PARAMETER ESTIMATION IN CARDIAC BIOMECHANICAL MODELS BASED ON PHYSICS-INFORMED NEURAL NETWORKS

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PINN-PAD
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Background and Motivation

- Great potential of biophysical models for **personalised medicine,** e.g. for cardiovascular diseases
- Parameter estimation and model calibration are challenging, due to the **complexity** of the cardiac function and availability of **clinical measurements**
- Parameter estimation methods can benefit from **machine learning**

- Aims of this work:
  - Extension of **physics-informed neural networks (PINN)** methodology to time-dependent 3D non-linear elasticity problems for **cardiac** applications
  - Investigation of training methodologies
  - Identification of **biophysical properties** of the myocardial tissue

Caforio et al, arXix 2023

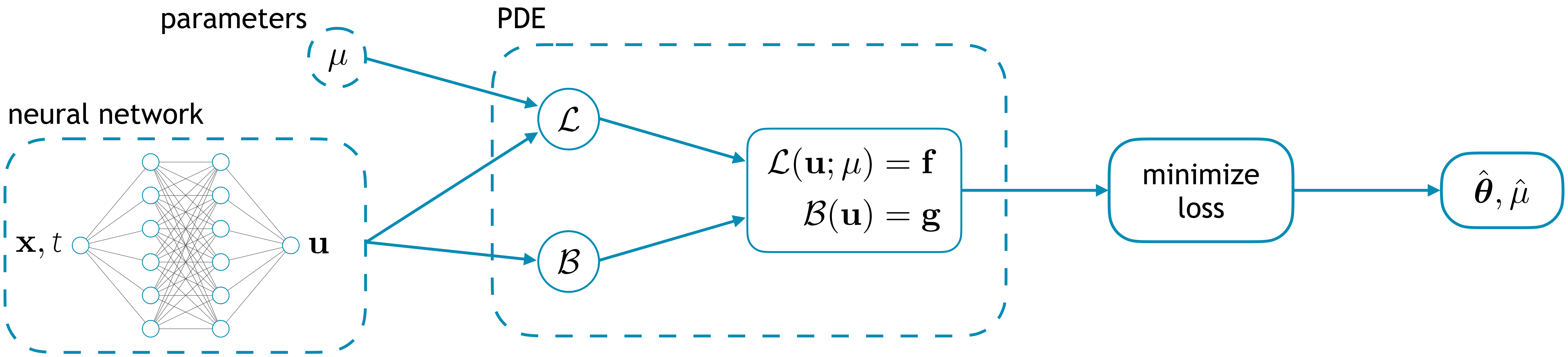
Methodology: PINNs

Objective: identify the **solution** $\mathbf{u}(\mathbf{x};\mu)$ and the unknown **parameters** μ given:

$$\begin{cases} \mathcal{L}(\mathbf{u};\mu) = \mathbf{f} & \text{in } \Omega \\ \mathcal{B}(\mathbf{u}) = \mathbf{g} & \text{on } \Gamma \end{cases} \qquad \text{or} \qquad \begin{cases} \mathcal{L}(\mathbf{u};\mu) = \mathbf{f} & \text{in } \Omega \times (0,T] \\ \mathcal{B}(\mathbf{u}) = \mathbf{g} & \text{on } \Gamma \end{cases}$$

with $\mathbf{f},\mathbf{g} : \Omega \longrightarrow \mathbb{R}$ — with $\mathbf{f},\mathbf{g} : \Omega \times (0,T] \longrightarrow \mathbb{R}$

considering **noisy observations** $\mathbf{u}_i^{\text{OBS}} = \mathbf{u}(\mathbf{x}_i^{\text{OBS}};\mu) + \epsilon$, for $i = 1, \dots, N_{\text{OBS}}$



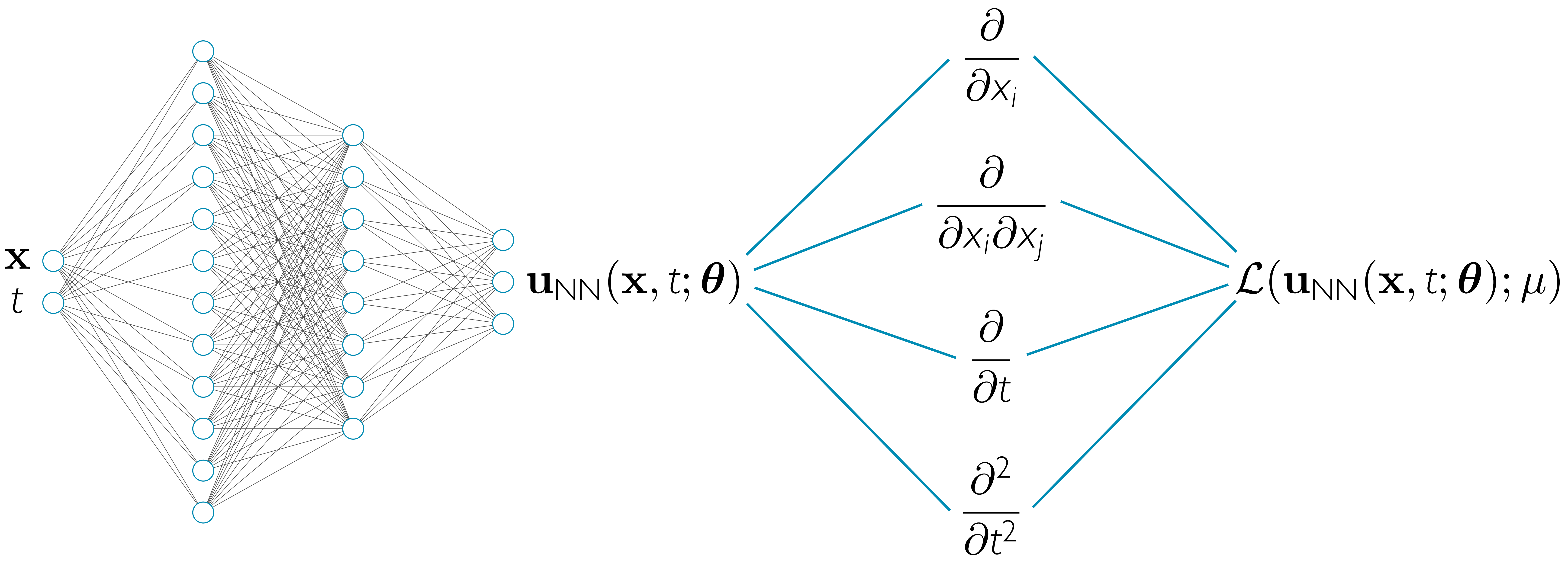
Methodology: PINNs

Objective: Find the weights and biases $\hat{\boldsymbol{\theta}}$ of a NN and the unknown parameters $\hat{\mu}$ s.t.

$$\hat{\mu}, \hat{\boldsymbol{\theta}} = \arg\min_{\mu,\theta} \left\| \mathbf{u}_{\mathrm{NN}}(\mathbf{x}^{\mathrm{OBS}}; \mu, \boldsymbol{\theta}) - \mathbf{u}^{\mathrm{OBS}} \right\|^2 + \mathcal{R}(\mathbf{u}_{\mathrm{NN}}(\mathbf{x}^{\mathrm{COL}}; \mu, \boldsymbol{\theta}))$$

OBJECTIVE FUNCTION

REGULARISATION



AUTOMATIC DIFFERENTIATION

Raissi et al, JCP 2019

Methodology: PINNs

Objective: Find the weights and biases $\hat{\boldsymbol{\theta}}$ of an ANN and the unknown parameters $\hat{\mu}$ s.t.

$$\min_{\mu,\boldsymbol{\theta}} \mathcal{J}_{\text{OBS}}(\boldsymbol{\theta}) + \mathcal{J}_{\text{PDE}}(\mu,\boldsymbol{\theta}) + \mathcal{J}_{\text{BC}}(\boldsymbol{\theta}) + \mathcal{R}(\boldsymbol{\theta})$$

with $$\mathcal{J}_{\text{OBS}}(\boldsymbol{\theta}) = \frac{\lambda_{\text{OBS}}}{N_{\text{OBS}}} \sum_{i=1}^{N_{\text{OBS}}} \left\| \mathbf{u}_i^{\text{OBS}} - \mathbf{u}_{\text{NN}}(\mathbf{x}_i^{\text{OBS}};\boldsymbol{\theta}) \right\|^2$$

$$\mathcal{J}_{\text{PDE}}(\mu,\boldsymbol{\theta}) = \frac{\lambda_{\text{PDE}}}{N_{\text{PDE}}} \sum_{i=1}^{N_{\text{PDE}}} \left\| \mathbf{f}(\mathbf{x}_i^{\text{PDE}}) - \mathcal{L}\big(\mathbf{u}_{\text{NN}}(\mathbf{x}_i^{\text{PDE}};\boldsymbol{\theta});\mu\big) \right\|^2$$

$$\mathcal{J}_{\text{BC}}(\boldsymbol{\theta}) = \frac{\lambda_{\text{BC},D}}{N_{\text{BC},D}} \sum_{i=1}^{N_{\text{BC, D}}} \left\| \mathbf{u}_{\Gamma_D}(\mathbf{x}_i^{\text{BC,D}}) - \mathbf{u}_{\text{NN}}(\mathbf{x}_i^{\text{BC,D}};\boldsymbol{\theta}) \right\|^2 + \frac{\lambda_{\text{BC},N}}{N_{\text{BC},N}} \sum_{i=1}^{N_{\text{BC, N}}} \left\| \nabla \mathbf{u}_{\text{NN}}(\mathbf{x}_i^{\text{BC, N}};\boldsymbol{\theta}) \cdot \mathbf{n}(\mathbf{x}_i^{\text{BC, N}}) - p\mathbf{n}(\mathbf{x}_i^{\text{BC, N}}) \right\|^2$$

and $$\mathcal{R}(\boldsymbol{\theta}) = \lambda_W \|\boldsymbol{\theta}\|^2$$

Methodology: Random Fourier Features

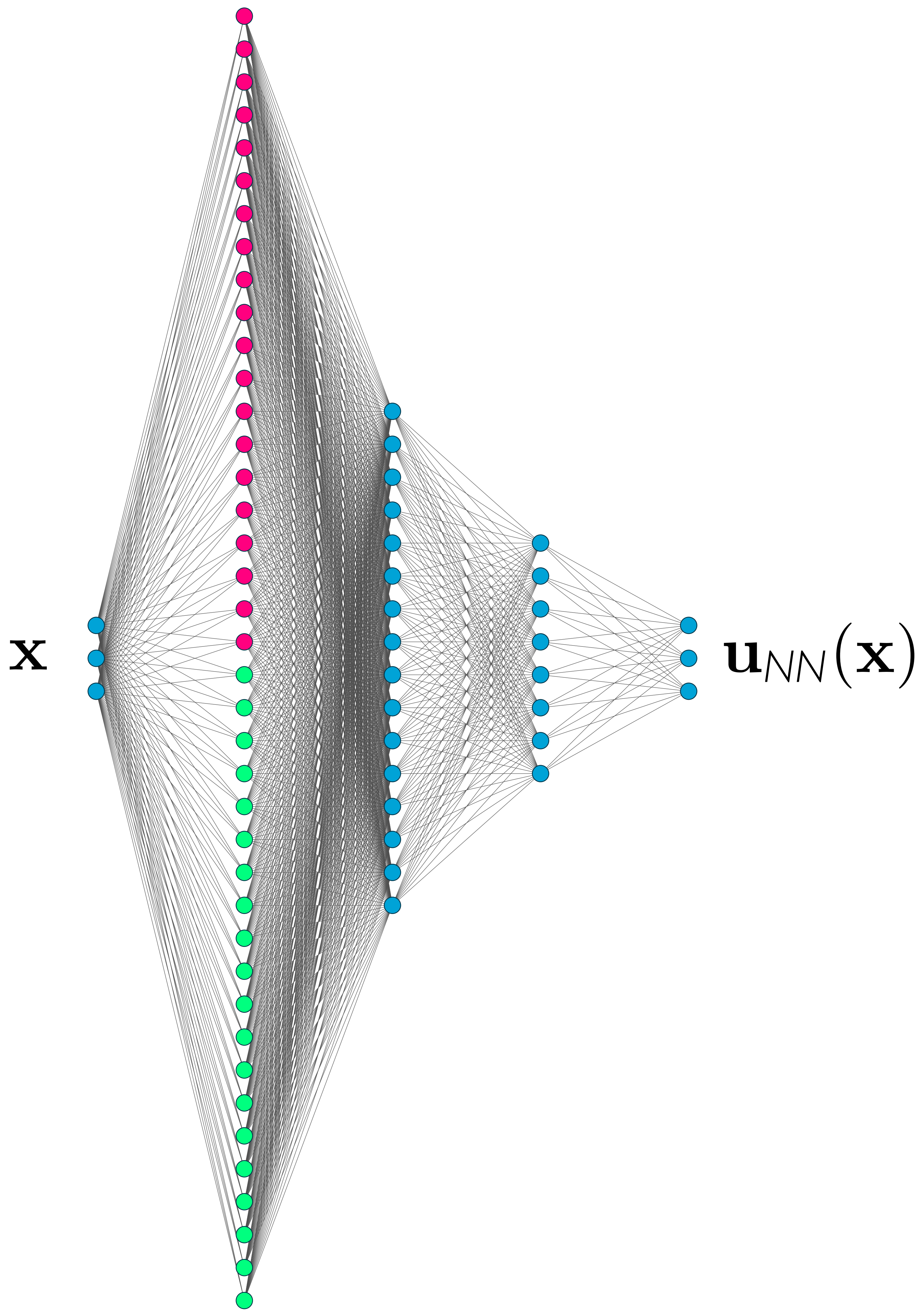
Idea: Replace first layer with non-trainable frequency features:

$$\begin{cases} \gamma : \mathbb{R}^{\text{input}} \longrightarrow \mathbb{R}^{2p} \\ \quad \mathbf{x} \mapsto \begin{pmatrix} \cos(\mathbf{B}\mathbf{x}) \\ \sin(\mathbf{B}\mathbf{x}) \end{pmatrix} \end{cases}$$

$$\mathbf{B} = (b_{ij}) \in \mathbb{R}^{p \times \text{input}} \quad \text{with} \quad b_{ij} \sim \mathcal{N}(0, \sigma_F)$$

Results in a network architecture

$$\mathbf{u}_{NN}(\mathbf{x}) = L_K \circ L_{K-1} \circ \ldots \circ L_1(\gamma(\mathbf{x})) \quad \text{with} \quad L_k(\mathbf{y}) = \sigma\left(\mathbf{W}_k\mathbf{y} + \mathbf{b}_k\right)$$

