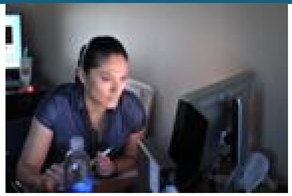
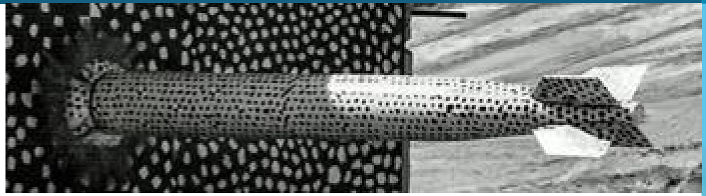
SAND2022-8261C

Sandia National Laboratories

Reduced order modeling with boosting Barlow Twins self-supervised learning for contact problem in a compressible hyperelastic material





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Why reduced order model?

Full order model (FOM) is computationally demanding.

This would take 1-2 hours[1,2].

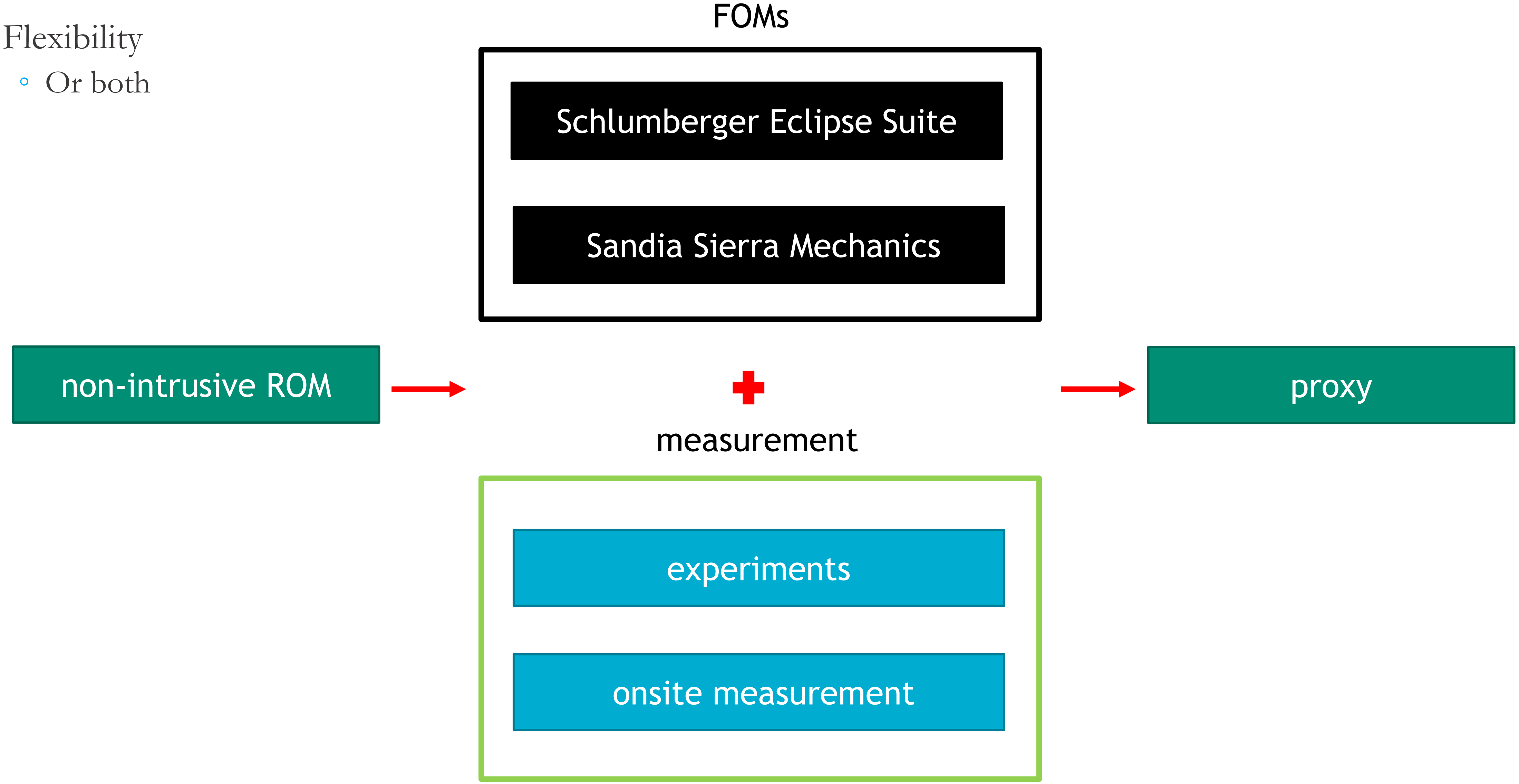
Imagine if you do 100,000 times of this type of simulation.

