Machine-Learning Error Models for Approximate Solutions to Parameterized Systems of Nonlinear Equations

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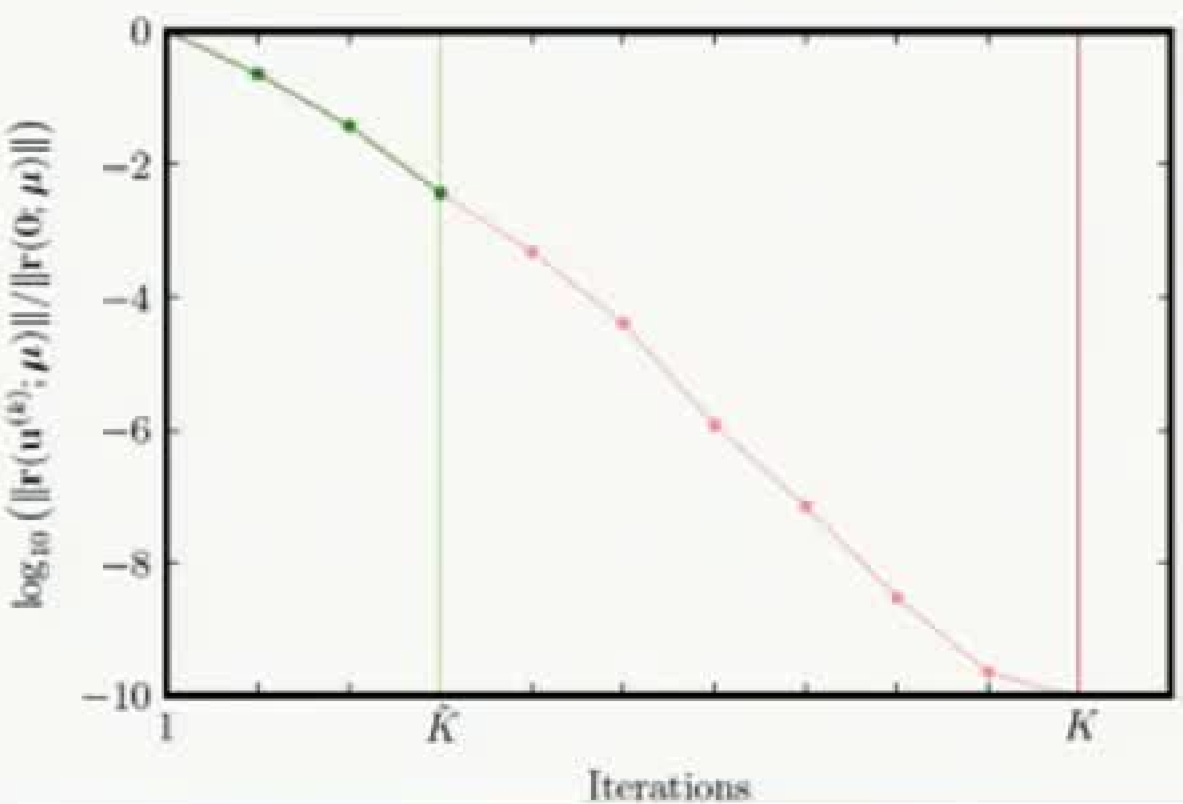
Solution Approximations

- **Inexact solutions:** When solving nonlinear equations, prematurely terminate iterations
- **Lower-fidelity models:** Neglect physical phenomena, coarsen the mesh, or use lower-order finite differences or elements
- **Reduced-order models:** Approximate solution with a linear combination of $m_{\mathbf{u}} \ll N_{\mathbf{u}}$ basis functions



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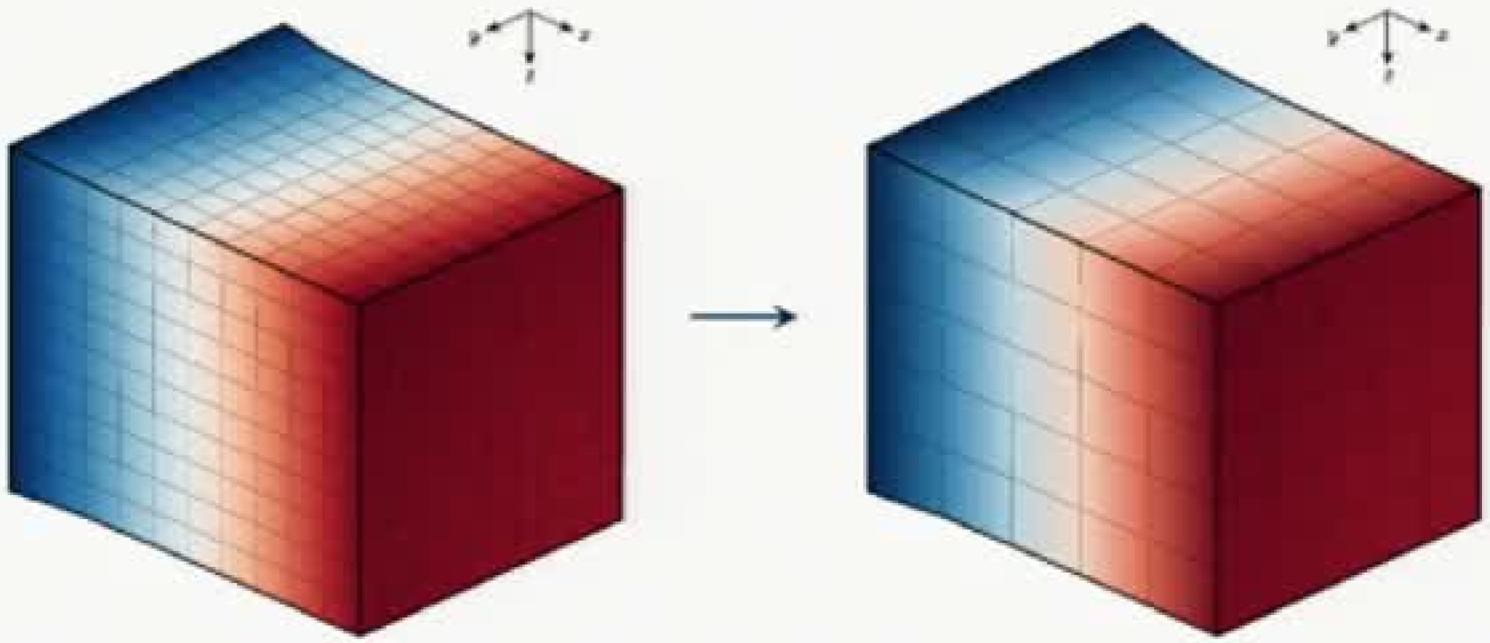