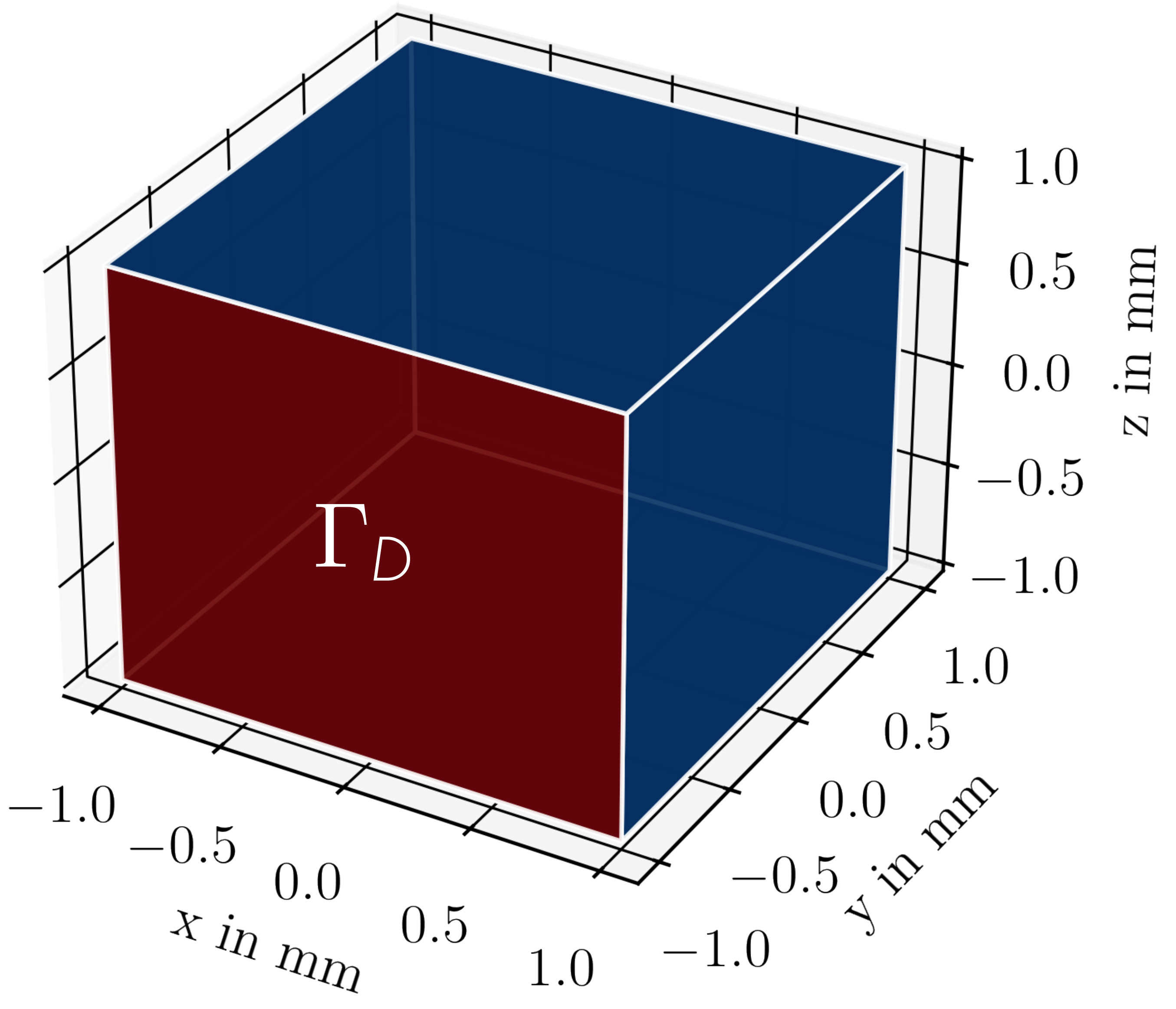


Tancik et al, AIPS 2020

Methodology: Exact Boundary Condition

Idea: Dirichlet boundary Γ_D can be explicitly imposed with a distance function:

$$\begin{cases} \phi : \mathbb{R}^{\text{input}} & \longrightarrow \mathbb{R} \\ \quad\quad \mathbf{x} & \mapsto \text{dist}(\mathbf{x}, \text{proj}_{\Gamma_D}(\mathbf{x})) \end{cases}$$



This results in a network architecture:

$$\mathbf{u}_{NN}^{\text{exact}}(\mathbf{x}) = \mathbf{u}_{NN}(\mathbf{x}) \cdot \phi(\mathbf{x}) + G(\mathbf{x}) \quad \text{with } G(\mathbf{x}) \text{ extension of boundary}$$

$$\phi_{\Gamma_D}(\mathbf{x}) = \left\| \mathbf{E}_y \mathbf{x} + \mathbf{e}_y \right\|^2$$

Especially for homogeneous boundary conditions:

$$\mathbf{u}_{NN}^{\text{exact}}(\mathbf{x}) = \mathbf{u}_{NN}(\mathbf{x}) \cdot \phi(\mathbf{x})$$

Sukumar et al, CMAME, 2022

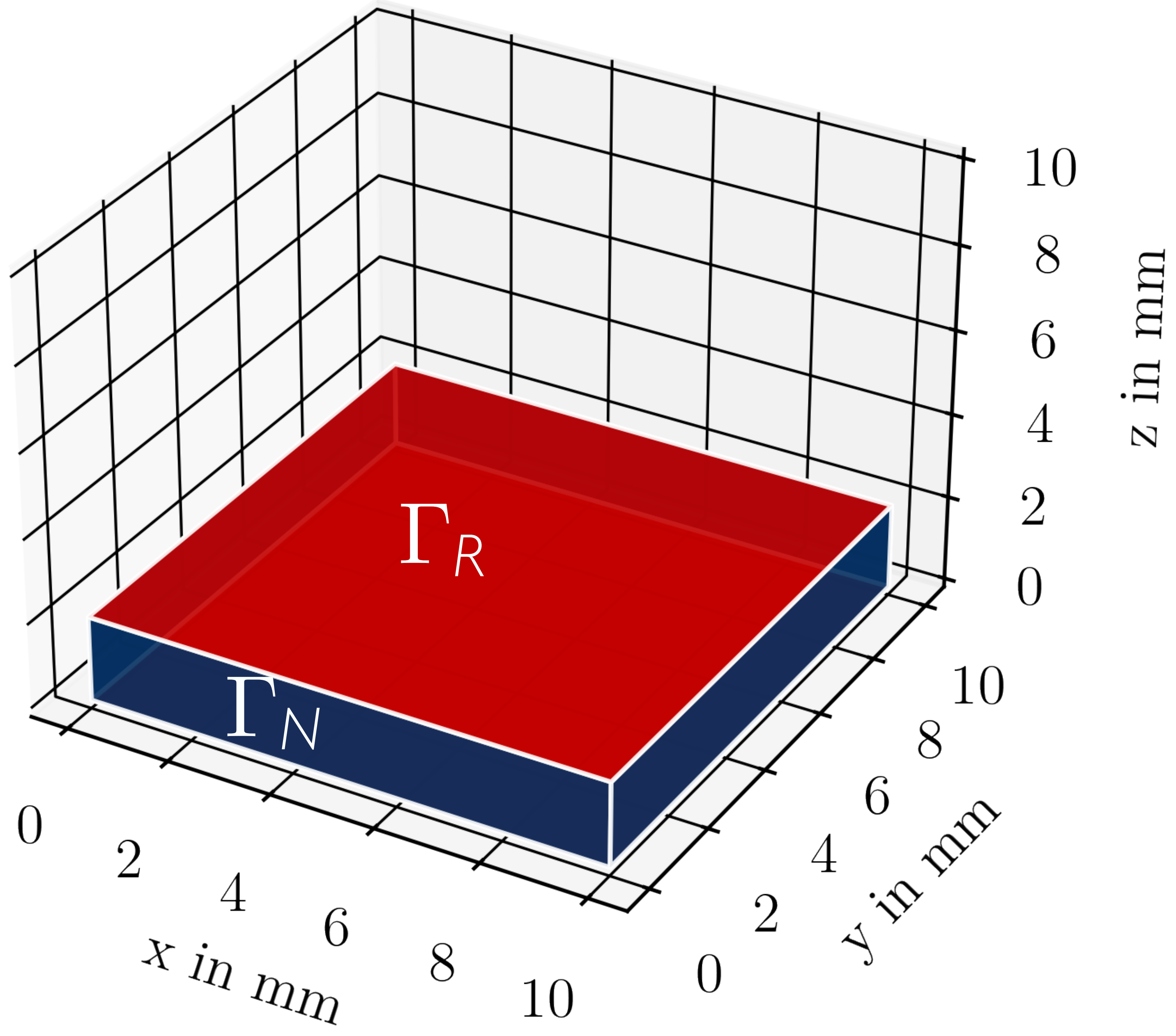
Guccione Model for Passive Stress

- Quasi-static problem:

Find $\mathbf{u}$ s.t.

$$\begin{cases} -\nabla \cdot \mathbf{P}(\mathbf{u}) = 0 & \text{in } \Omega \\ \mathbf{P}(\mathbf{u})\,\mathbf{n} = -pJ\,\mathbf{F}^{-T}\,\mathbf{n} & \text{on } \Gamma_N \\ \mathbf{P}(\mathbf{u})\,\mathbf{n} + k\,\mathbf{u} = 0 & \text{on } \Gamma_R \end{cases}$$

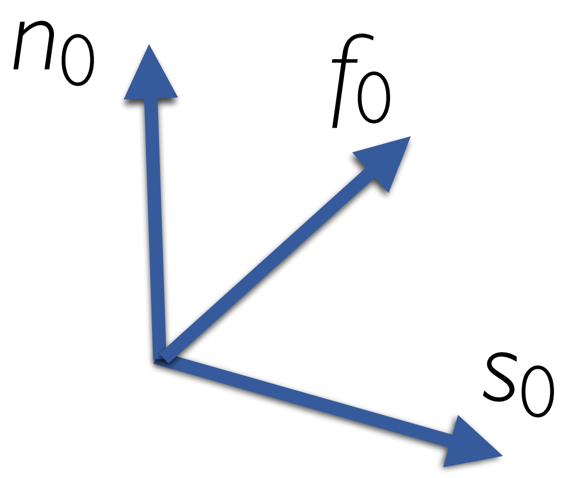
$$\text{with } \mathbf{P} = \frac{\partial \mathcal{W}}{\partial \mathbf{F}}$$



- Transverse-isotropic material:

$$\mathcal{W} = \frac{\mu}{2}\left(\exp \bar{Q} - 1\right) + \frac{\lambda}{2}\left(\log J\right)^2$$

$$\text{with } \bar{Q} = b_f\left(\mathbf{f}_0 \cdot \overline{\mathbf{E}}\,\mathbf{f}_0\right)^2 + b_t\left[\left(\mathbf{s}_0 \cdot \overline{\mathbf{E}}\,\mathbf{s}_0\right)^2 + \left(\mathbf{n}_0 \cdot \overline{\mathbf{E}}\,\mathbf{n}_0\right)^2 + 2\left(\mathbf{s}_0 \cdot \overline{\mathbf{E}}\,\mathbf{n}_0\right)^2\right] + 2\,b_{fs}\left[\left(\mathbf{f}_0 \cdot \overline{\mathbf{E}}\,\mathbf{s}_0\right)^2 + \left(\mathbf{f}_0 \cdot \overline{\mathbf{E}}\,\mathbf{n}_0\right)^2\right]$$



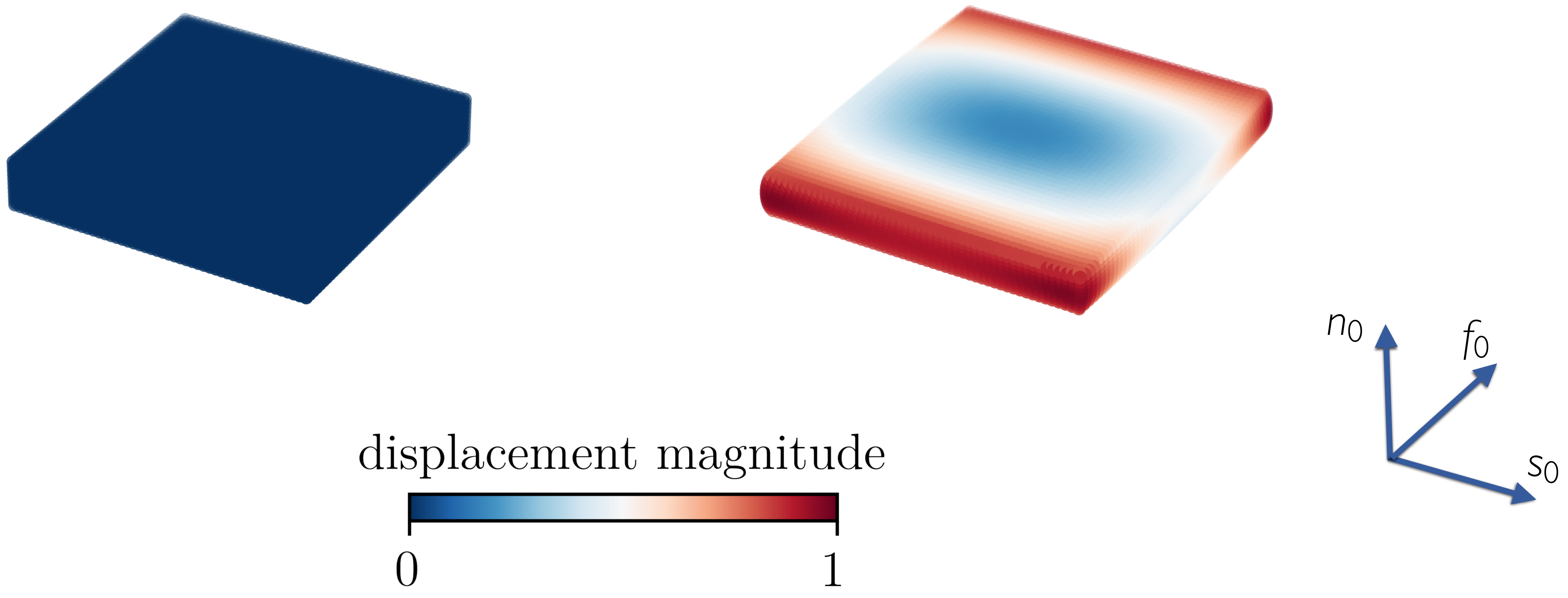
- Geometry: Parallelepiped

- Parameters:

b_f	b_t	b_{fs}
18,48	3,58	1,627

Guccione model for Passive Stress: Forward Solution

- stiffness: $\mu = 10\,\mathrm{kPa}$, nearly-incompressible material : $\lambda = 1000\,\mathrm{kPa}$



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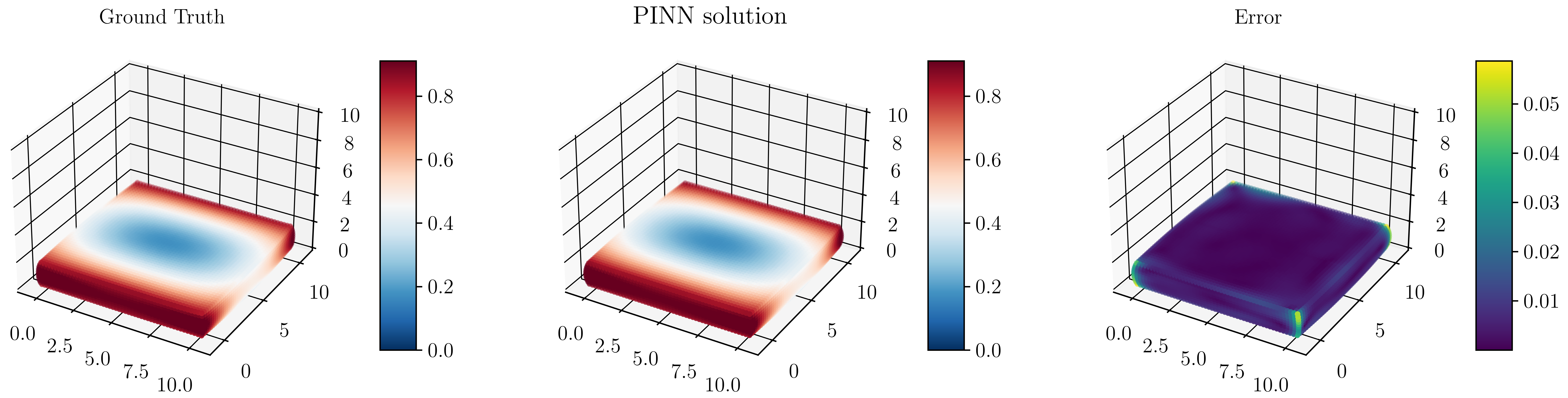
Guccione Model for Passive Stress:
PINN-based Reconstruction of Forward Solution