FOM is computationally very expensive for high fidelity simulations, uncertainty quantification, optimization, or inverse modeling

[1]Kadeethum et al. (2022, Advances in Water Resources)
[2]Kadeethum et al. (2021, Computers & Geosciences)

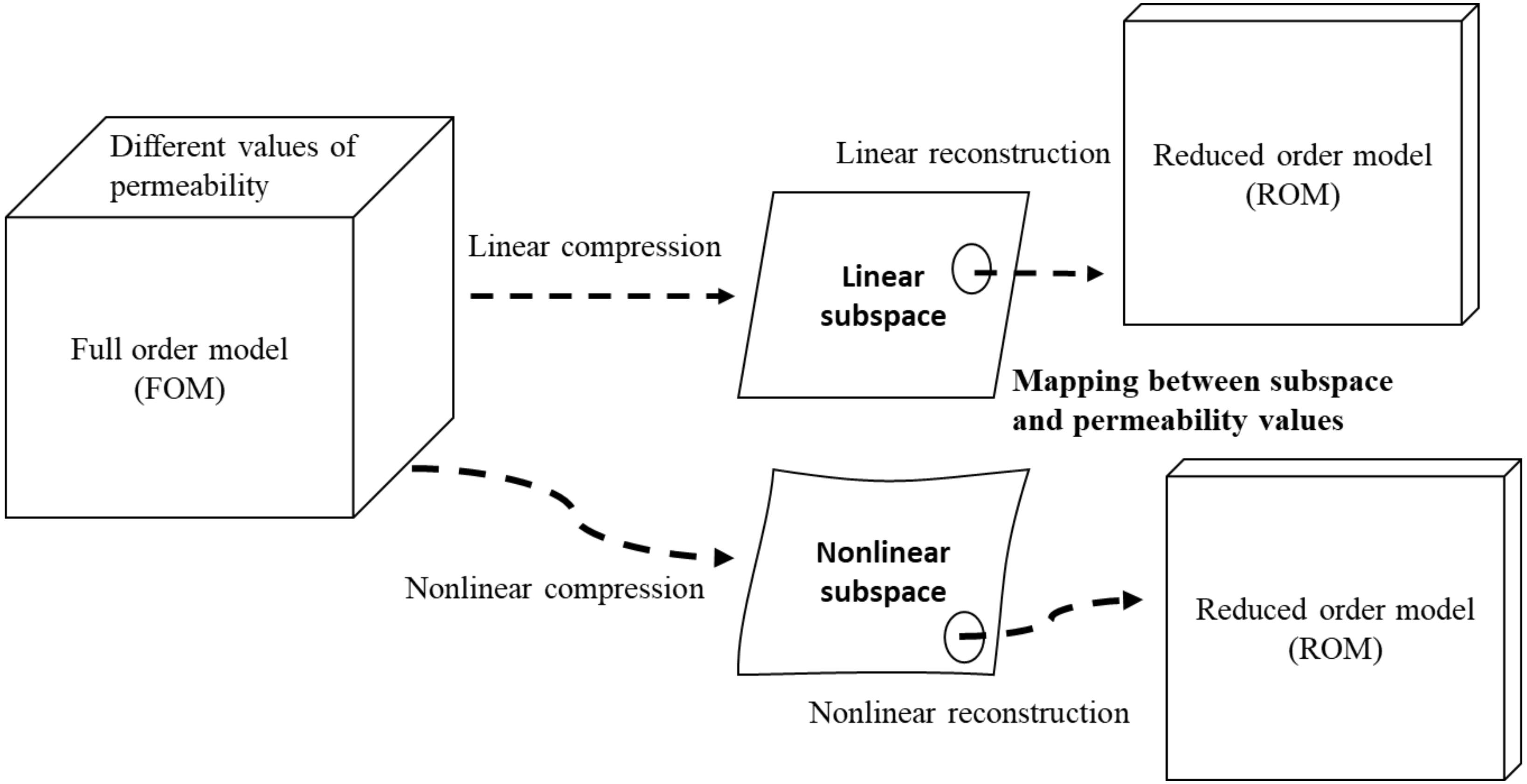
Why non-intrusive approach?