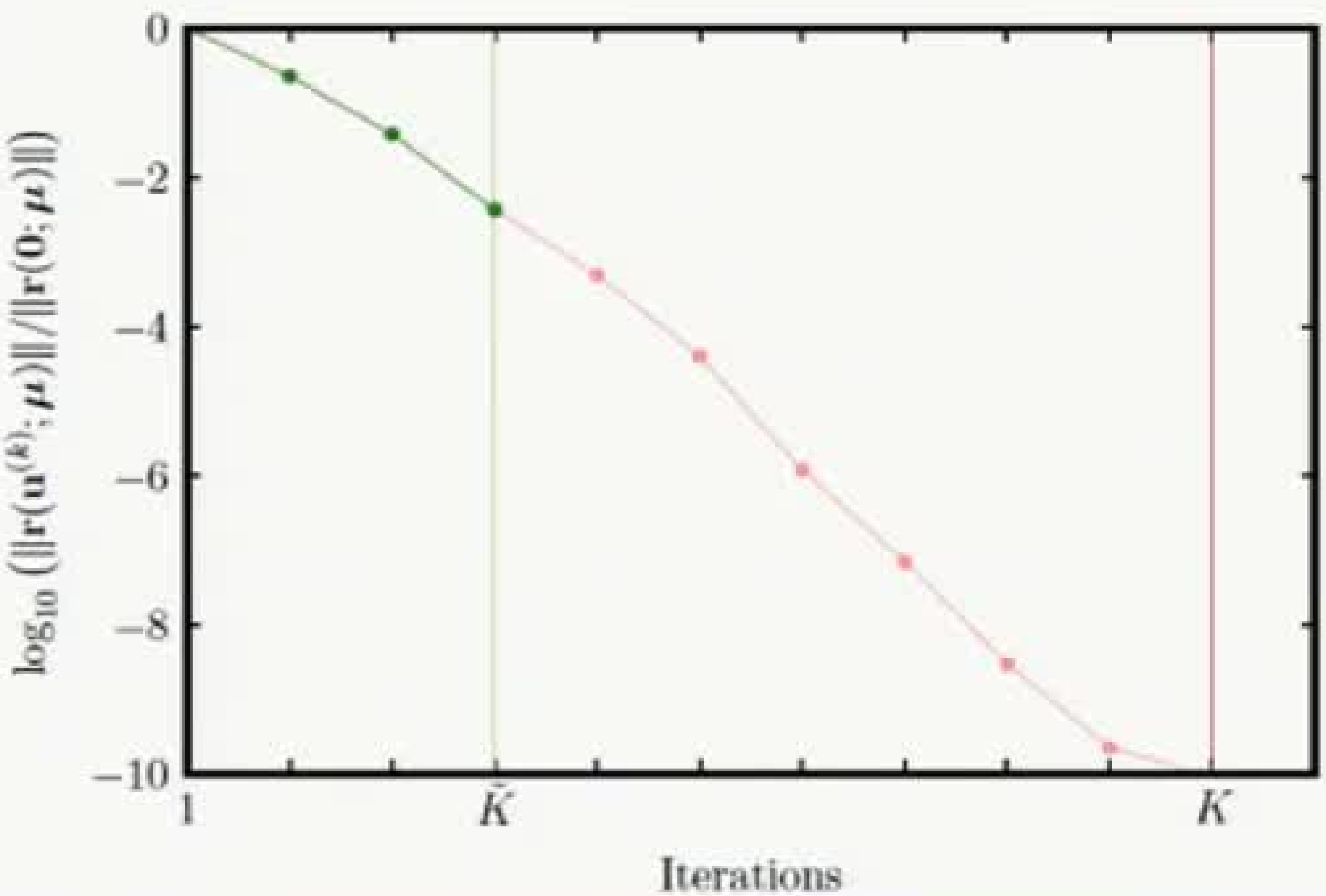
Inexact Solutions

- Iterative solution to nonlinear equations: sequence of approximations

$$\mathbf{u}^{(k)}, \quad k = 0, \ldots, K$$

- Approximate solution $\mathbf{u}^{(\tilde{K})}$ can be obtained after iteration $\tilde{K}$