- $C = 0$

500 data points



No Fourier features | 900 boundary points | 500 data points | Sobol sampling

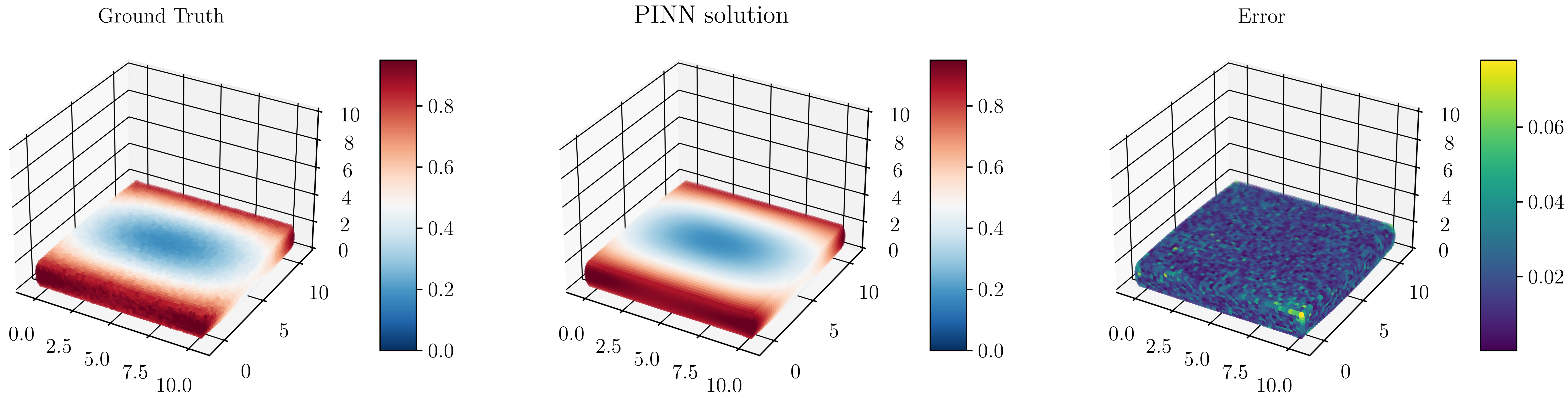
$$\tilde{\mathbf{u}} = \mathbf{u} + \epsilon$$

$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

$$C = \frac{3\sigma}{\max(\mathbf{u})}$$

- $C = 0.05$

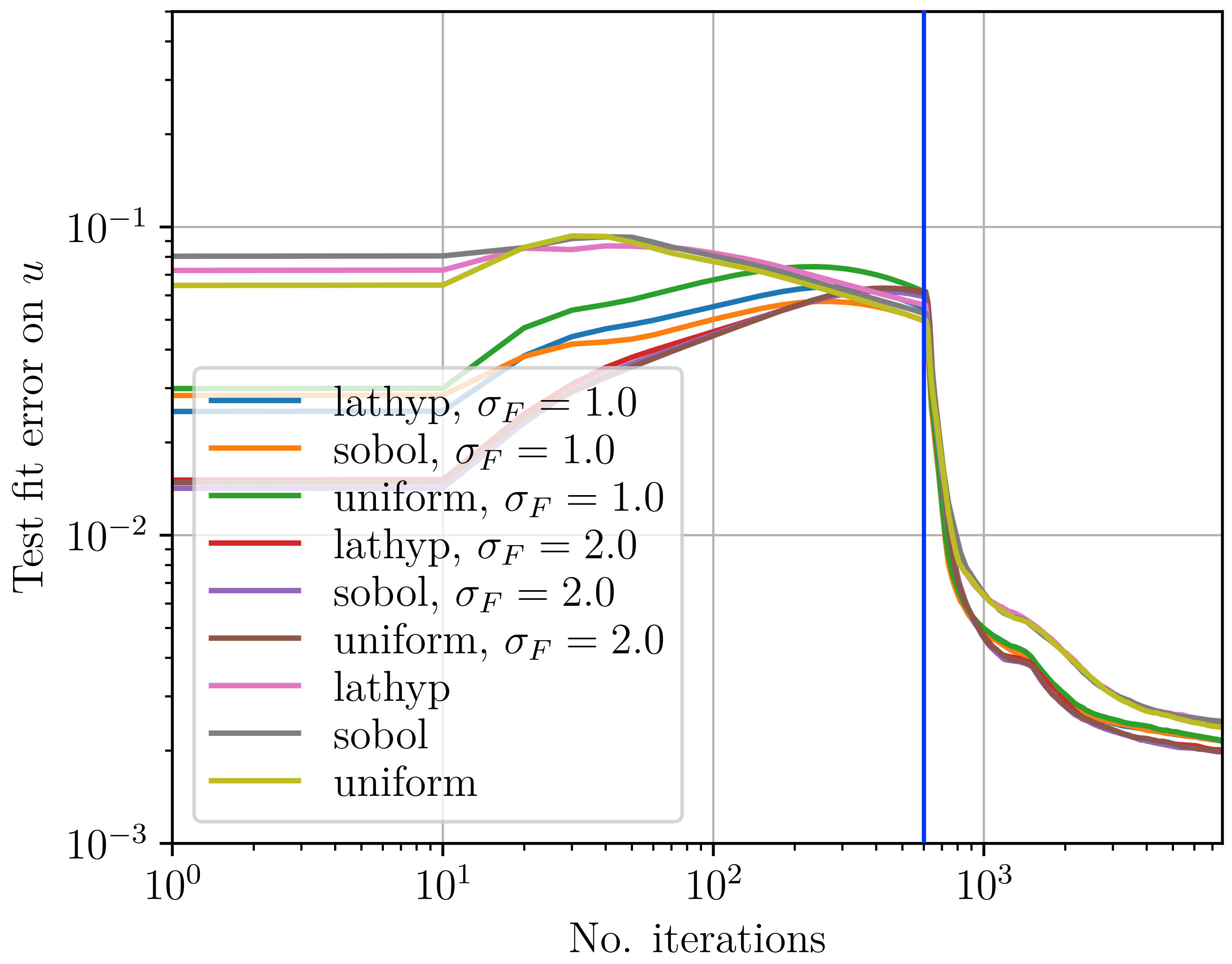
1000 data points



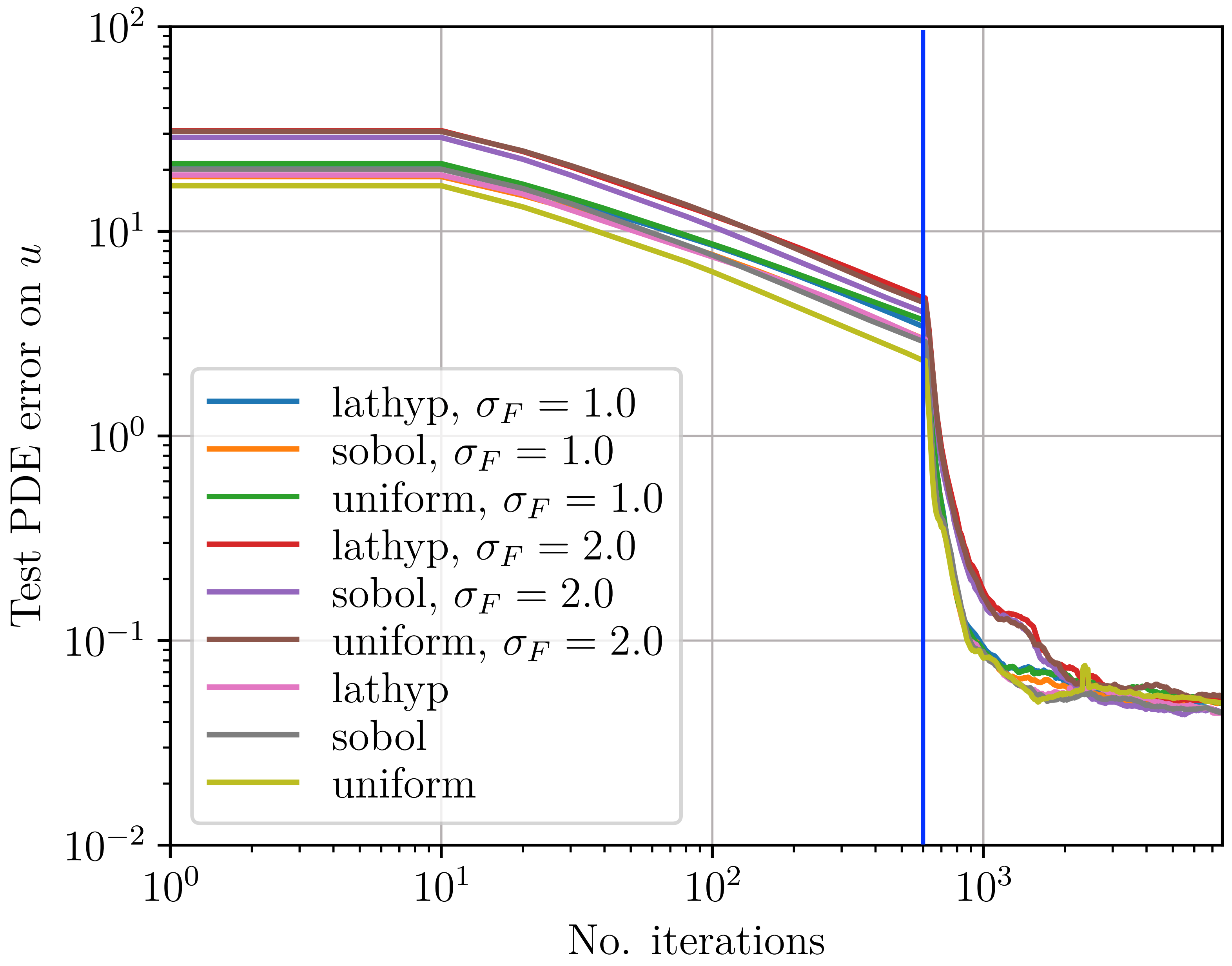
No Fourier features | 2100 boundary points | 1000 data points | Sobol sampling

Guccione Model for Passive Stress: Loss Terms

- Fit loss $\sqrt{\mathcal{J}_{\text{OBS}}(\boldsymbol{\theta})}$ on test points, $C = 0$



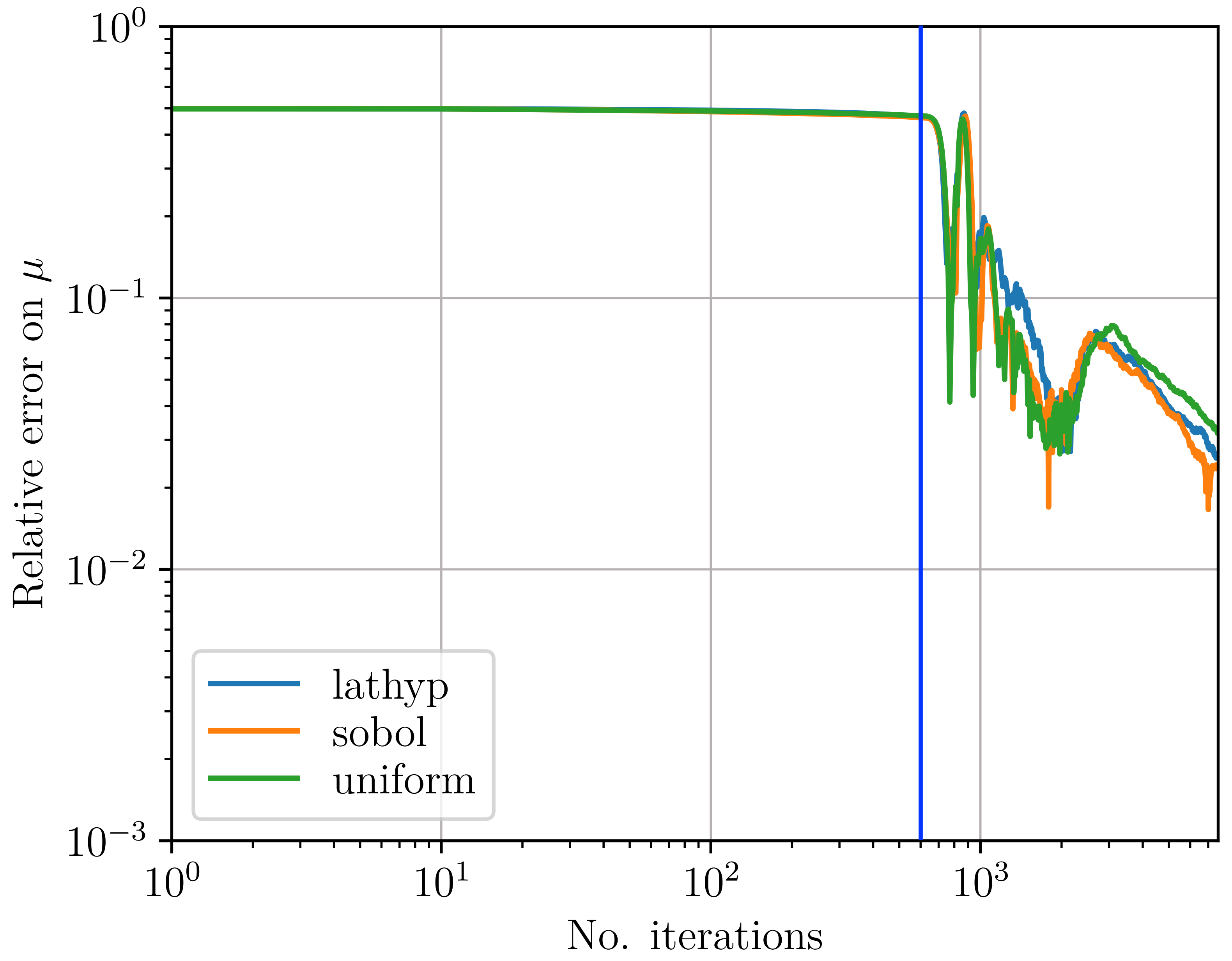
- PDE loss $\sqrt{\mathcal{J}_{\text{PDE}}(\boldsymbol{\theta})}$ on test points, $C = 0$



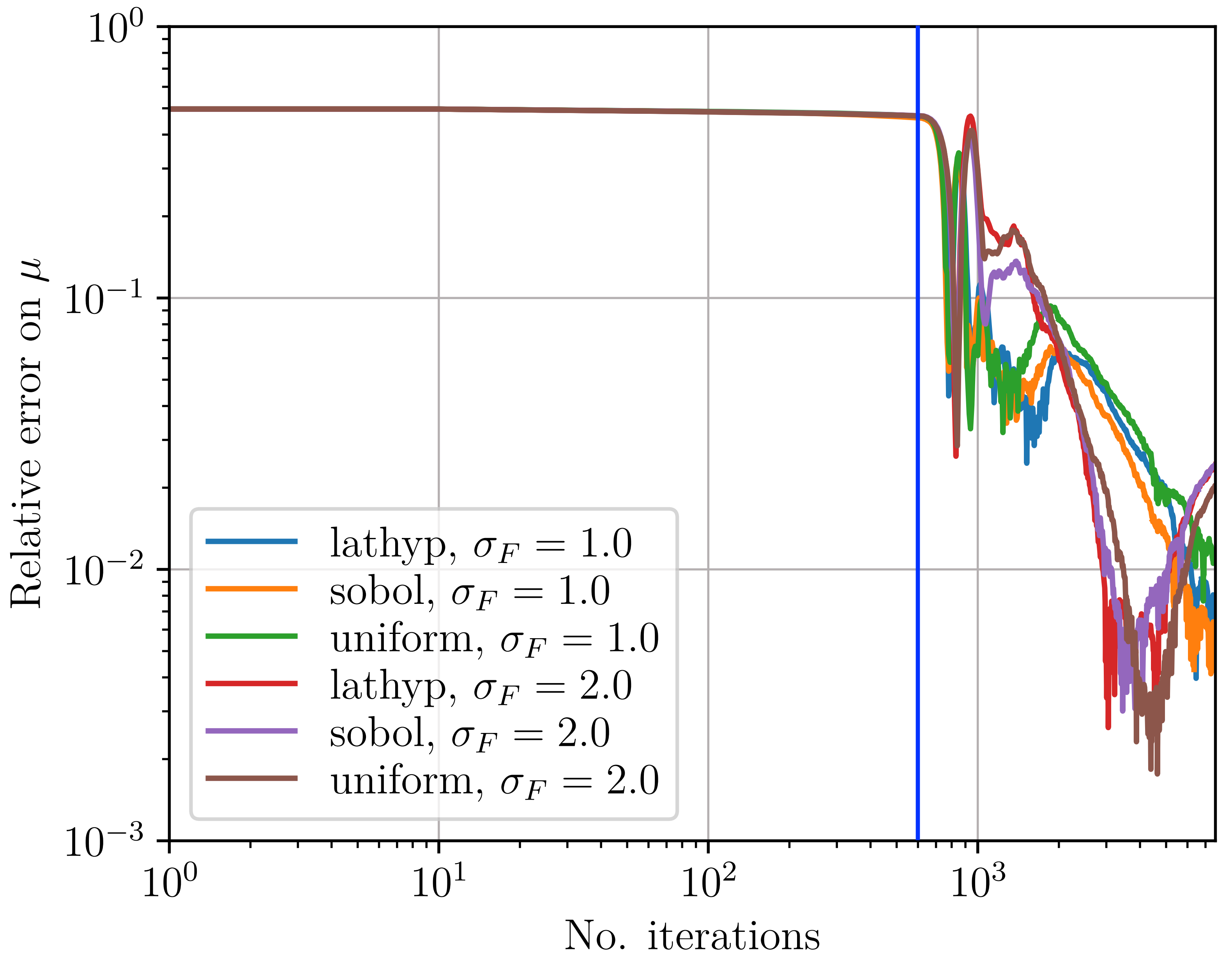
- 500 test points
- 10 seeds
- 600 Adam + 7000 BFGS