Flexibility
- Or both



Motivation

ROM typically works on ‘parameterized PDEs’ and ‘reduced subspace’

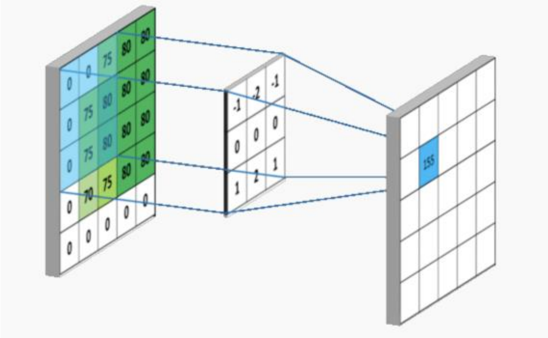


Motivation - continued

1. A unified framework suitable for problems that lie within both **linear** and **nonlinear** manifolds

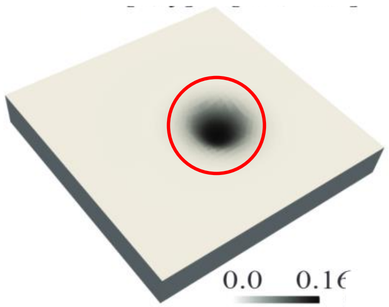
(proper orthogonal decomposition (POD) yields optimal data compression for linear manifolds) [1]

2. A framework that does not rely on 'convolutional layers,' which makes our framework applicable to both **structured** and **unstructured** meshes [1, 2]



[3]

3. Applying machine learning techniques for the physics-based problems with point source (or Dirac delta distribution) such as contact problems or subsurface flow with wells ➔ how to deal with imbalanced training data?