$$\tilde{\mathbf{u}}(\boldsymbol{\mu}) = \mathbf{u}^{(\tilde{K})}$$

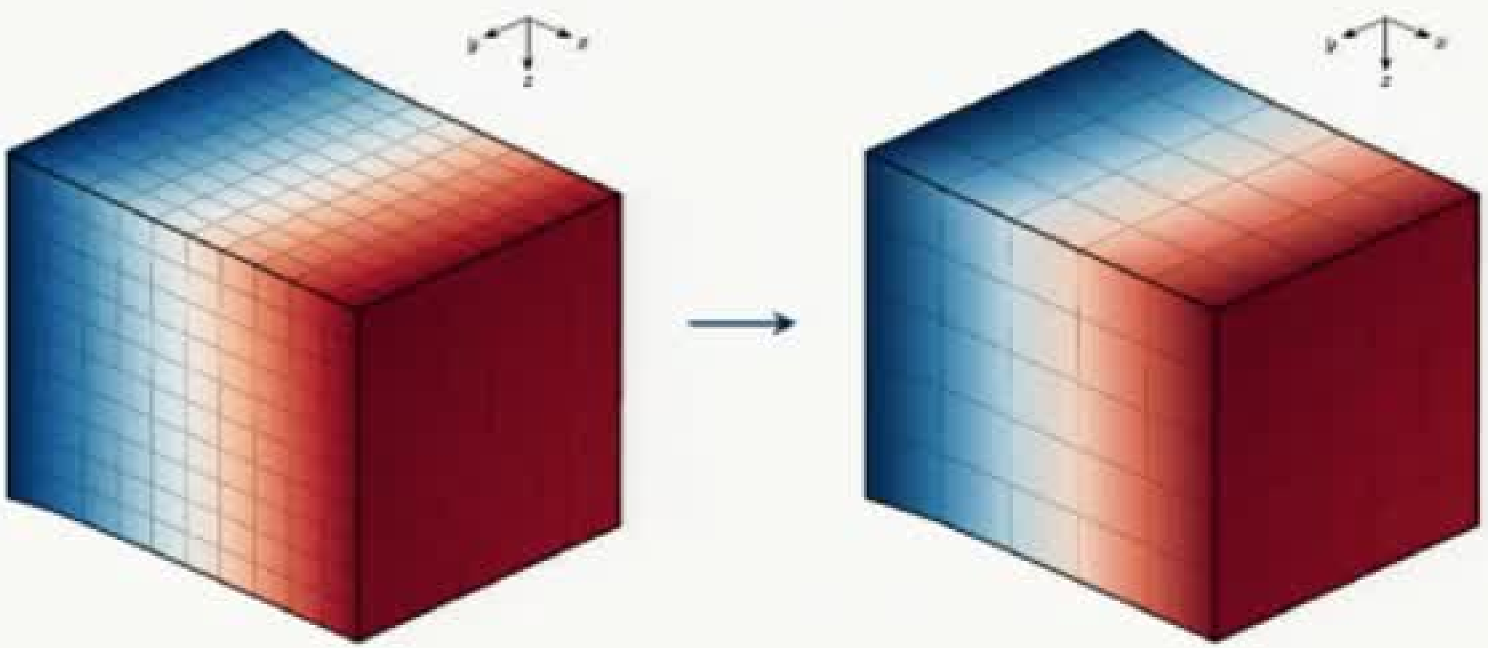


Lower-Fidelity Models

Fidelity reduction approaches

- Neglect physical phenomena
- Reduce spatial accuracy
  - Use lower-order finite differences or elements
  - Coarsen the mesh and prolongate (interpolate) the solution:

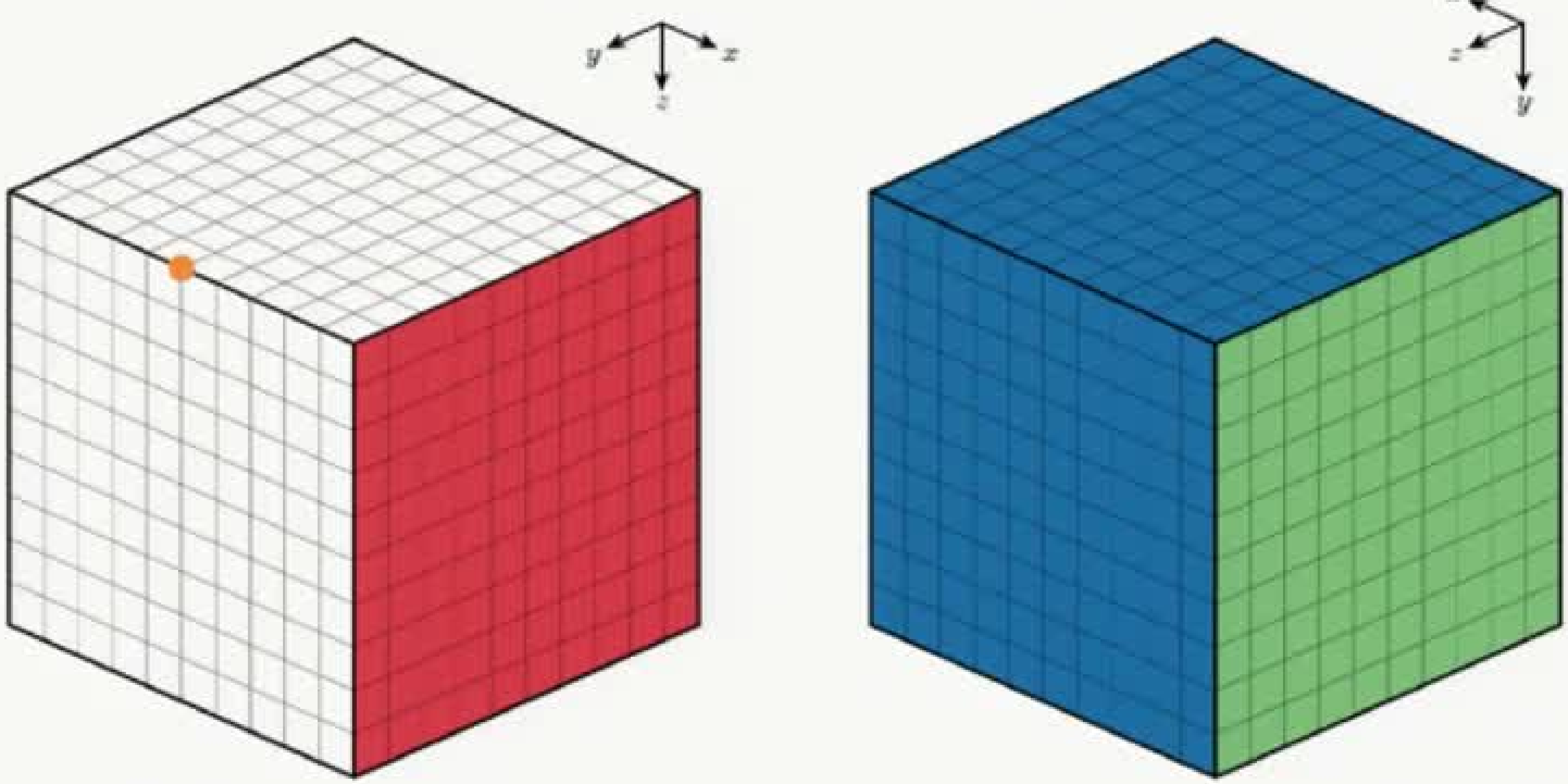
$$\tilde{\mathbf{u}} = \mathbf{p}(\mathbf{u}_{\mathrm{LF}}), \quad \mathbf{p} : \mathbb{R}^{N_{\mathbf{u}_{\mathrm{LF}}}} \to \mathbb{R}^{N_{\mathbf{u}}}$$



