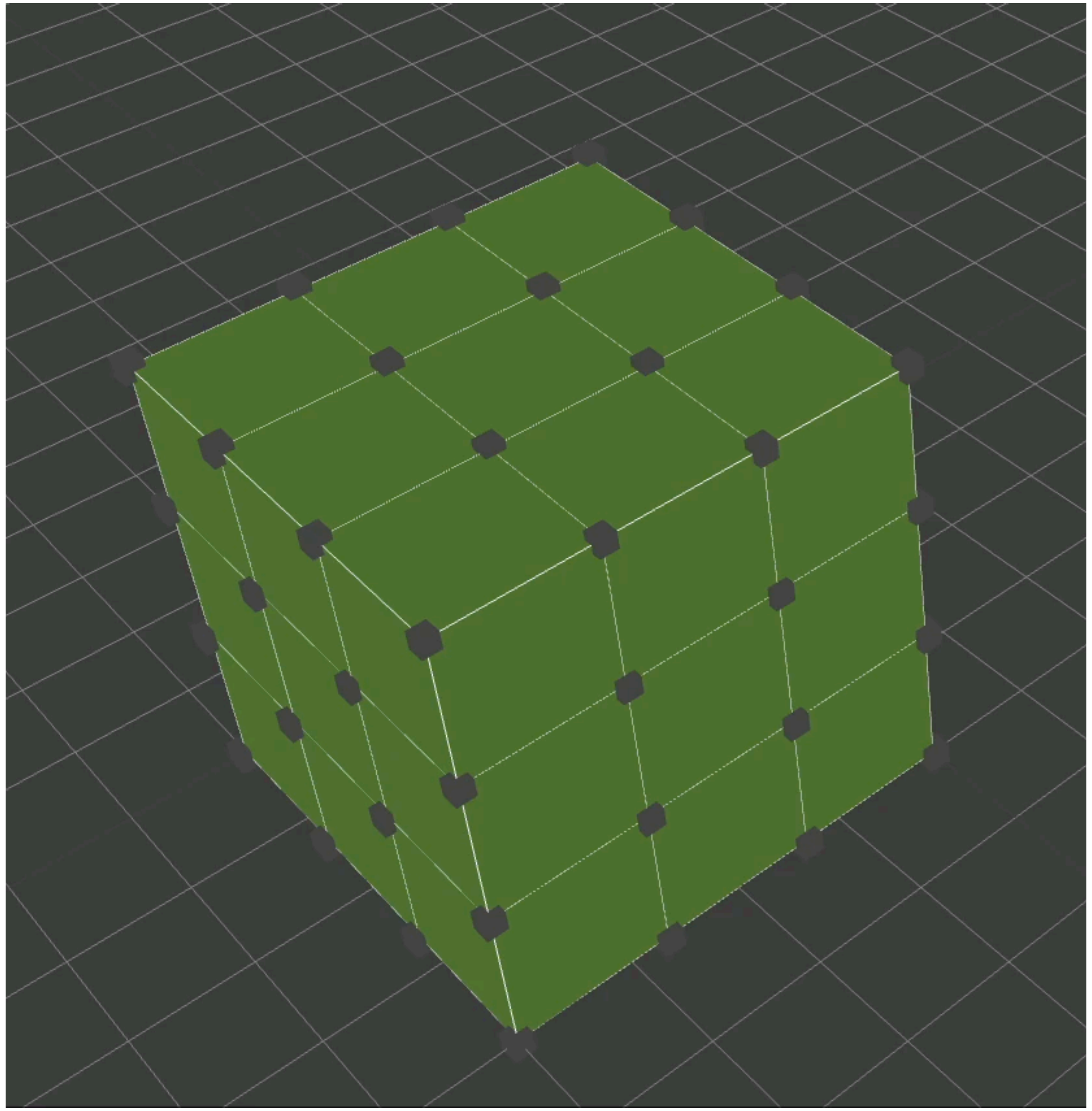
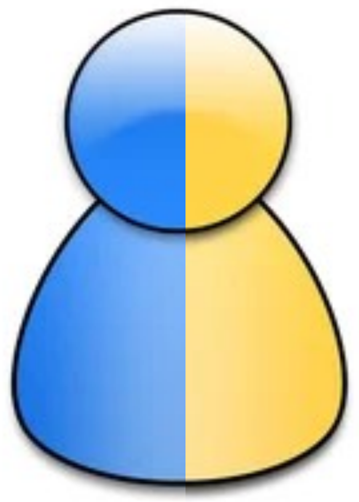




CAD

FEA



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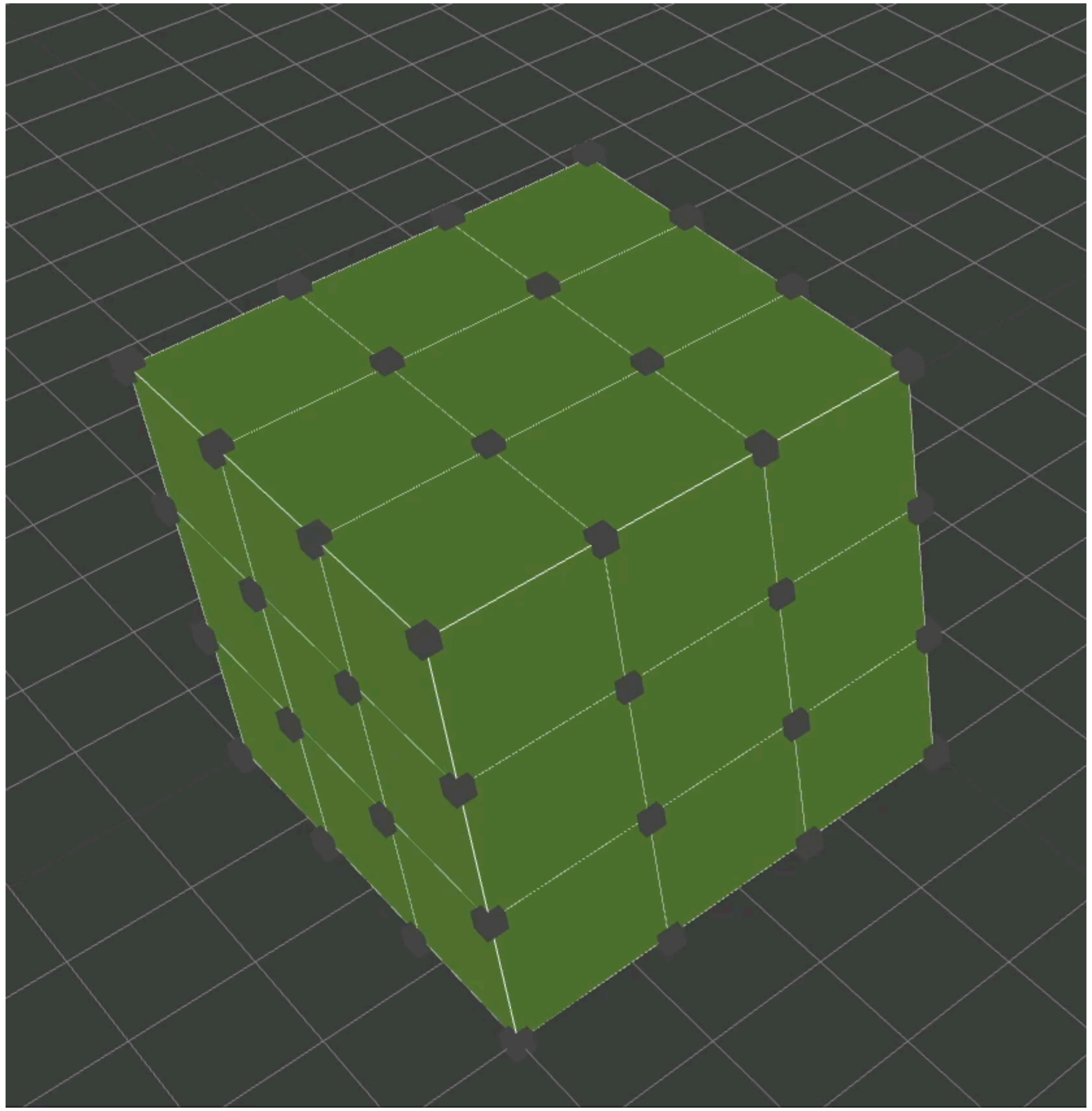


Automatic placement of interior control points!

FEA

Creation of analysis-suitable parameterizations

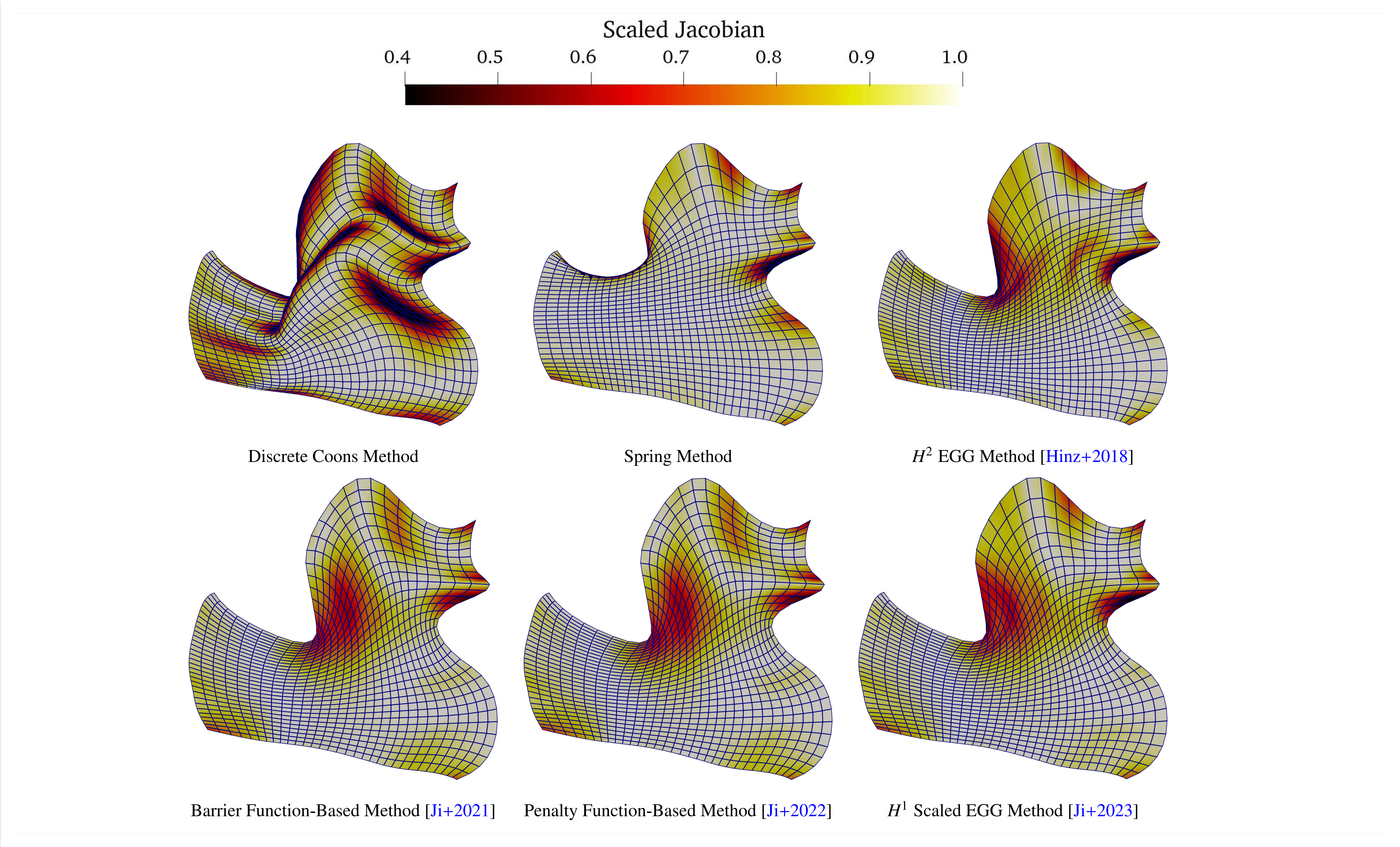
Algebraic methods

- Coons patch [Farin et al. 1999]
- spring patch [Gravesen et al. 2012], …

Nonlinear methods

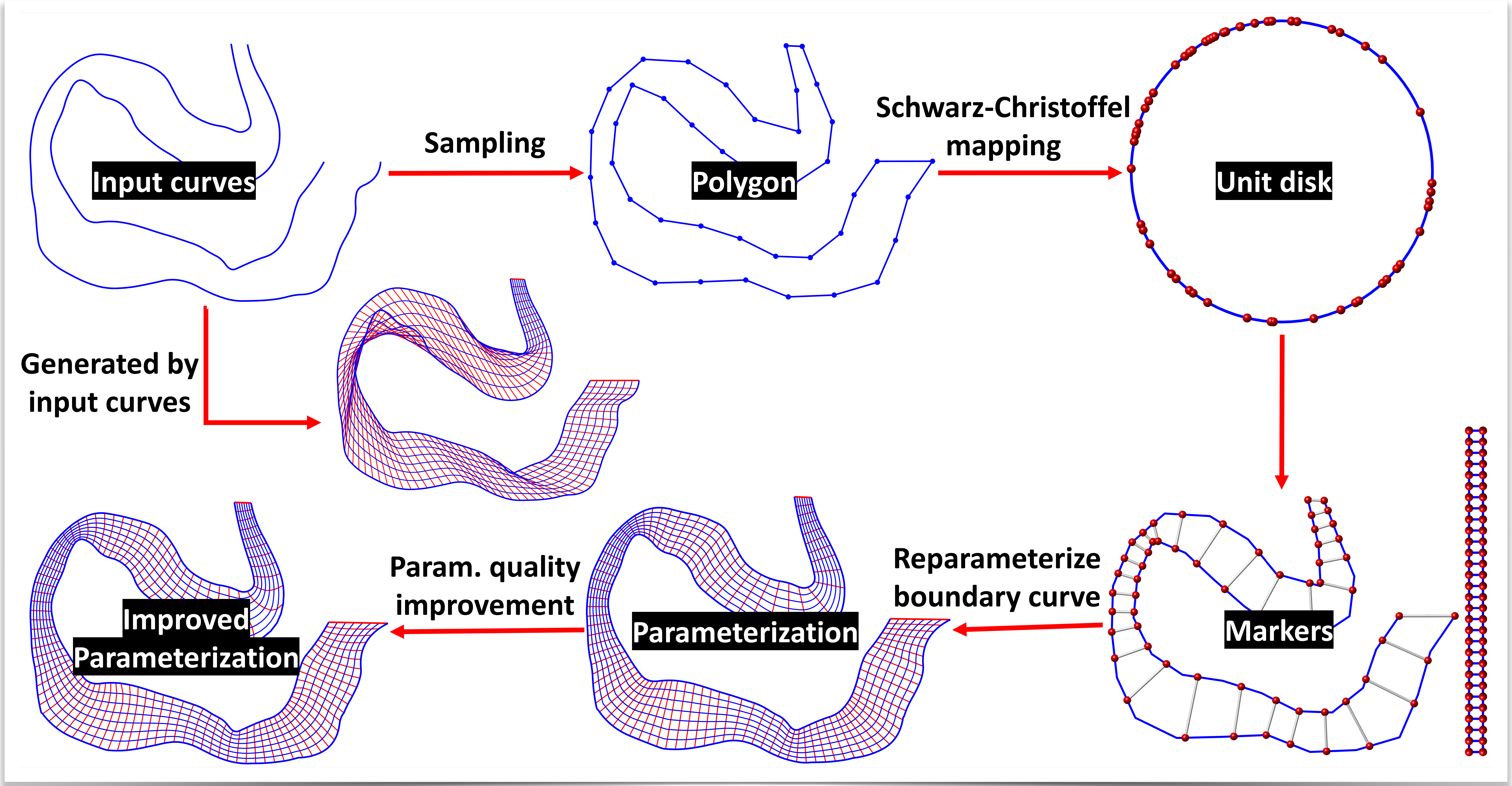
- constrained optimization [Wang et al. 2014, Pan et al. 2020],
- unconstrained optimization: barrier functions [Ji et al. 2021], penalty functions [Wang 2021, Ji 2022]
- Teichmüller mappings [Chen et al. 2016], low-rank quasi-conformal mappings [Pan et al. 2024], harmonic mappings [Martin et al. 2009, Nguyen et al. 2010, Xu et al. 2013, Falini et al. 2015]
- PDE-based methods [Hinz et al. 2018 & 2020, Ji et al. 2023]
- …

Comparison of methods



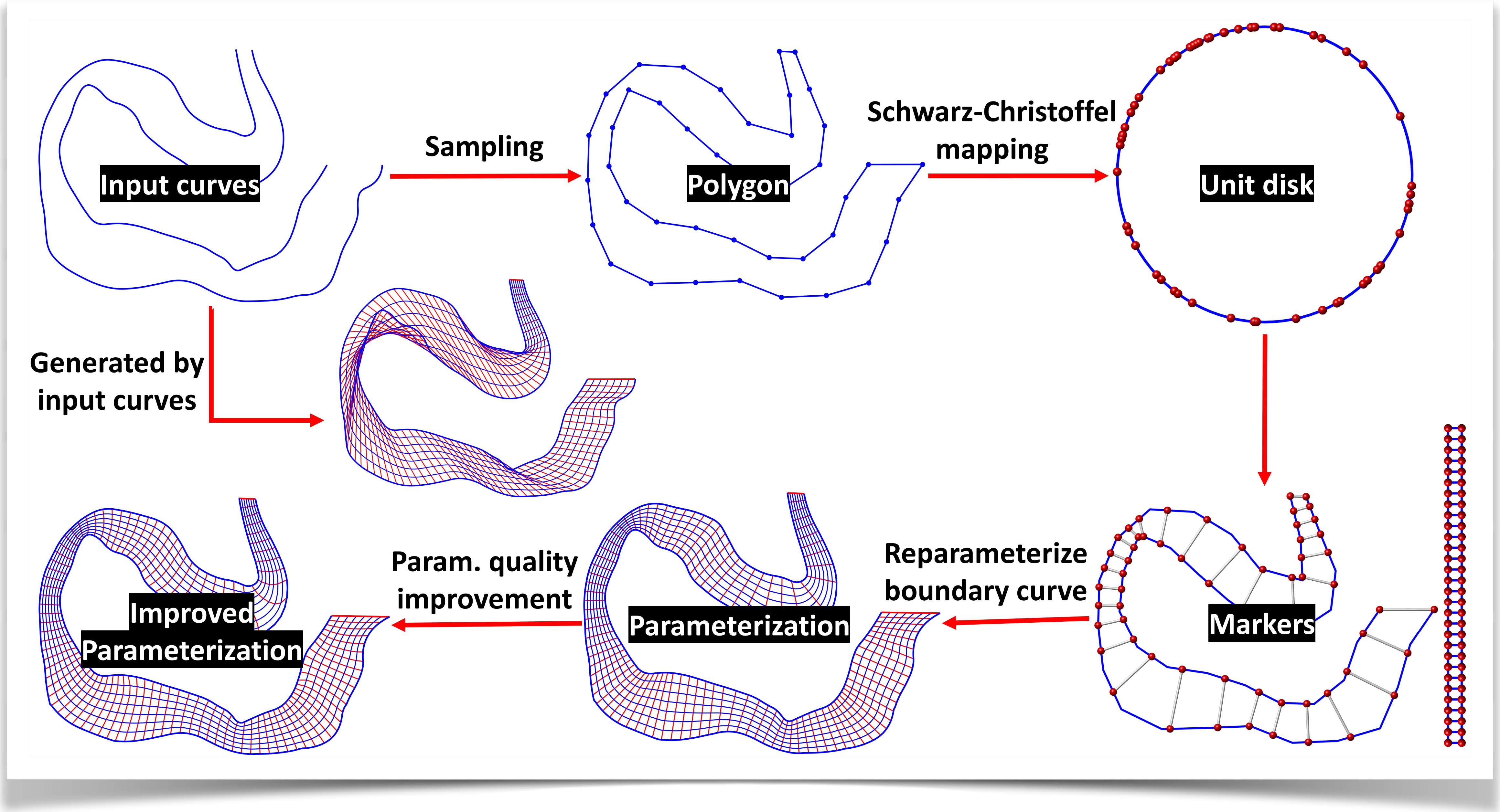
Ye Ji

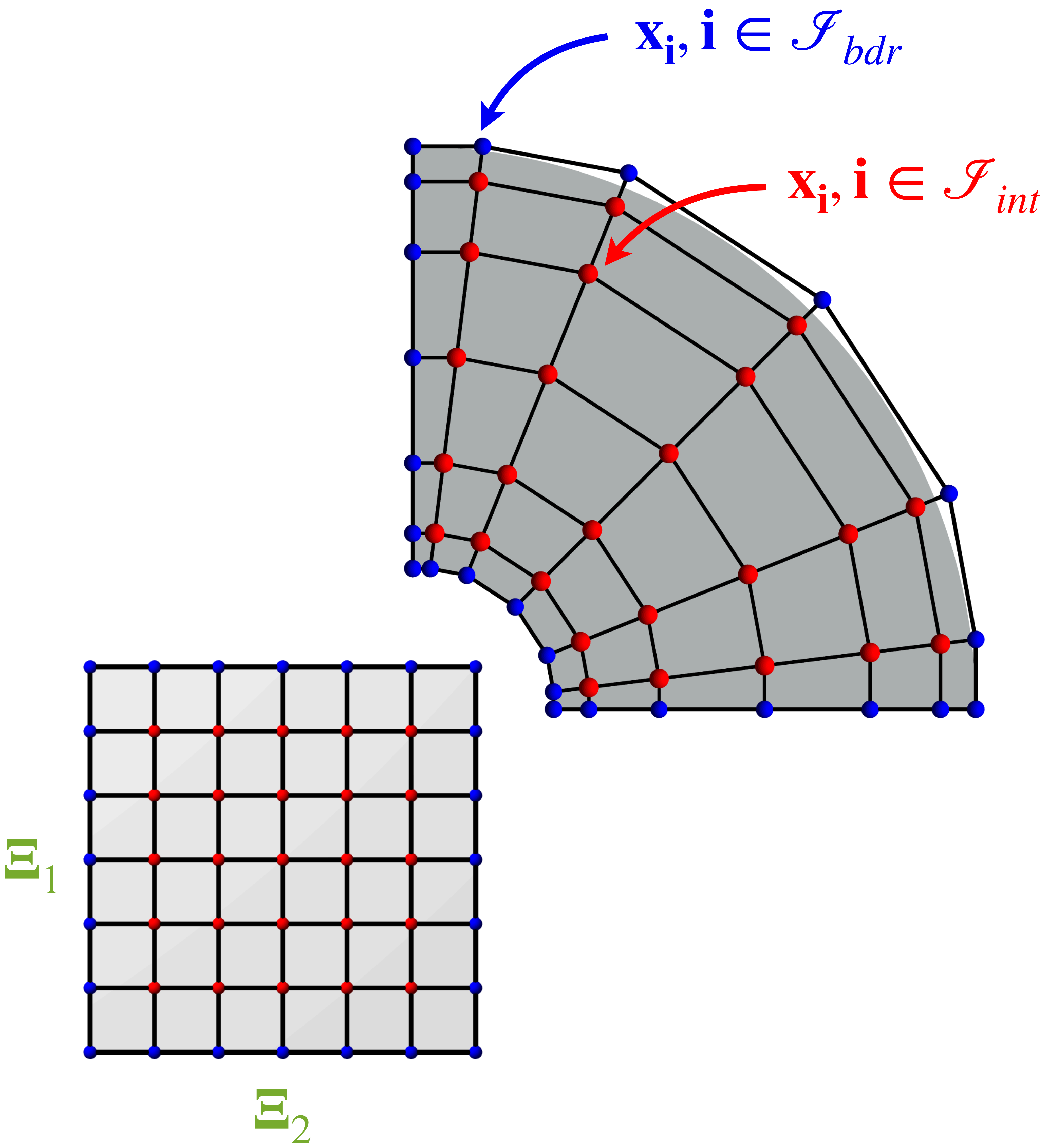
Workflow for planar domains



Ye Ji, Wed 10:30 - 12:30 in #MS012A

Workflow for planar domains





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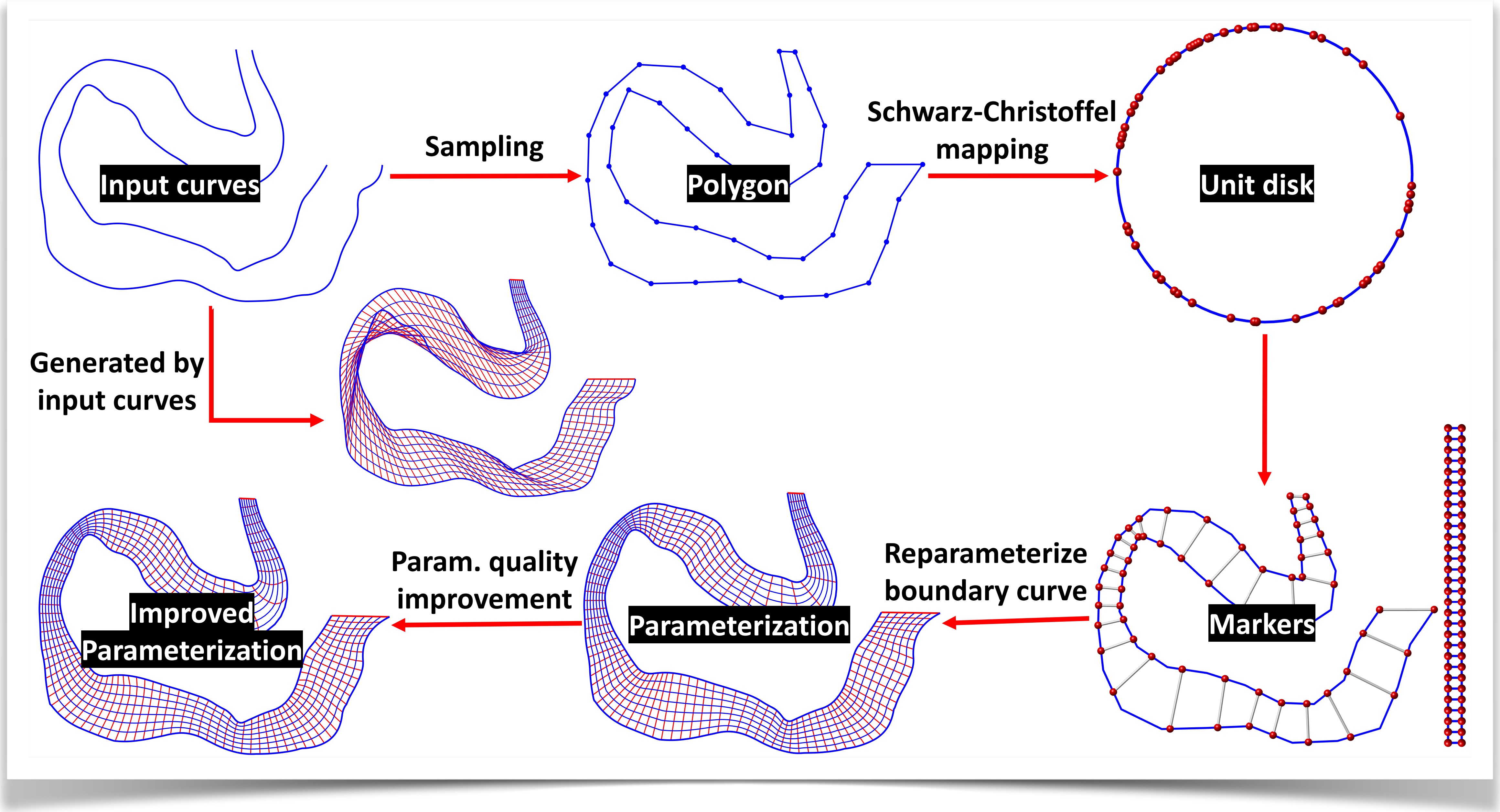
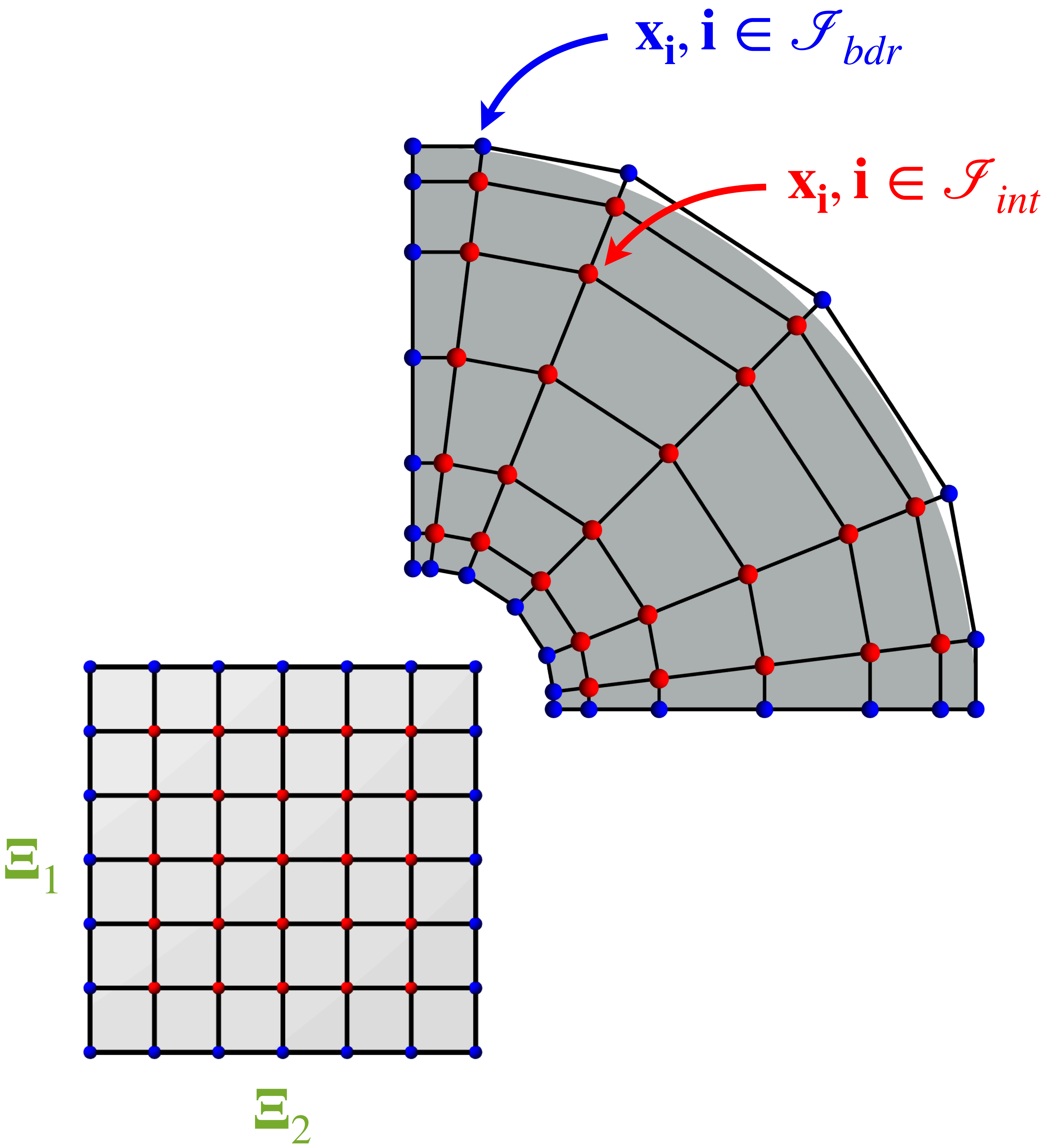
Workflow for planar domains