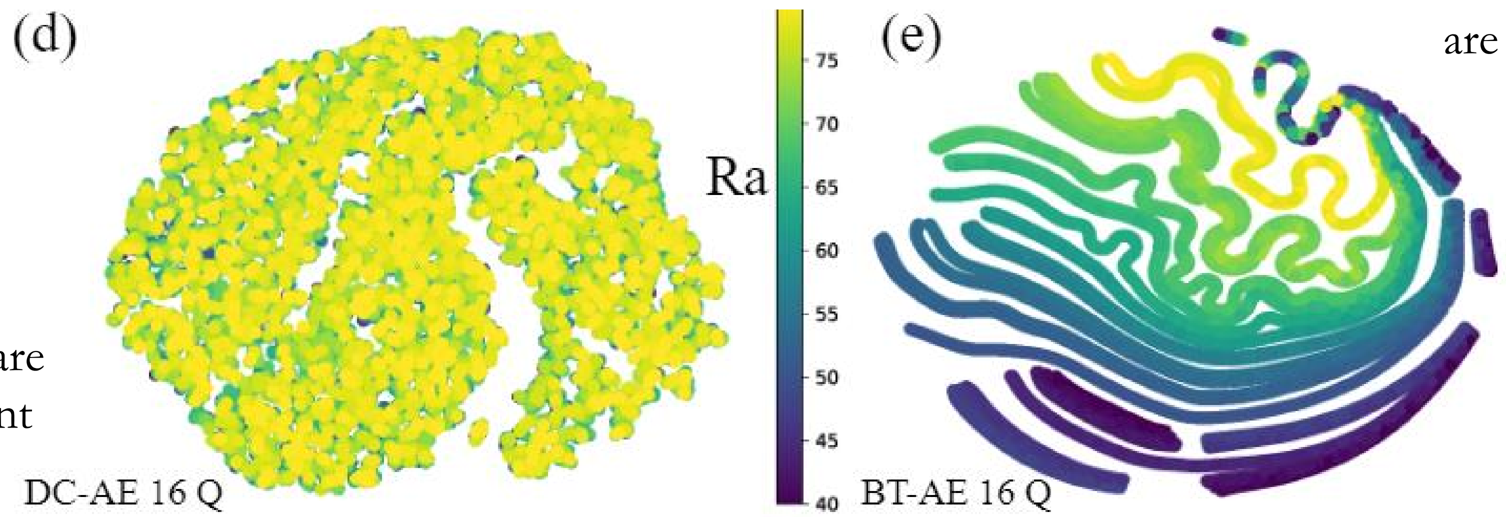
[1]Kadeethum et al. (2022, Advances in Water Resources)
[2]Kadeethum et al. (2021, Nature Computational Science)
[3]https://towardsdatascience.com/simple-introduction-to-convolutional-neural-networks-cdf8d3077bac

Idea

1.A key to develop a good ROM is to produce **better reduced manifolds** [1].

2. We apply Barlow Twins (BT) self-supervised learning [1,2], where BT maximizes the information content of the embedding with the latent space through a **joint embedding architecture**

The nonlinear manifolds are well structure



The nonlinear manifolds are not well structured in latent space

[1]Kadeethum et al. (2022, Scientific Report , accepted)
[2]Zbontar et al. (2021, arXiv:2103.03230)

Idea - continued

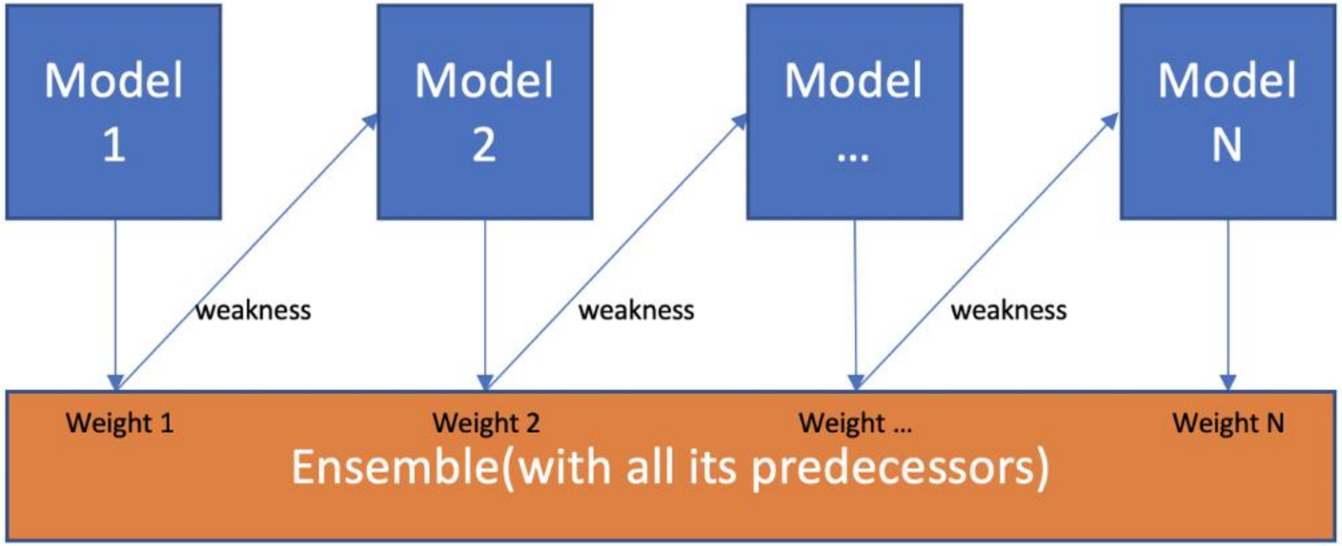
3. We apply a boosting concept for our previous BT-ROM [1]