Guccione Model for Passive Stress: PINN-based Estimation of Stiffness

- Without Fourier features, $C = 0$



- With Fourier features, $C = 0$

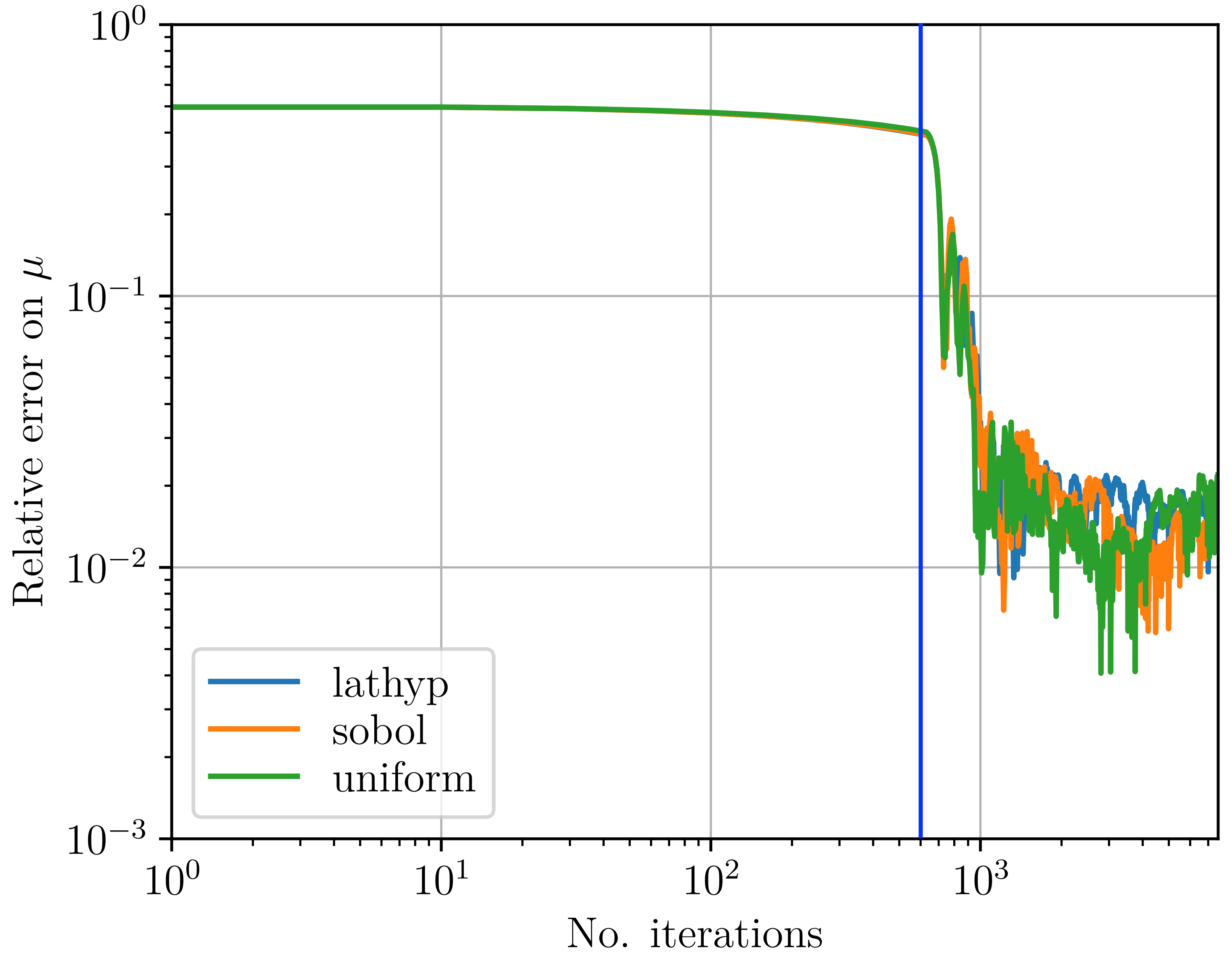


- 500 data points
- 10 seeds
- 600 Adam + 7000 BFGS

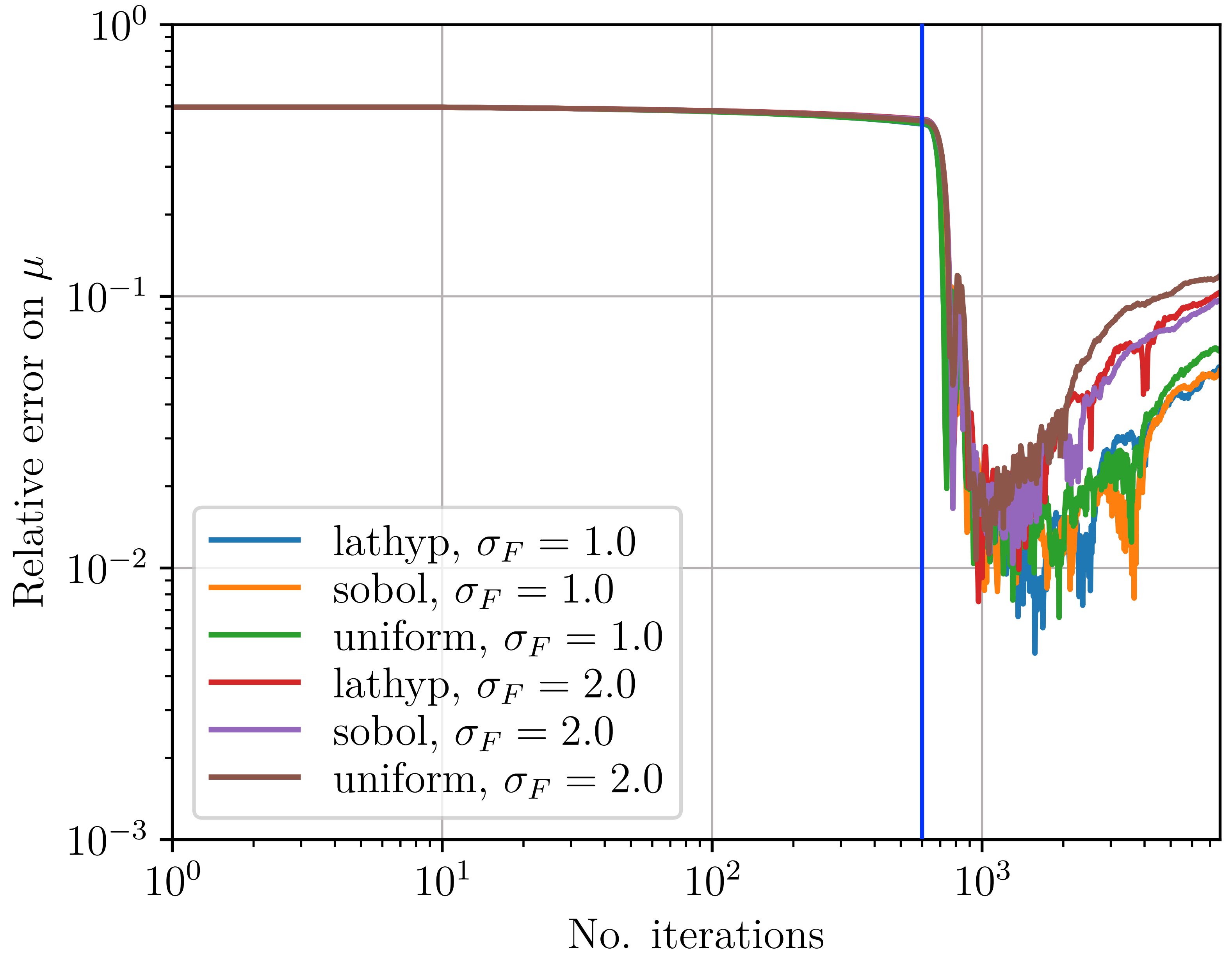
Sampling	Vanilla Net	Fourier Layer $\sigma_F = 1$	Fourier Layer $\sigma_F = 2$
Uniform	3.4E-02	1.5E-02	2.1E-02
Sobol	2.9E-02	1.3E-02	2.9E-02
LatHyp	3.2E-02	1.3E-02	2.7E-02

Guccione Model for Passive Stress: PINN-based Estimation of Stiffness

- Without Fourier features, $C = 0.05$



- With Fourier features, $C = 0.05$

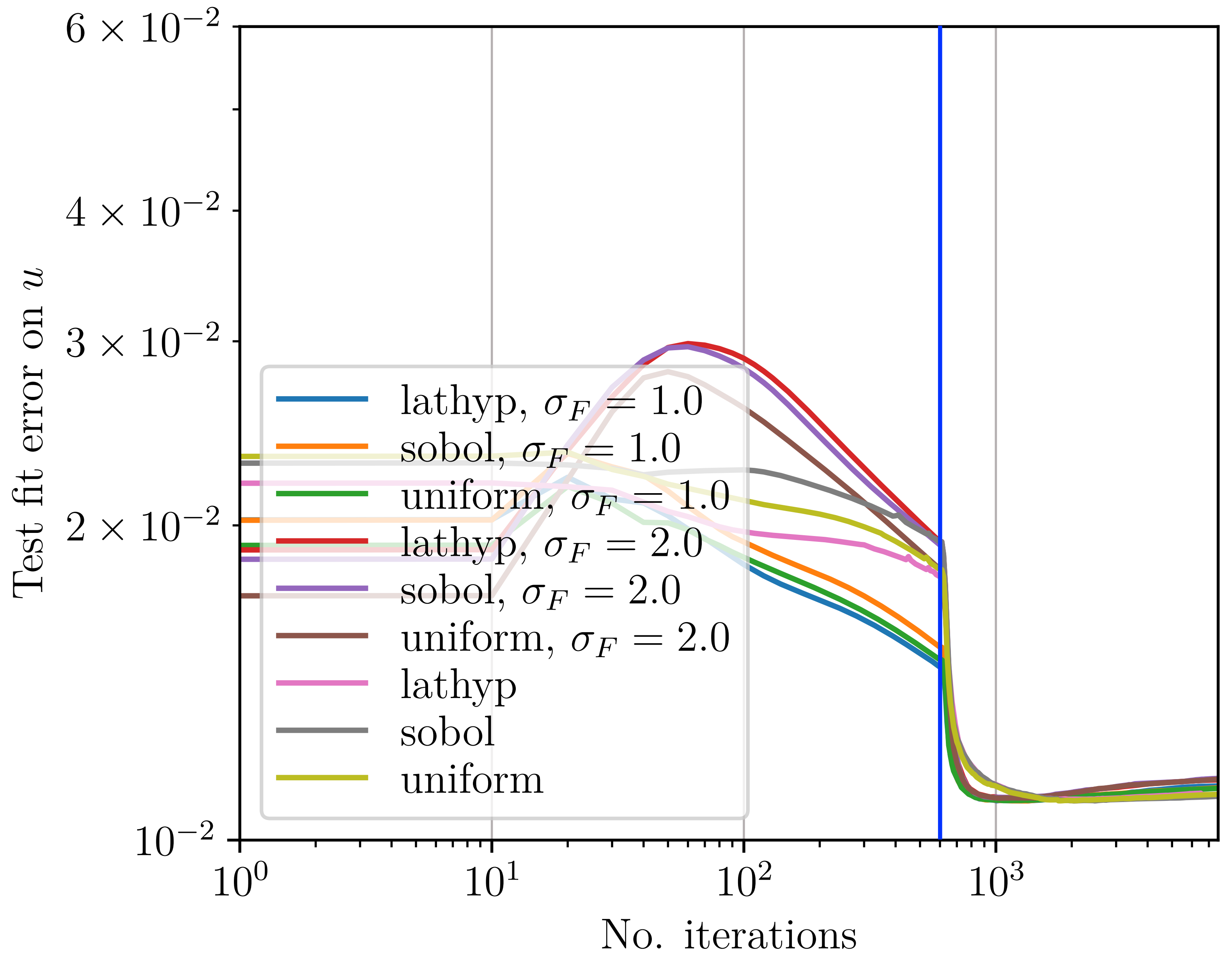


- 1000 data points
- 10 seeds
- 600 Adam + 7000 BFGS

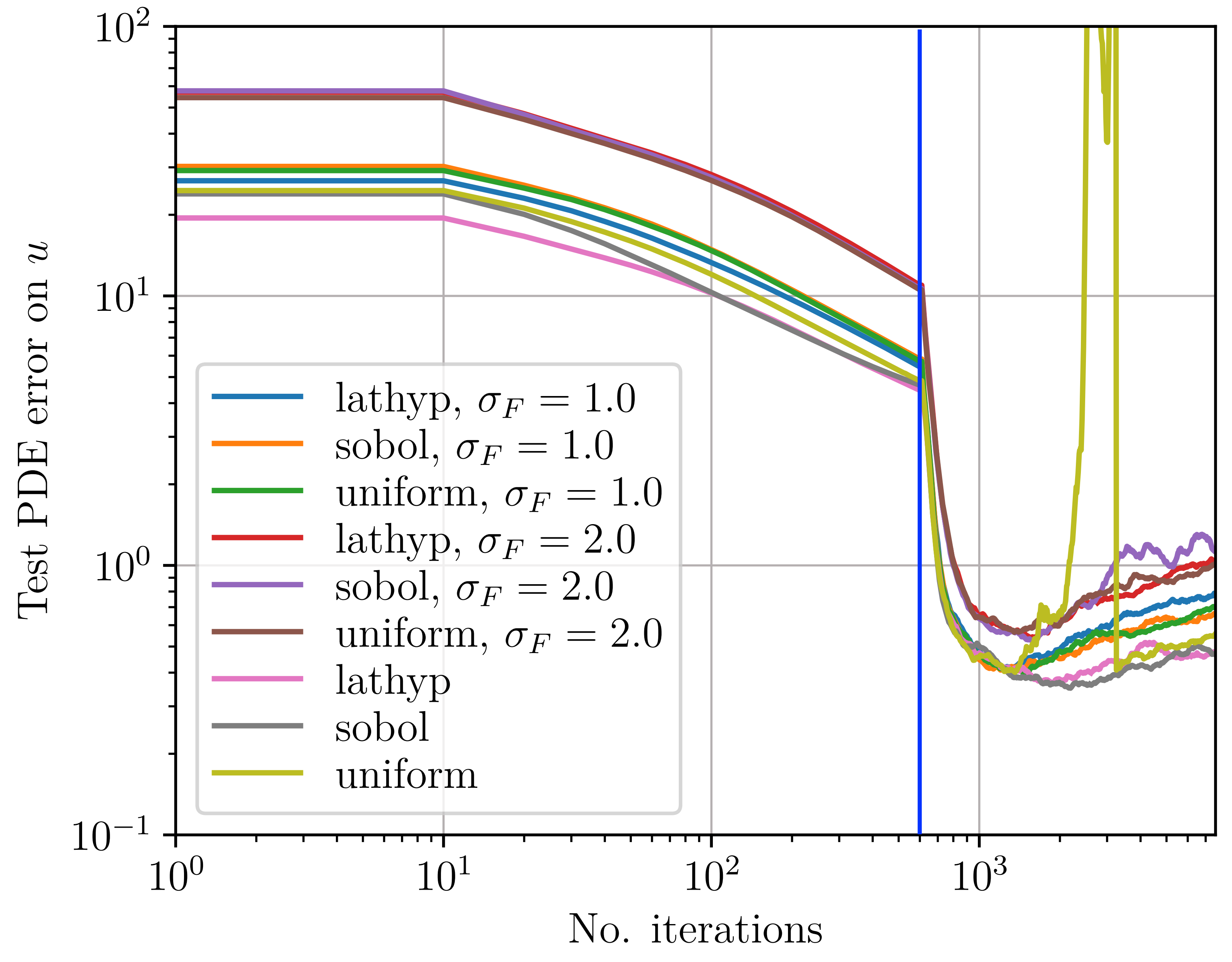
Sampling	Vanilla Net	Fourier Layer $\sigma_F = 1$	Fourier Layer $\sigma_F = 2$
Uniform	4.6E-02	8.4E-02	1.3E-01
Sobol	3.5E-02	7.6E-02	1.1E-01
LatHyp	3.9E-02	6.9E-02	1.3E-01