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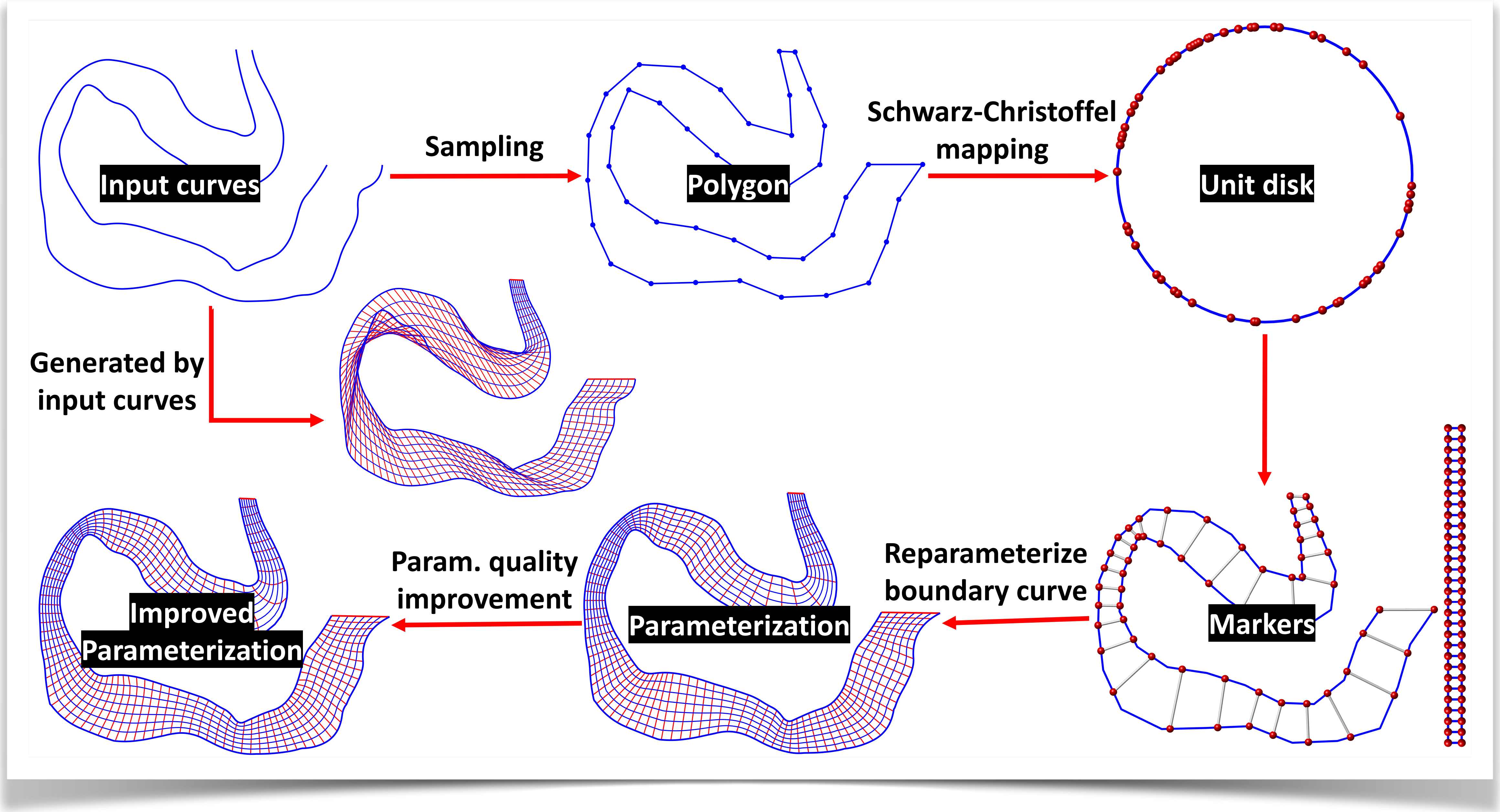
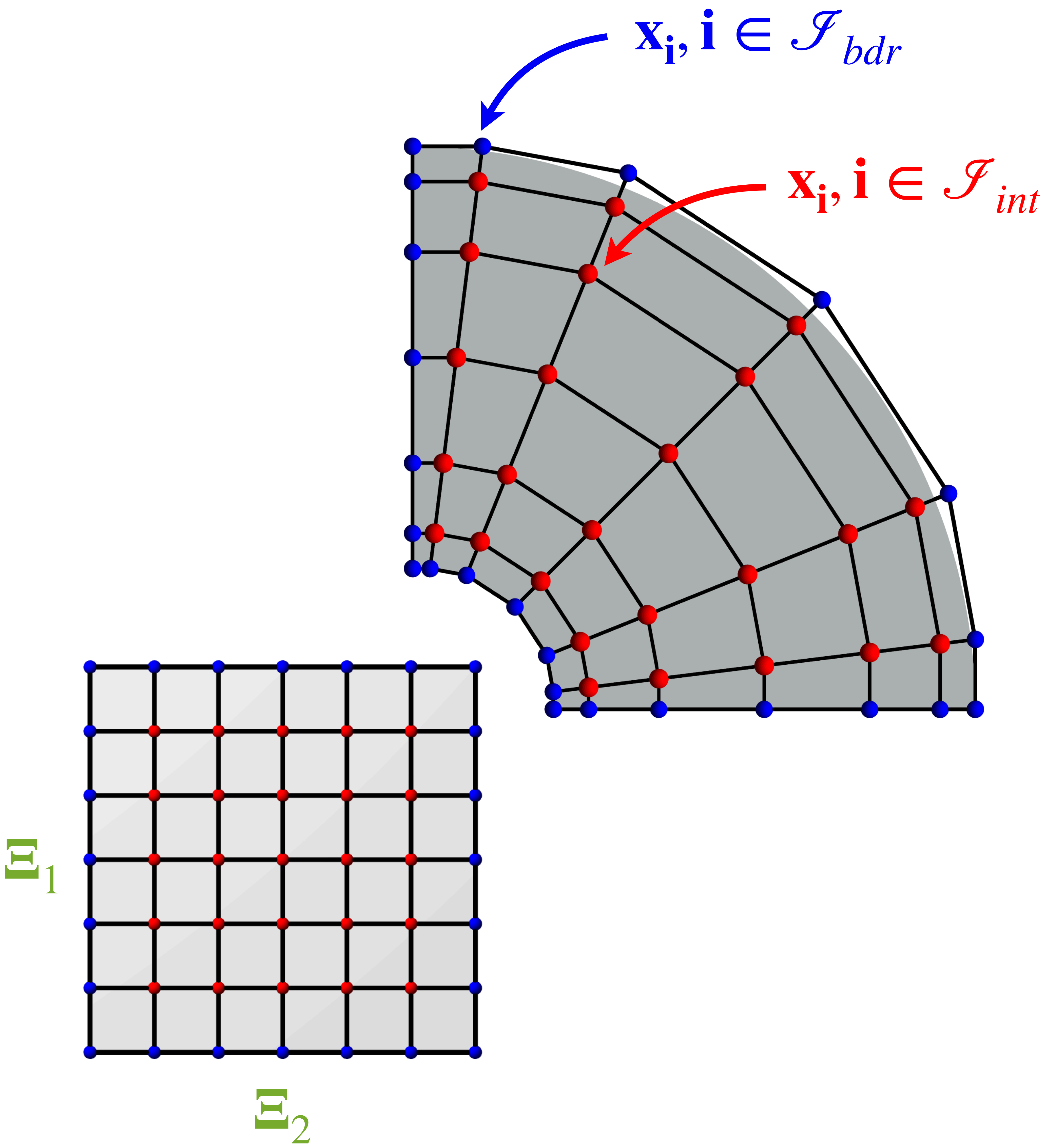
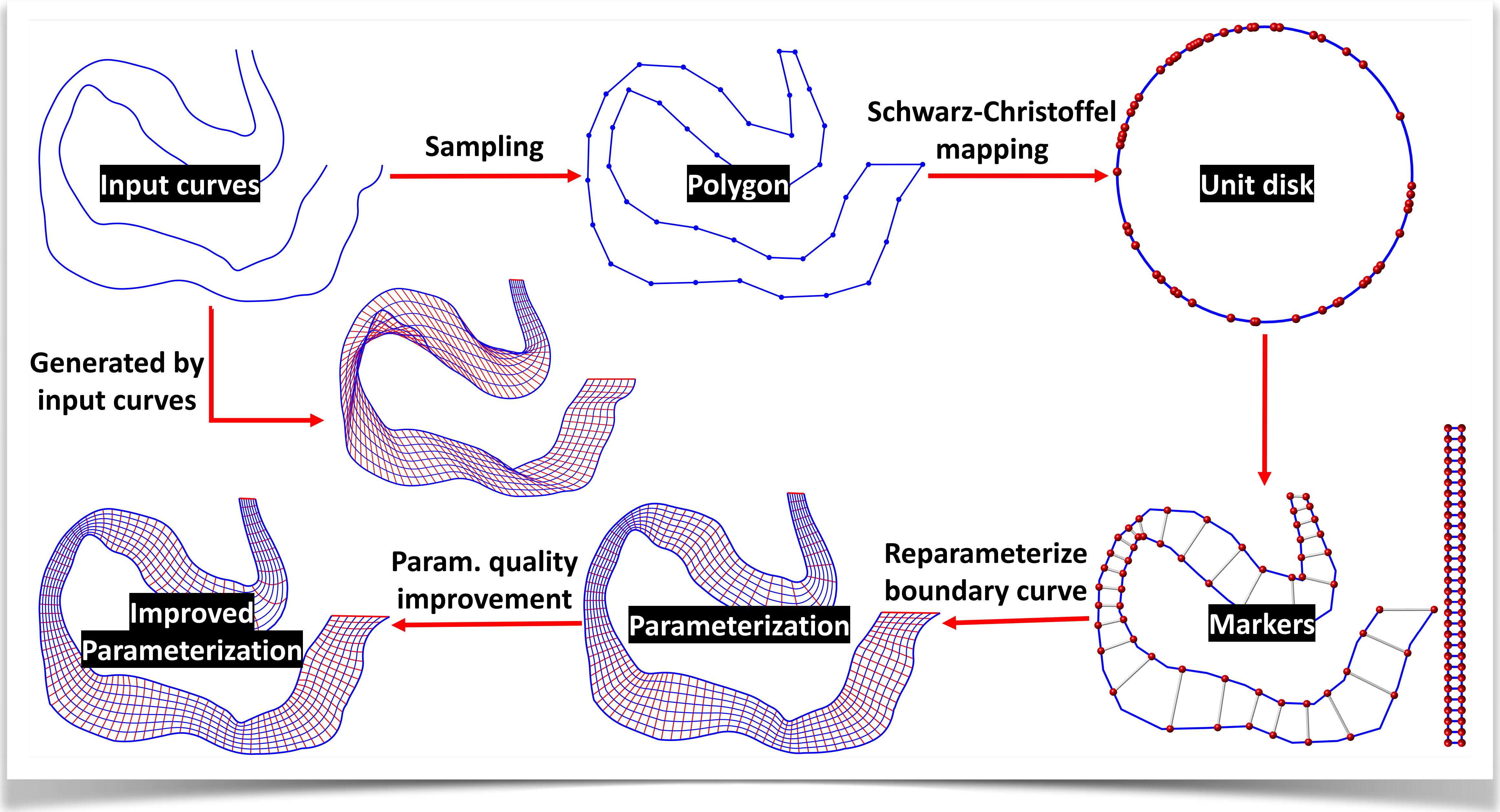
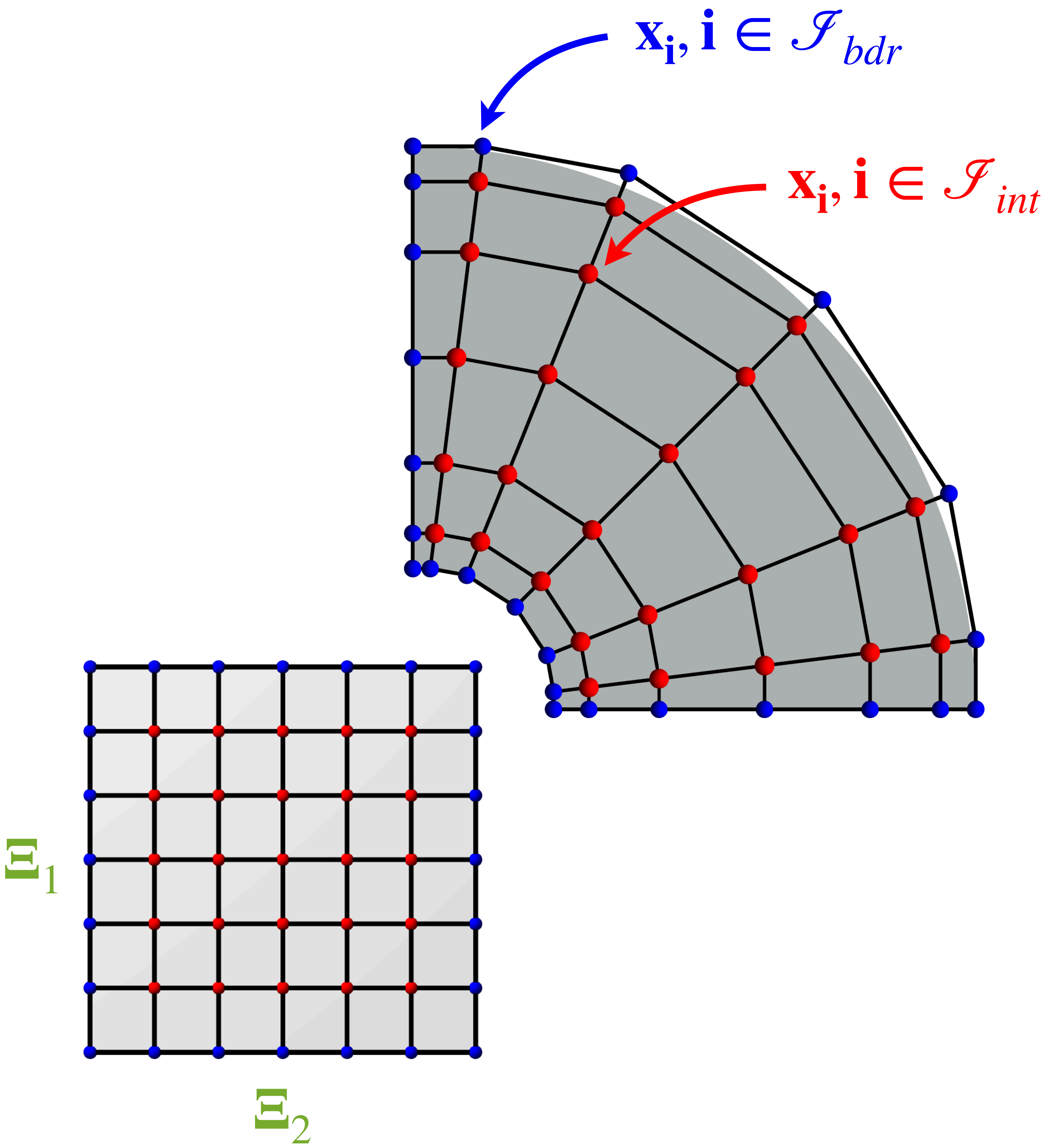




Ye Ji, Wed 10:30 - 12:30 in #MS012A

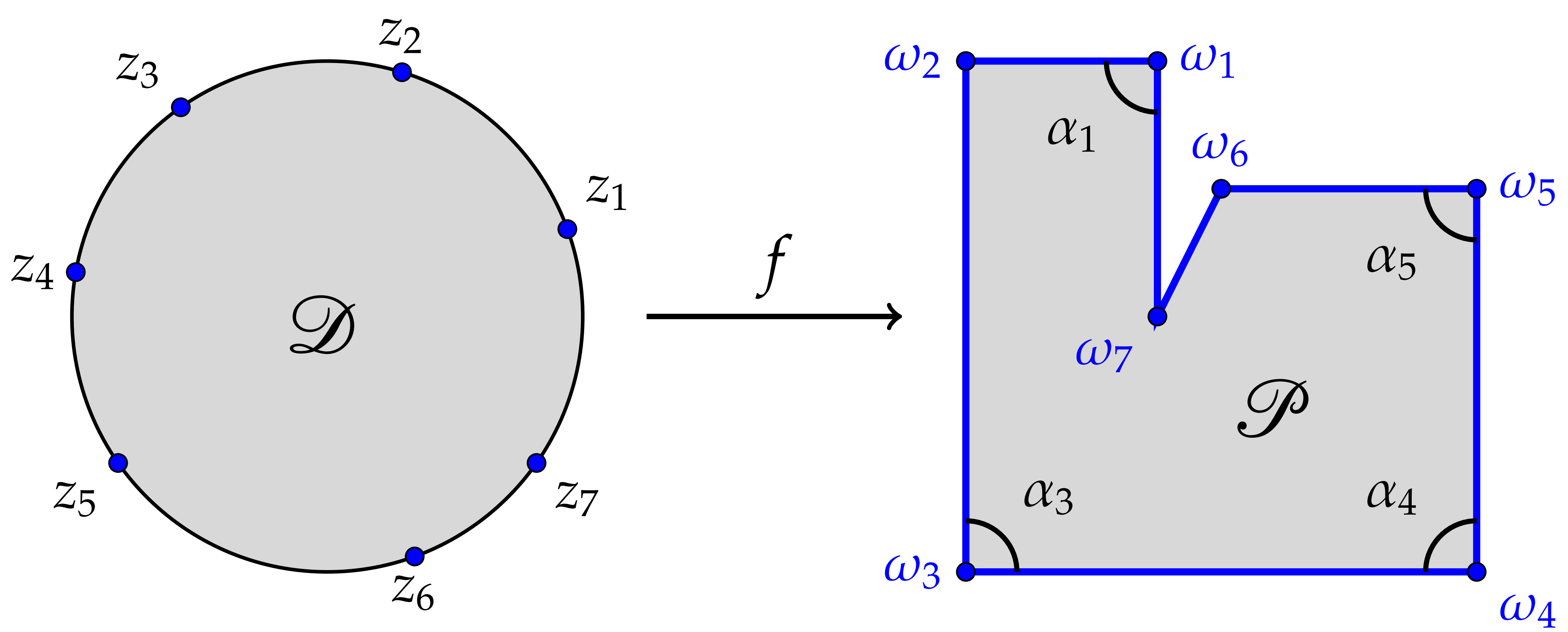
Workflow for planar domains





Ye Ji, Wed 10:30 - 12:30 in #MS012A

Schwarz-Christoffel mapping

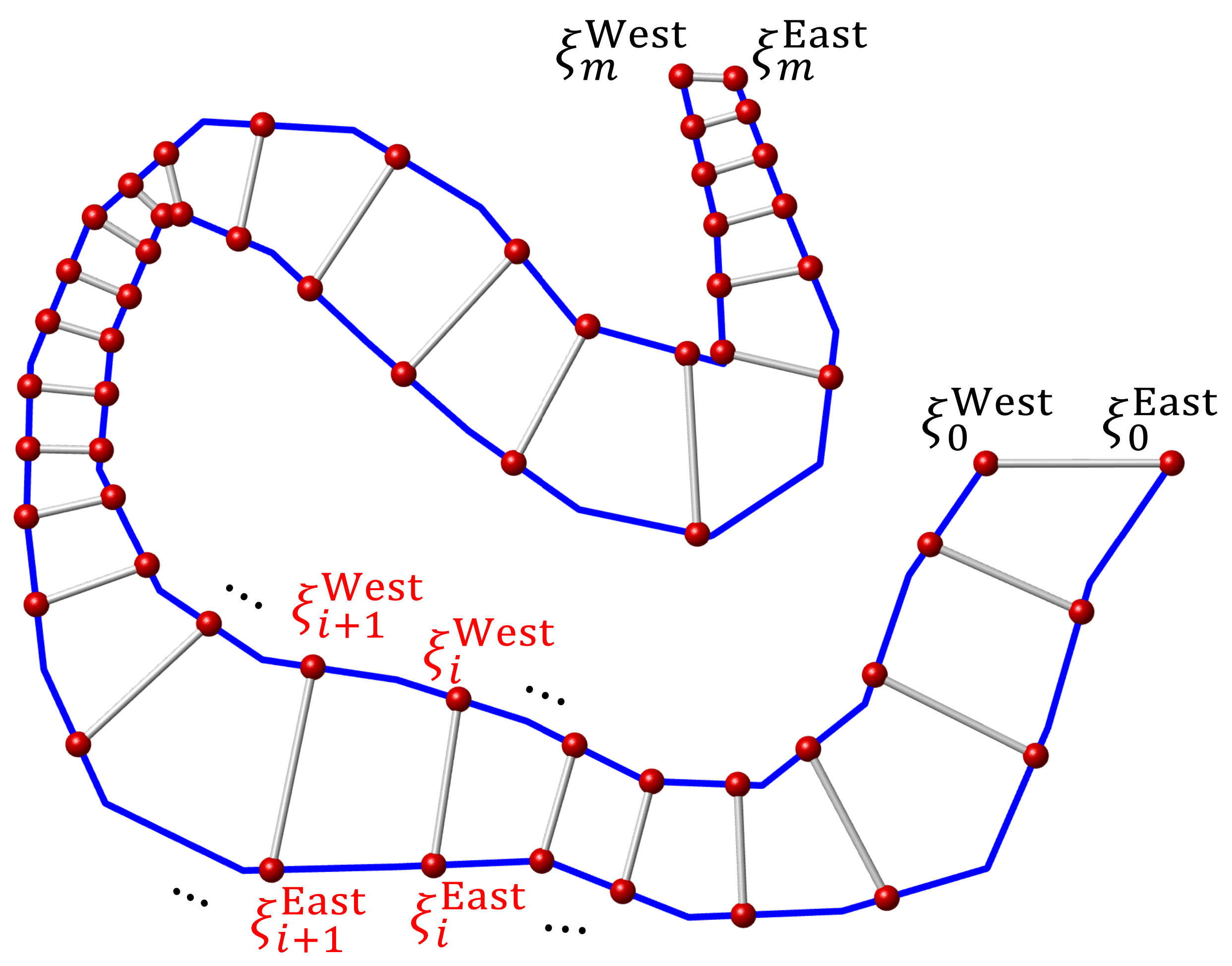


Riemann mapping theorem: $\exists$ analytic function f with non-zero derivative such that $f(\mathscr{D}) = \mathscr{P}$.

Scharz-Christoffel formula

$$f(z) = f(z_0) + C \int_{z_0}^{z} \prod_{j=1}^{n} \left(1 - \frac{\zeta}{z_j}\right)^{\alpha_j/\pi - 1} d\zeta$$

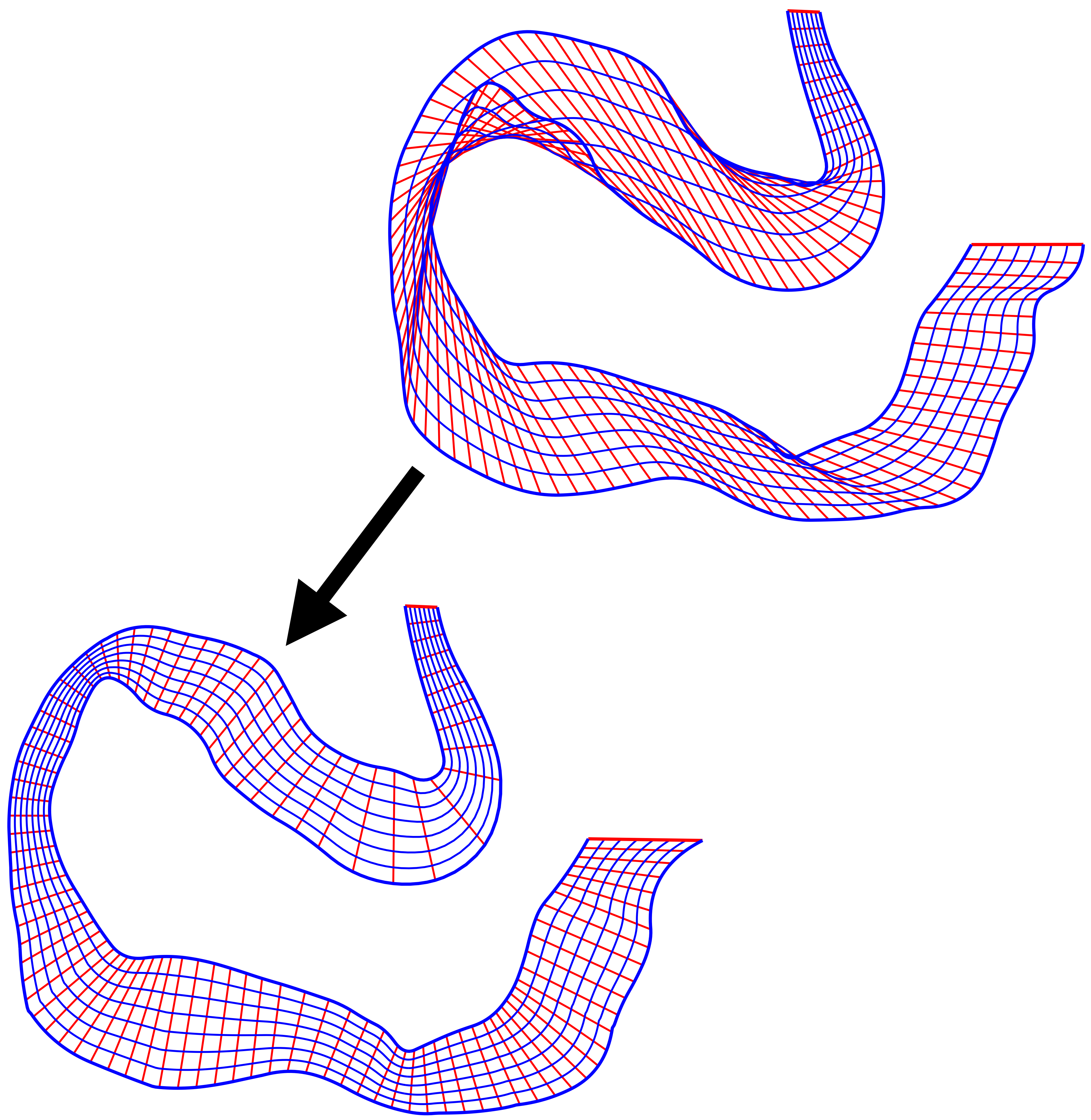
Solving the Schwarz-Christoffel parameter problem for $\{z_j\}$ numerically allows us to calculate sets of markers $\{\mathbf{P}_i^{West}\}$ and $\{\mathbf{P}_i^{East}\}$ on the two opposite curves C^{West} and C^{East} that can be used to reparameterize one curve w.r.t. the other



Y. Ji, MM, Y. Yu, Ch. Zhu, arXiv: 2403.10284

Boundary reparameterization

Theorem [Ji et al. 2024]: B-spline and NURBS basis functions are invariant under scaling and translation of the knot vector, i.e. $b^d_{i,\Xi}(\xi) = b^d_{i,\hat{\Xi}}(s\xi + t)$ with $\hat{\Xi} = s\Xi + t, \quad s > 0$



Sketch of the reparameterization algorithm

- For each pair of markers $(\mathbf{P}_i^{East}, \mathbf{P}_i^{West})$ identify the pair of parameters $(\xi_i^{East}, \xi_i^{West})$ by solving the nonlinear equation $\left(C^*(\xi) - \mathbf{P}_i^*\right) \cdot \partial C^*(\xi)/\partial\xi = 0$ using Newton's method

- Without loss of generality, align the segment of curve C^{East} defined over the parameter interval $[\xi_i^{East}, \xi_{i+1}^{East}]$ with C^{West} by applying an affine transformation

Y. Ji, MM, Y. Yu, Ch. Zhu, arXiv: 2403.10284

From boundary to planar domain parameterizations

Given: $\Gamma = C^{North} \cup C^{South} \cup C^{East} \cup C^{West}$ as push-forward from $\hat{\Gamma}$

Harmonic mapping: compute $\mathbf{x} : \hat{\Omega} \to \Omega$ by solving Laplace problems for $\mathbf{x}^{-1} = \boldsymbol{\xi} : \Omega \to \hat{\Omega}$

$$\begin{aligned} \nabla \cdot \left[\mathbb{A} \, \nabla \xi_1(x_1, x_2) \right] &= 0 \\ \nabla \cdot \left[\mathbb{A} \, \nabla \xi_2(x_1, x_2) \right] &= 0 \end{aligned} \qquad \text{s.t. } \mathbf{x}^{-1} \Big|_{\Gamma} = \hat{\Gamma}$$

with $\mathbb{A} = 1$ [Hinz et al. 2018] or $\mathbb{A} = \mathrm{diag}(1/|\mathbf{J}|)$, Jacobian $\mathbf{J}(\xi_1, \xi_2)$ [Ji et al. 2023]

Radó-Kneser-Choquet theorem: convexity of $\hat{\Omega}$ ensures one-to-one mapping between $\hat{\Omega}$ and Ω

Y. Ji, MM, Proc. 13th Int. Conf. On Compressors and Their Systems 2023

Computation of planar parameterization

Weak form in H^2 [Hinz et al. 2018]

$$\int_{\hat{\Omega}} \mathbf{w} \tilde{\mathscr{L}} \xi_1 \, \mathrm{d}\hat{\Omega} = \mathbf{0}$$
$$\int_{\hat{\Omega}} \mathbf{w} \tilde{\mathscr{L}} \xi_2 \, \mathrm{d}\hat{\Omega} = \mathbf{0}$$