4. Each model (in general sense) is trained **sequentially** using **subsample** from the training set with **weights**

6. The weights are calculated based on the current model's performance (i.e., **more error more weights**)

5. This way, the $\mathbf{model}^{n+1}$ is forced to learn the samples that $\mathbf{model}^{n}$ fails to mimic

[2]



[1] Kadeethum et al. (2022, Scientific Report, accepted)
[2] https://towardsdatascience.com/boosting-algorithms-explained-d38f56ef3f30

Methodology

1. Initialization

Training set: $\boldsymbol{\mu} = \left[\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \cdots, \boldsymbol{\mu}^{(M-1)}, \boldsymbol{\mu}^{(M)}\right]$

Validation set: $\boldsymbol{\mu}_{\text{validation}}$ = randomly select 5% of MN^t

Testing set: $\boldsymbol{\mu}_{\text{test}} = \left[\boldsymbol{\mu}^{(1)}_{\text{test}}, \boldsymbol{\mu}^{(2)}_{\text{test}}, \cdots, \boldsymbol{\mu}^{(M_{\text{test}}-1)}_{\text{test}}, \boldsymbol{\mu}^{(M_{\text{test}})}_{\text{test}}\right]$

We first initialize training, validation, and testing sets.

These parameters could be material properties, boundary conditions, or parameterized geometry representation.

Methodology

1. Initialization

Training set: $\boldsymbol{\mu} = [\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \cdots, \boldsymbol{\mu}^{(M-1)}, \boldsymbol{\mu}^{(M)}]$

Validation set: $\boldsymbol{\mu}_{\text{validation}} =$ randomly select 5% of MN^t

Testing set: $\boldsymbol{\mu}_{\text{test}} = [\boldsymbol{\mu}_{\text{test}}^{(1)}, \boldsymbol{\mu}_{\text{test}}^{(2)}, \cdots, \boldsymbol{\mu}_{\text{test}}^{(M_{\text{test}}-1)}, \boldsymbol{\mu}_{\text{test}}^{(M_{\text{test}})}]$

2. Full order model (FOM)

FOM = $\boldsymbol{X}_h(\boldsymbol{\mu}^{(1)}), \ldots, \boldsymbol{X}_h(\boldsymbol{\mu}^{(M)})$

Same goes for $\boldsymbol{\mu}_{\text{v}}, \boldsymbol{\mu}_{\text{t}}$

We then build the training set through by querying full order model for each parameter.

*This is the major cost of building data-driven model.

Methodology

Data compression: training BBT-AE model

The machine learning model has one encoder, decoder, and projector.

The main goal is to maximizes the information content of the embedding with the latent space through a joint embedding architecture.