Outline

- Introduction
- Parameterized Systems of Nonlinear Equations
- Machine-Learning Error Models
- Numerical Experiments
  - Cube: Reduced-Order Modeling
  - PCAP: Reduced-Order Modeling
  - Burgers' Equation: Inexact Solutions and Coarse Solution Prolongation
- Summary

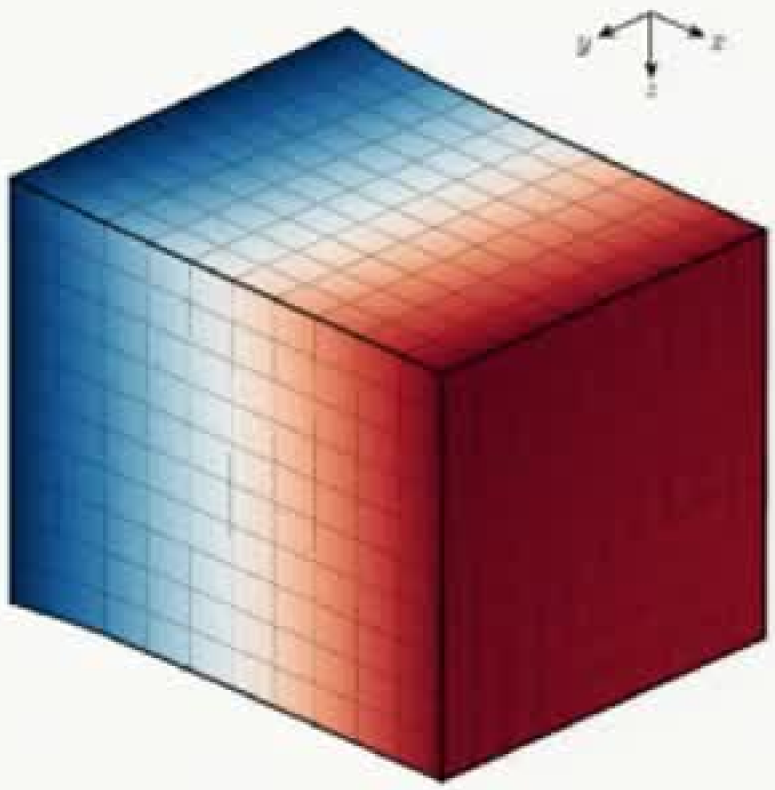
Cube: Reduced-Order Modeling

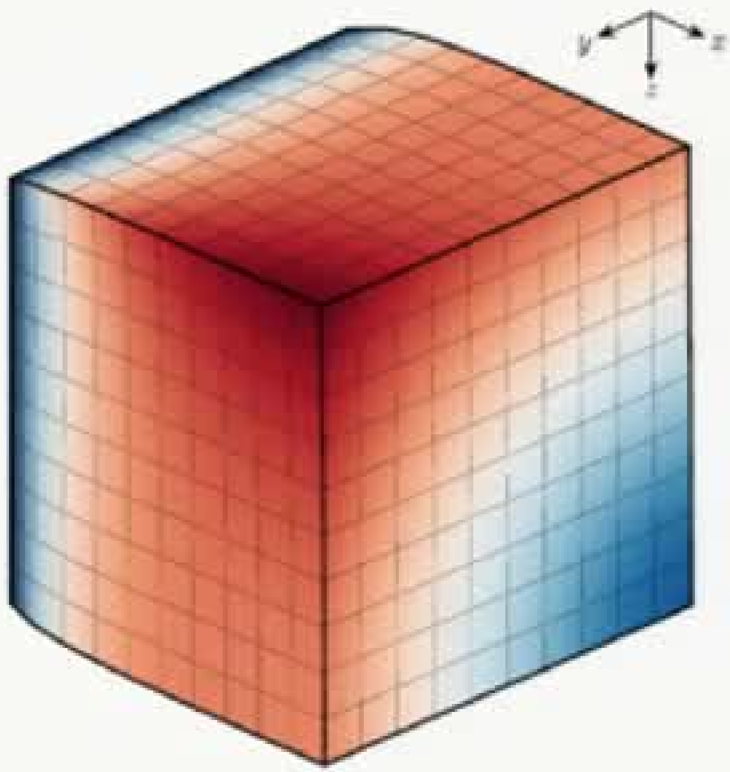


- Applied traction (Neumann boundary condition)
- Planar constraint (Dirichlet boundary condition)
- Complete constraint (Dirichlet boundary condition)
- Node of interest