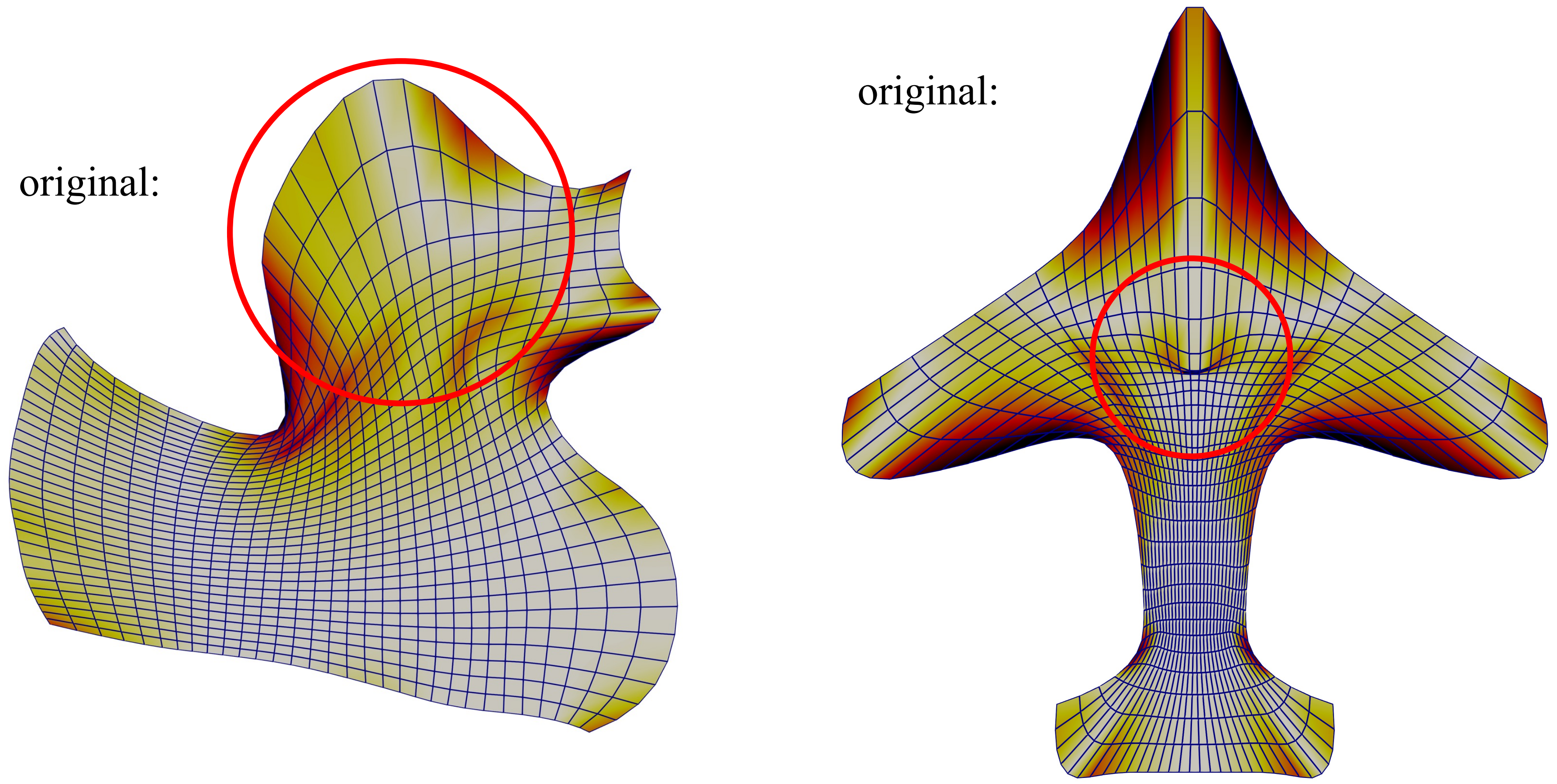
s.t. $\mathbf{x}^{-1}|_{\Gamma} = \hat{\Gamma}$

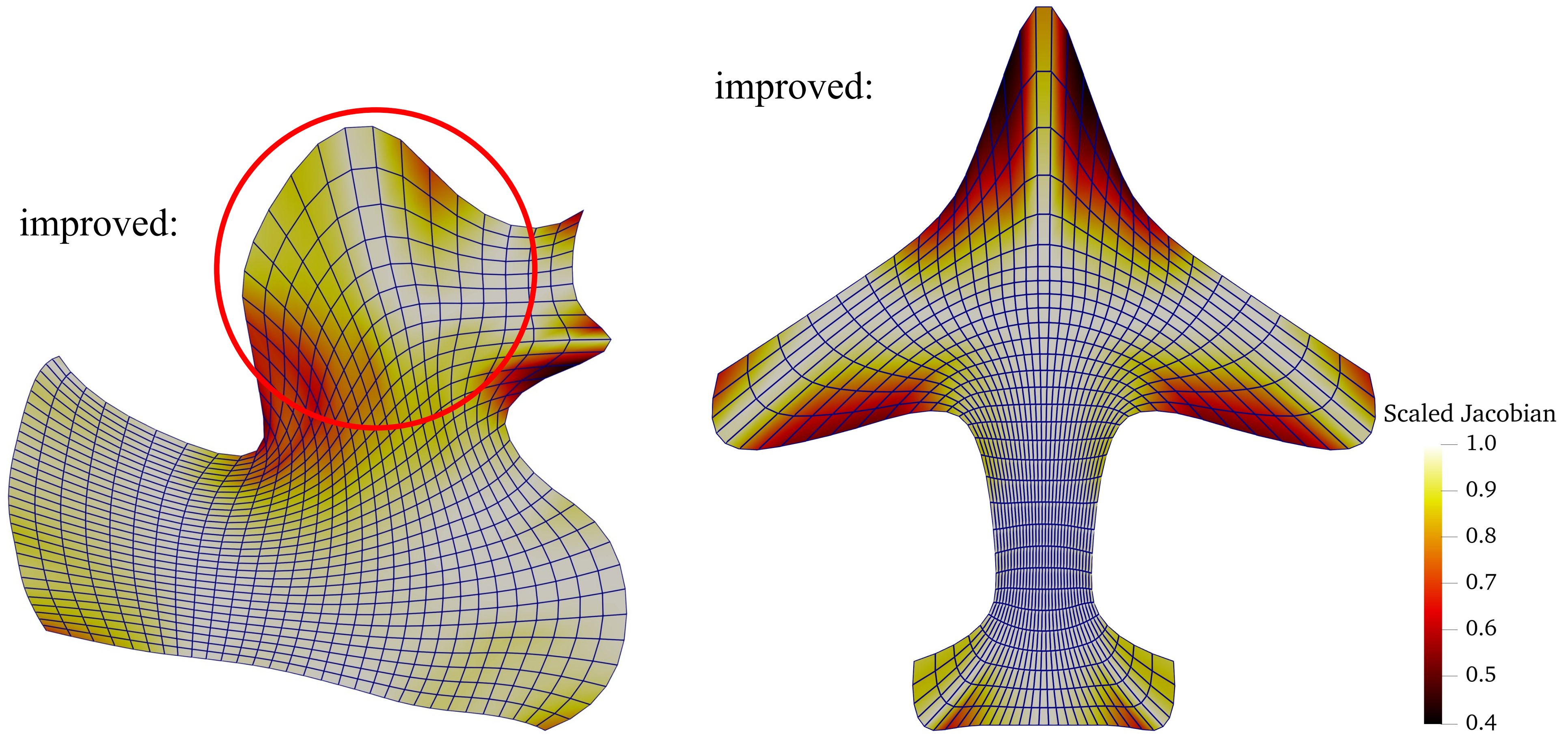
where $\tilde{\mathscr{L}} = \left(g_{22} \frac{\partial^2}{\partial \xi_1^2} - 2 g_{12} \frac{\partial^2}{\partial \xi_1 \partial \xi_2} + g_{11} \frac{\partial^2}{\partial \xi_2^2} \right) / (g_{11} + g_{22})$

Weak form in H^1 [Ji et al. 2023]

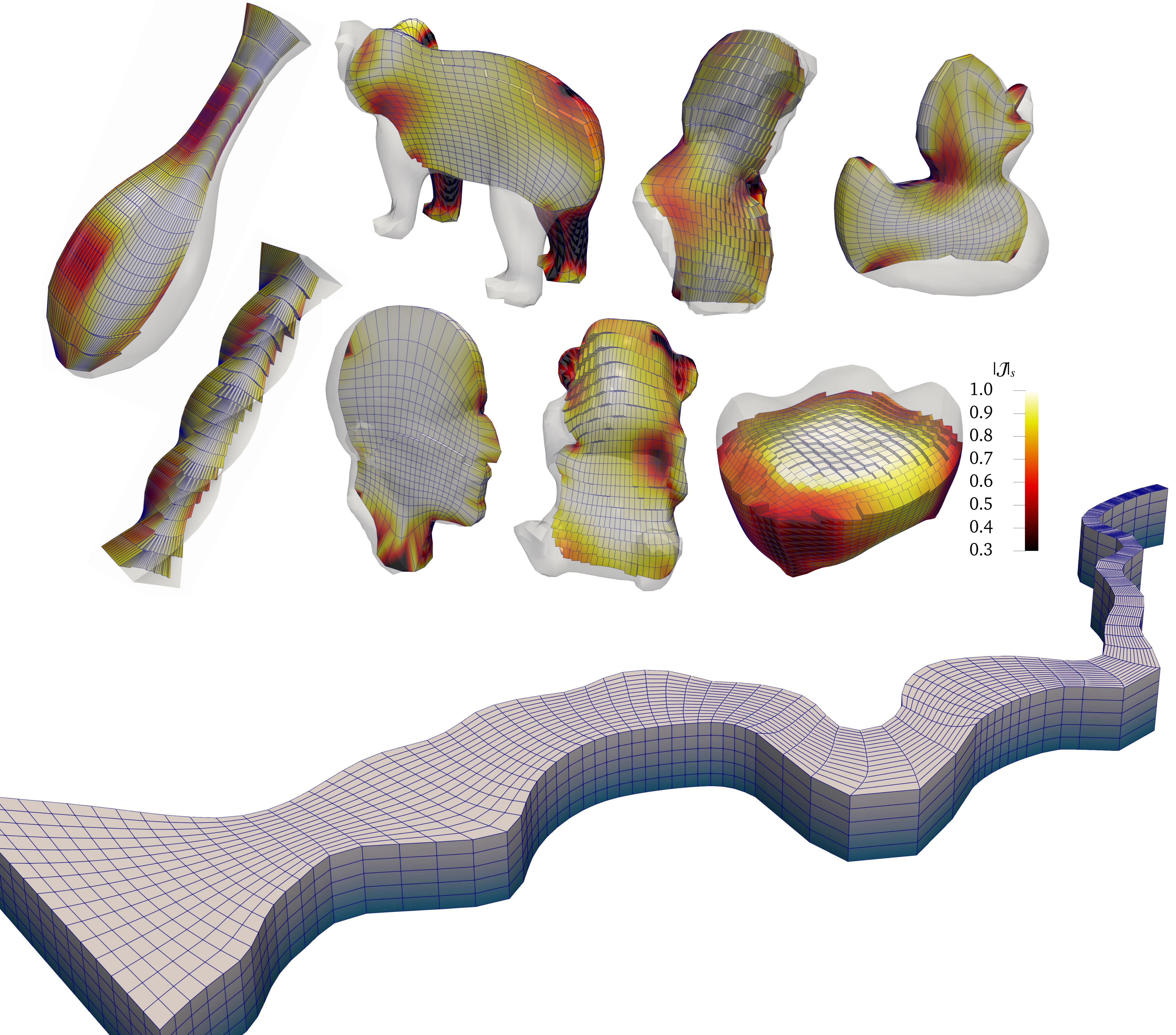
$$\int_{\hat{\Omega}} \nabla \mathbf{w} \cdot \mathbb{A} \nabla \xi_1 \, \mathrm{d}\hat{\Omega} = \mathbf{0}$$
$$\int_{\hat{\Omega}} \nabla \mathbf{w} \cdot \mathbb{A} \nabla \xi_2 \, \mathrm{d}\hat{\Omega} = \mathbf{0}$$

s.t. $\mathbf{x}^{-1}|_{\Gamma} = \hat{\Gamma}$

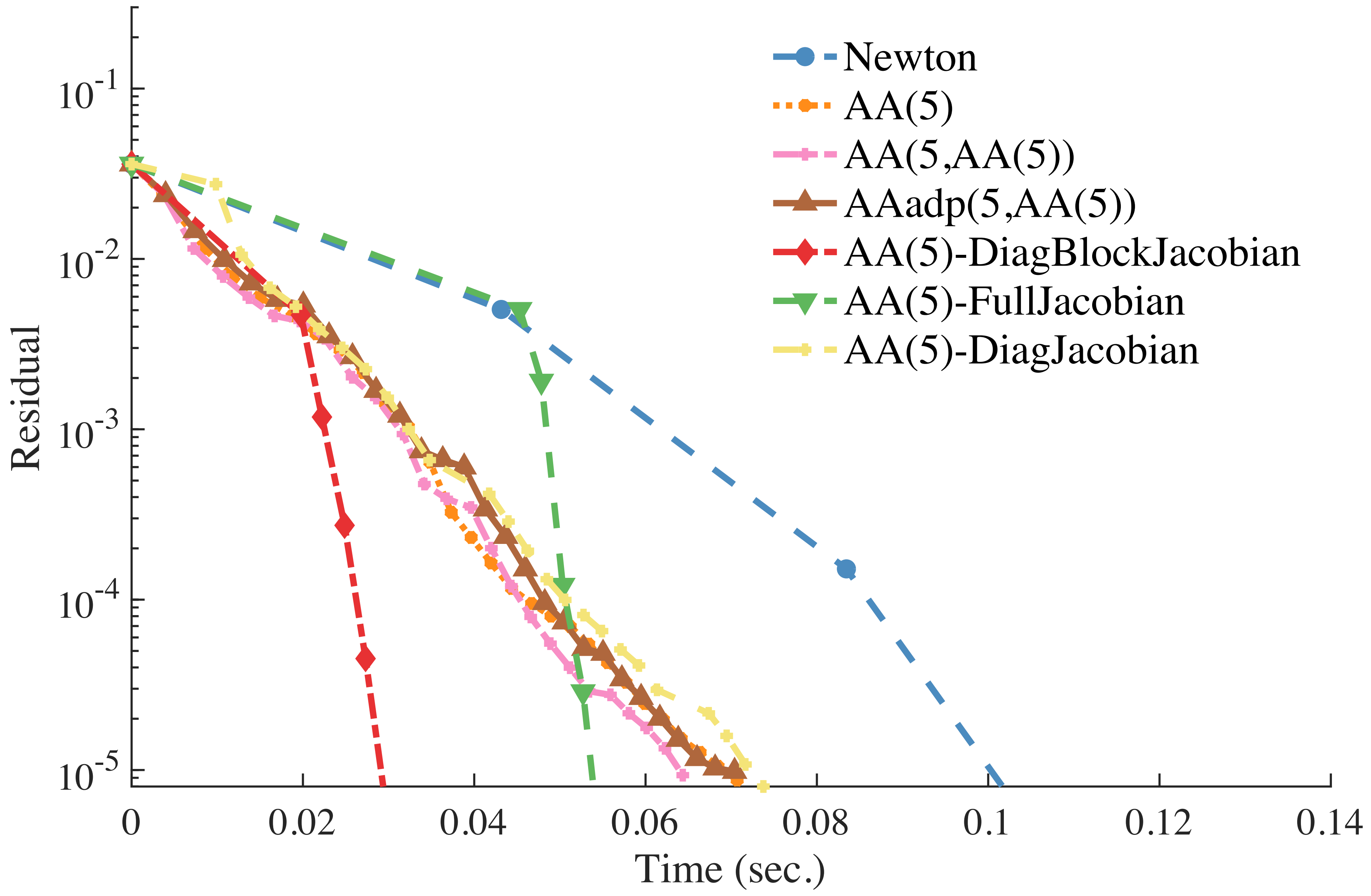




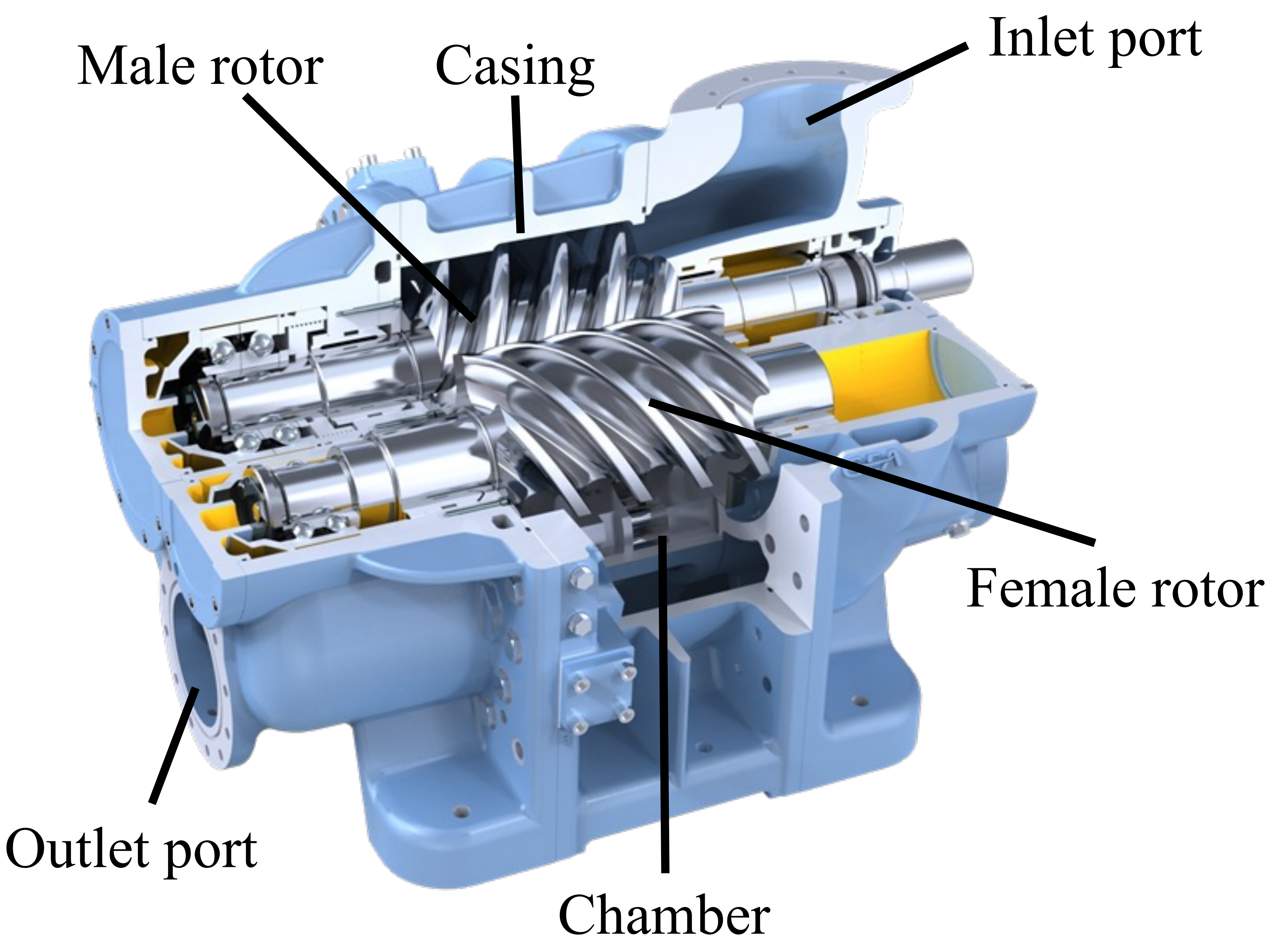
Extension to trivariate parameterizations



Existence of one-to-one mapping is no longer ensured by RKC theorem for non-planer domains but our **approach is efficient and robust in practice** when the nonlinear problems are solved with a preconditioned Anderson accelerator

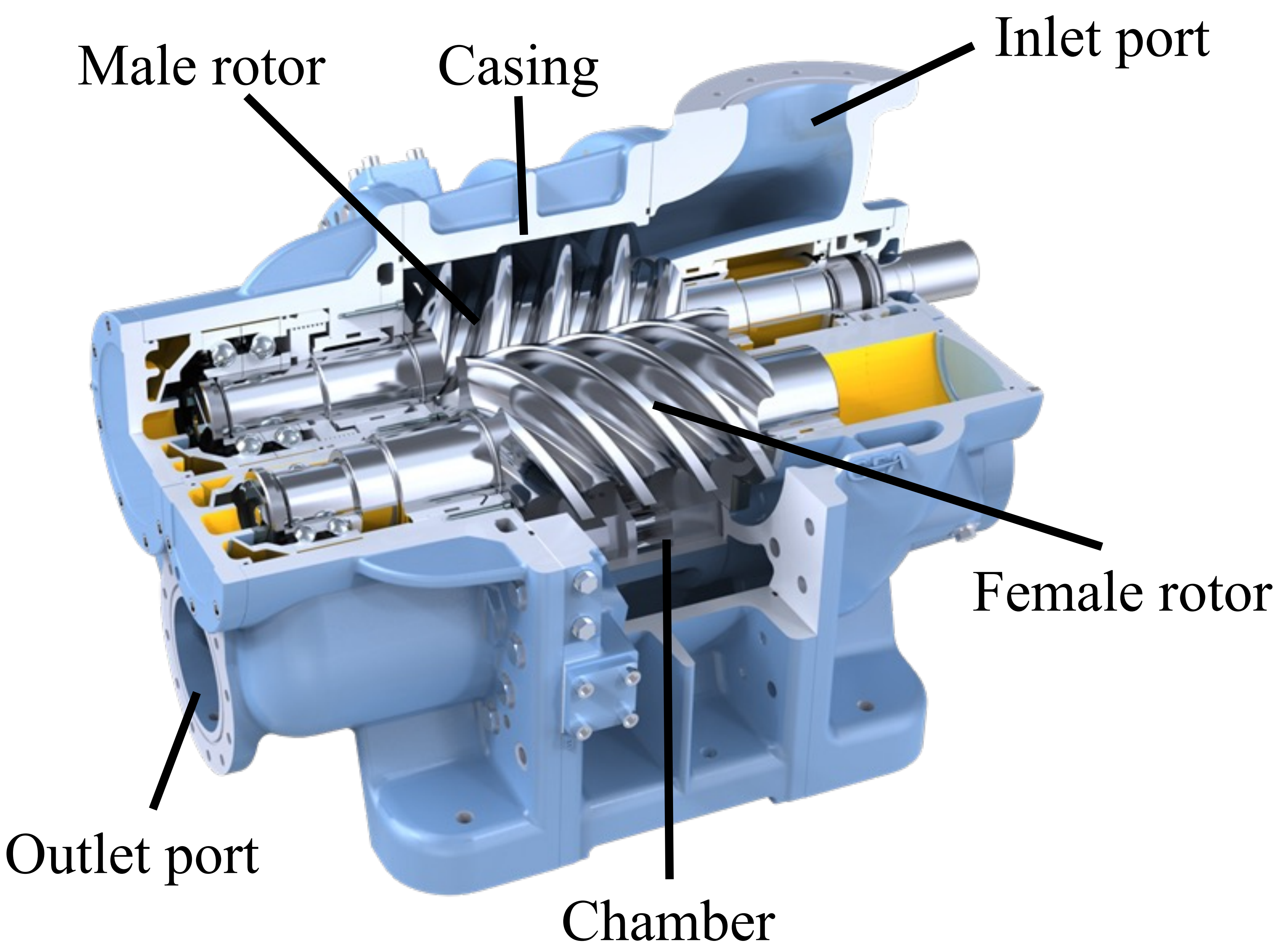


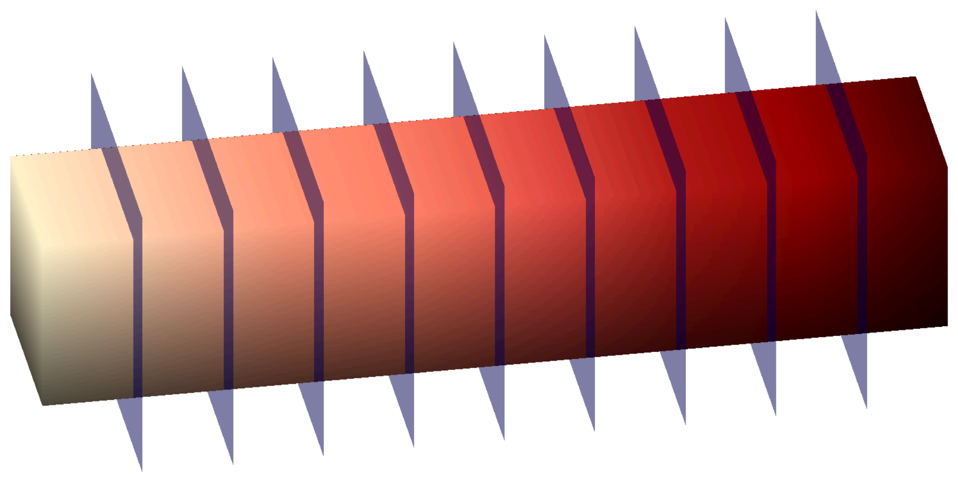
Intermezzo: spline-based mesh generation