Resulting in a **better reduced manifolds**

<u>If we have 1 encoder, our model is BT-ROM</u>
<u>If we have more than 1 encoders, our model is BBT-ROM</u>

<u>1. Initialization</u>

Training set: $\boldsymbol{\mu} = [\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \cdots, \boldsymbol{\mu}^{(M-1)}, \boldsymbol{\mu}^{(M)}]$

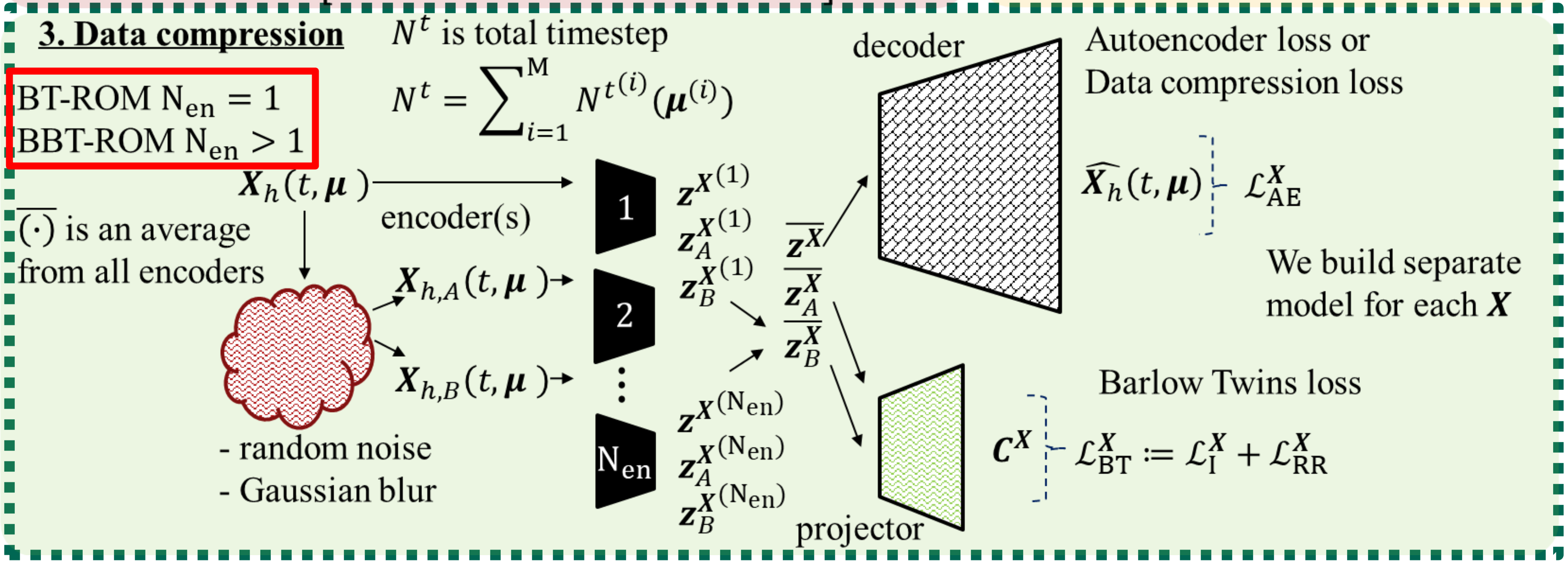
Validation set: $\boldsymbol{\mu}_{\text{validation}}$ = randomly select 5% of MN^t

Testing set: $\boldsymbol{\mu}_{\text{test}} = [\boldsymbol{\mu}^{(1)}_{\text{test}}, \boldsymbol{\mu}^{(2)}_{\text{test}}, \cdots, \boldsymbol{\mu}^{(M_{\text{test}}-1)}_{\text{test}}, \boldsymbol{\mu}^{(M_{\text{test}})}_{\text{test}}]$

<u>2. Full order model (FOM)</u>

FOM = $\boldsymbol{X}_h(\boldsymbol{\mu}^{(1)}), \ldots, \boldsymbol{X}_h(\boldsymbol{\mu}^{(M)})$

Same goes for $\boldsymbol{\mu}_{\text{v}}, \boldsymbol{\mu}_{\text{t}}$



Methodology

We then map our parameters to reduced manifolds using ANN.