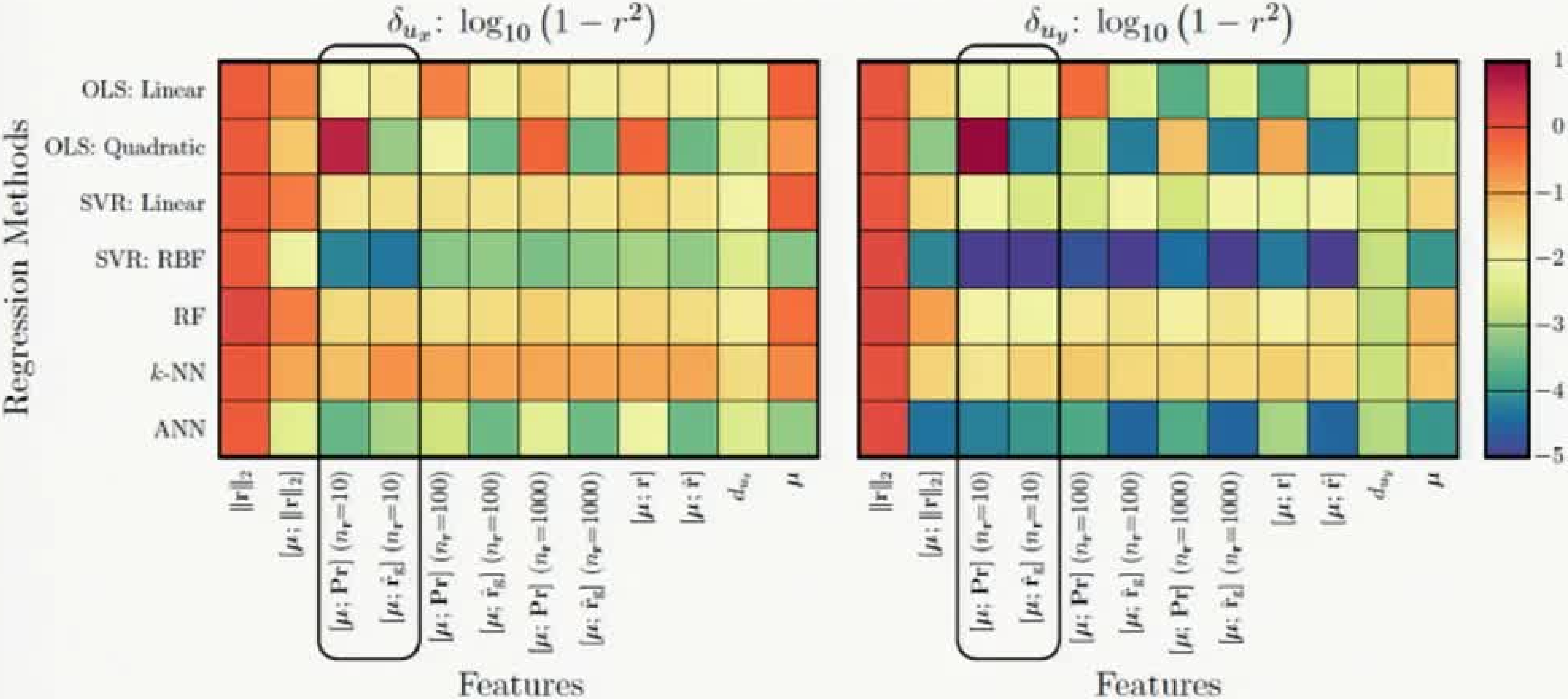
Cube: Overview

- $N_{\mathbf{u}} = 3410$ – deliberately small to compute $d(\boldsymbol{\mu})$ and use $\mathbf{r}(\boldsymbol{\mu})$
- $N_{\boldsymbol{\mu}} = 3$ parameters: $\boldsymbol{\mu} = [E; \nu; t]$
  - $E \in [75, 125]$ GPa, $\nu \in [0.20, 0.35]$, $t \in [40, 60]$ GPa
- 8 HF runs → up to $m_{\mathbf{u}} = 8$ ROM basis vectors (2 used – 99.49%)