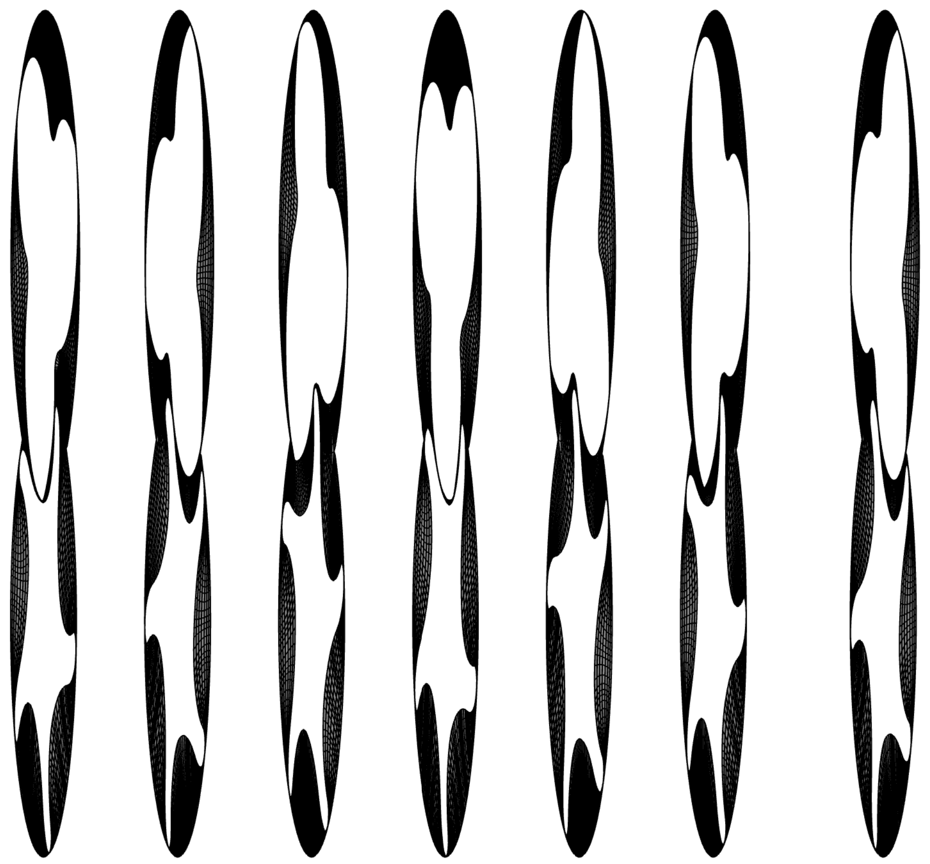


Y. Ji, 2024

Intermezzo: spline-based mesh generation

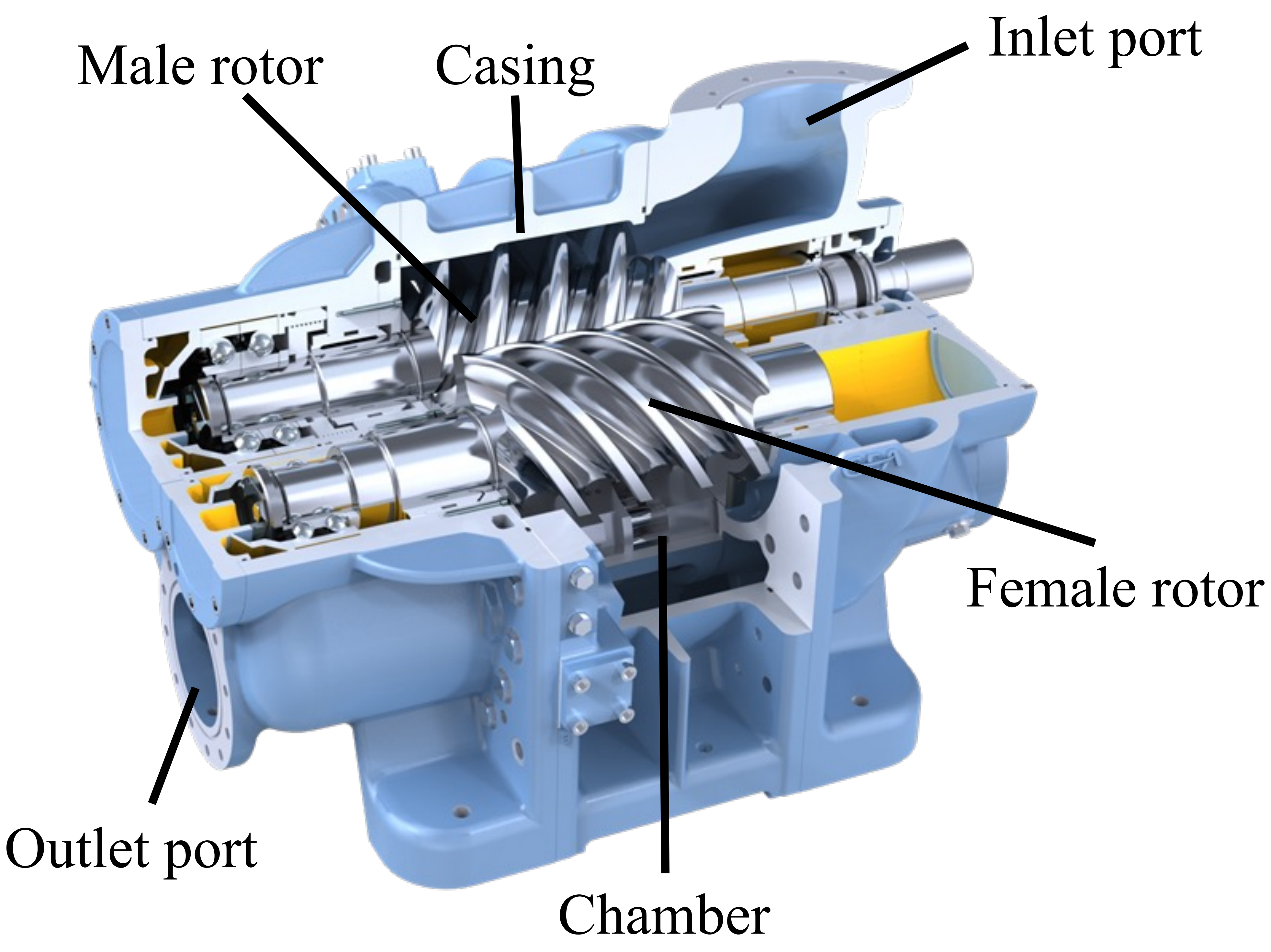


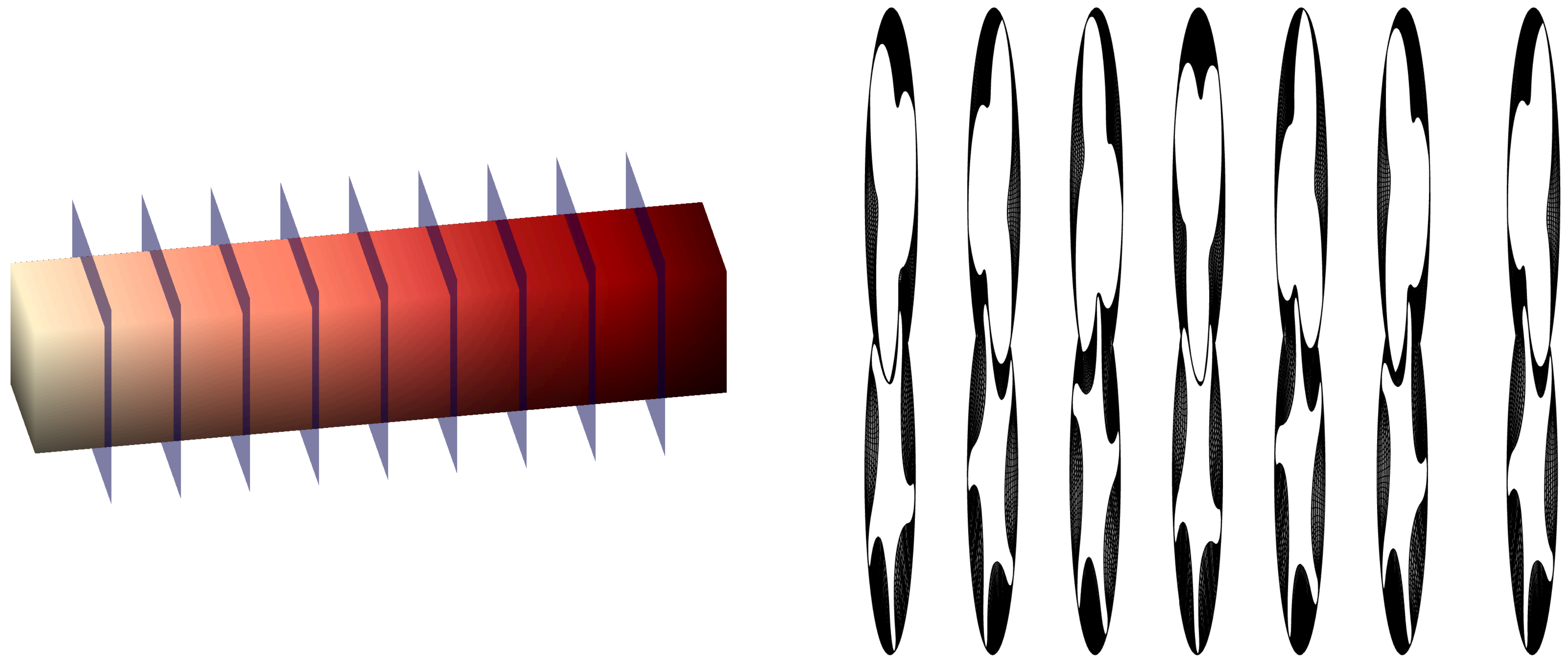


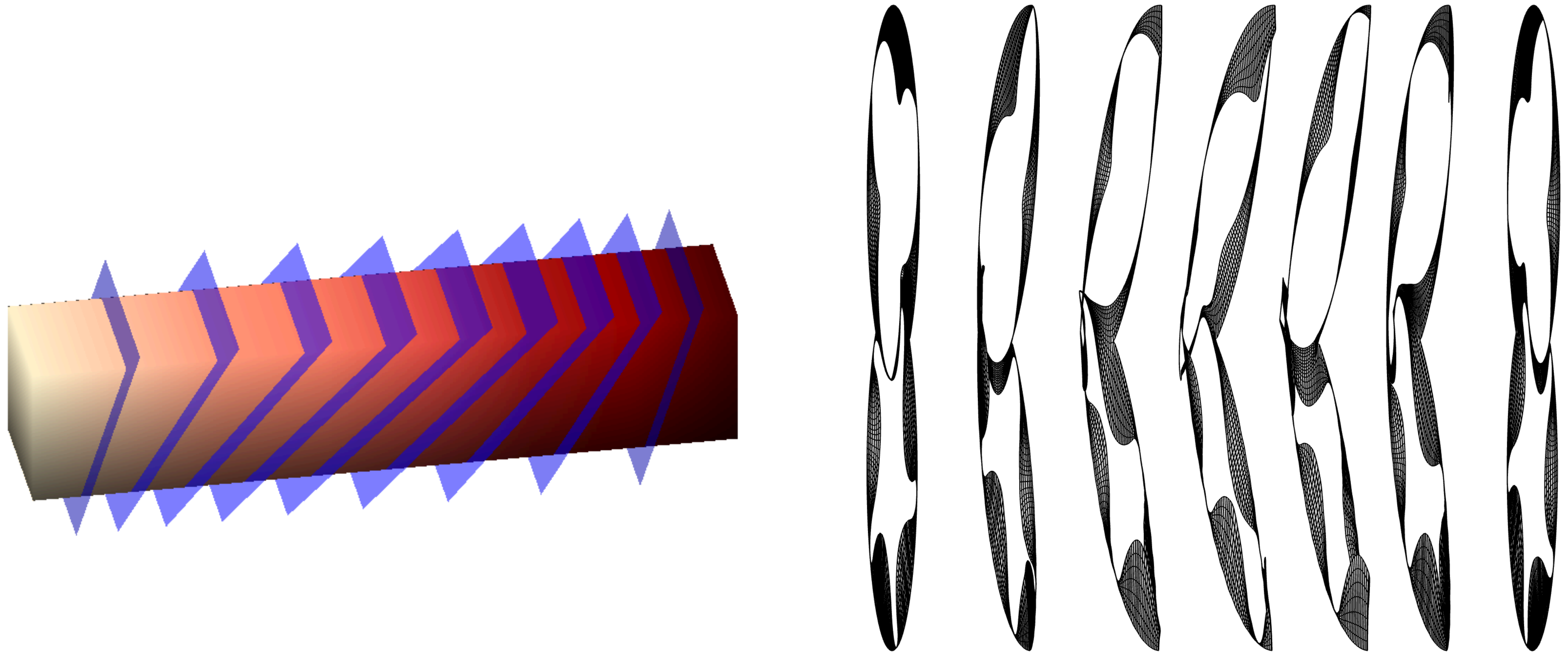


Y. Ji, 2024

Intermezzo: spline-based mesh generation







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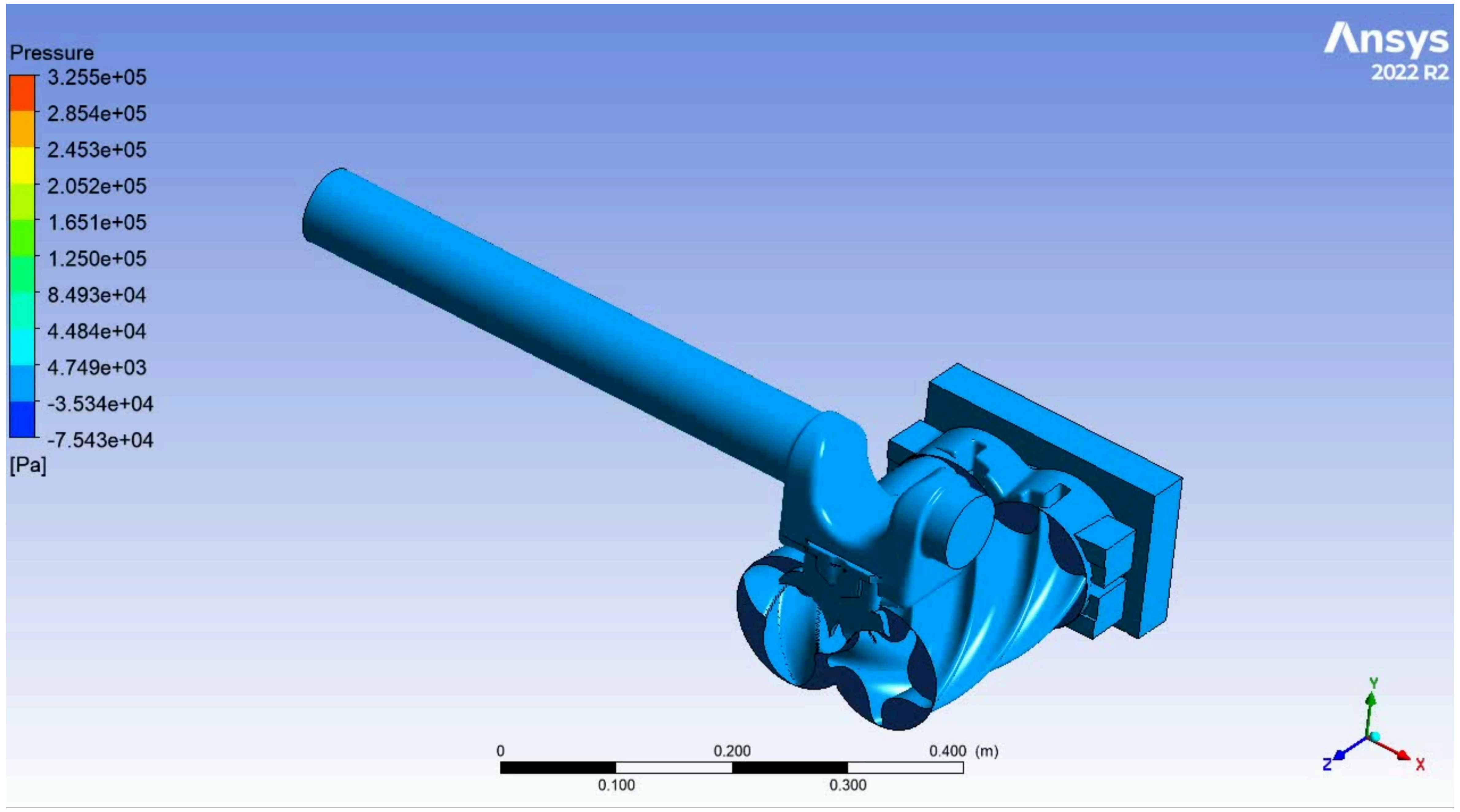
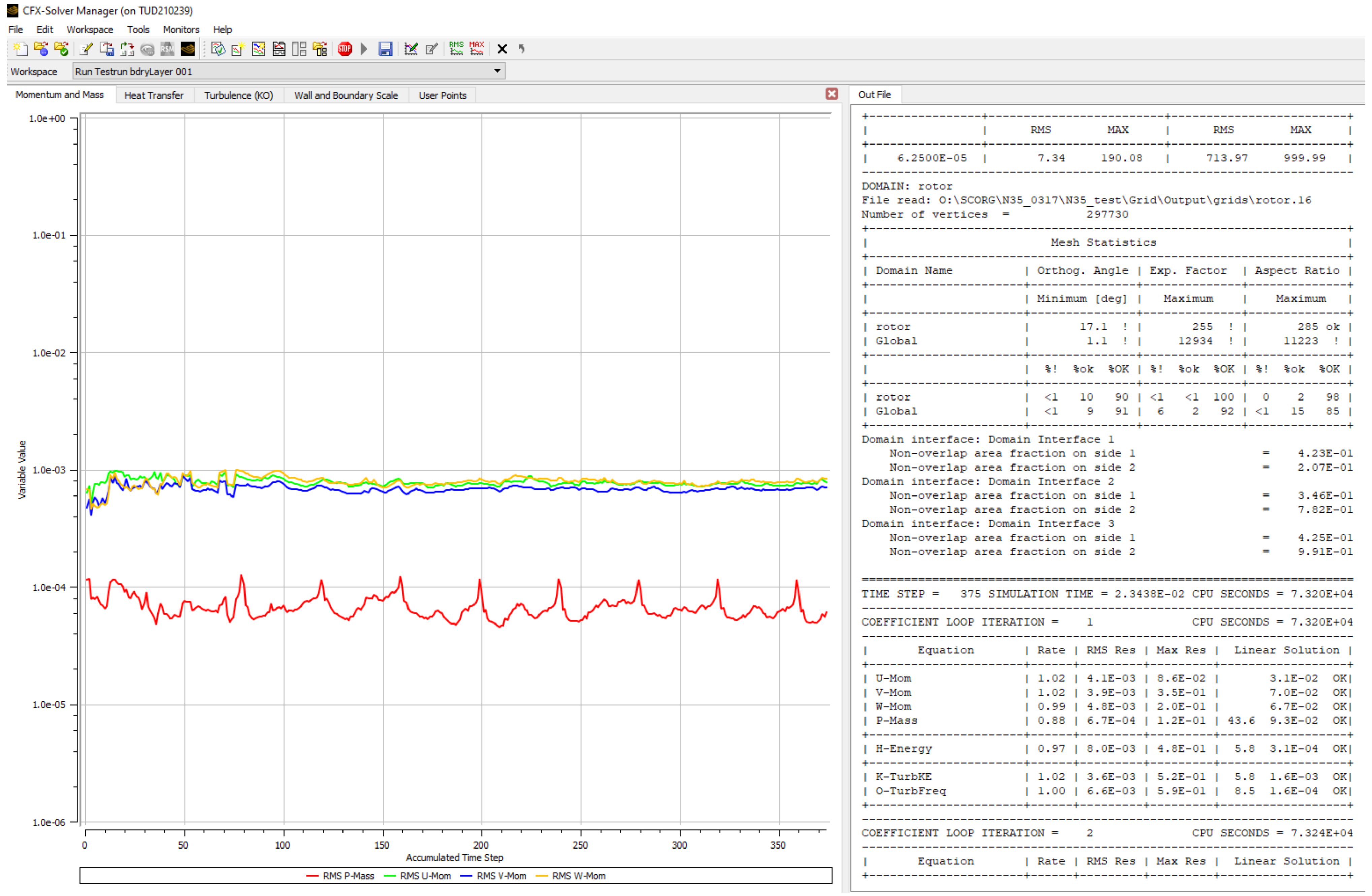
Intermezzo: spline-based mesh generation + simulation





Y. Ji, 2024

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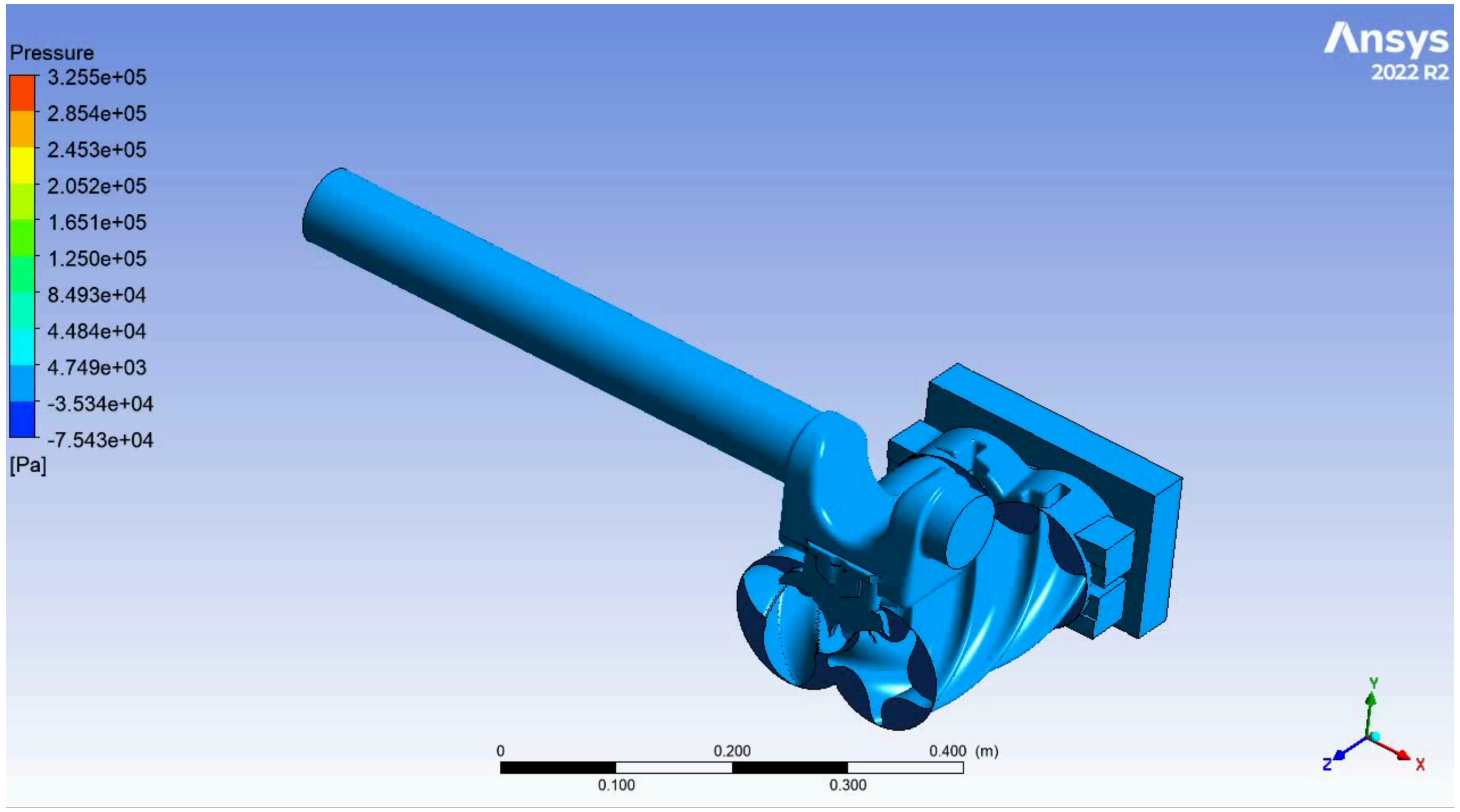
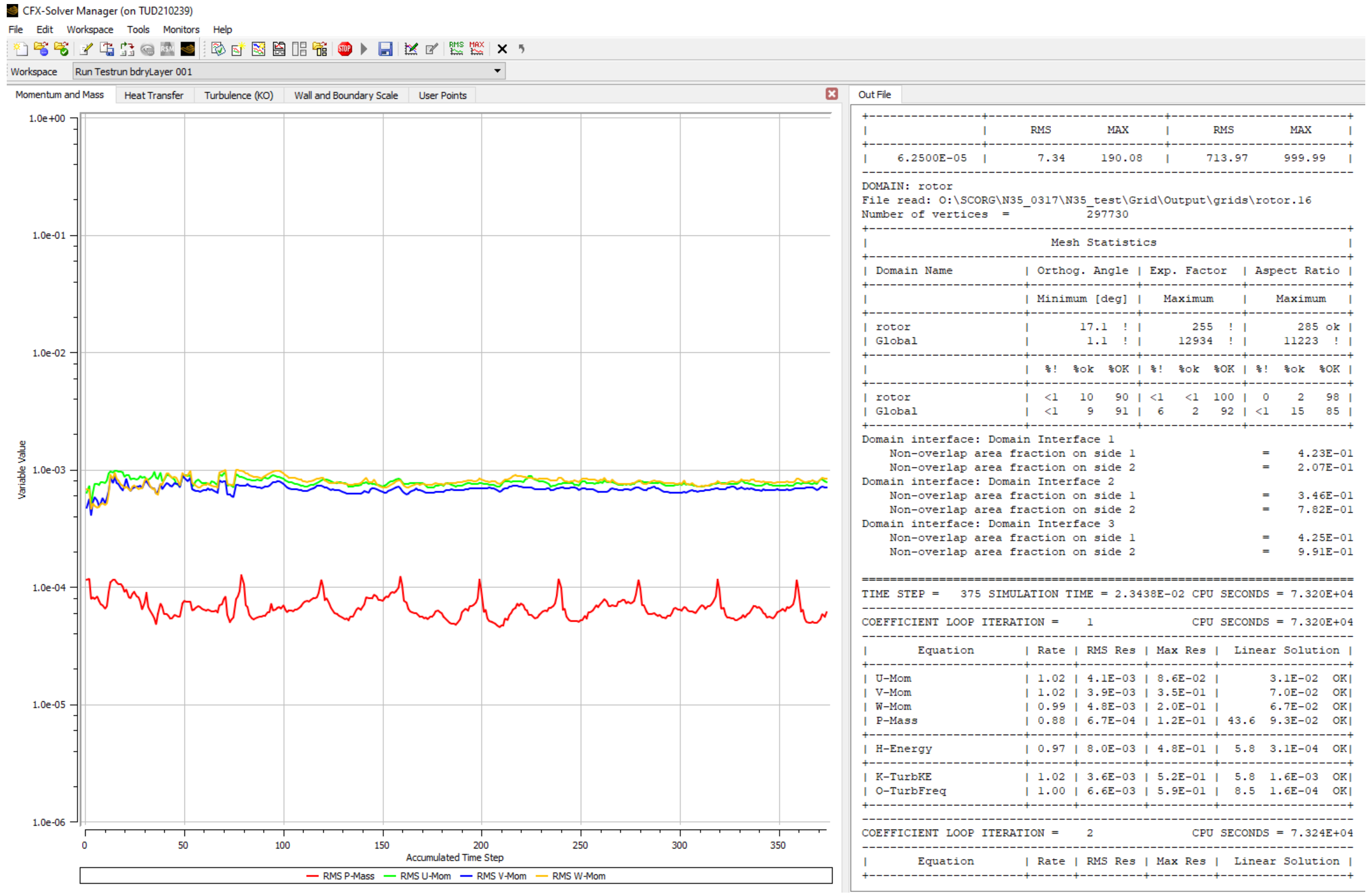
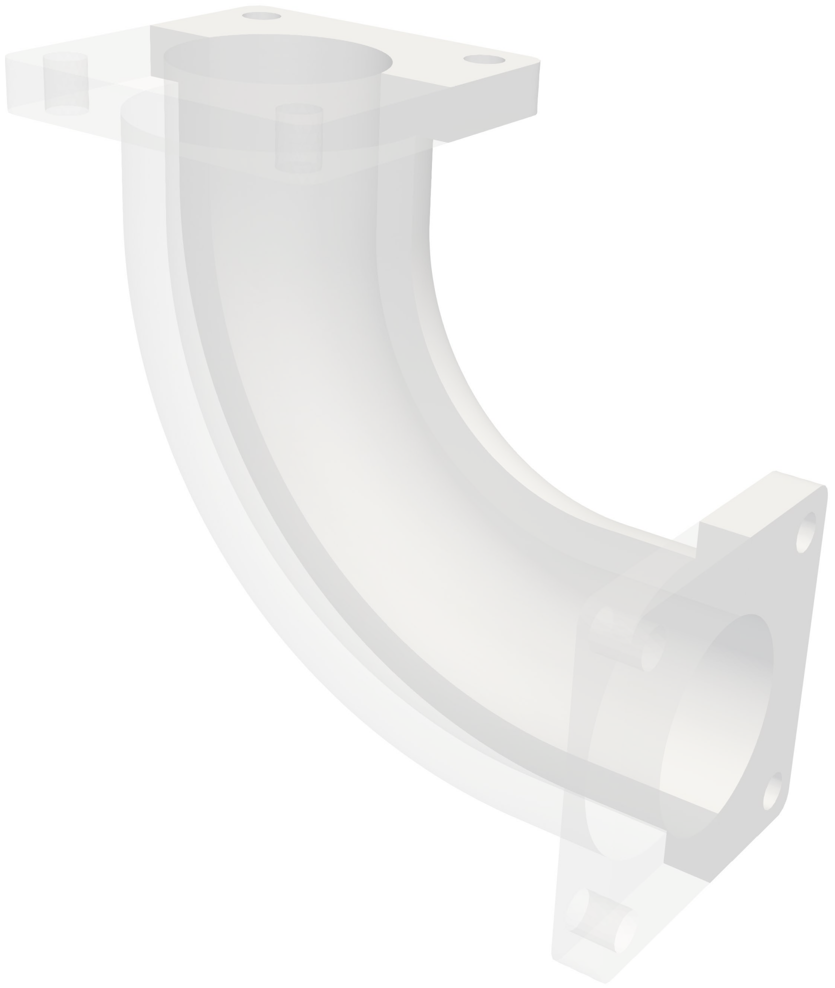
EST 1894

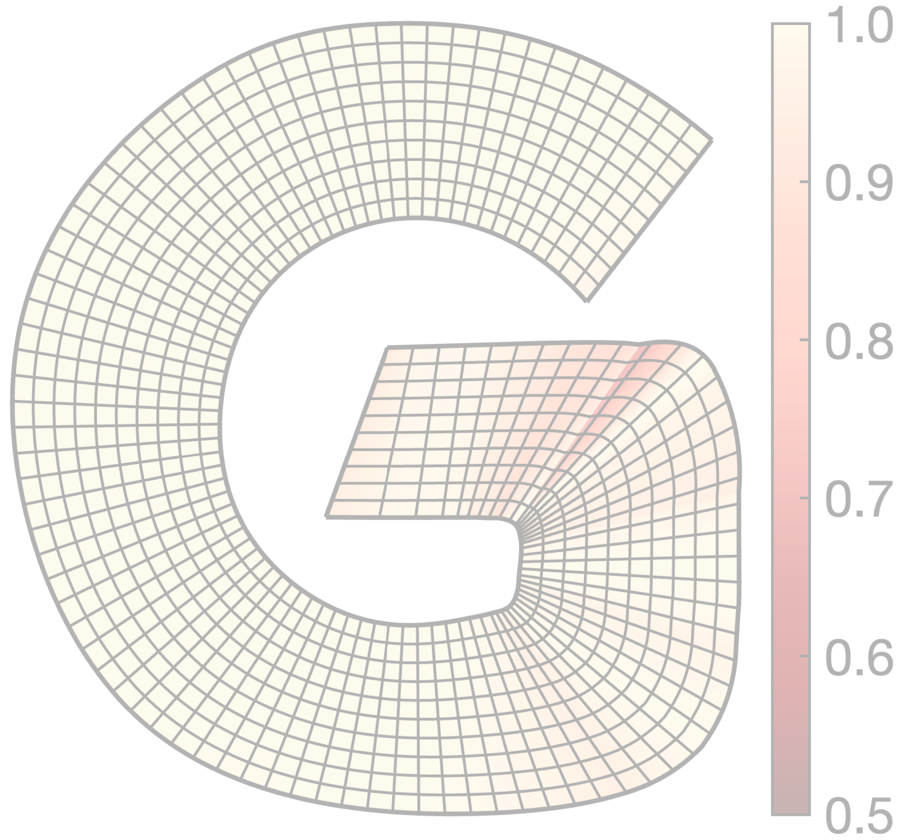
Intermezzo: spline-based mesh generation + simulation

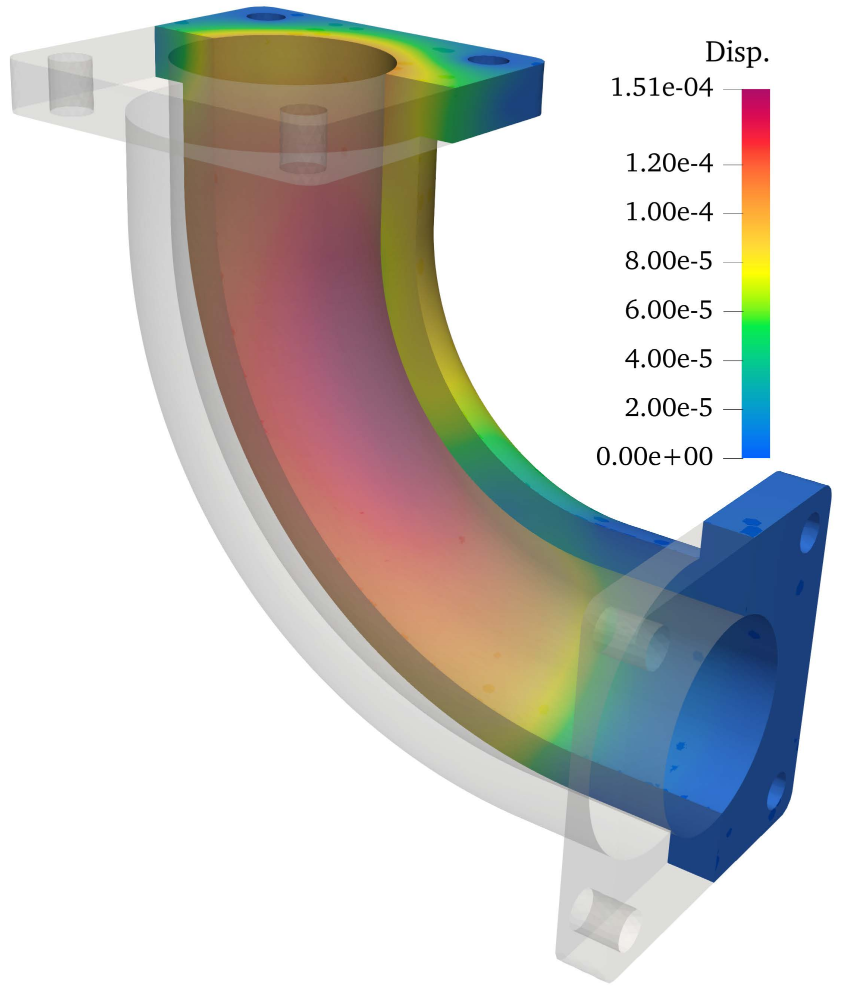


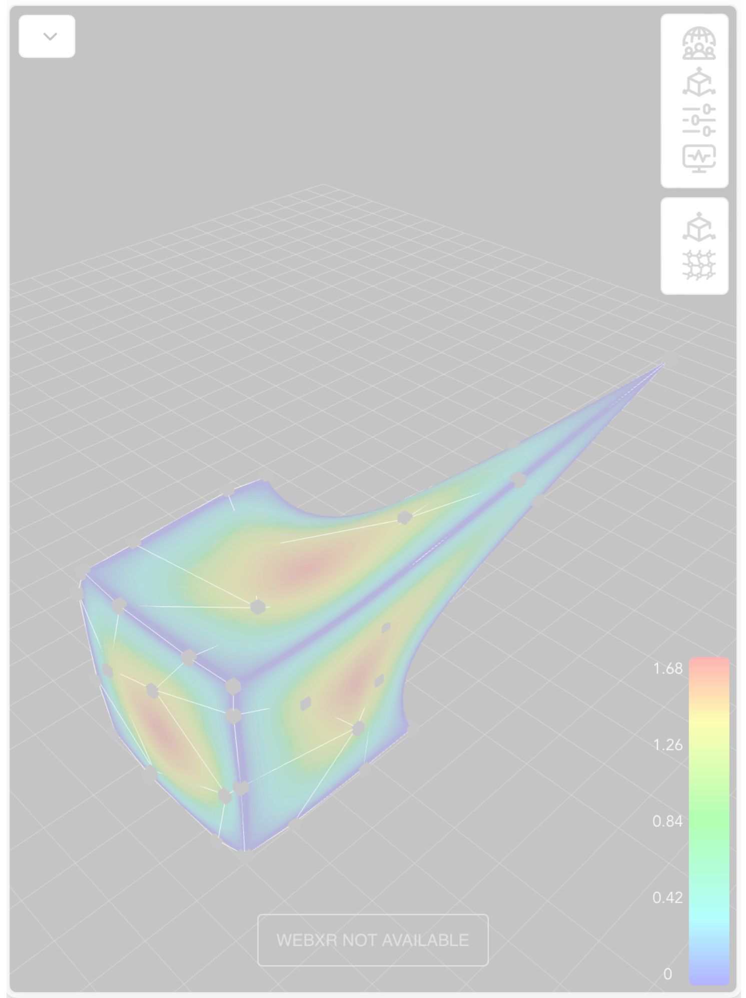


Y. Ji, 2024









1. Creation of VReps from BReps

2. Reparameterization techniques

3. Isogeometric Analysis and IgANets

4. Interactive Design-through-Analysis

Galerkin IgA

Model problem

$$\mathscr{L}u = f \quad \text{in } \Omega$$
$$\mathscr{B}u = g \quad \text{on } \Gamma$$