Guccione Model for Passive Stress: Loss Terms

- Fit loss $\sqrt{\mathcal{J}_{\mathrm{OBS}}(\boldsymbol{\theta})}$ on test points, $C = 0.05$



- PDE loss $\sqrt{\mathcal{J}_{\mathrm{PDE}}(\boldsymbol{\theta})}$ on test points, $C = 0.05$



- 1000 test points
- 10 seeds
- 600 Adam + 7000 BFGS

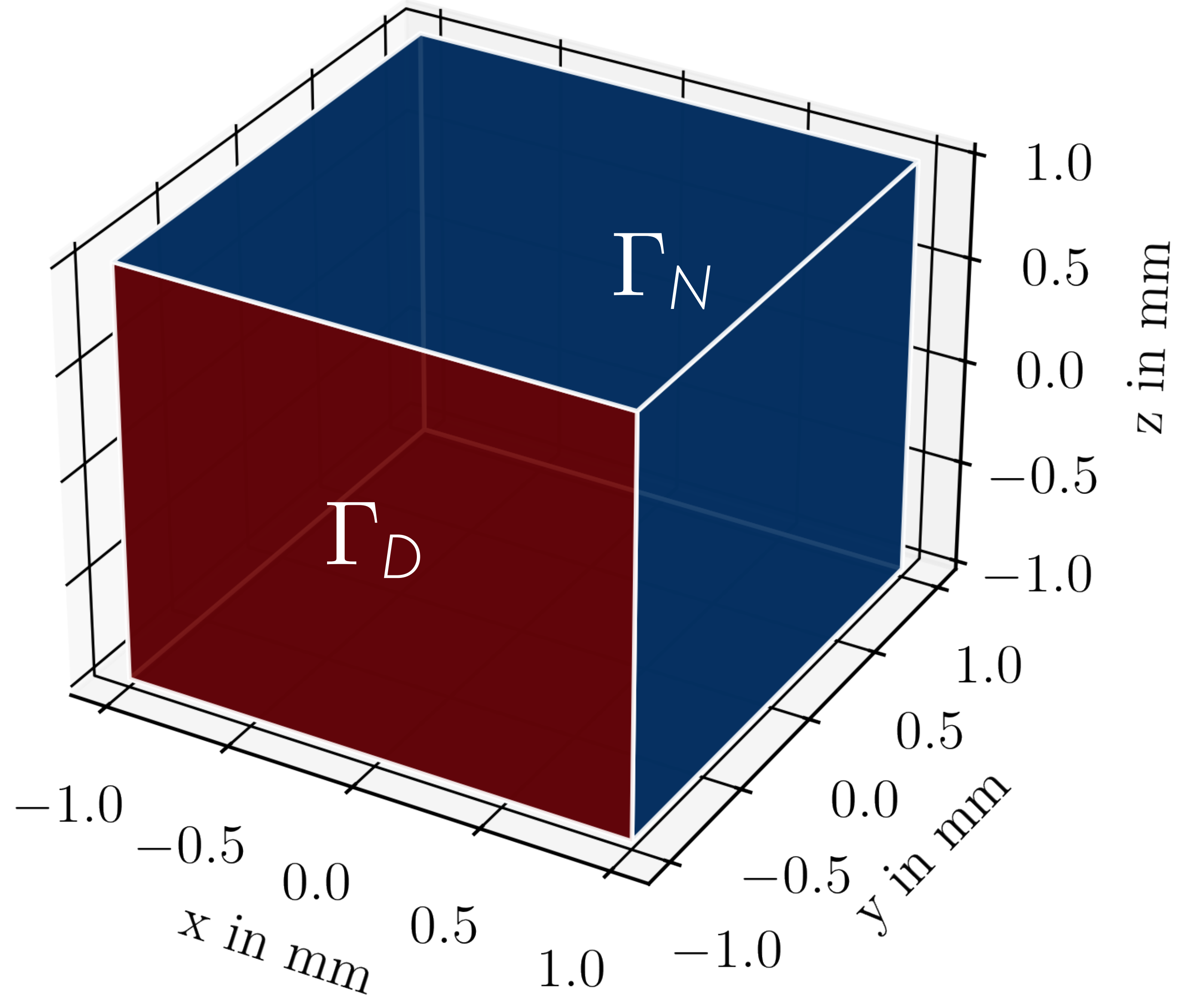
Ambrosi Pezzuto Model for Active Stress

- Quasi-static problem:

Find $\mathbf{u}$ s.t.

$$\begin{cases} -\nabla \cdot \mathbf{P}(\mathbf{u}) = 0 & \text{in } \Omega \\ \mathbf{P}(\mathbf{u})\,\mathbf{n} = 0 & \text{on } \Gamma_N \\ \mathbf{u} = 0 & \text{on } \Gamma_D \end{cases}$$

$$\text{with } \mathbf{P} = \frac{\partial \mathcal{W}_{\text{pas}}}{\partial \mathbf{F}} + \mathbf{P}_{\text{act}}$$

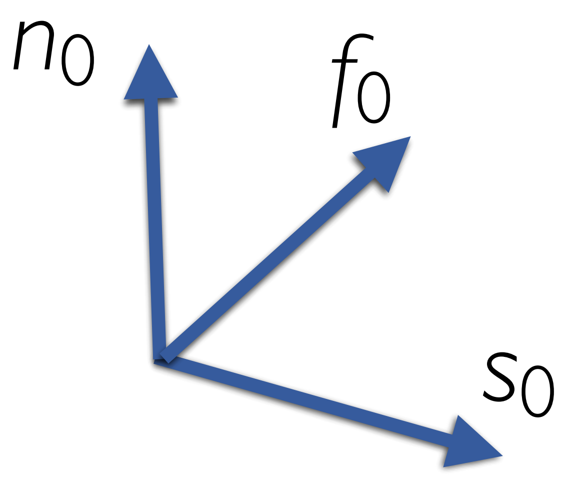


- Transverse-isotropic material:

$$\mathcal{W}_{\text{pas}} = \frac{\mu}{2}\left(\exp \bar{Q} - 1\right) + \frac{\lambda}{2}\left(\log J\right)^2$$

- Active stress:

$$\mathbf{P}_{\text{act}} = S_a \frac{\mathbf{F}\mathbf{f}_0 \otimes \mathbf{f}_0}{\sqrt{\mathbf{F}\mathbf{f}_0 \cdot \mathbf{F}\mathbf{f}_0}}$$

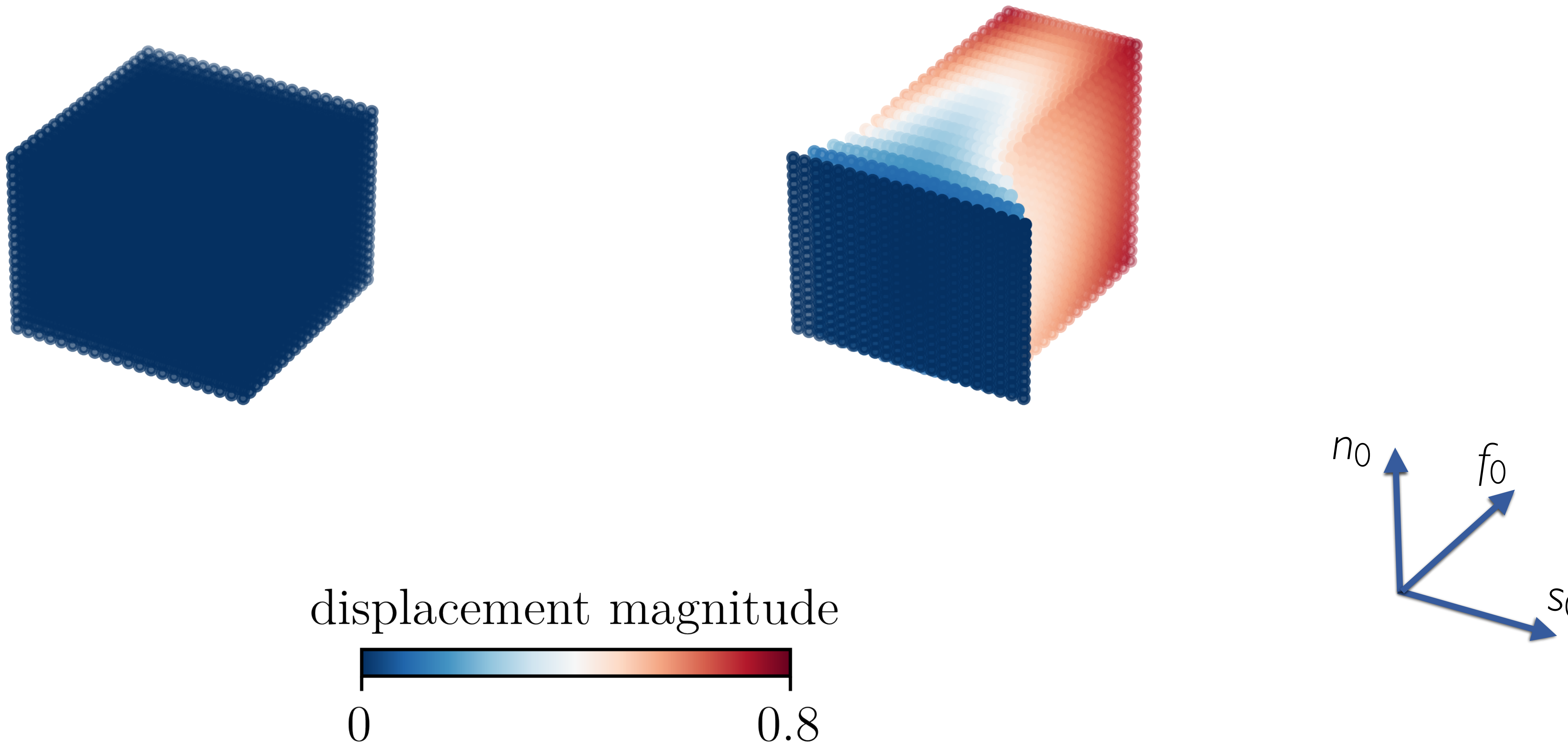


- Geometry: Cube

Ambrosi et al, JE 2012

Ambrosi Pezzuto Model for Active Stress: Forward Solution

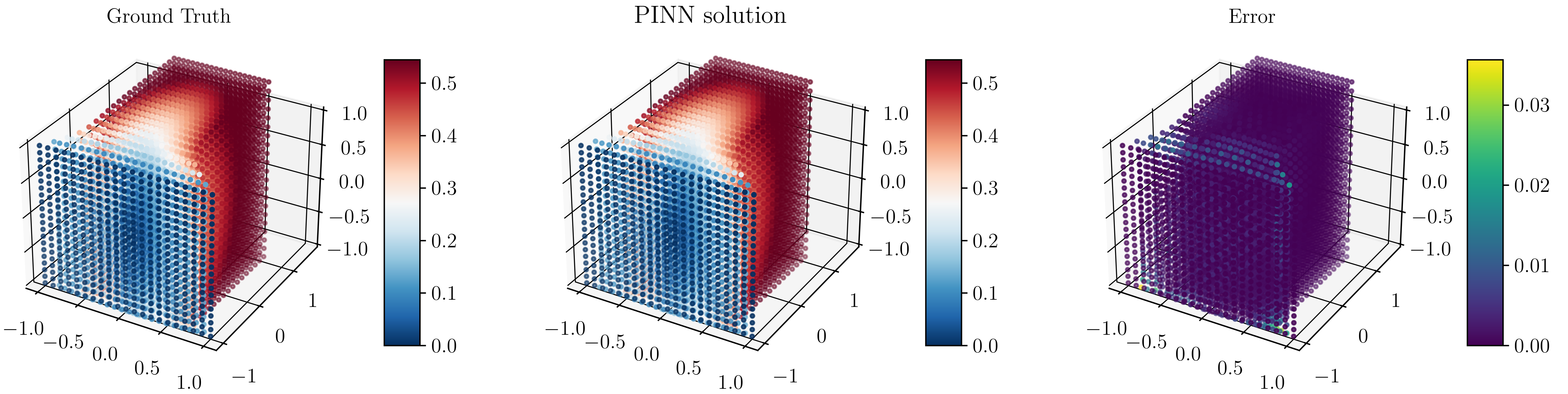
- stiffness: $\mu = 0.8$ kPa, nearly-incompressible material: $\lambda = 650$ kPa
- active stress parameter: $S_a = 118$ kPa



Ambrosi Pezzuto Model for Active Stress: PINN-based Reconstruction of Forward Solution

- $C = 0$

500 data points



Boundary layer | 500 boundary points | 500 data points | Sobol sampling

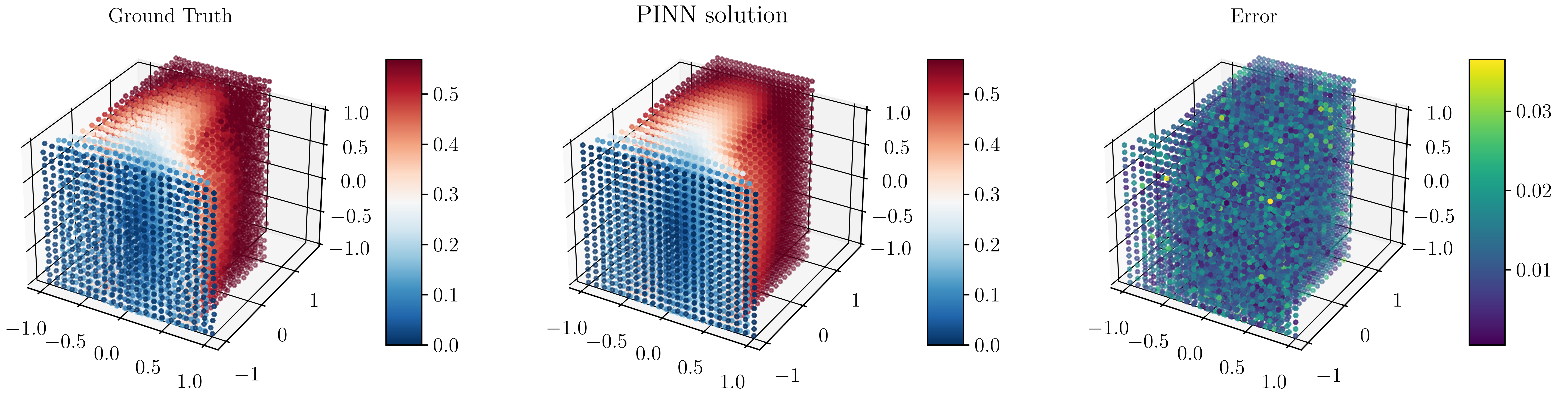
$$\tilde{\mathbf{u}} = \mathbf{u} + \epsilon$$