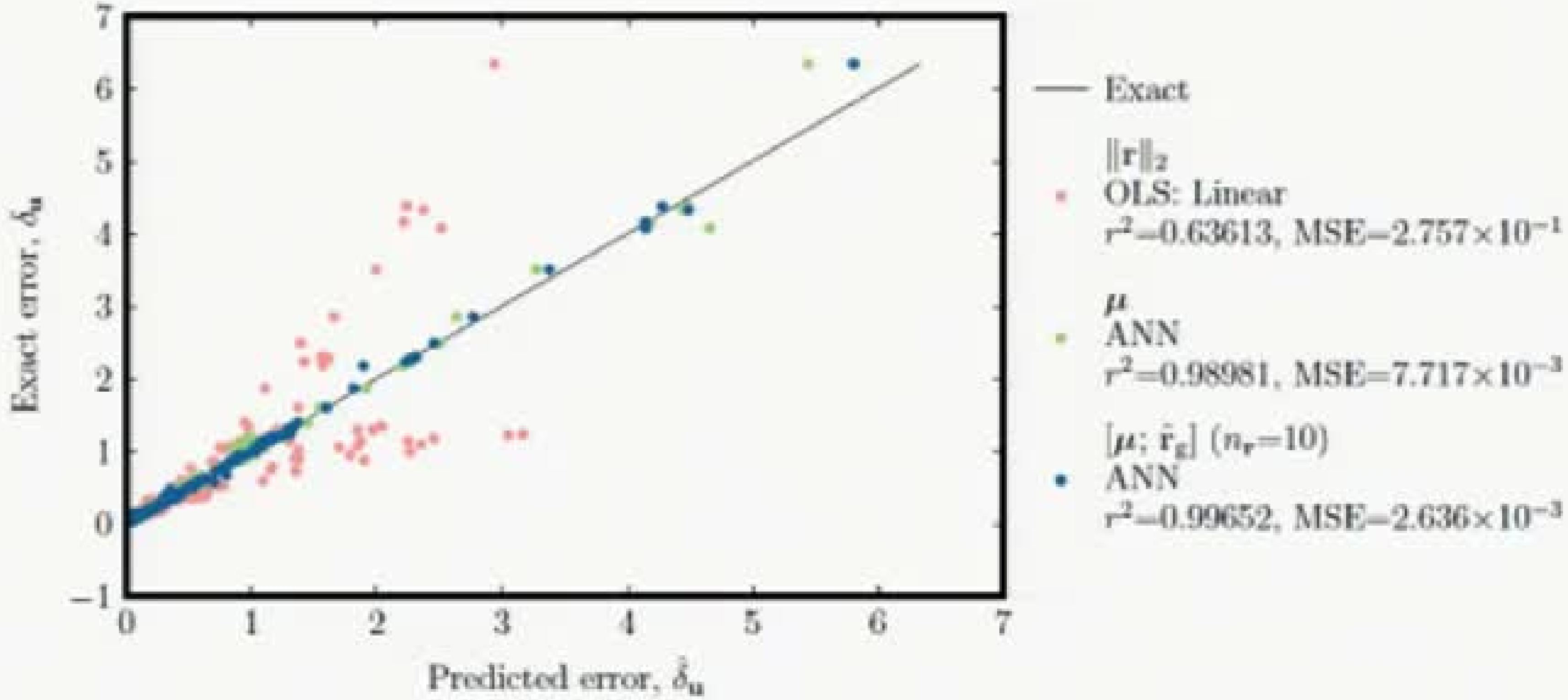


Cube: Variance Unexplained for QoI Error Prediction



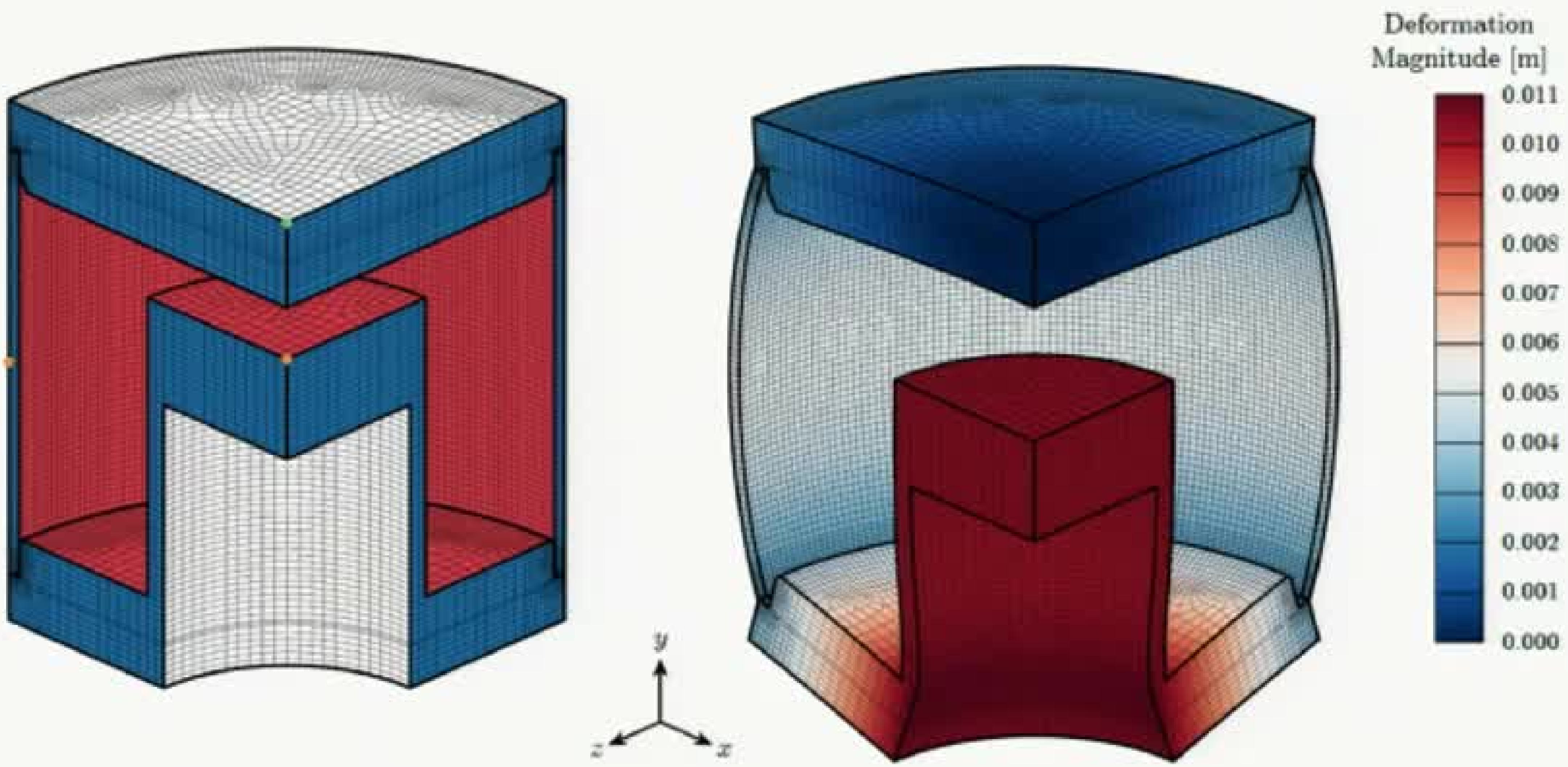
- $\|\mathbf{r}\|_2$ yields highest variance unexplained
- d_{u_x} and d_{u_y} yield moderate variance unexplained, but are costly
- SVR: RBF and ANN yield lowest variance unexplained
- $[\boldsymbol{\mu}; \hat{\mathbf{r}}_g]$ and $[\boldsymbol{\mu}; \mathbf{Pr}]$ yield low variance unexplained with only 10 samples (compared to $N_{\mathbf{u}} = 3410$)