Weighted residual form

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

Procedure

1. Integrate by parts to equilibrate C^ℓ between test and trial functions
2. Integrate natural boundary conditions into boundary integral term
3. Discretize (evaluate integrals on parametric domain) + solve

Collocation IgA

Model problem

$$\mathscr{L}u = f \quad \text{in } \Omega$$
$$\mathscr{B}u = g \quad \text{on } \Gamma$$

Weighted residual form

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

Let

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

then

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

Collocation IgA

As the coefficients c_i are arbitrary we obtain

$$\begin{aligned} \mathscr{L}u(\mathbf{x}_i) &= f(\mathbf{x}_i) \qquad && i = 1,\ldots,k \\ \mathscr{B}u(\mathbf{x}_i) &= g(\mathbf{x}_i) \qquad && i = k+1,\ldots,n \end{aligned}$$

replacing $u \approx u_h = \sum_{j=1}^{n} u_j b_j(\mathbf{x})$ yields

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

Collocation IgA

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- basis functions b_i need to be at least C^ℓ such that application of $\mathscr{L}$ and $\mathscr{B}$ is well-defined

- non-singular system matrix requires

  #coll. pts = #basfunc

  and all coll. points must be pairwise distinct

Collocation IgA

As the coefficients c_i are arbitrary we obtain

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

replacing $u \approx u_h = \sum_{j=1}^{n} u_j b_j(\mathbf{x})$ yields

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- basis functions b_i need to be at least C^ℓ such that application of $\mathscr{L}$ and $\mathscr{B}$ is well-defined

- non-singular system matrix requires

  #coll. pts = #basfunc

  and all coll. points must be pairwise distinct

- B-spline basis functions are defined on the parametric domain $\hat{\Omega} = (0,1)^d$, hence

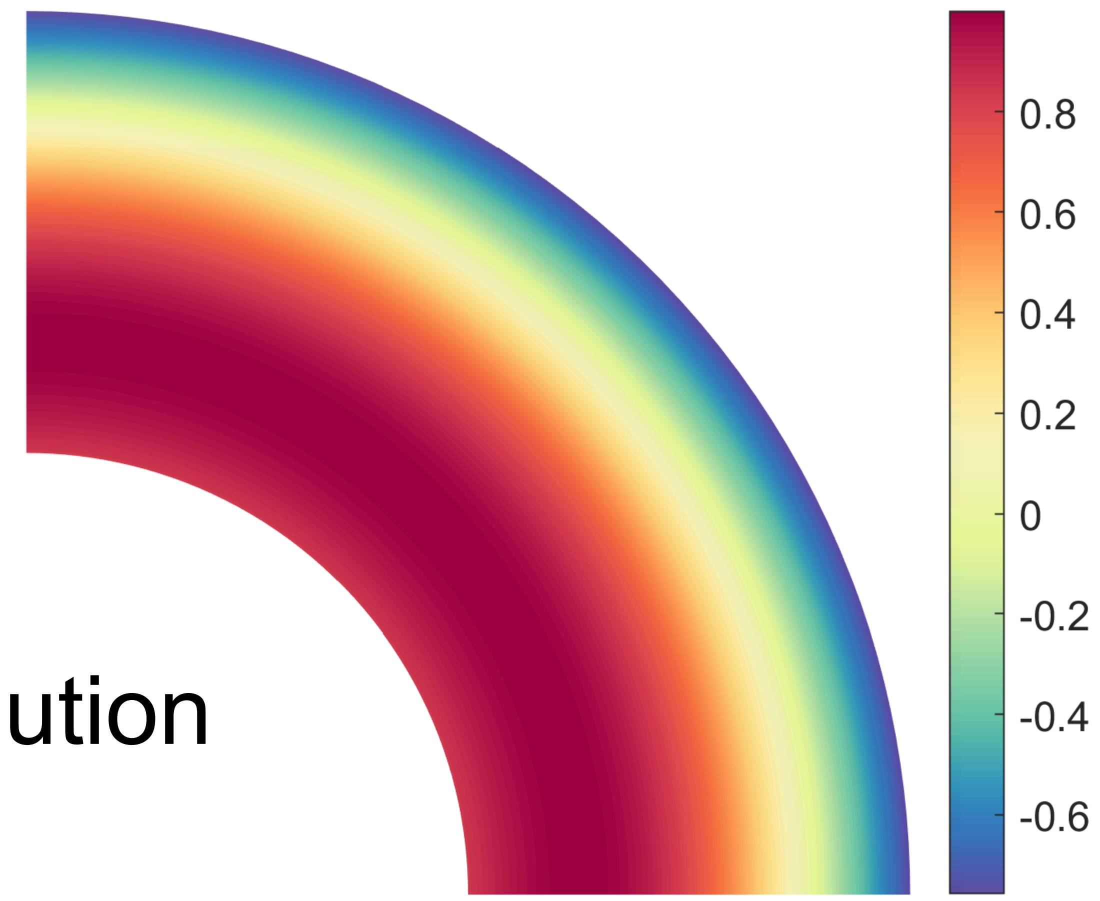
$$\mathscr{L}_{\mathbf{x}} b_i(\mathbf{x}) \to \mathscr{L}_{\boldsymbol{\xi}} b_i(\boldsymbol{\xi})$$
$$\mathscr{B}_{\mathbf{x}} b_i(\mathbf{x}) \to \mathscr{B}_{\boldsymbol{\xi}} b_i(\boldsymbol{\xi})$$

and define $\mathbf{x}_i := \mathbf{x}_h(\boldsymbol{\xi}_i)$

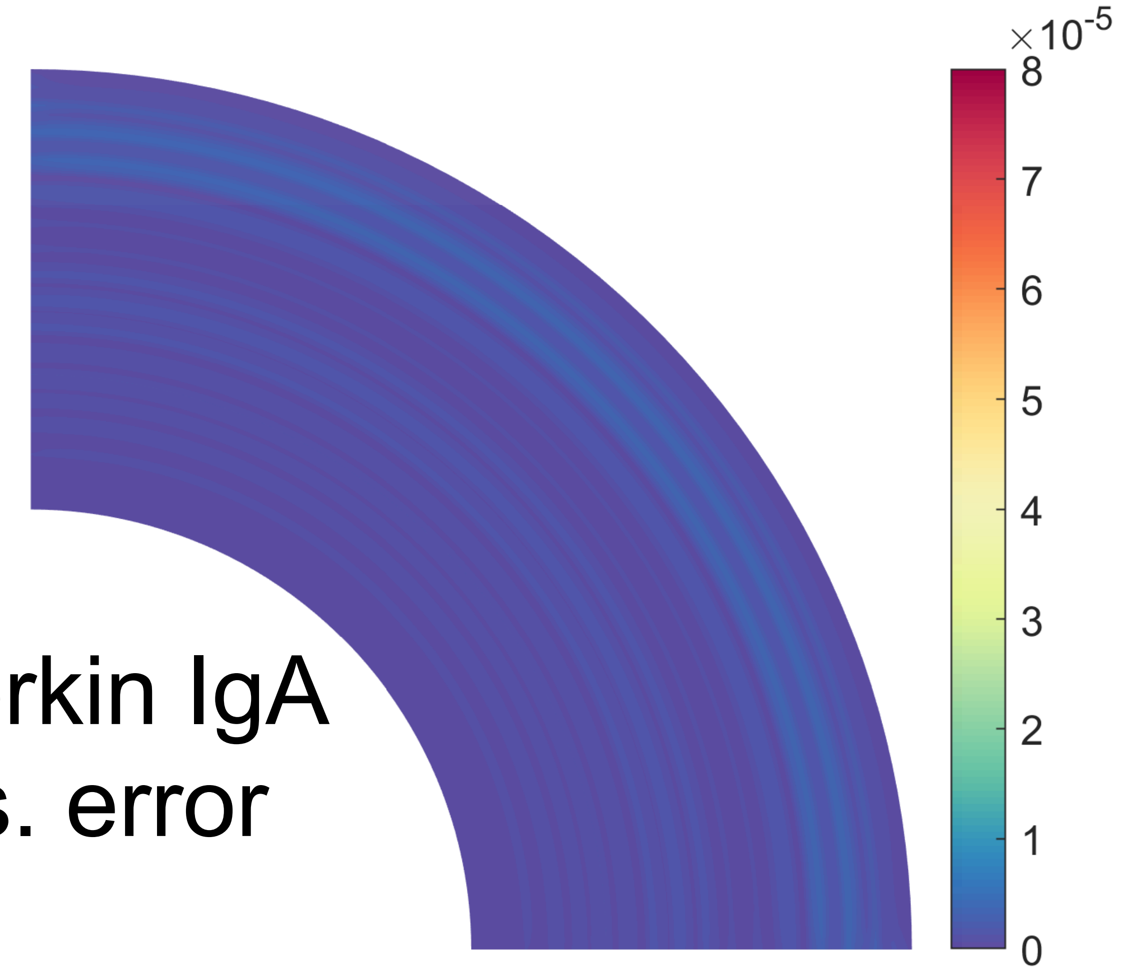
Galerkin vs. collocation IgA

Model problem

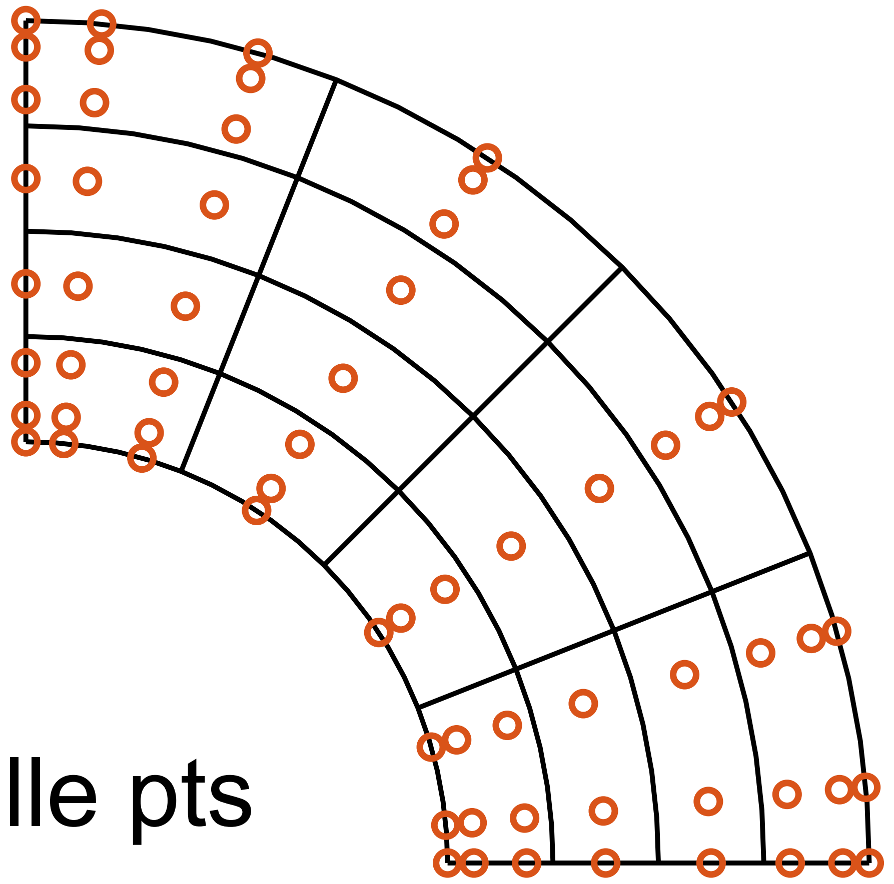
$$-\Delta u = f \quad \text{in } \Omega$$
$$u = g \quad \text{on } \Gamma$$



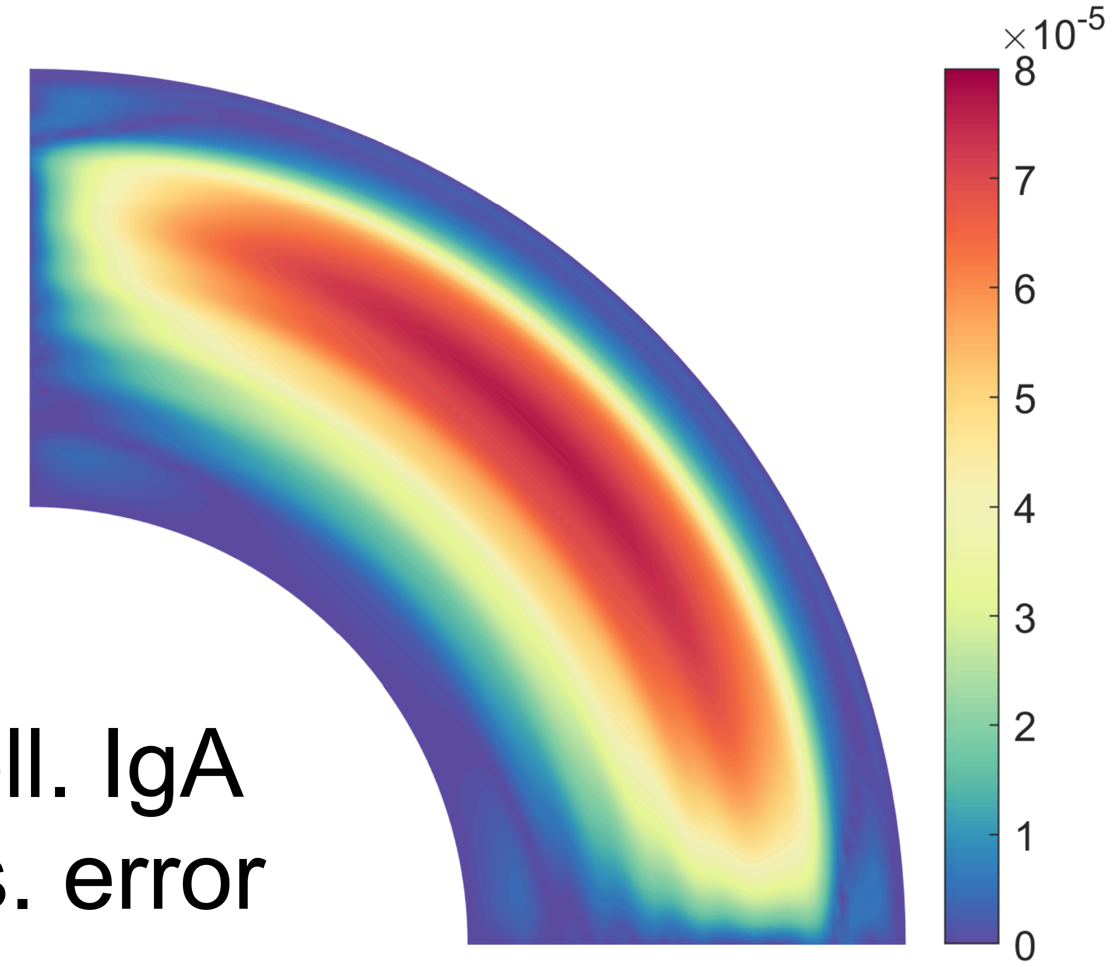
solution



Galerkin IgA
abs. error



Greville pts



Coll. IgA
abs. error

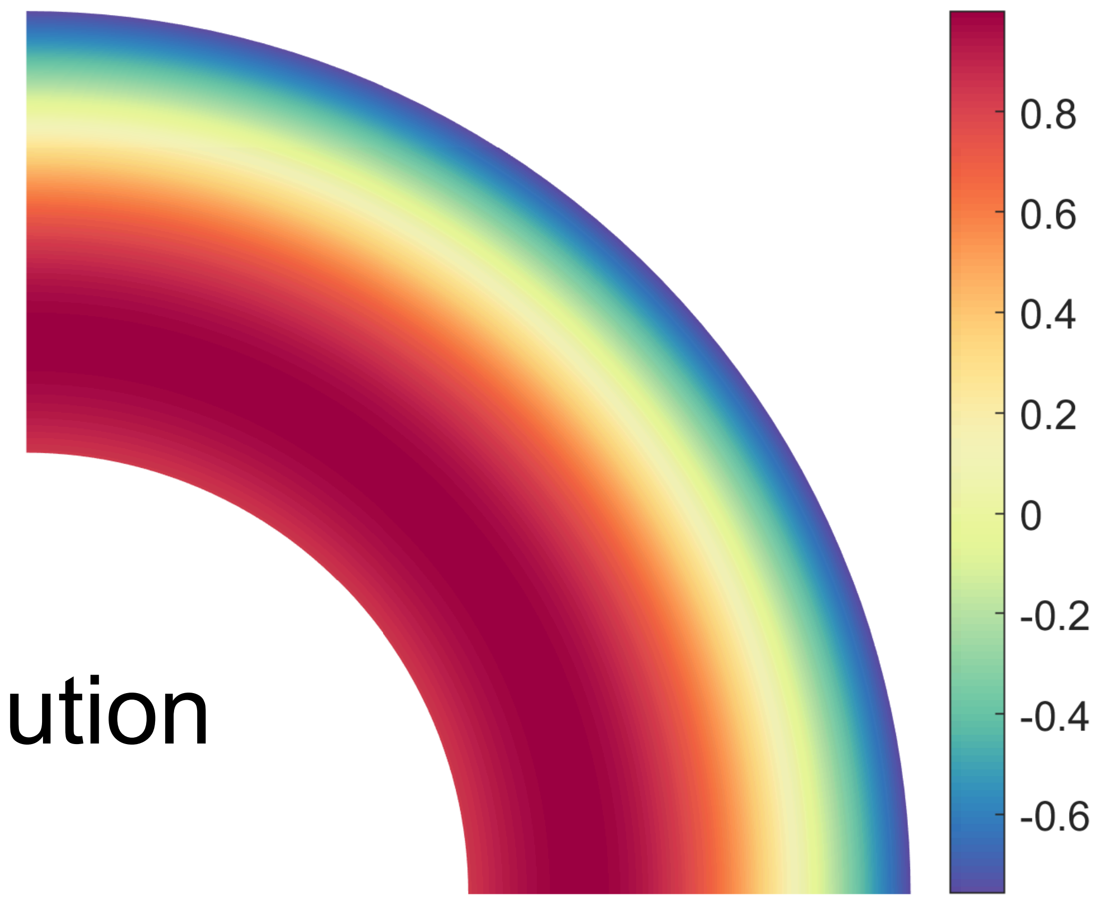
M. Wang, 2023

Galerkin vs. collocation IgA

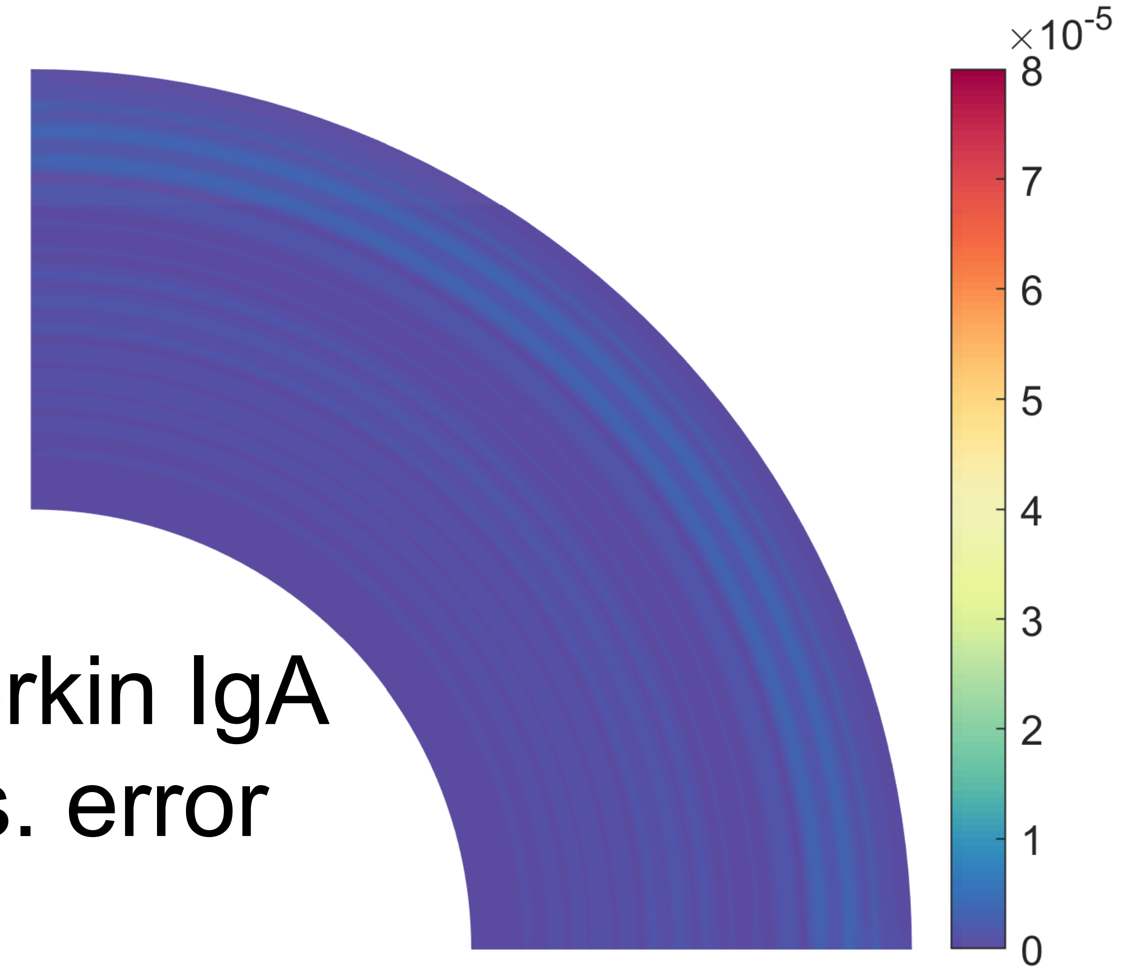
Model problem

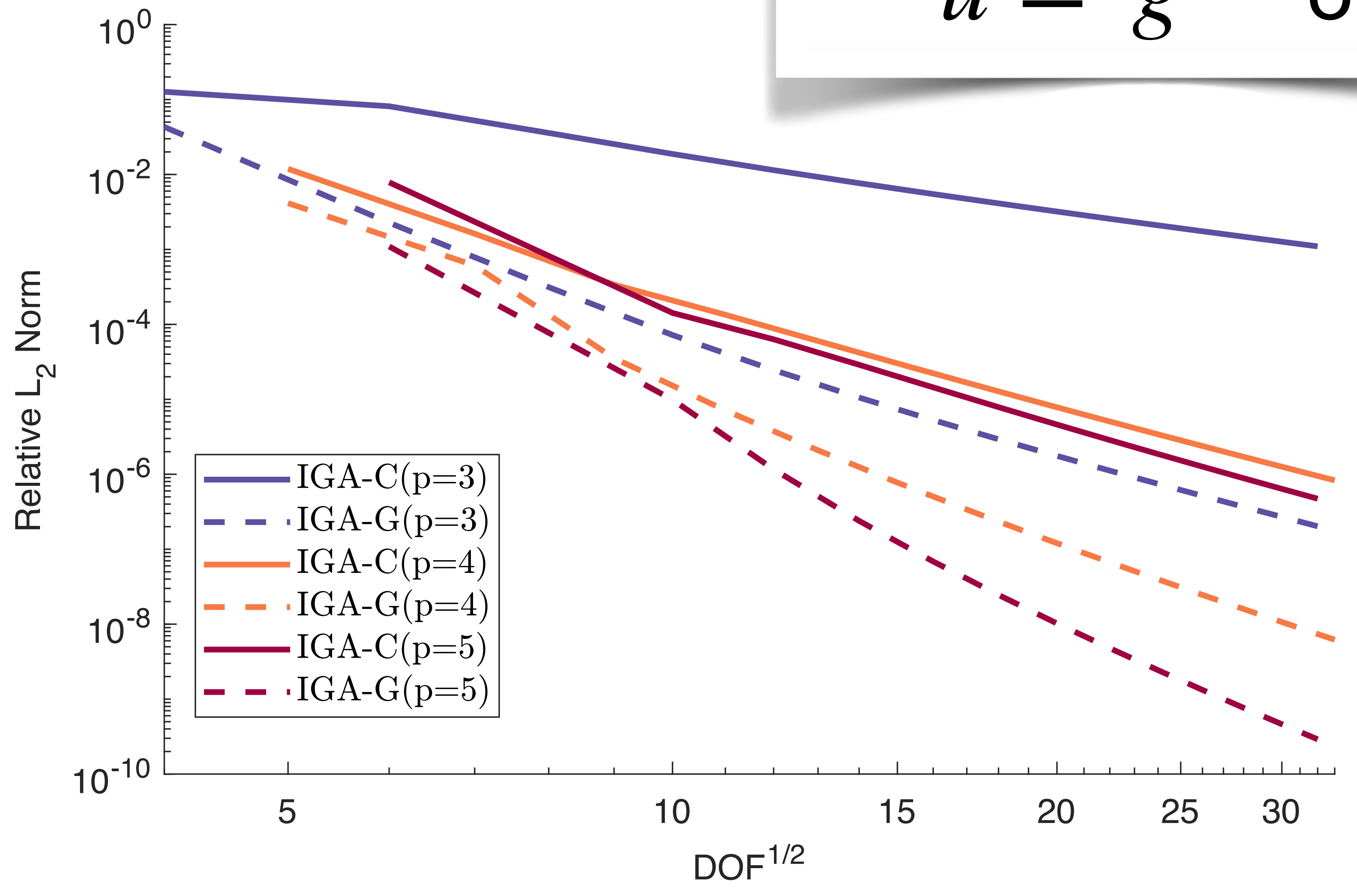
$$-\Delta u = f \quad \text{in } \Omega$$
$$u = g \quad \text{on } \Gamma$$