$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

$$C = \frac{3\sigma}{\max(\mathbf{u})}$$

- $C = 0.05$

2000 data points

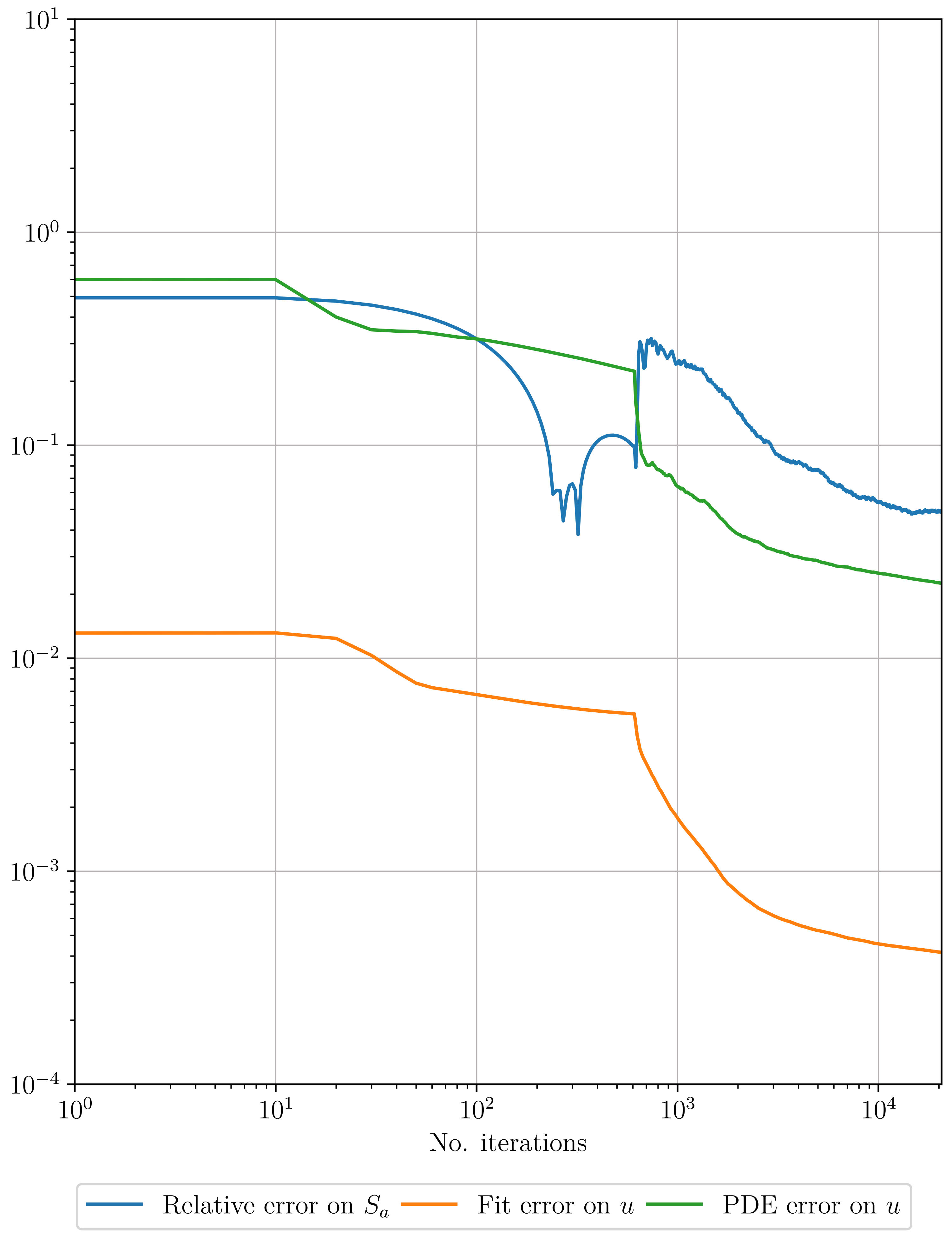


Boundary layer | 750 boundary points | 2000 data points | Sobol sampling

Ambrosi Pezzuto Model for Active Stress: PINN-based Reconstruction of Stress

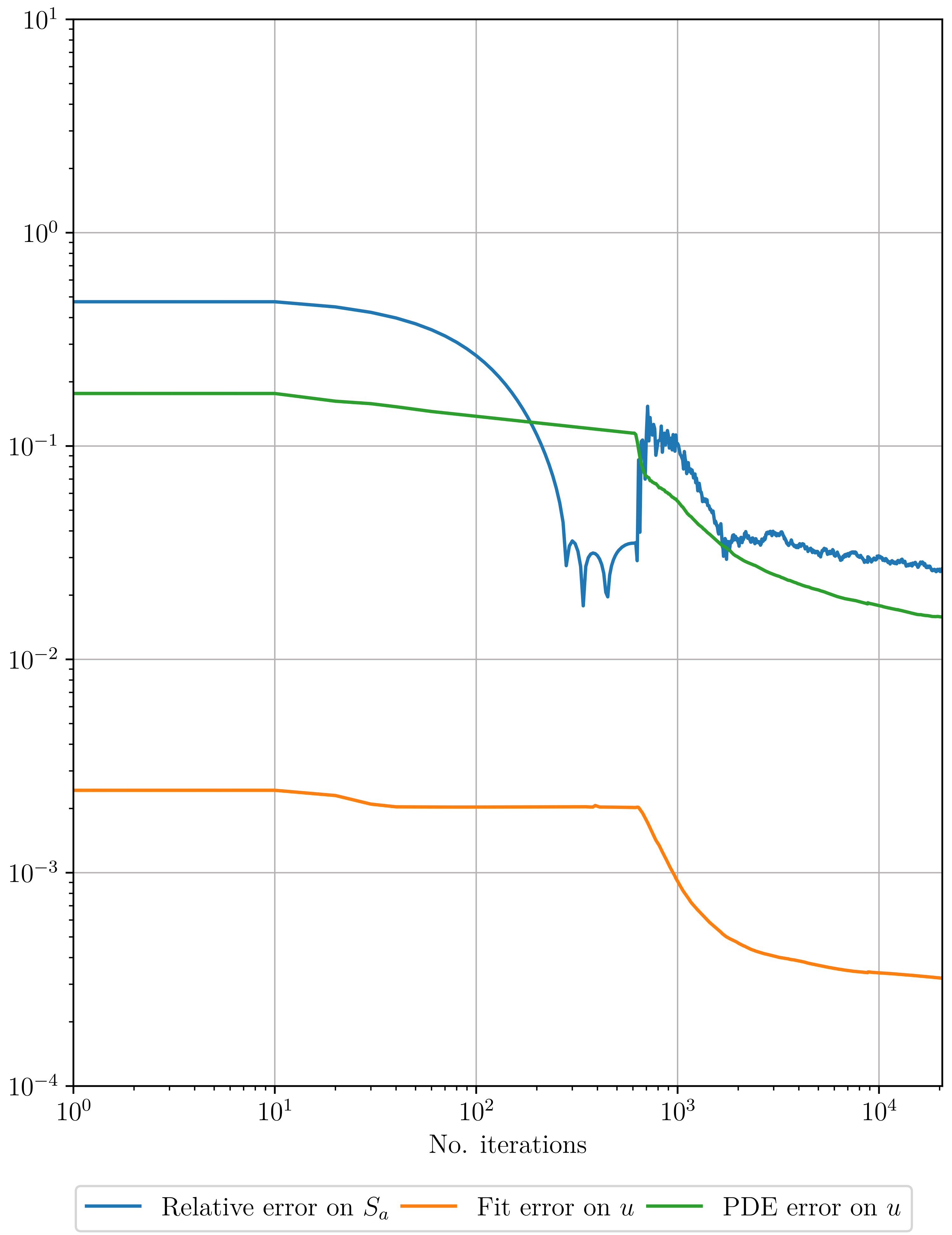
- With implicit Dirichlet boundary, $C = 0$

Relative error on S_a: 4.9E-02



- With explicit Dirichlet boundary, $C = 0$

Relative error on S_a: 2.6E-02

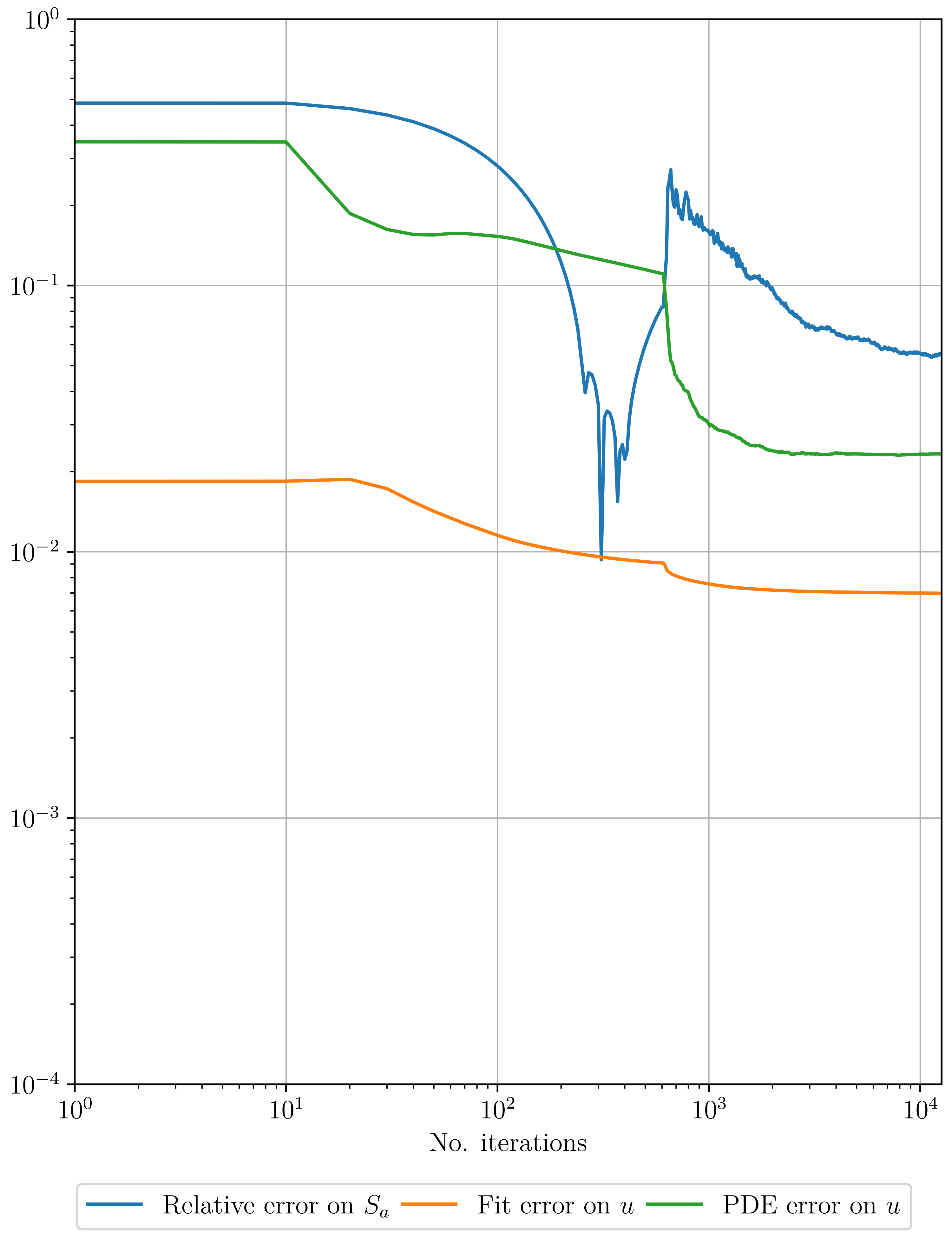


- 500 data points
- Sobol sampling
- 5 seeds

Ambrosi Pezzuto Model for Active Stress: PINN-based Reconstruction of Stress

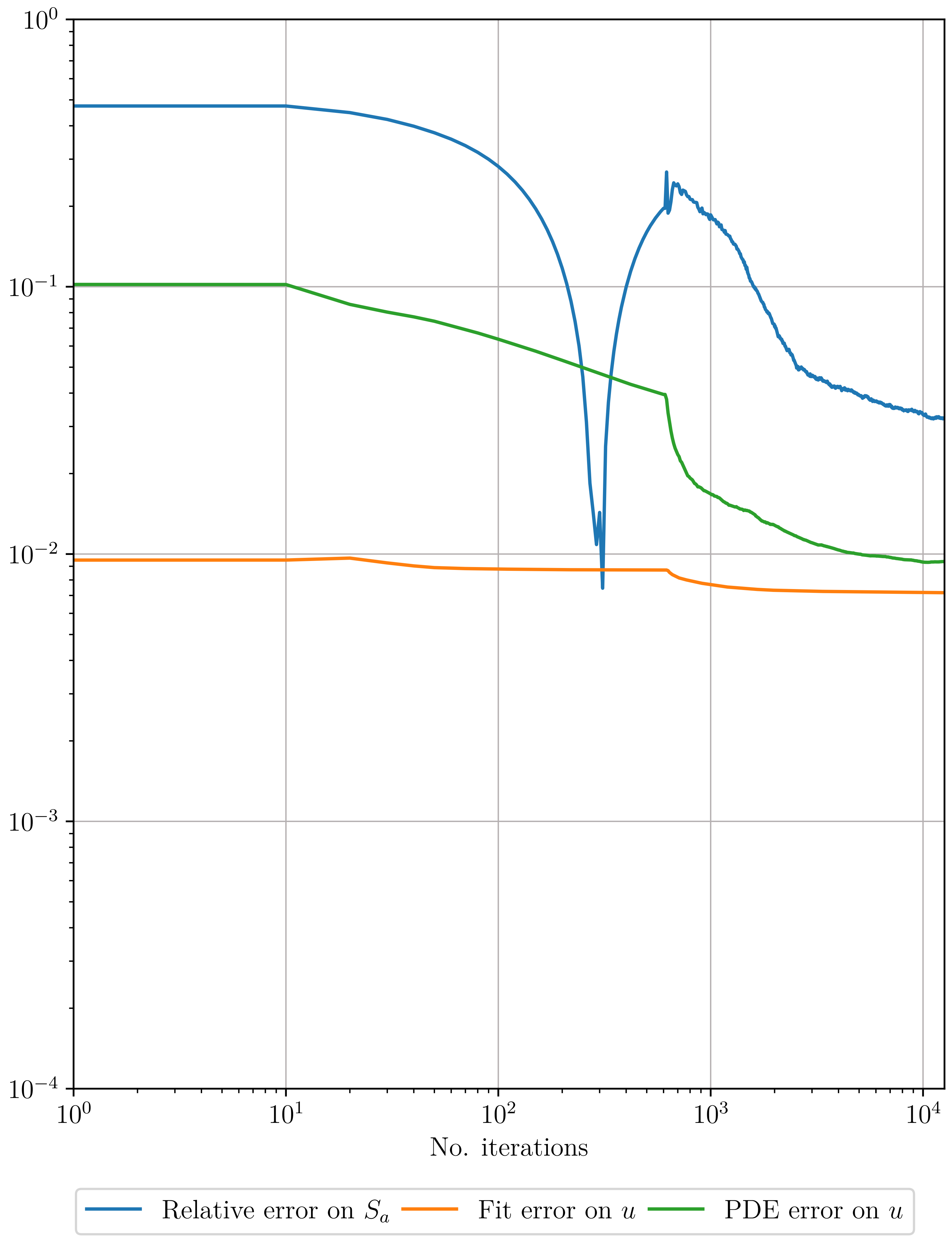
- With implicit Dirichlet boundary, $C = 0.05$