Cube: Normed State-Space Error Predictions



- Our method beats previous state-of-the-art methods with $r^2 > 0.996$

Predictive Capability Assessment Project: Reduced-Order Modeling

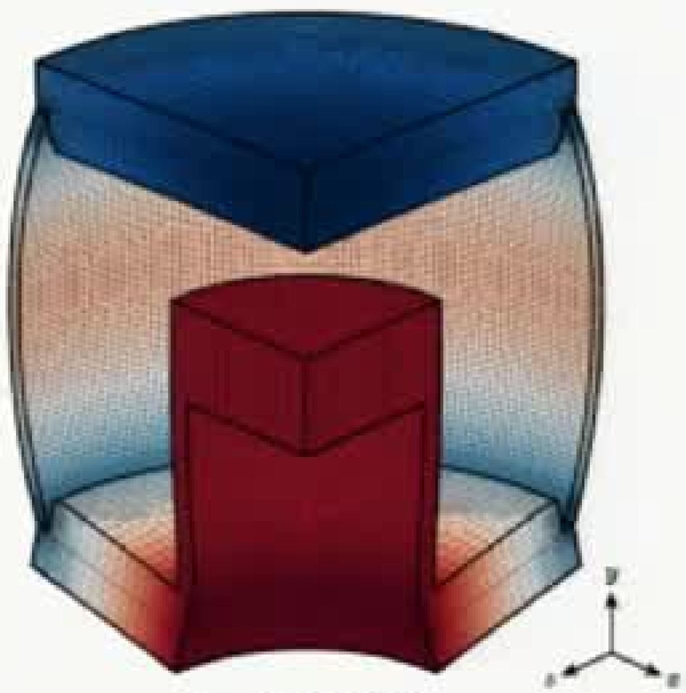


- Applied pressure (Neumann boundary condition)
- Planar constraint (Dirichlet boundary condition)
- Complete constraint (Dirichlet boundary condition)
- Nodes of interest

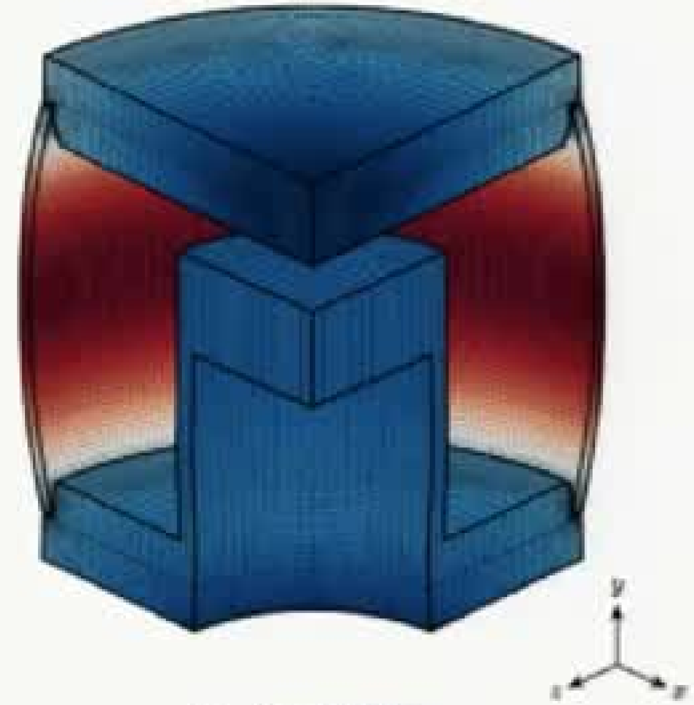
PCAP: Overview

- $N_{\mathbf{u}} = 274,954$ for quarter of domain
- $N_{\boldsymbol{\mu}} = 3$ parameters: $\boldsymbol{\mu} = [E; \nu; p]$
  - $E \in [50, 100]$ GPa, $\nu \in [0.20, 0.35]$, $p \in [6, 10]$ GPa
- 8 HF runs $\rightarrow$ up to $m_{\mathbf{u}} = 8$ ROM basis vectors (5 used – 99.90%)
- 30 parameter training instances for regression model