solution

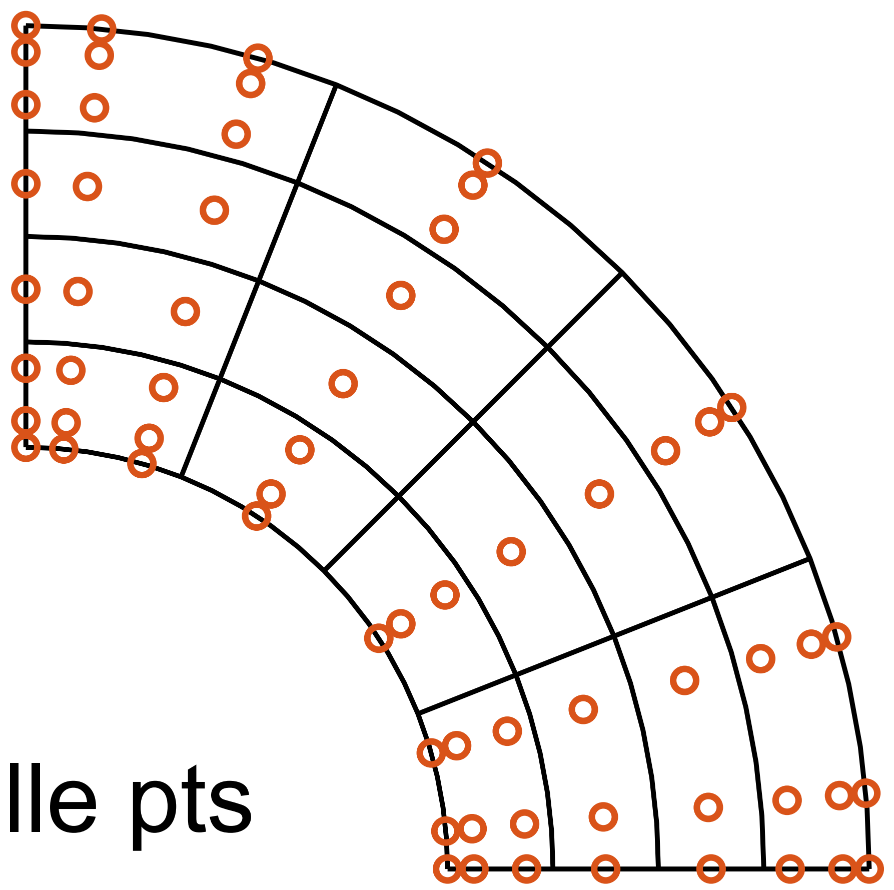


Galerkin IgA
abs. error

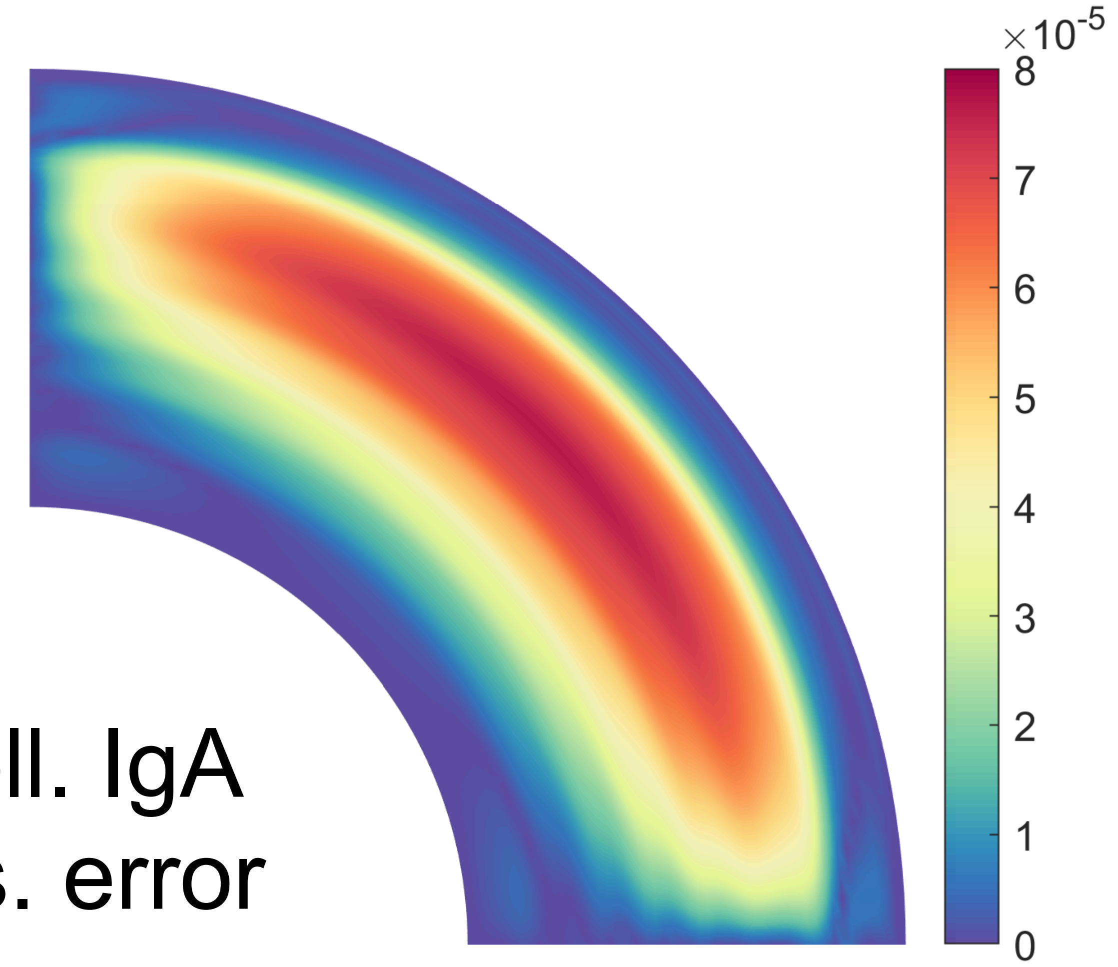


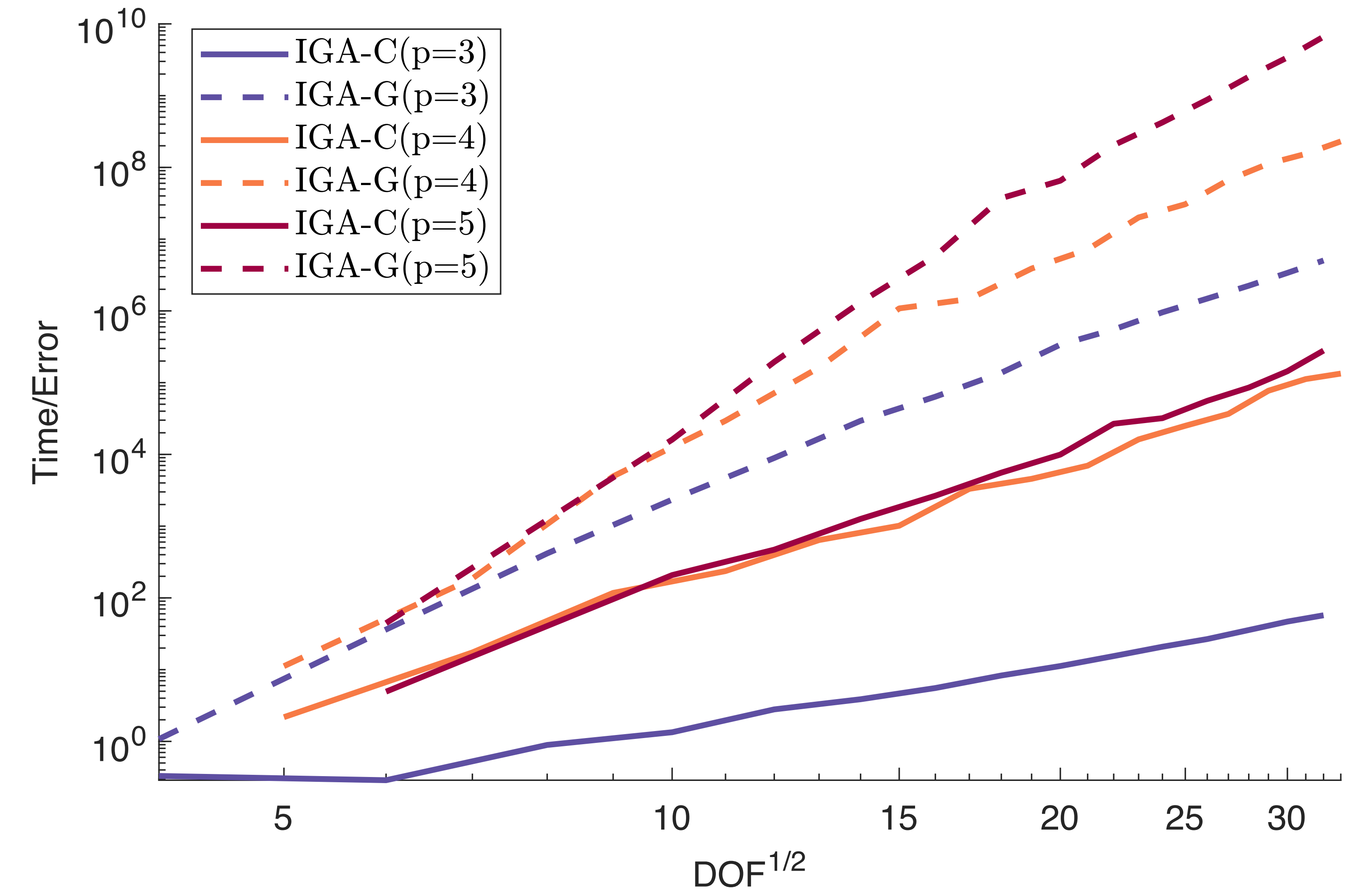


Greville pts



Coll. IgA
abs. error



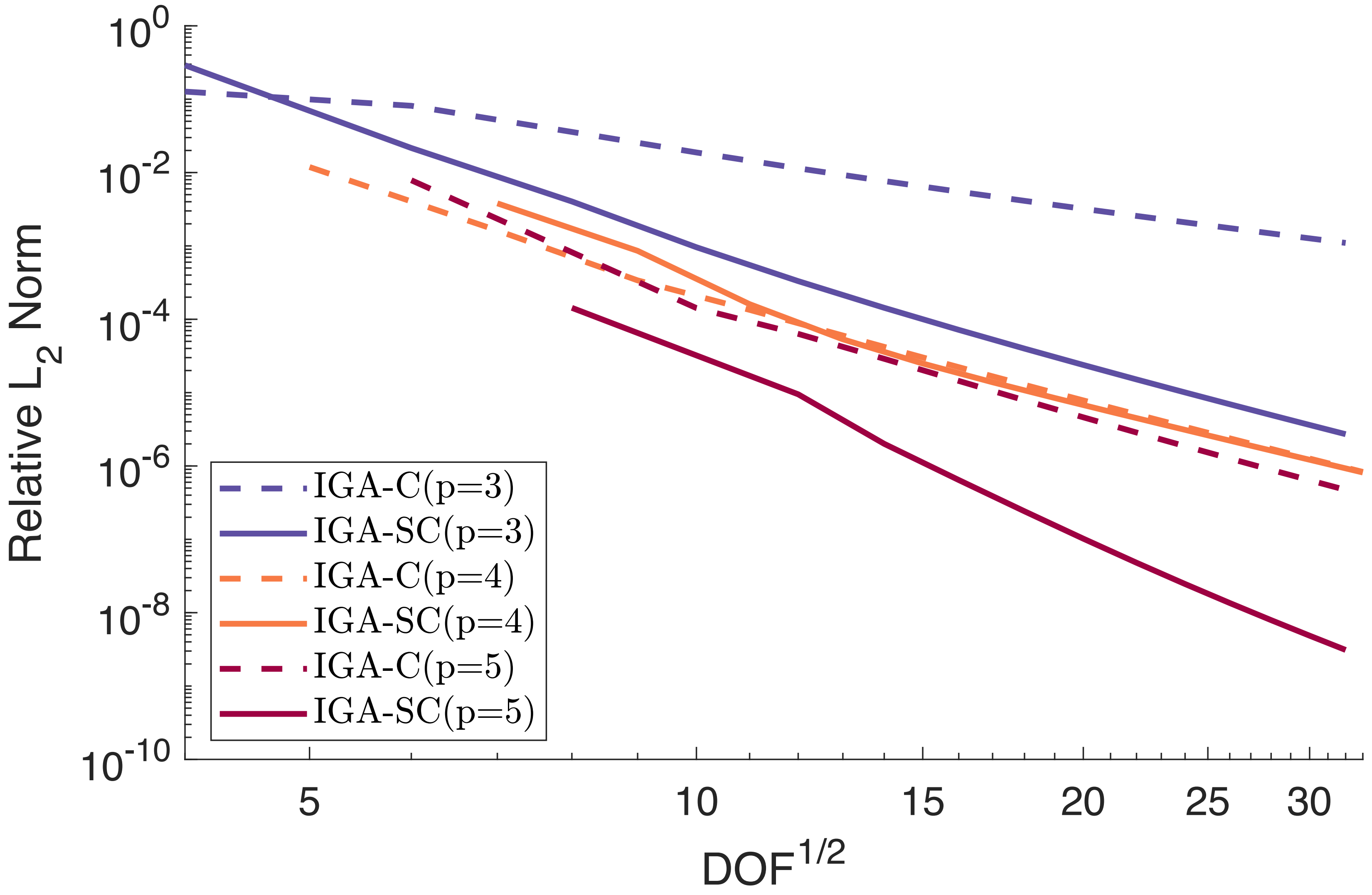


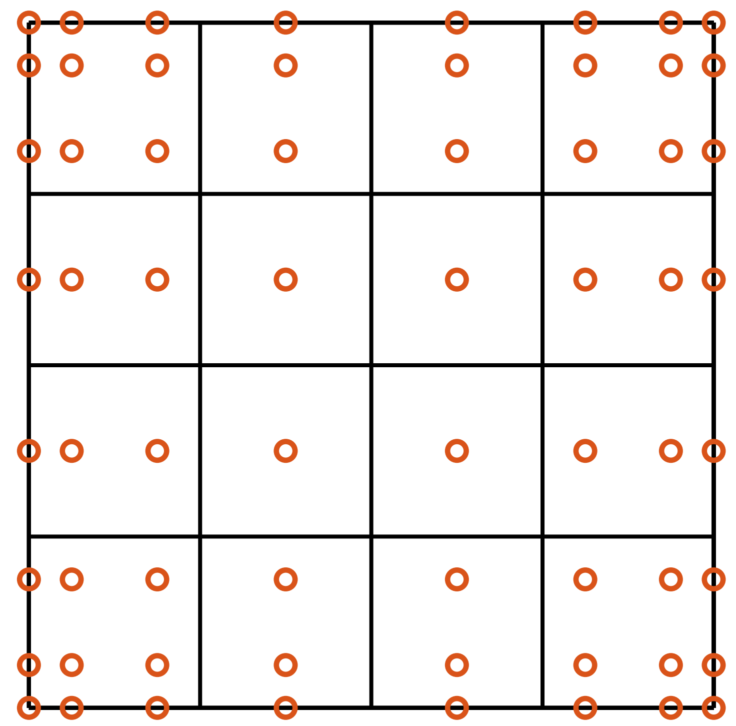
M. Wang, 2023

Influence of collocation points

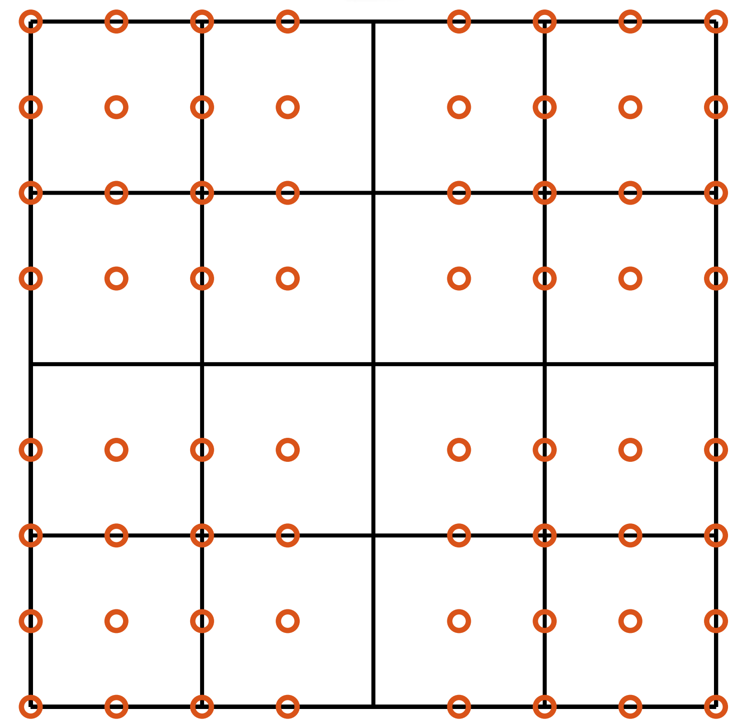
Model problem

$$
\begin{aligned}
-\Delta u &= f \quad \text{in } \Omega \\
u &= g \quad \text{on } \Gamma
\end{aligned}
$$

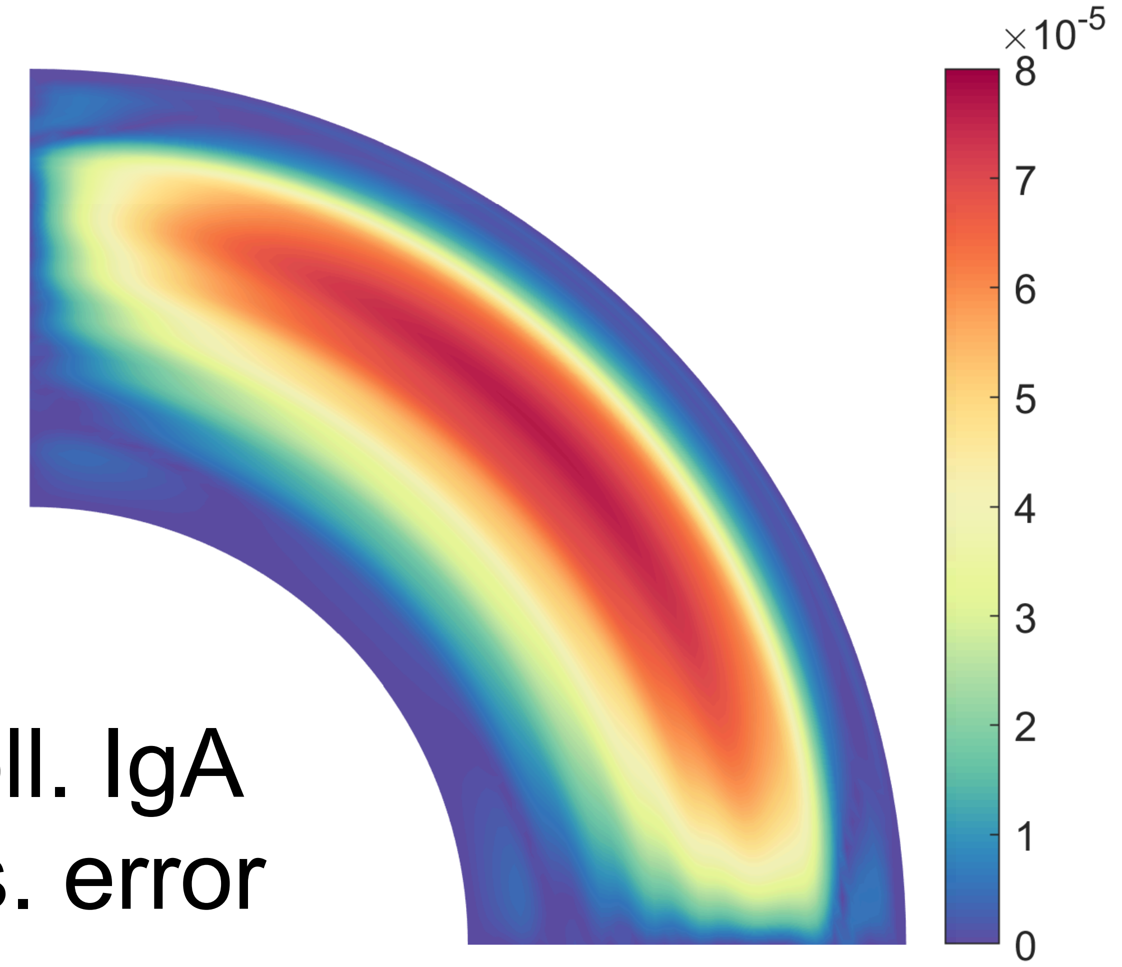




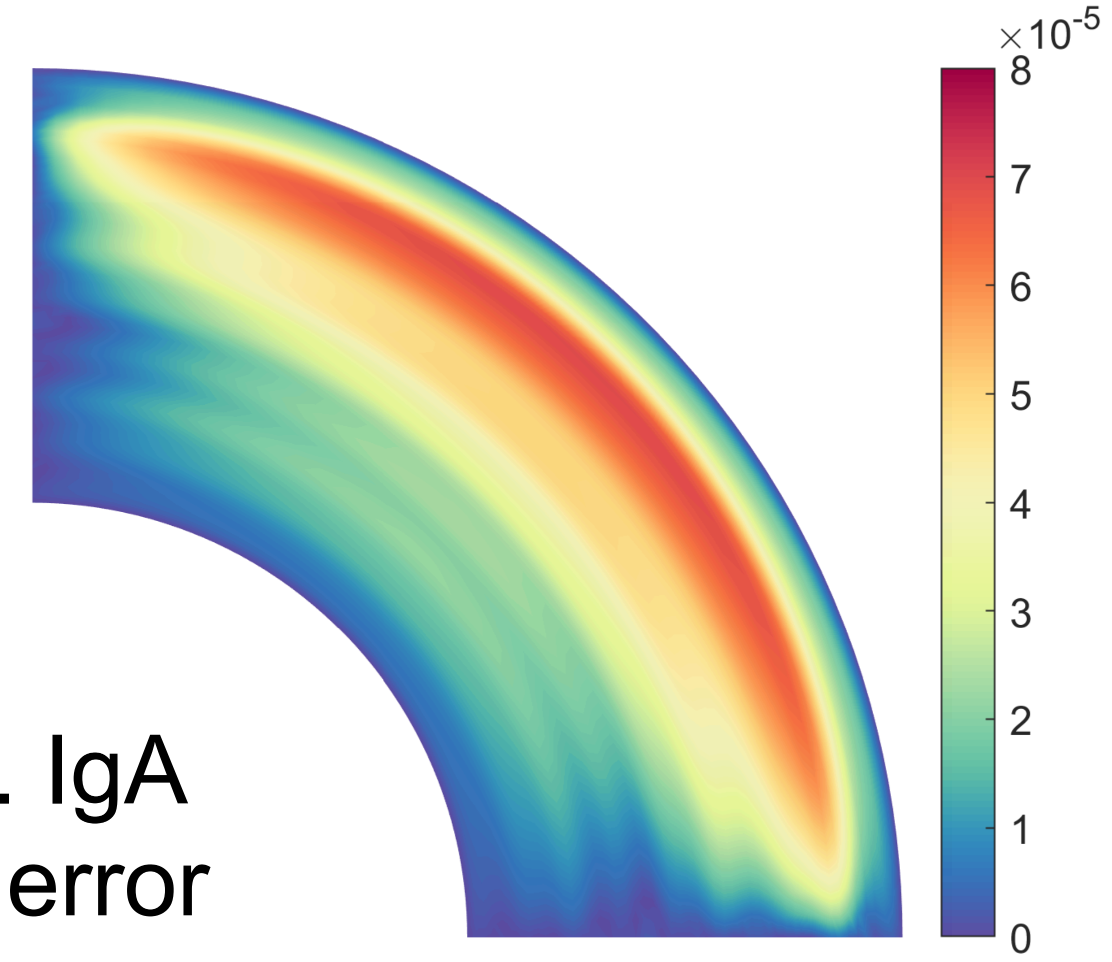
Greville pts



Clustered SC pts



Coll. IgA abs. error



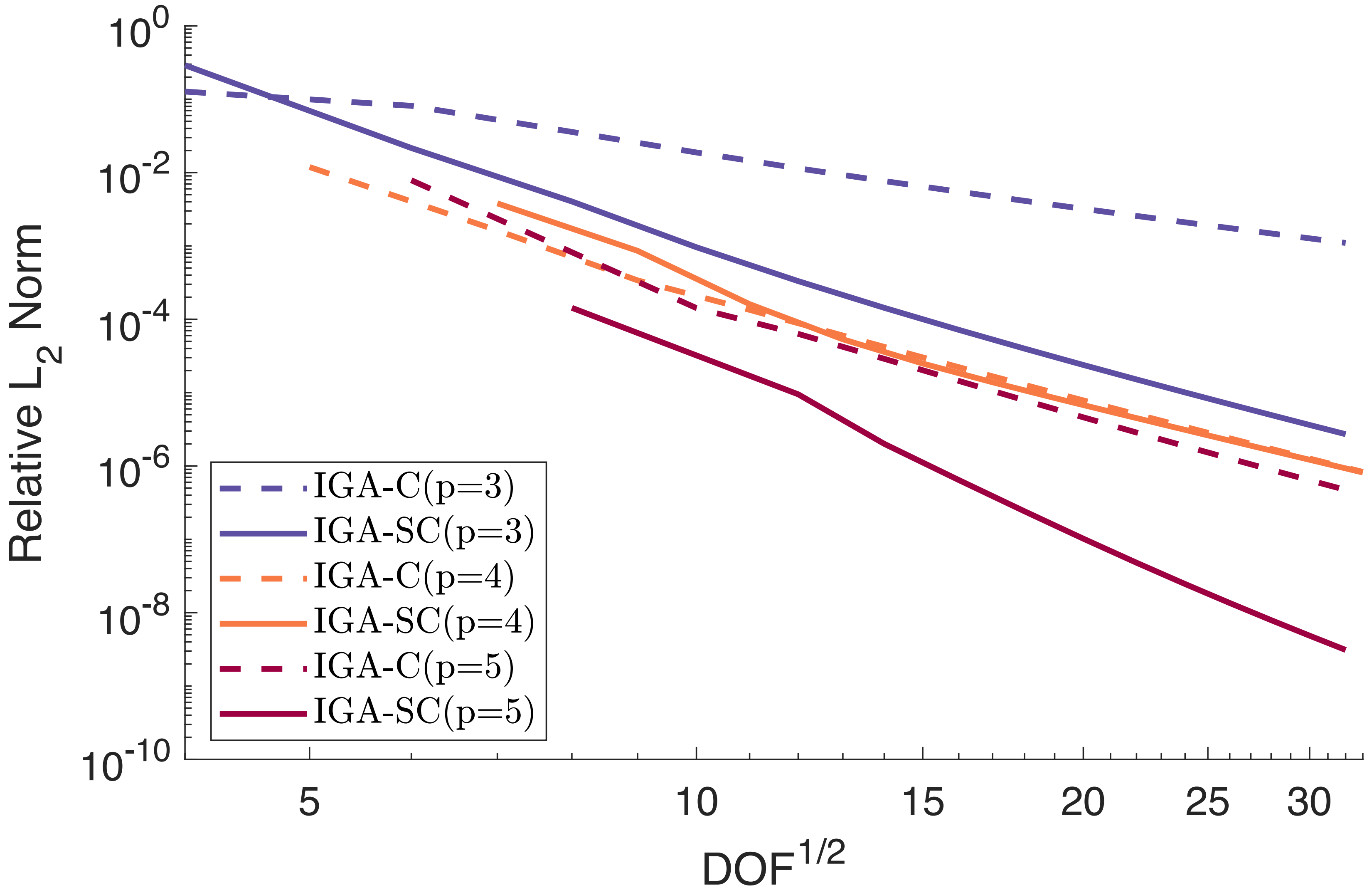
Coll. IgA abs. error

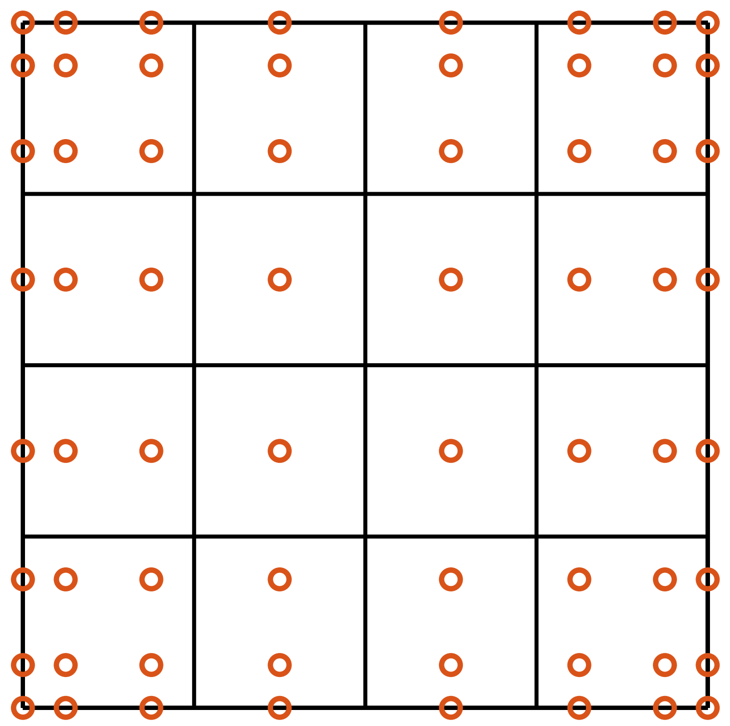
M. Wang, 2023

Influence of collocation points

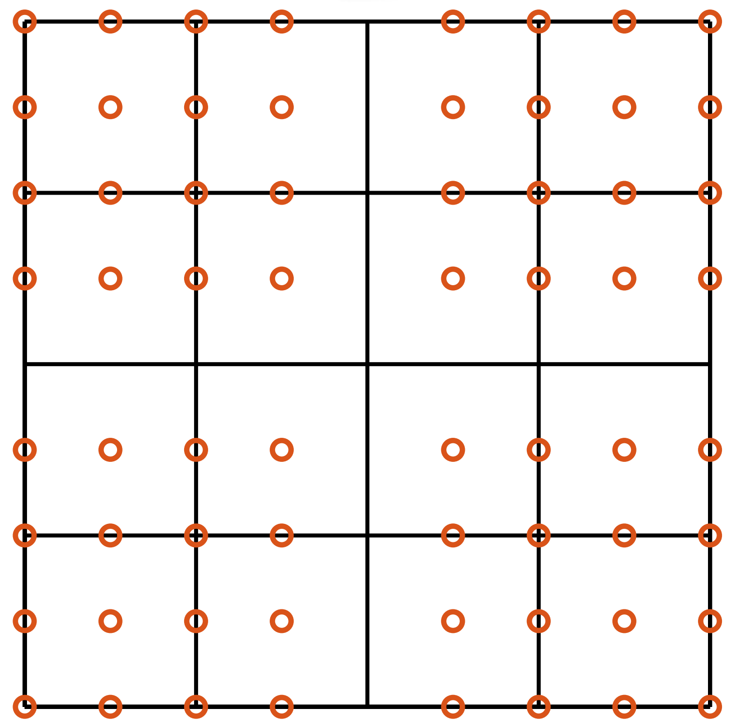
Model problem

$$-\Delta u = f \quad \text{in } \Omega$$
$$u = g \quad \text{on } \Gamma$$

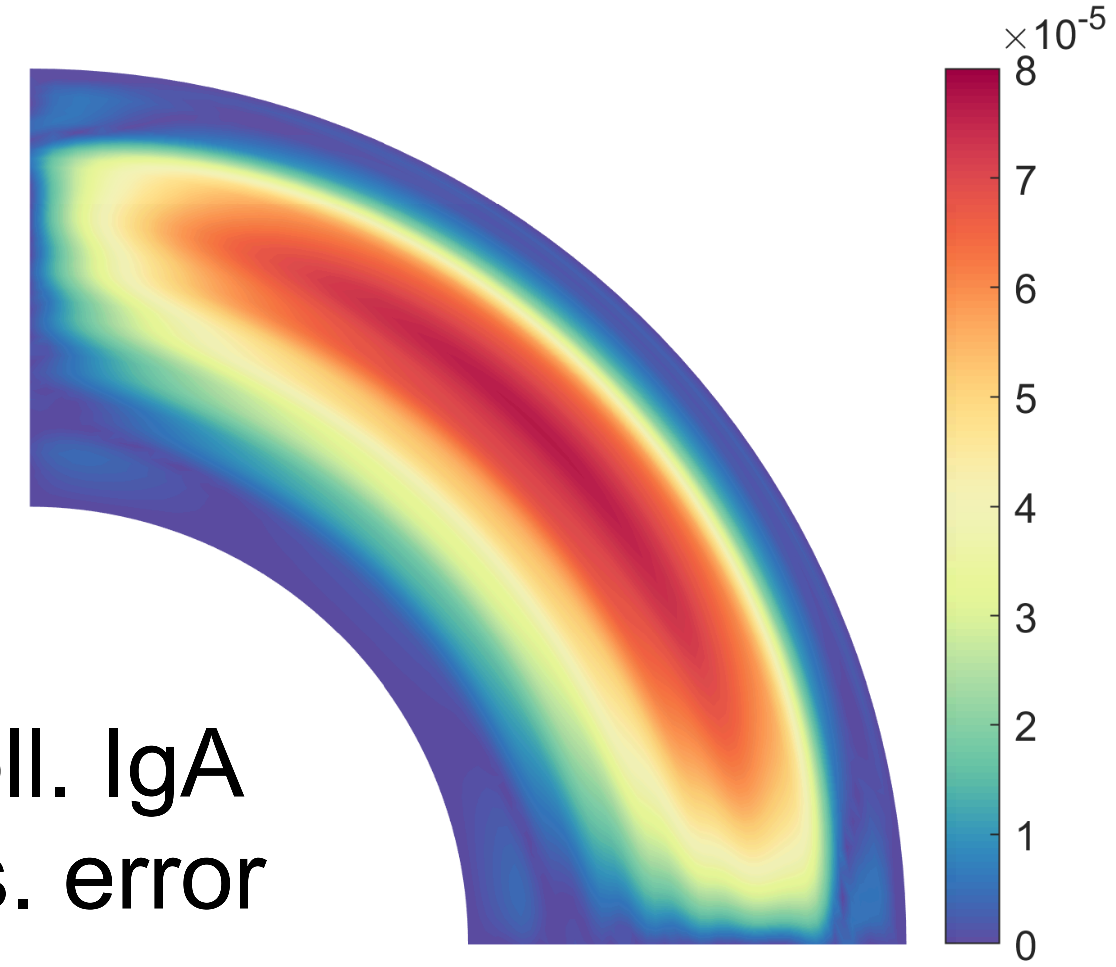




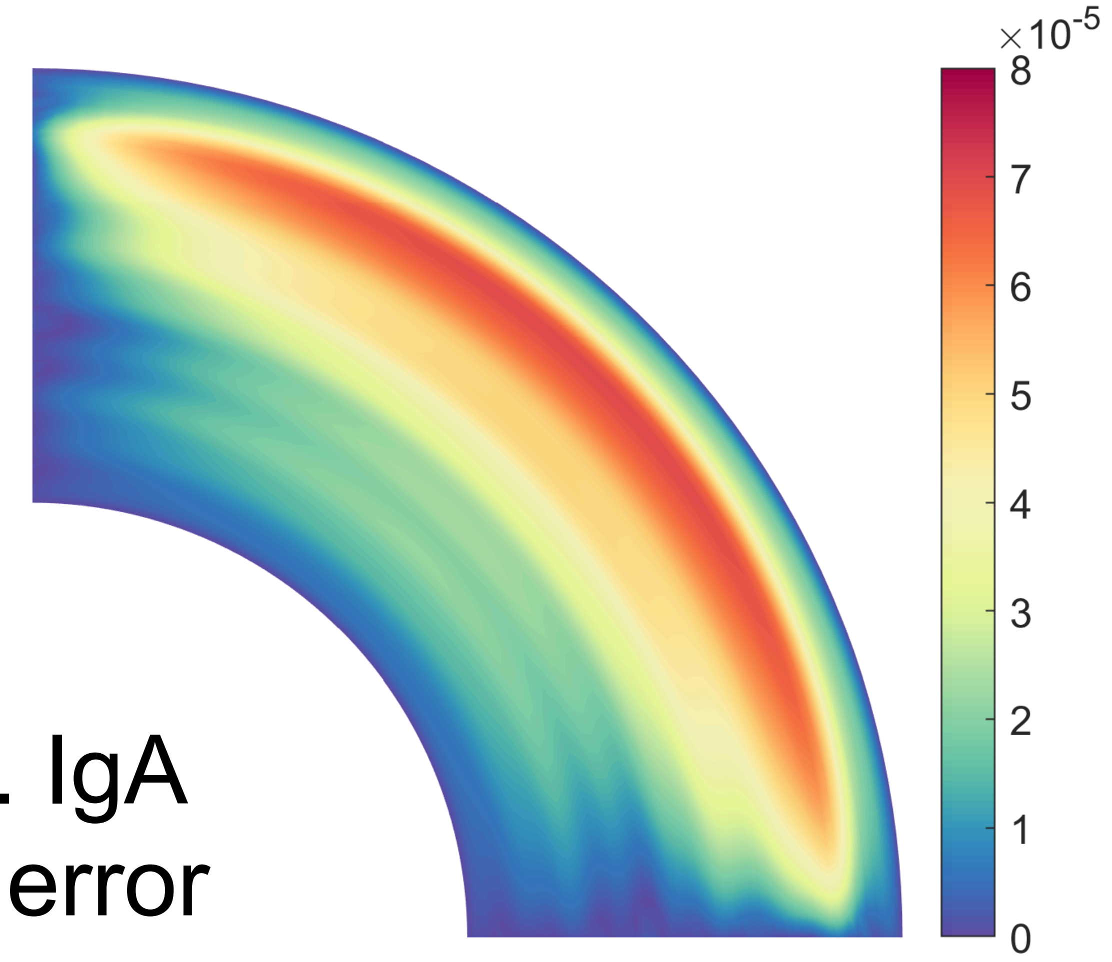
Greville pts



Clustered SC pts



Coll. IgA abs. error



Coll. IgA abs. error

As finding the **optimal position of collocation points** is difficult, can't we instead increase their number to reduce the error?