Relative error on S_a: 5.5E-02



- With explicit Dirichlet boundary, $C = 0.05$

Relative error on S_a: 3.2E-02



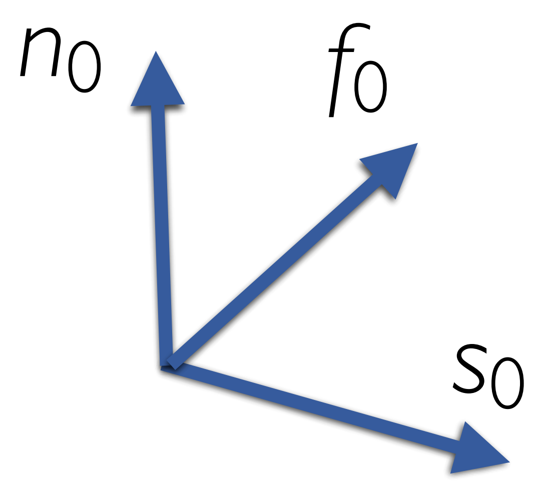
- 2000 data points
- Sobol sampling
- 5 seeds

Bestel-Clément-Sorine Model for Active Stress

- Time-dependent problem: Find $\mathbf{u}$ s.t.

$$\begin{cases} \partial_t^2 \mathbf{u} - \nabla \cdot \mathbf{P}(\mathbf{u}) = 0 & \text{in } \Omega \times (0, T] \\ \mathbf{P}(\mathbf{u})\,\mathbf{n} = 0 & \text{on } \Gamma_N \\ \mathbf{u} = 0 & \text{on } \Gamma_D \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0 & \text{in } \Omega \end{cases}$$

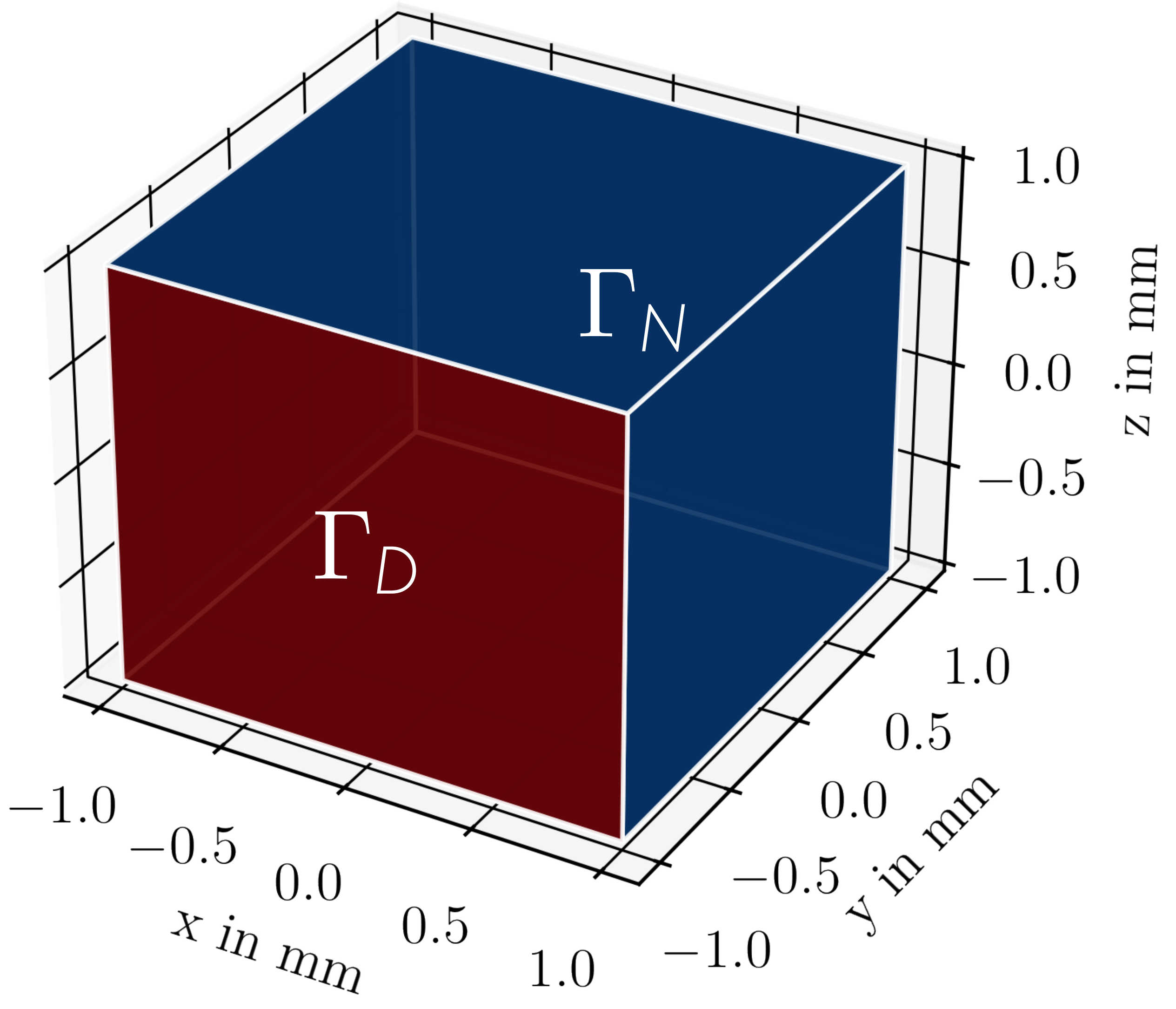
$$\text{with } \mathbf{P} = \frac{\partial \mathcal{W}_{\text{pas}}}{\partial \mathbf{F}} + \mathbf{P}_{\text{act}}$$



- Transverse-isotropic material: $$\mathcal{W}_{\text{pas}} = \frac{\mu}{2}\left(\exp \bar{Q} - 1\right) + \frac{\lambda}{2}(\log J)^2$$

- Active stress: $$\mathbf{P}_{\text{act}} = S_a(t) \frac{\mathbf{F}\mathbf{f}_0 \otimes \mathbf{f}_0}{\sqrt{\mathbf{F}\mathbf{f}_0 \cdot \mathbf{F}\mathbf{f}_0}}$$

- Geometry: Cube



Bestel-Clément-Sorine Model for Active Stress

- ODE for active stress:

Find S_a s.t.

$$\begin{cases} \dot{S}_a(t) = -|a(t)|S_a(t) + \sigma_0 |a(t)|_+ & \text{for } t \text{ in } (0, T] \\ S_a(0) = 0 \end{cases}$$

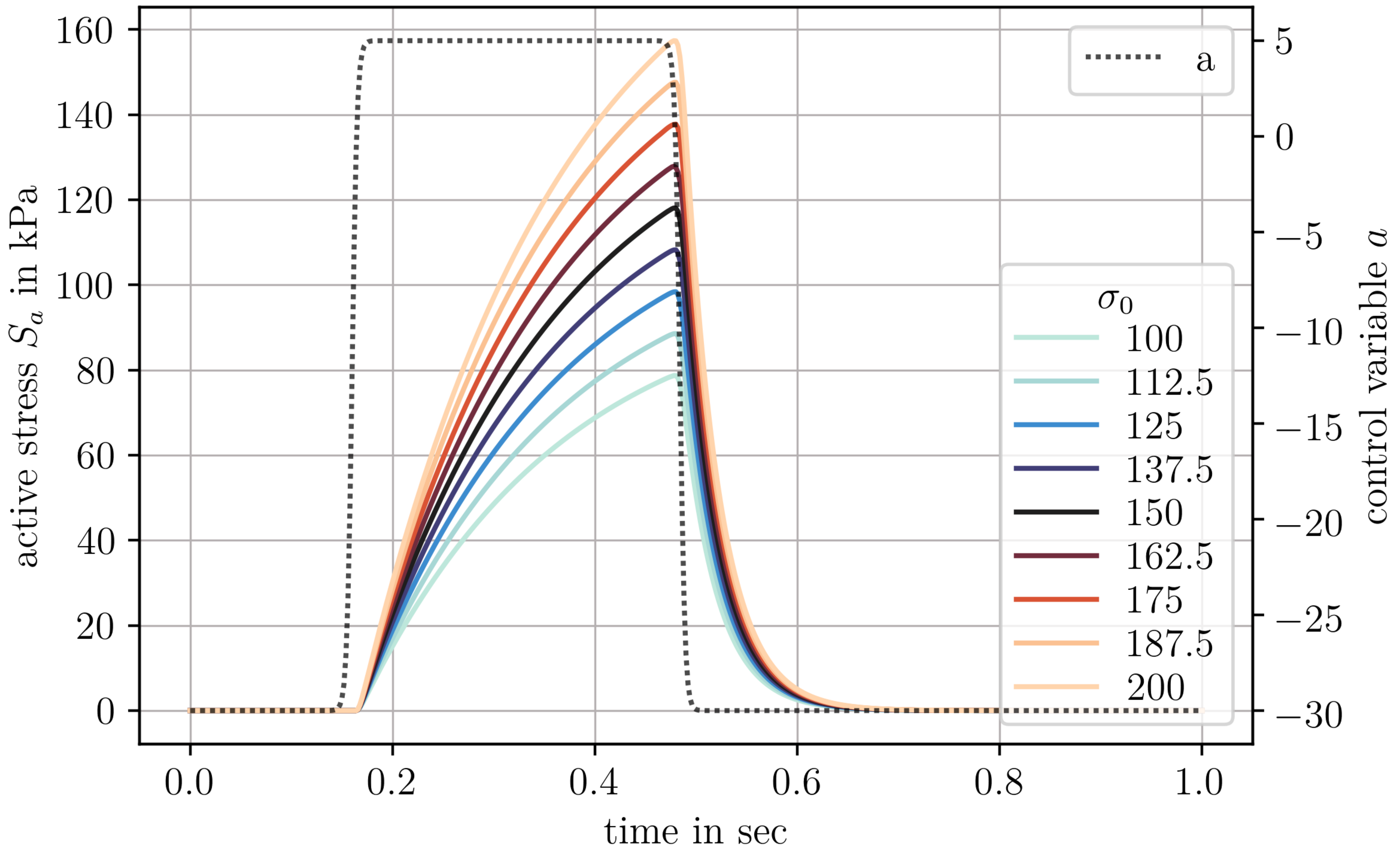
with

$$|a(t)|_+ = \max\{a(t), 0\}$$

$$a(t) = \alpha_{\max} f(t) + \alpha_{\min} \cdot (1 - f(t))$$

$$f(t) = S^+(t - t_{sys}) \cdot S^-(t - t_{dias}))$$

$$S^{\pm}(\Delta t) = \frac{1}{2}\left(\pm \tanh\left(\frac{\Delta t}{\gamma}\right)\right)$$



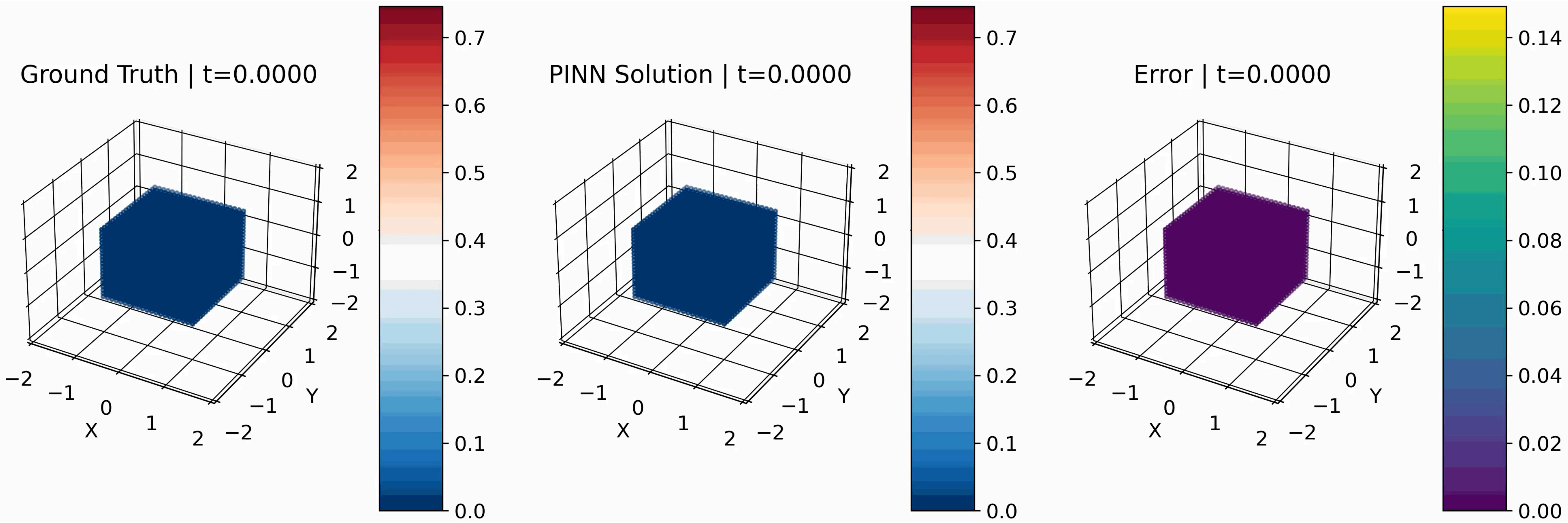
- **Parameters:**

$\alpha_{\min}$	$\alpha_{\max}$	t_{sys}	t_{dias}	σ_0
-30	5	0,161 s	0,484 s	150 kPa

Bestel et al, MICCAI 2001

Bestel-Clément-Sorine Model for Active Stress: PINN-based Reconstruction of Forward Solution

- stiffness: $\mu = 0.8$ kPa , nearly-incompressible material: $\lambda = 650$ kPa , maximal stiffness $\sigma_0 = 150$ kPa



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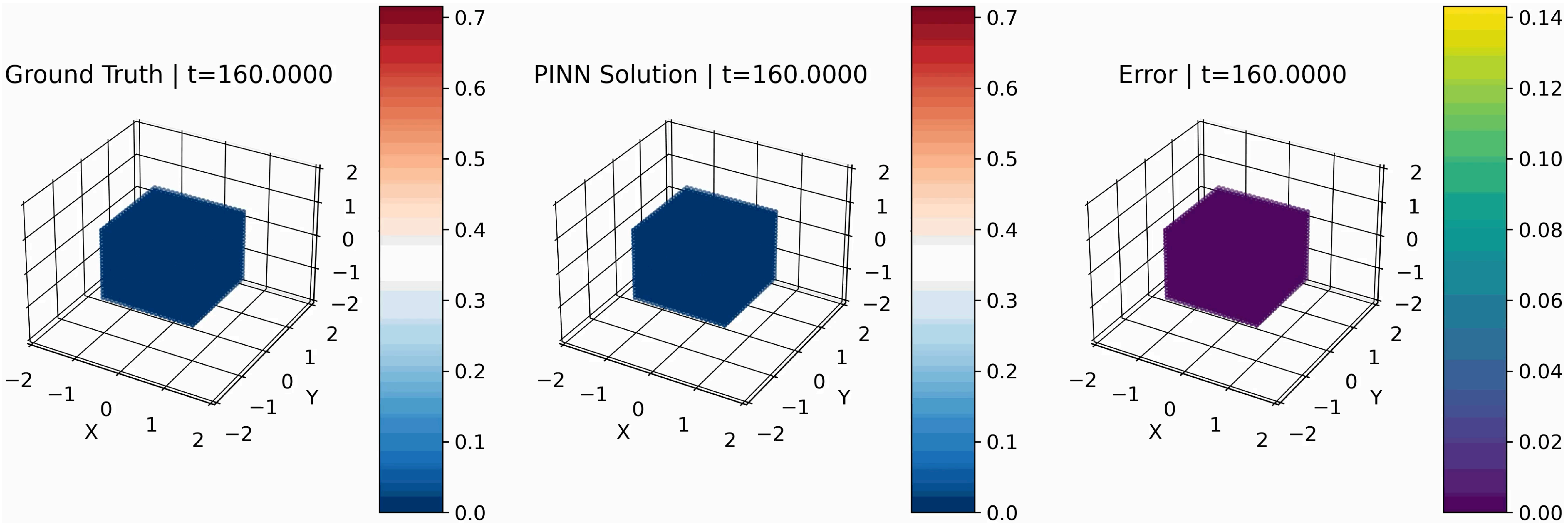
Bestel-Clément-Sorine Model for Active Stress: PINN-based Reconstruction of Stiffness