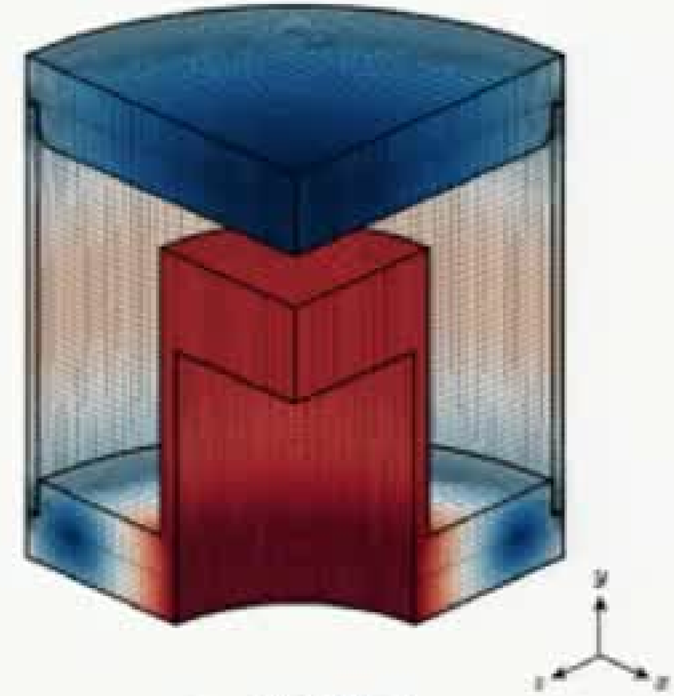
PCAP: Basis Vectors



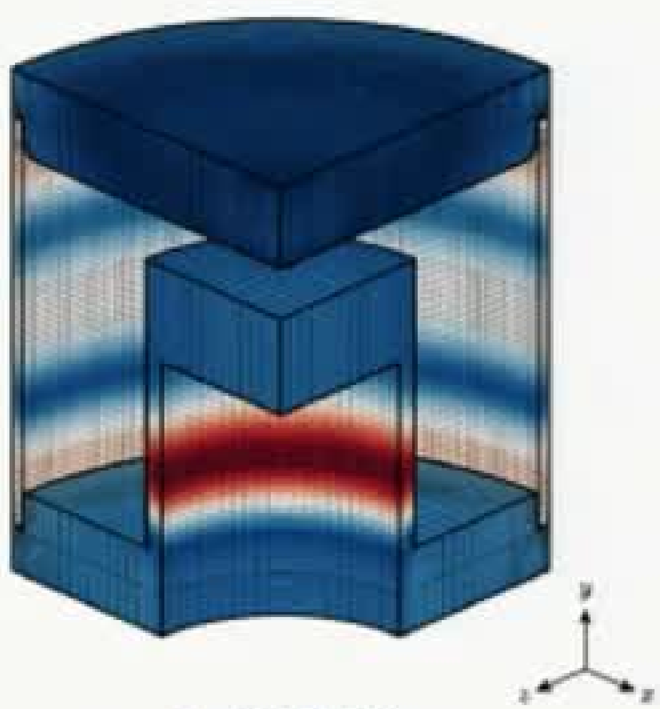
1: 85.03%



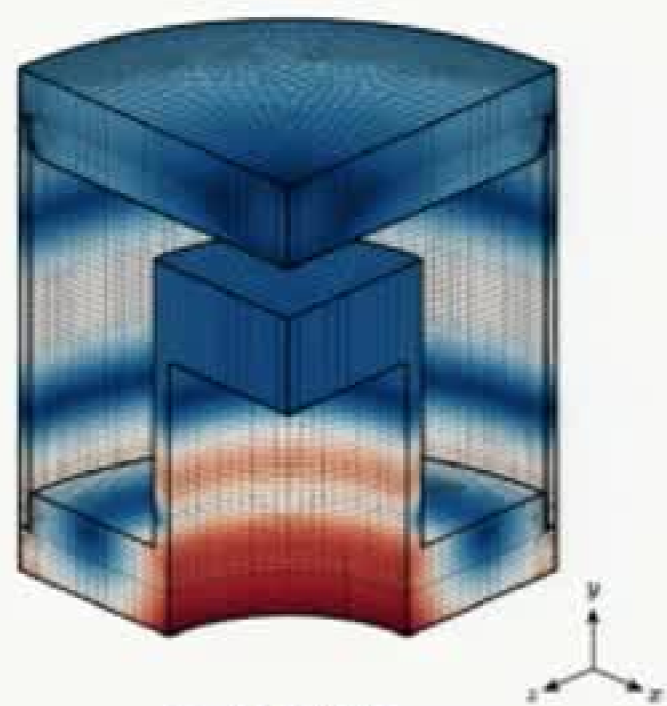
2: 95.69%



3: 99.35%

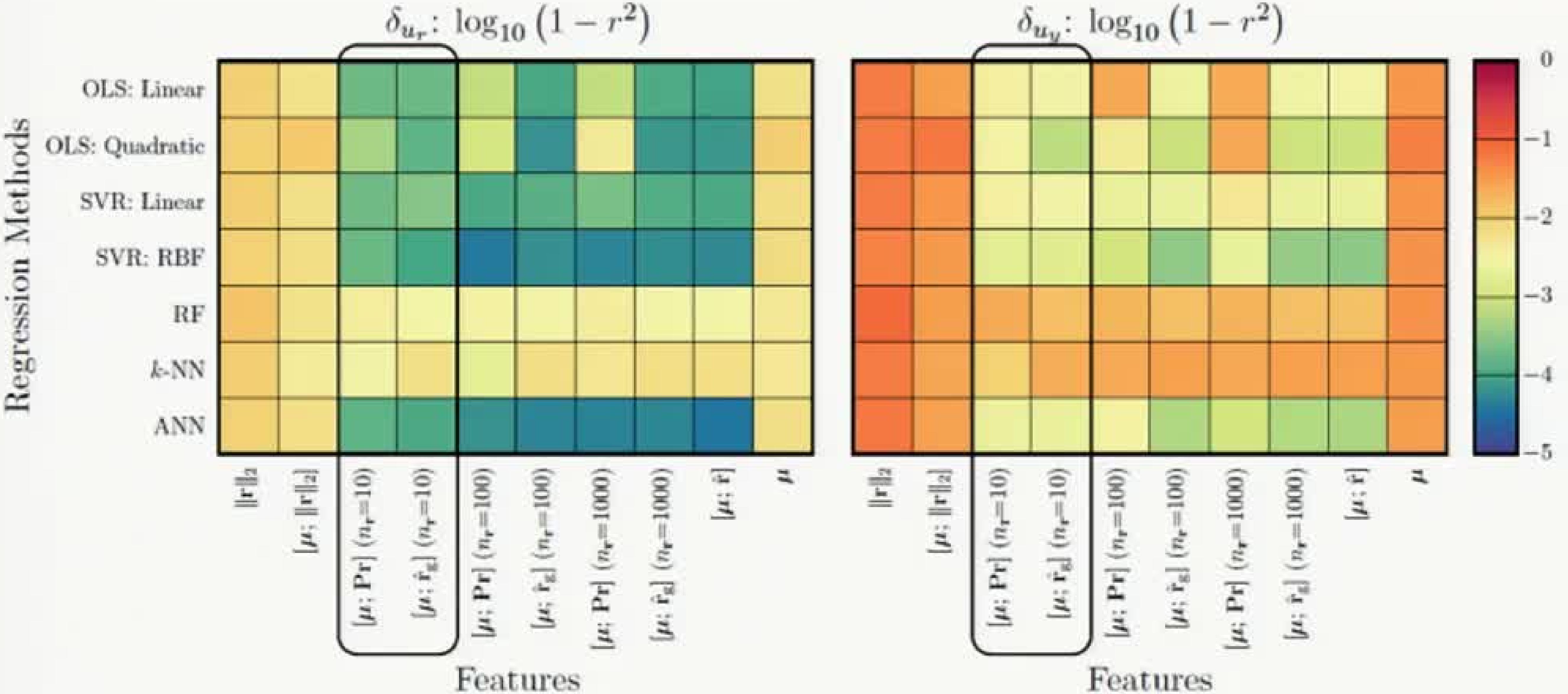


4: 99.77%



5: 99.90%

PCAP: Variance Unexplained for QoI Error Prediction



- $\|\mathbf{r}\|_2$, $[\boldsymbol{\mu}; \|\mathbf{r}\|_2]$, and $\boldsymbol{\mu}$ yield highest variance unexplained
- RF and k-NN yield highest variance unexplained
- SVR: RBF and ANN yield lowest variance unexplained
- $[\boldsymbol{\mu}; \hat{\mathbf{r}}_g]$ and $[\boldsymbol{\mu}; \mathbf{Pr}]$ yield low variance unexplained with only 10 samples (compared to $N_\mathbf{u} = 274,954$)