M. Wang, 2023

Least-squares collocation IgA

When #collocation points ($m_1 + m_2$) > #degrees of freedom (n) then the system matrix is over-determined and the system cannot be solved regularly. However, we can solve it in **least-squares sense**

$$\min_{u_h} \frac{1}{m_1} \sum_{i=1}^{m_1} \|\mathscr{L}_{\mathbf{x}} u_h(\mathbf{x}_i) - f(\mathbf{x}_i)\|^2 + \frac{1}{m_2} \sum_{i=m_1+1}^{m_1+m_2} \|\mathscr{B}_{\mathbf{x}} u_h(\mathbf{x}_i) - g(\mathbf{x}_i)\|^2$$

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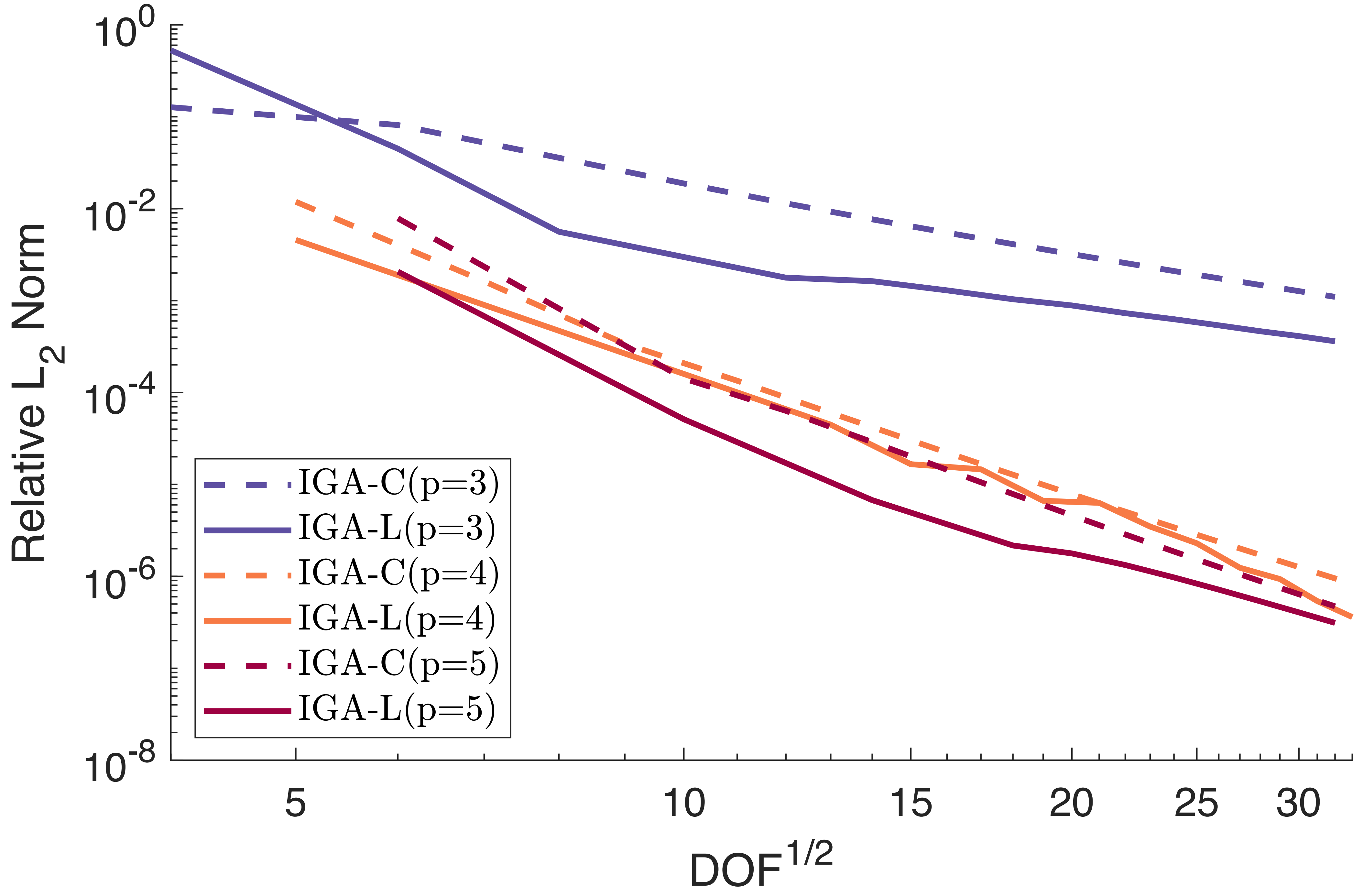
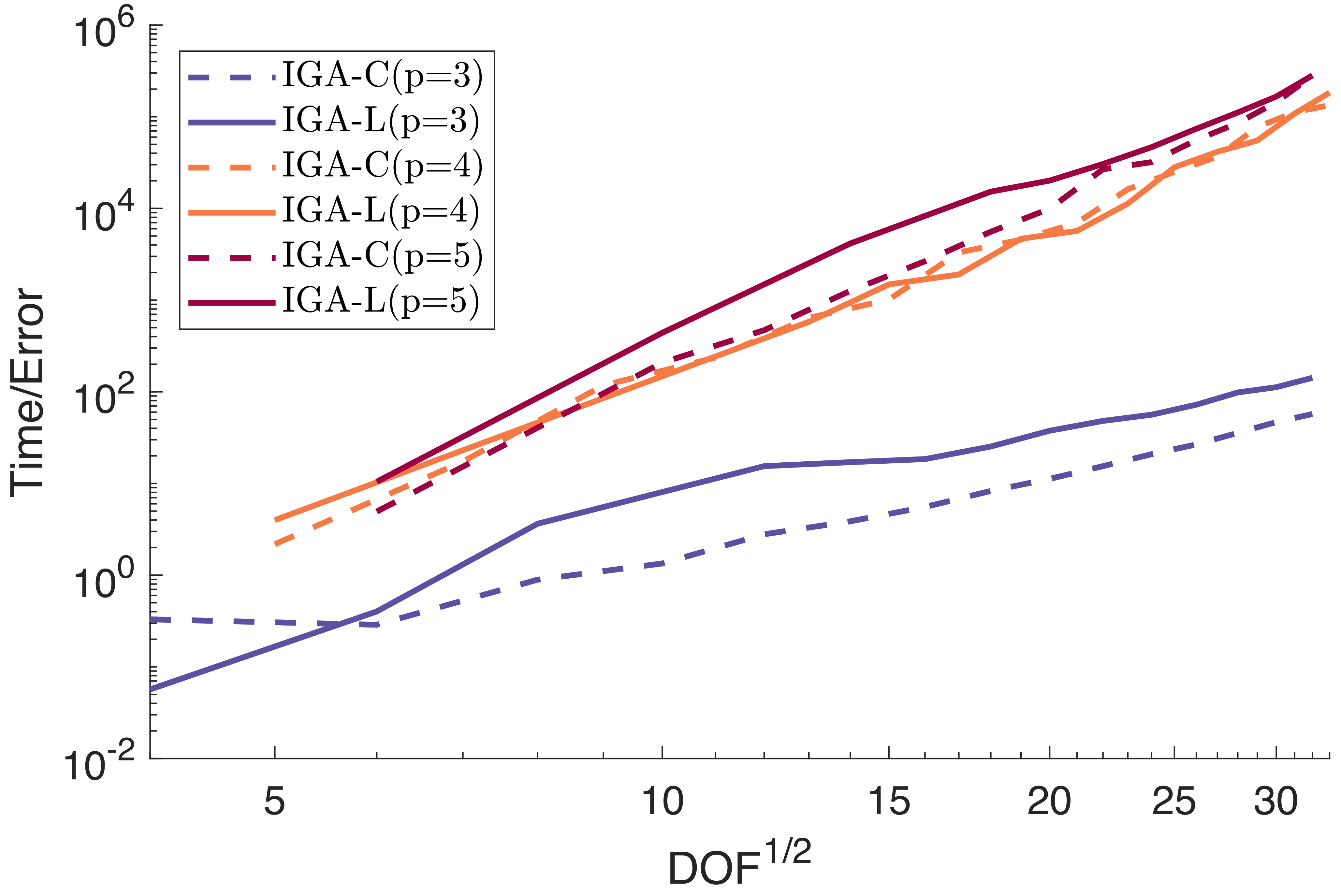
Theoretical justification [Lin et al. 2020]: under certain conditions, the least-squares collocation IgA method is consistent and convergent. In essence, there must be at *least one collocation point per element* (e.g., Greville point) but we can use more to increase the sampling resolution.

Least-squares collocation IgA





From least-squares collocation IgA to IgANets

$$\min_{u_h} \frac{1}{m_1} \sum_{i=1}^{m_1} \|\mathscr{L}_{\mathbf{x}} u_h(\mathbf{x}_i) - f(\mathbf{x}_i)\|^2 + \frac{1}{m_2} \sum_{i=m_1+1}^{m_1+m_2} \|\mathscr{B}_{\mathbf{x}} u_h(\mathbf{x}_i) - g(\mathbf{x}_i)\|^2$$

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$$\mathbf{x}_h(\boldsymbol{\xi}) = \sum_{j=1}^{n} b_j(\boldsymbol{\xi})\, \mathbf{x}_j$$

From least-squares collocation IgA to IgANets

$$\min_{u_h} \frac{1}{m_1} \sum_{i=1}^{m_1} \|\mathscr{L}_{\mathbf{x}} u_h(\mathbf{x}_i) - f(\mathbf{x}_i)\|^2 + \frac{1}{m_2} \sum_{i=m_1+1}^{m_1+m_2} \|\mathscr{B}_{\mathbf{x}} u_h(\mathbf{x}_i) - g(\mathbf{x}_i)\|^2$$

$$\min_{\boxed{\{u_j\}_j}} \frac{1}{m_1} \sum_{i=1}^{m_1} \| \sum_{j=1}^{n} \mathscr{L}_{\boldsymbol{\xi}} b_j(\boldsymbol{\xi}_i) u_j - b_j(\boldsymbol{\xi}_i) \boxed{f_j} \|^2 + \frac{1}{m_2} \sum_{i=m_1+1}^{m_1+m_2} \| \sum_{j=1}^{n} \mathscr{B}_{\boldsymbol{\xi}} b_j(\boldsymbol{\xi}_i) u_j - b_j(\boldsymbol{\xi}_i) \boxed{g_j} \|^2$$

solution

rhs

bc cond.

$$\mathbf{x}_h(\boldsymbol{\xi}) = \sum_{j=1}^{n} b_j(\boldsymbol{\xi}) \boxed{\mathbf{x}_j}$$

geometry

From least-squares collocation IgA to deep operator learning

$$\min_{\{u_j\}_j} \boxed{\frac{1}{m_1}\sum_{i=1}^{m_1} \| \sum_{j=1}^{n} \mathscr{L}_{\xi} b_j(\boldsymbol{\xi}_i) u_j - b_j(\boldsymbol{\xi}_i) f_j \|^2} + \boxed{\frac{1}{m_2}\sum_{i=m_1+1}^{m_1+m_2} \| \sum_{j=1}^{n} \mathscr{B}_{\xi} b_j(\boldsymbol{\xi}_i) u_j - b_j(\boldsymbol{\xi}_i) g_j \|^2}$$

PDE loss function

boundary loss function

From least-squares collocation IgA to deep operator learning

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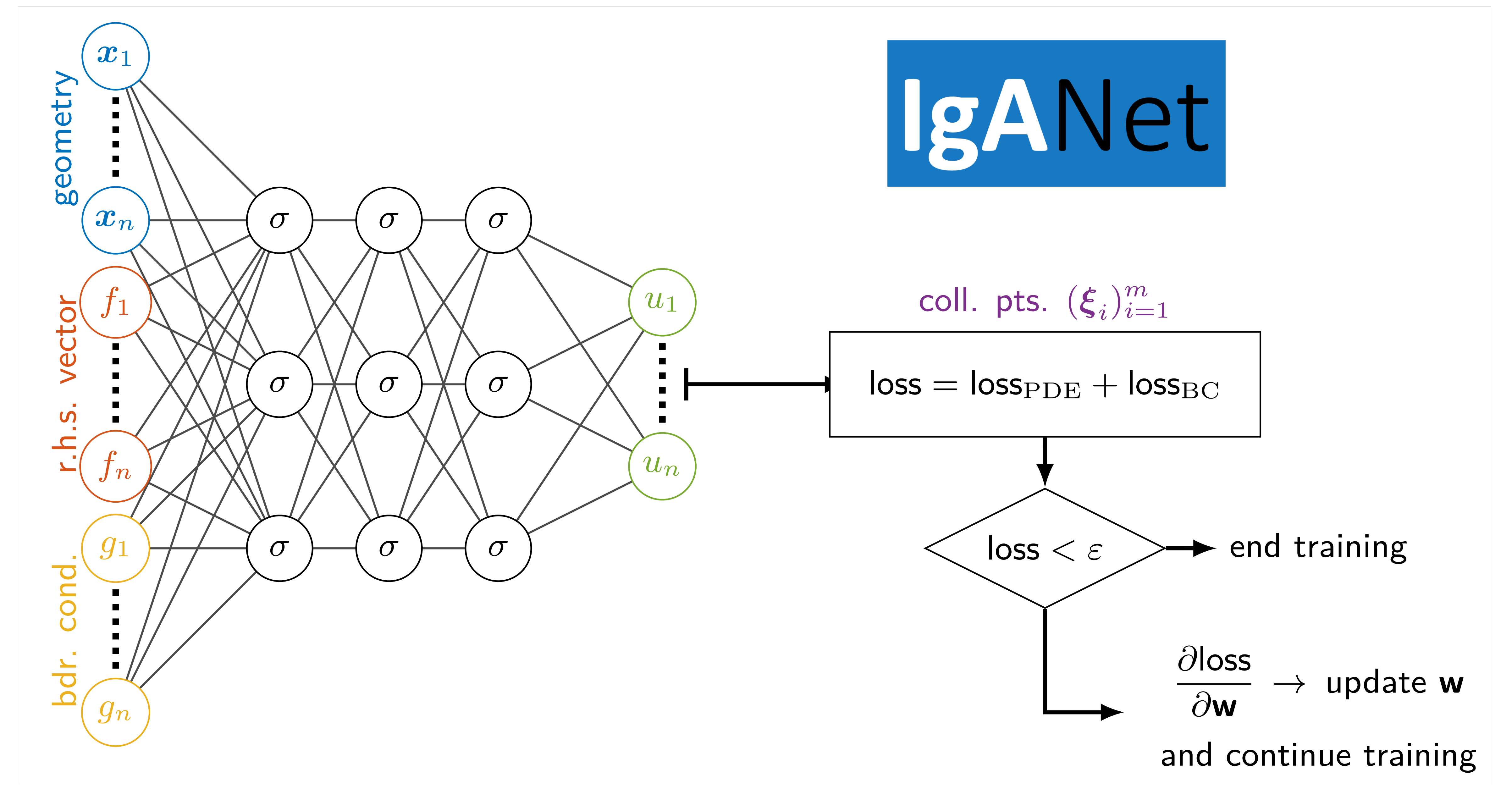

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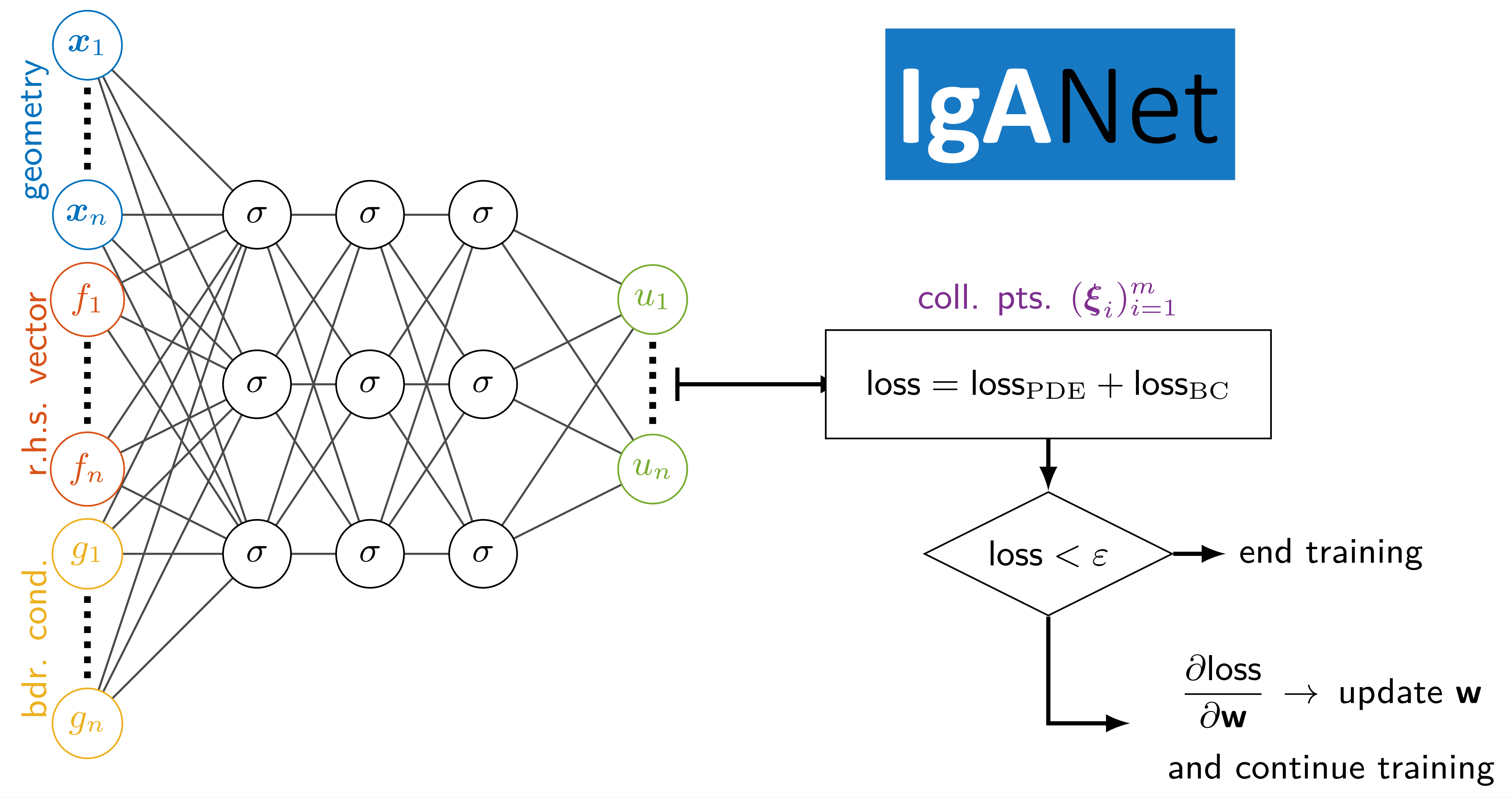

How is this related to PINNs, DeepONets, etc.?

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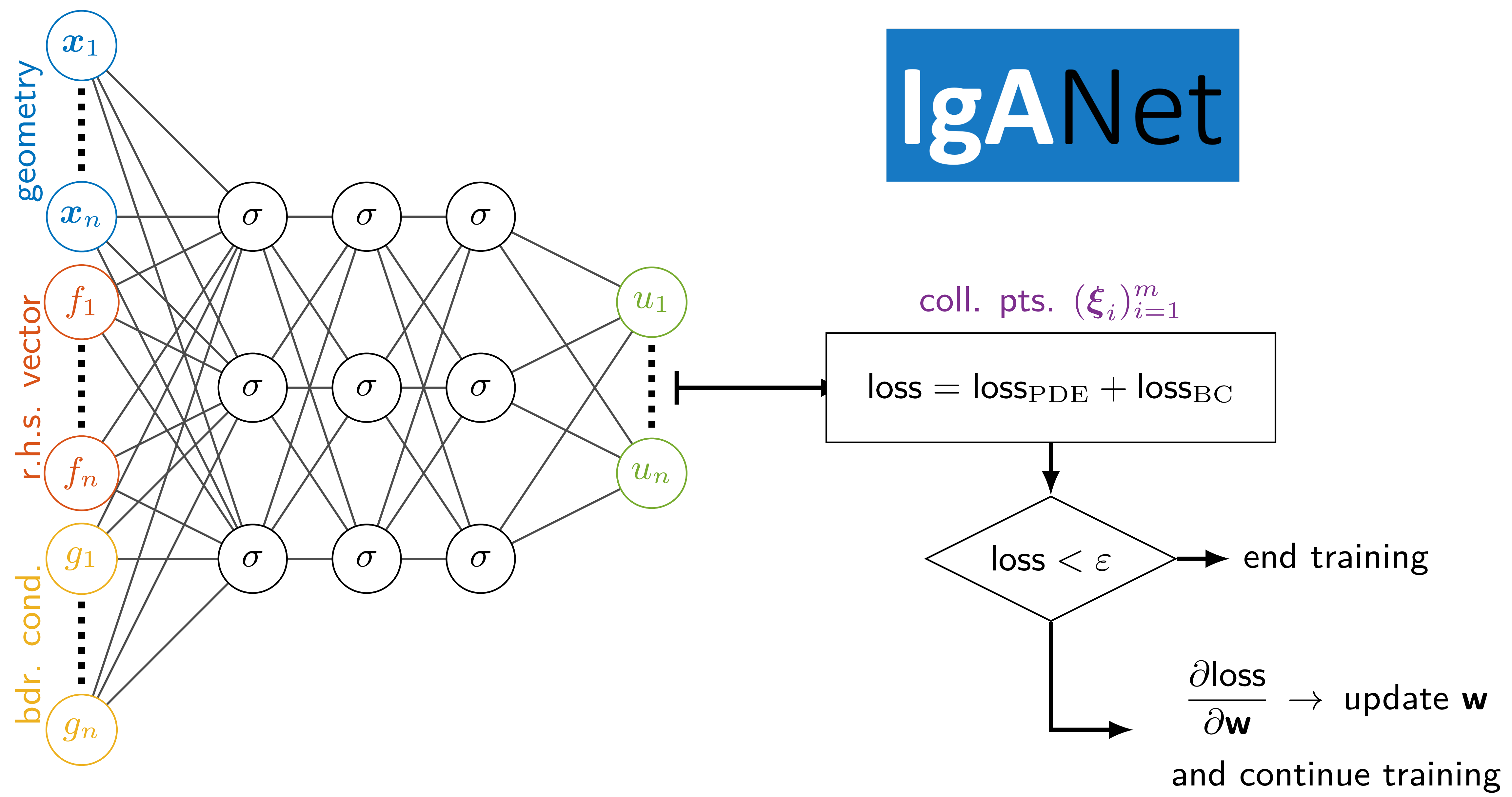

How is this related to PINNs, DeepONets, etc.?

Can be seen as deep operator network with *given* B-spline/NURBS basis!

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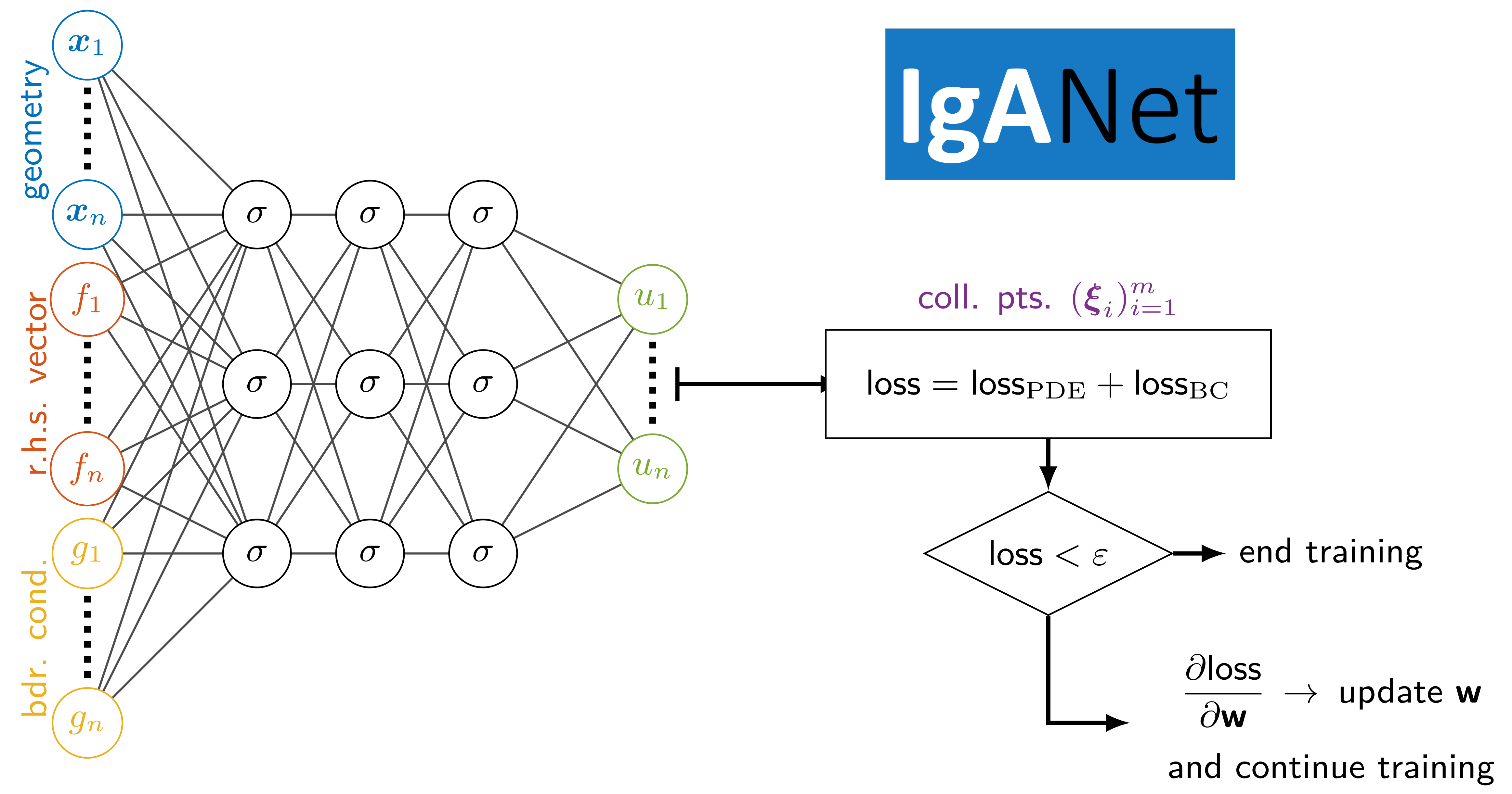

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PDE loss function

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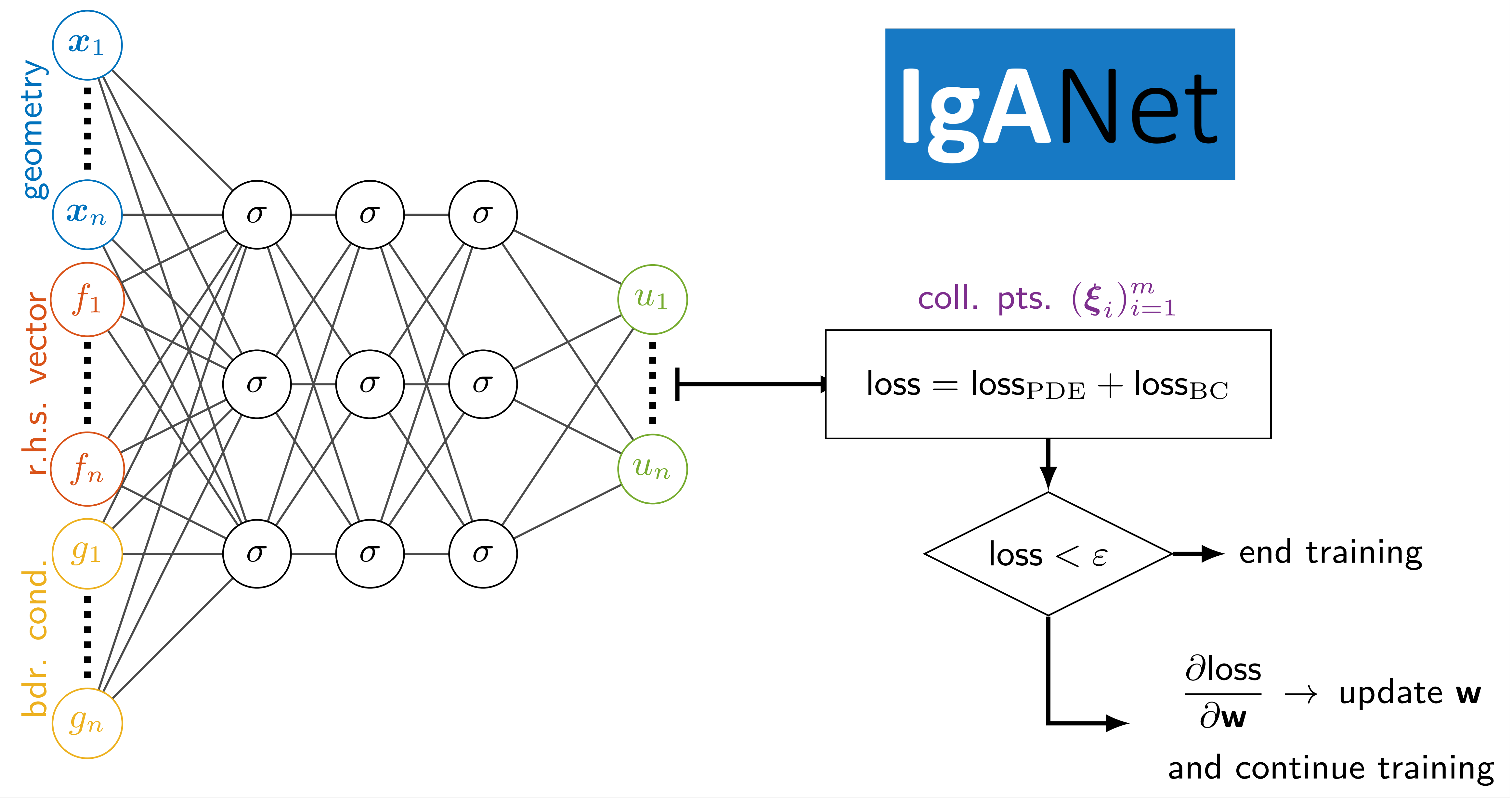


How is this related to PINNs, DeepONets, etc.?