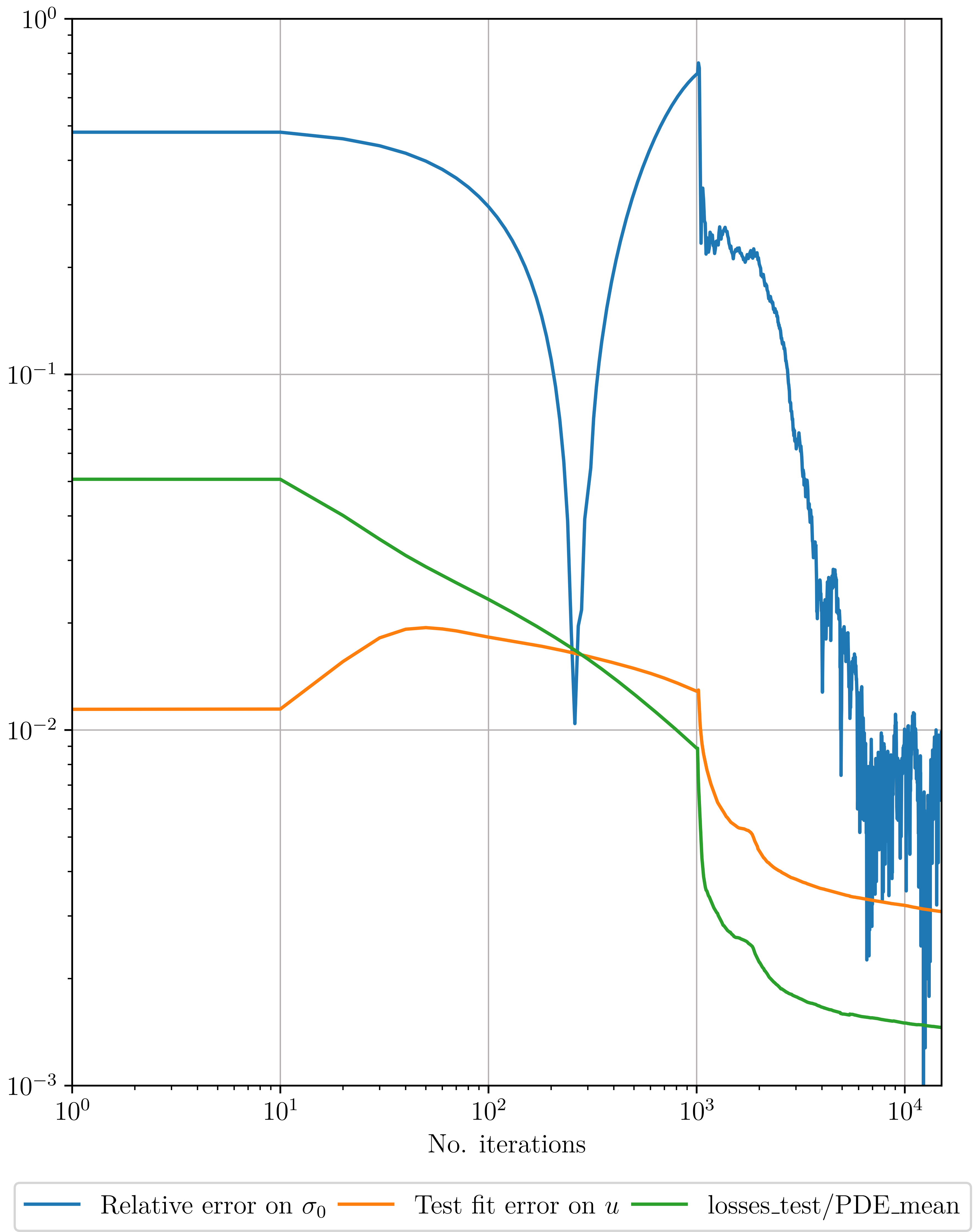
- With Dirichlet boundary layer, $C = 0$

Relative error on σ_0 : 0.9E-02



- 10000 data points
- 160-350ms
- 5 seeds
- 1000 Adam + 14000 BFGS

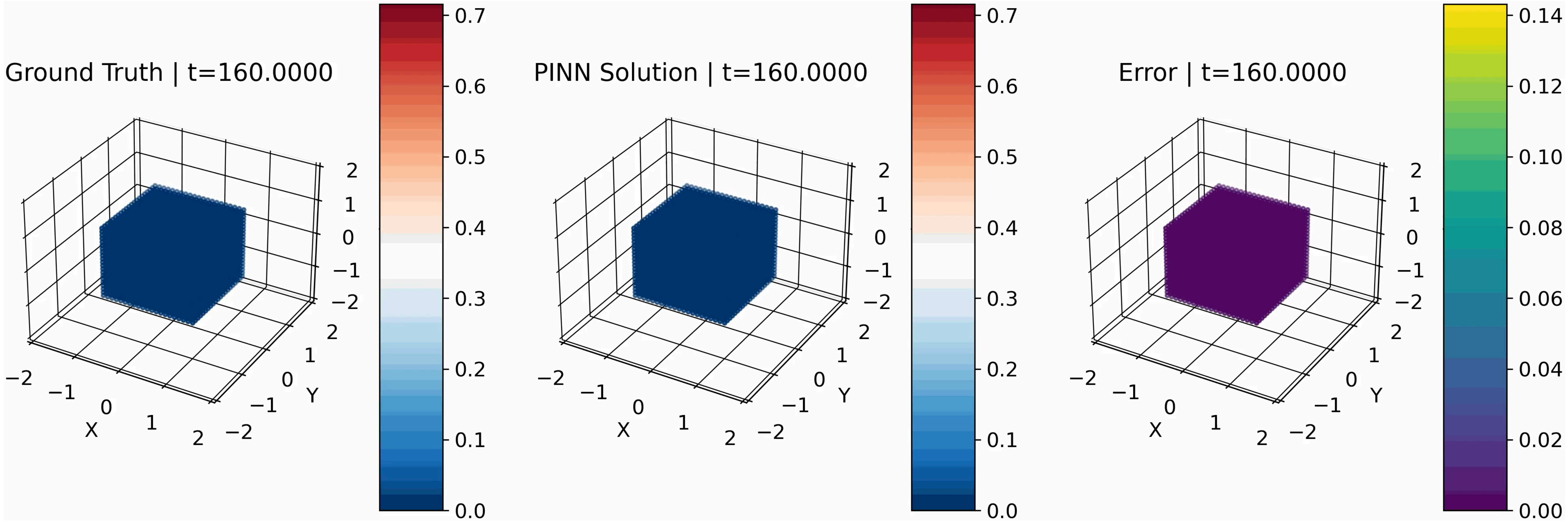
} 52 data points per ms



Bestel-Clément-Sorine Model for Active Stress: PINN-based Reconstruction of Stiffness

- With Dirichlet boundary layer, $C = 0.05$

Relative error on σ_0 : 1.3E-02



- 10000 data points
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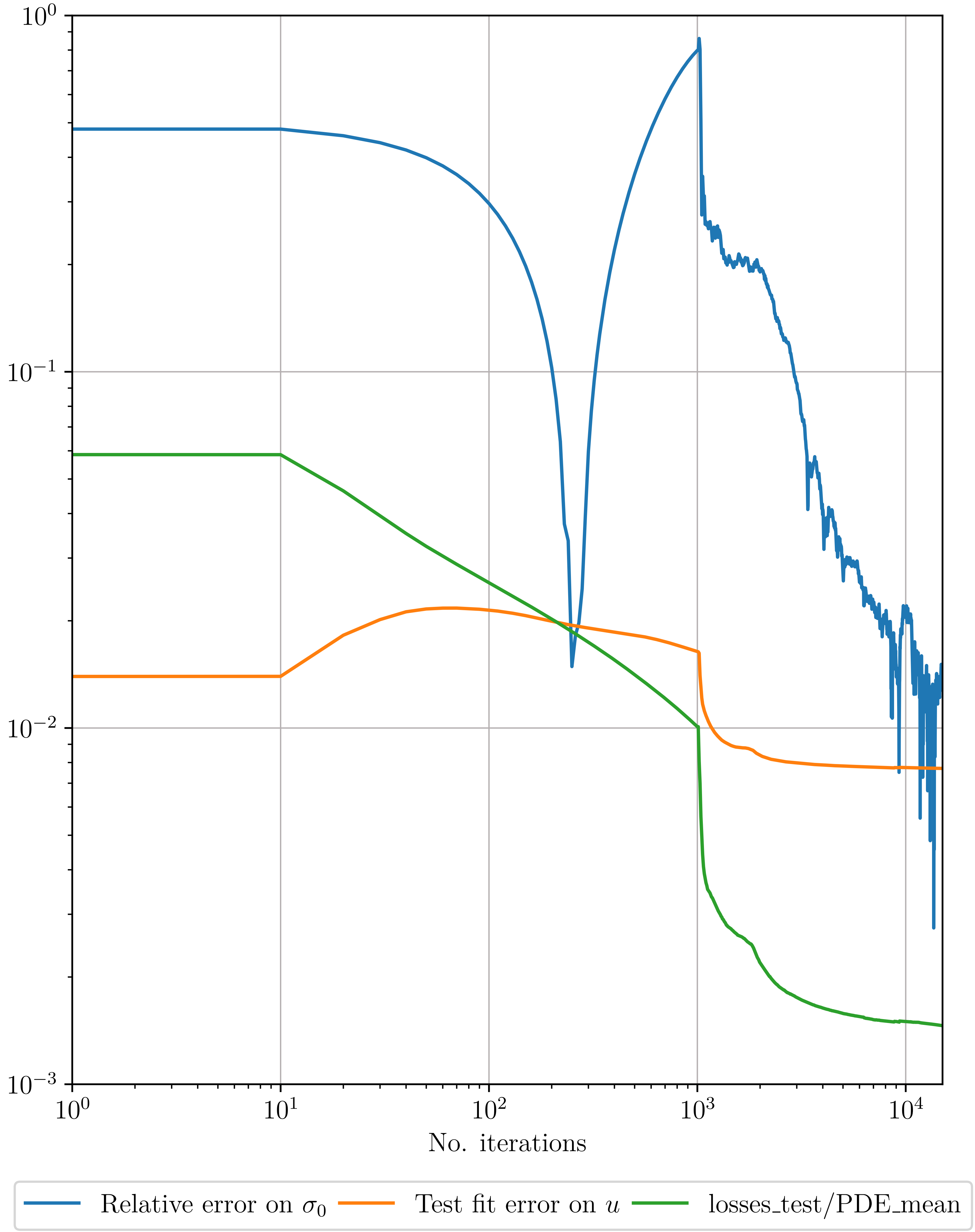
- 5 seeds
- 1000 Adam + 14000 BFGS



Discussion and Future Steps:

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- Efficient and versatile algorithm
- Robustness and convergence properties empirically proved in different testcases

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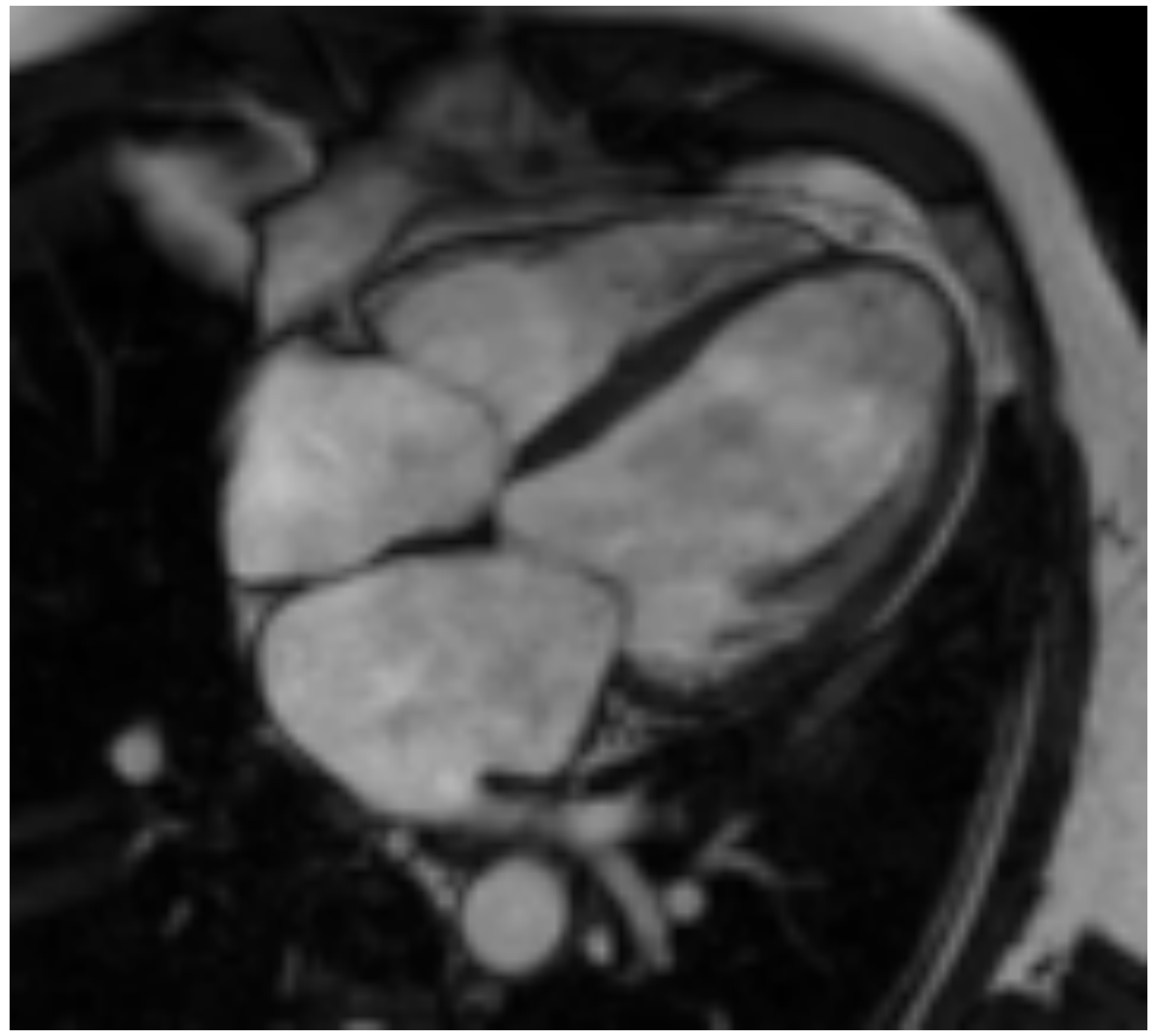
Future developments:

- Accelerate training for time-dependent case
- Realistic geometries



Thank you for your attention.

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