Can be seen as deep operator network with *given* B-spline/NURBS basis!

Do we need to separate training from inference?

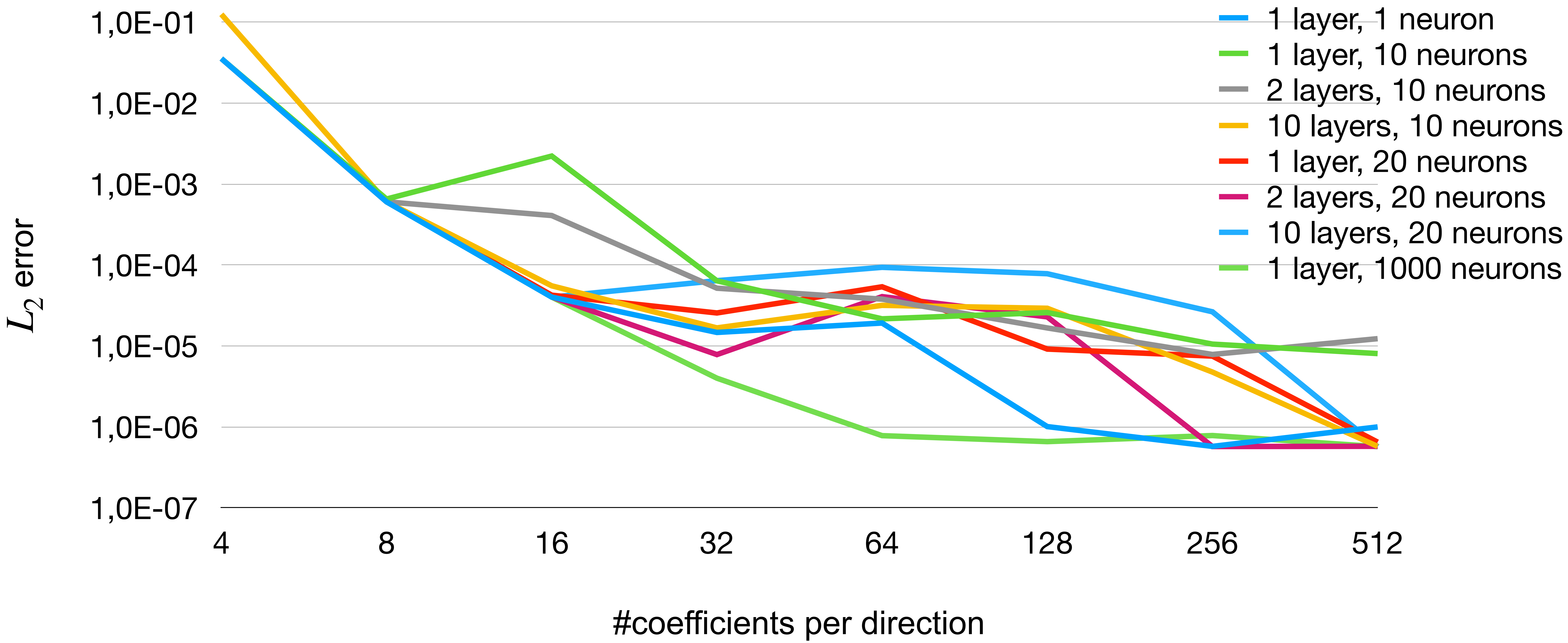
No, the network learns on the fly. But we can also pre-train it.

IgANet

GitHub.com/IgANets

- C++17 (soon open-source) library implemented atop LibTorch 2.x (C++ API of PyTorch)
- Dimension-independent B-splines and NURBS and a customisable IgANets deep learning framework
- Distributed computing on CPUs and GPUs (NVIDIA & AMD, Google TPUs WIP)
- Coupled with G+Smo (Geometry plus Simulation Modules) as IgA reference library and as toolkit with surface and volume reparameterization techniques

Hyper-parameter tuning (loss function tolerance 10^{-12})



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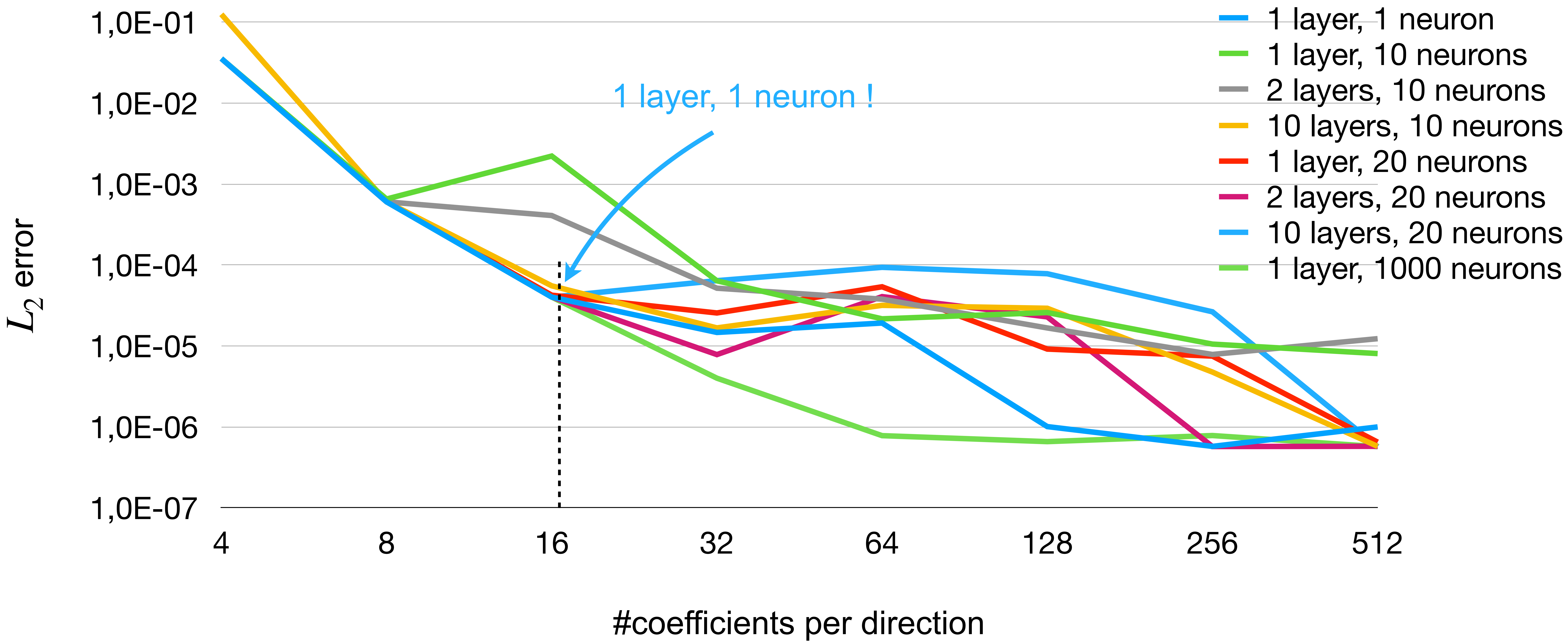

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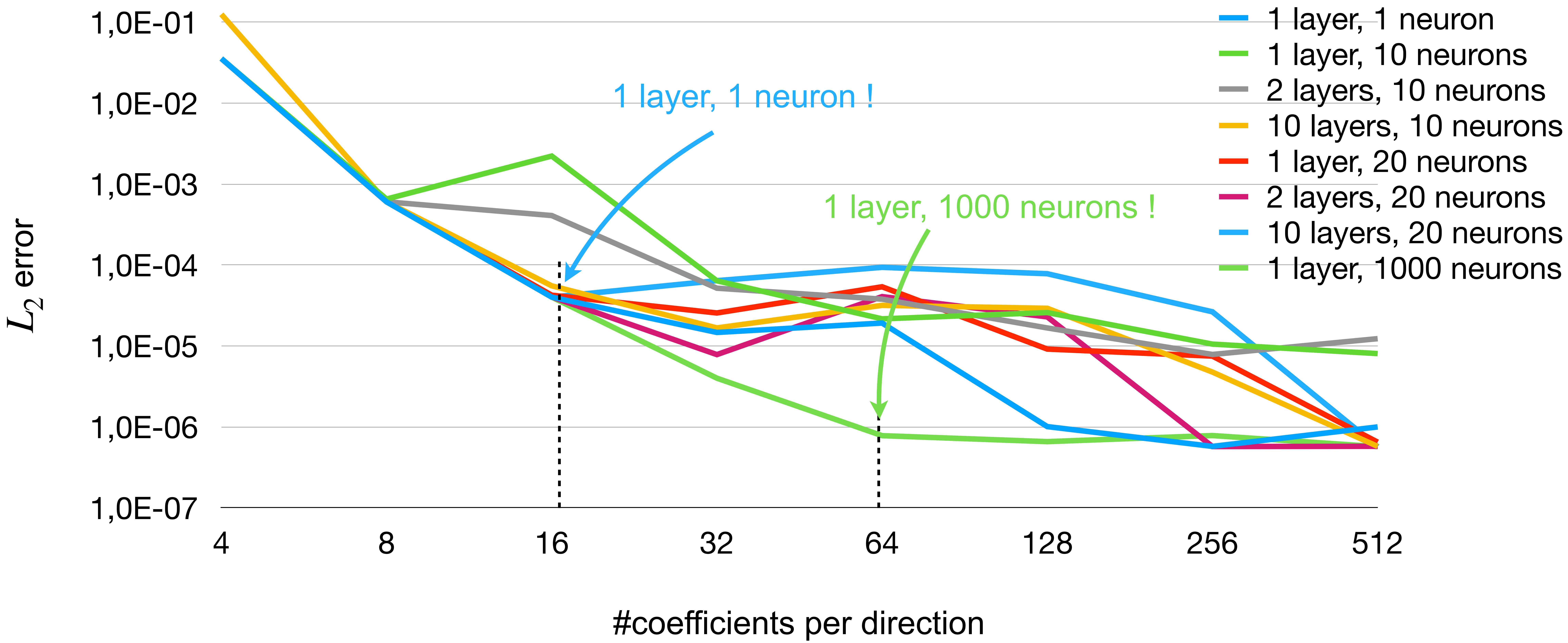


Cost analysis

$$\mathrm{loss}_{\mathrm{PDE}} = \frac{1}{m_1} \sum_{i=1}^{m_1} \left| \Delta \left[u_h \circ \mathbf{x}_h \left(\boldsymbol{\xi}_i \right) \right] - f_h \circ \mathbf{x}_h \left(\boldsymbol{\xi}_i \right) \right|^2$$

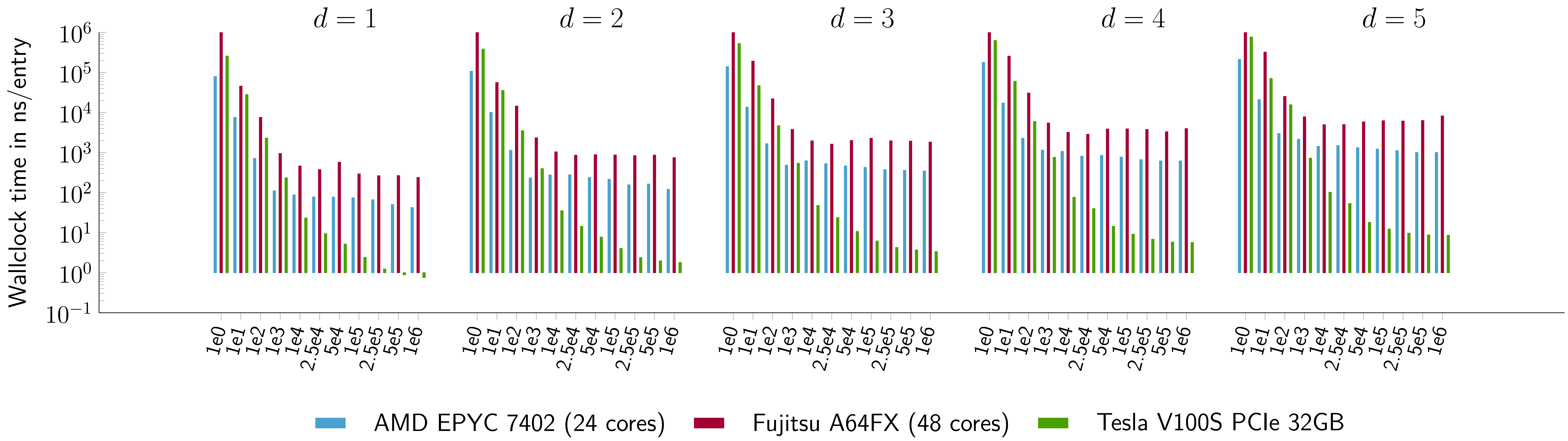
Differential operators in the loss function are computed efficiently in the ‘traditional’ IgA manner by differentiating the B-spline basis functions (no need to differentiate the network as in PINNs!)

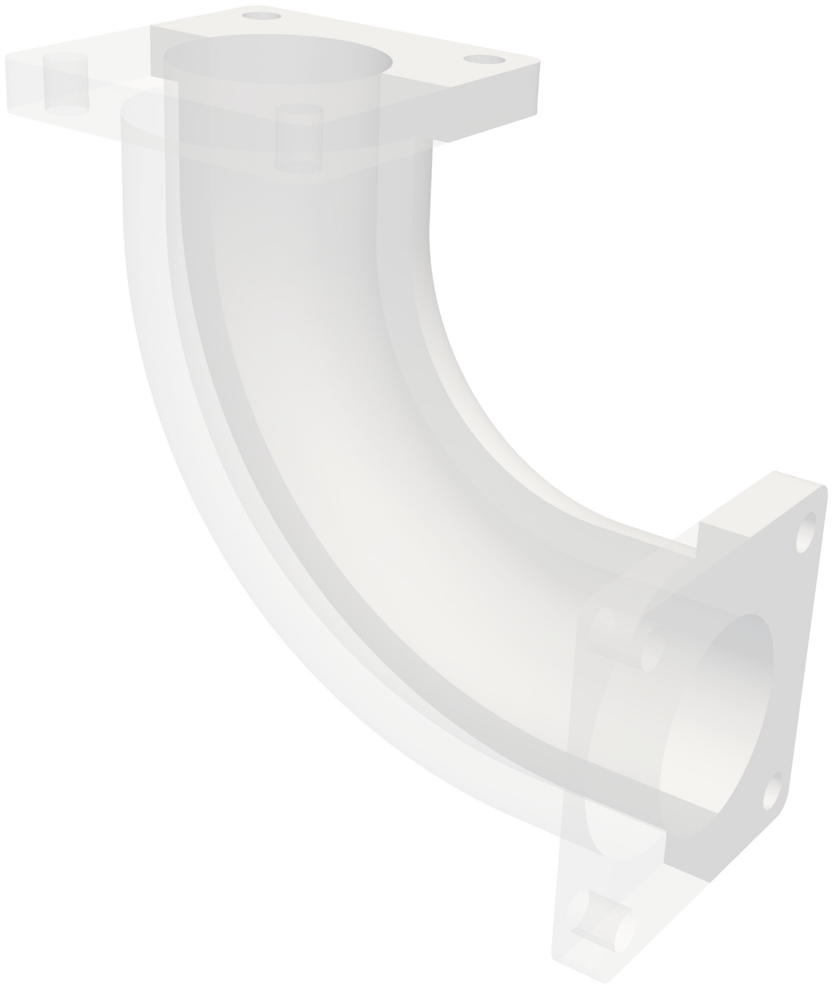
```
bspline.ilaplace(Geo, Cpts);
```

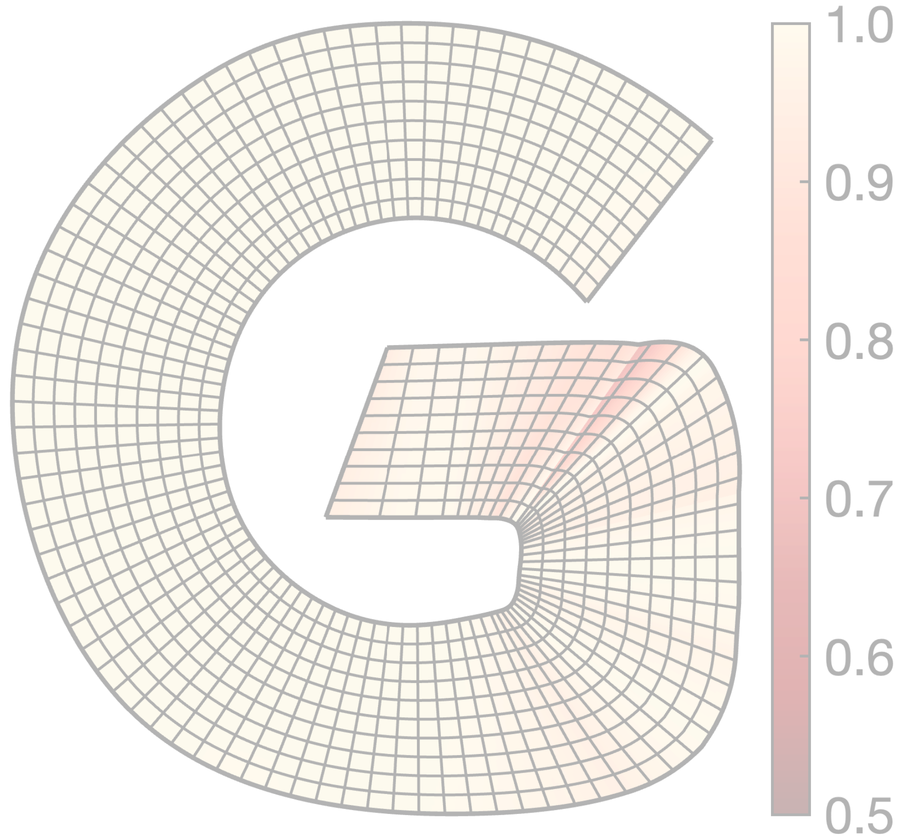
Derivatives of the loss function w.r.t. to the weights and biases are computed via back propagation

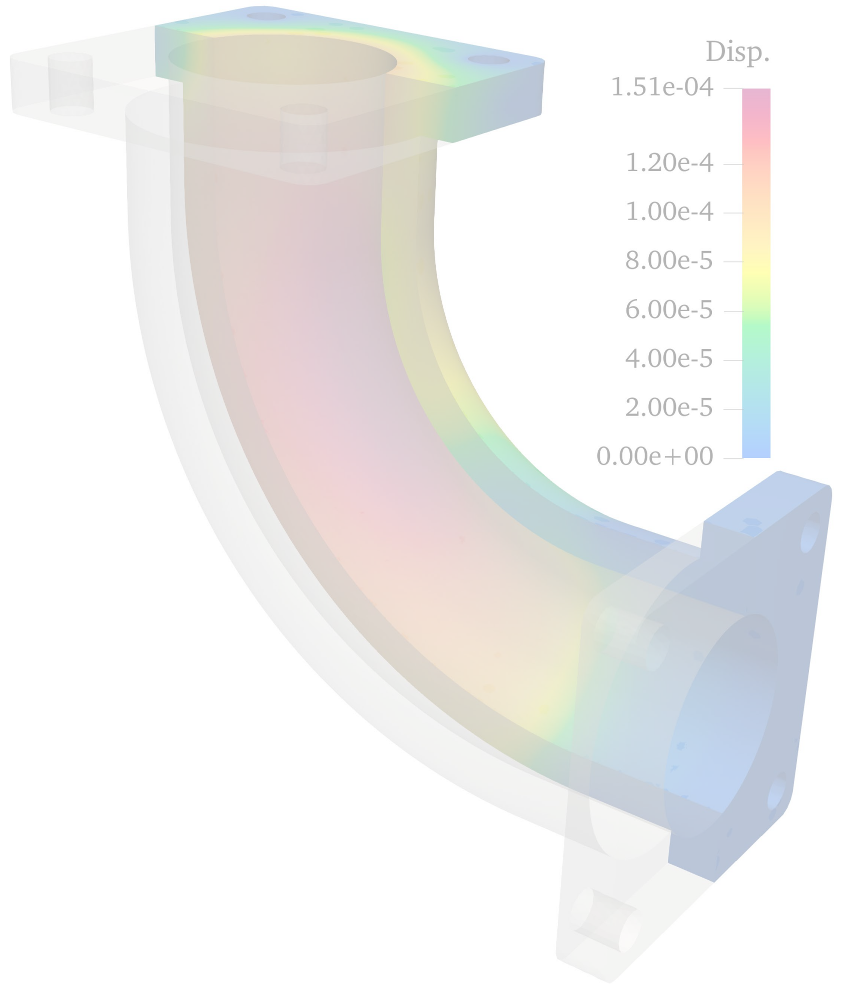
```
nn.zero_grad(); loss = L(nn.forward(Geo, Cpts),…); loss.backward();
```

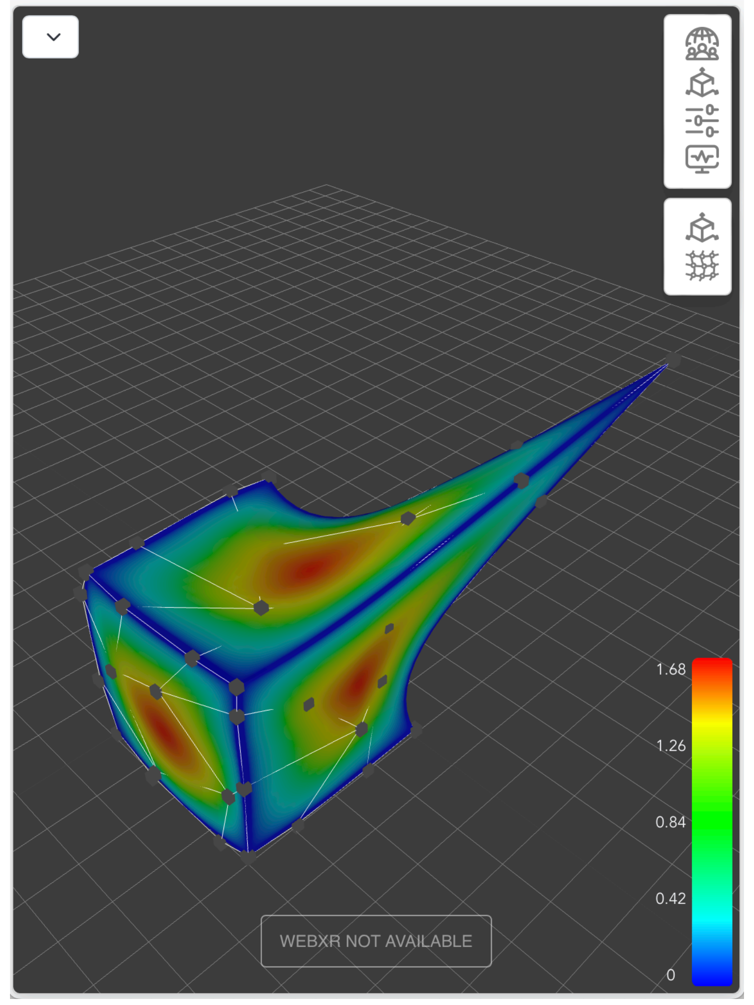
Cost analysis











1. Creation of VReps from BReps

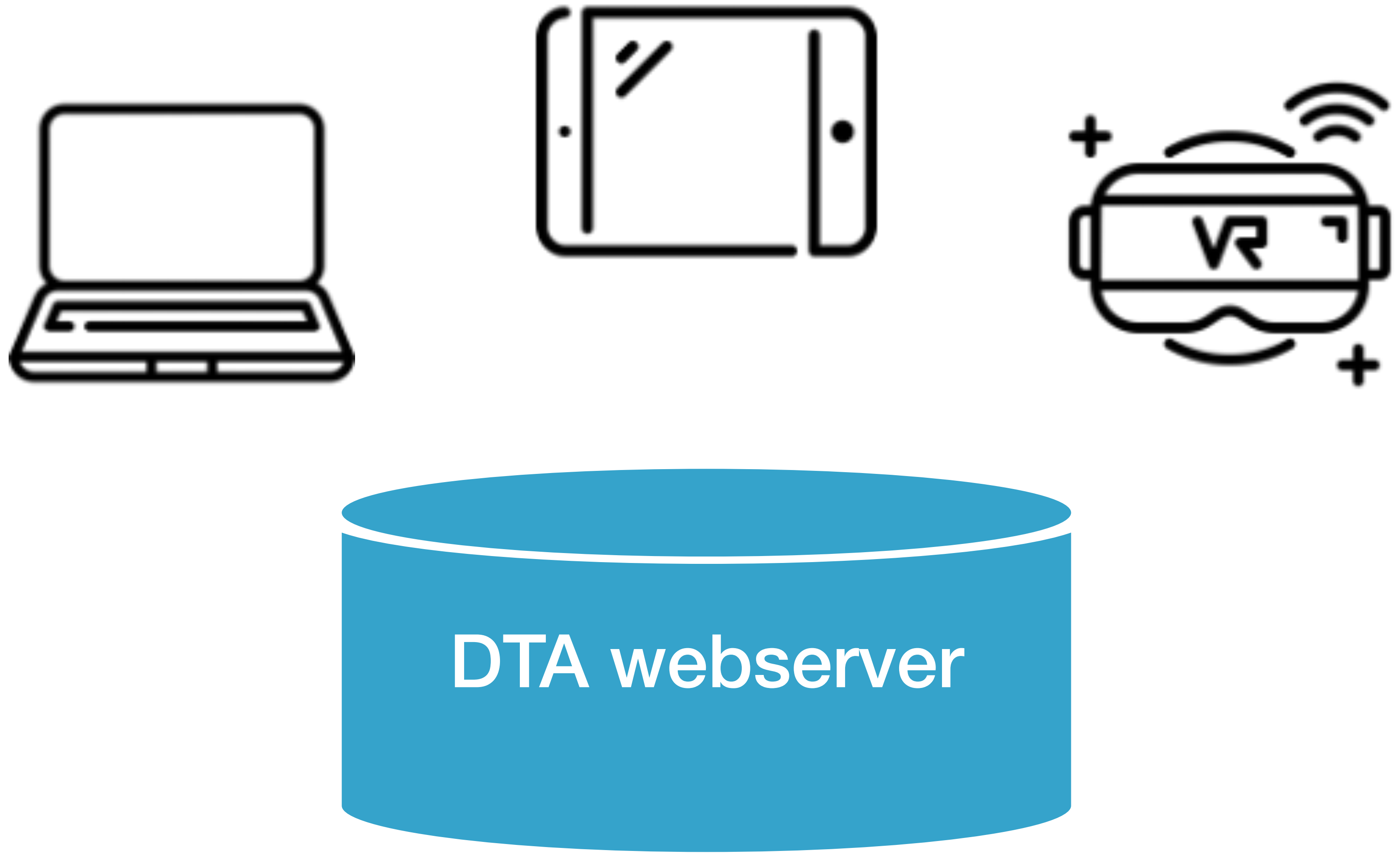
2. Reparameterization techniques

3. Isogeometric Analysis and IgANets

4. Interactive Design-through-Analysis

Interactive design-through-analysis

Vision: Enable CAD and CAE experts to collaborate in a distributed DTA framework



IgANet

https://visualization.surf.nl/iganet

Summary

Seamless **in-paradigm integration** of deep learning techniques into the IgA framework

Concept of an **interactive Design-through-Analysis** pipeline for CAD and CAE experts

Software toolbox for **automatic (re-)parameterization** to motivate CAD expert use VReps

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H2020: MOTOR (GA No. 678727), SURF: EINF-3689, EINF-7907, ETP-0001