*We note that we could use other regressors such as GP or RBF.

1. Initialization

Training set: $\boldsymbol{\mu} = [\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \cdots, \boldsymbol{\mu}^{(M-1)}, \boldsymbol{\mu}^{(M)}]$

Validation set: $\boldsymbol{\mu}_{\text{validation}}$ = randomly select 5% of MN^t

Testing set: $\boldsymbol{\mu}_{\text{test}} = [\boldsymbol{\mu}_{\text{test}}^{(1)}, \boldsymbol{\mu}_{\text{test}}^{(2)}, \cdots, \boldsymbol{\mu}_{\text{test}}^{(M_{\text{test}}-1)}, \boldsymbol{\mu}_{\text{test}}^{(M_{\text{test}})}]$

2. Full order model (FOM)

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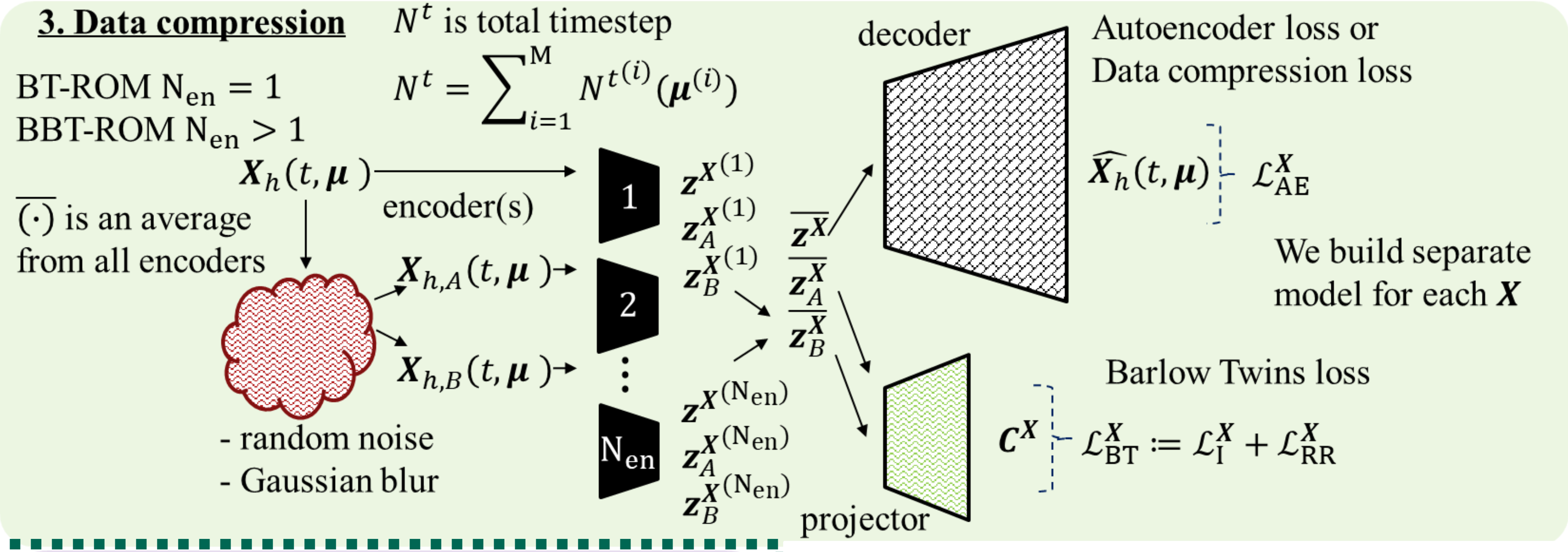
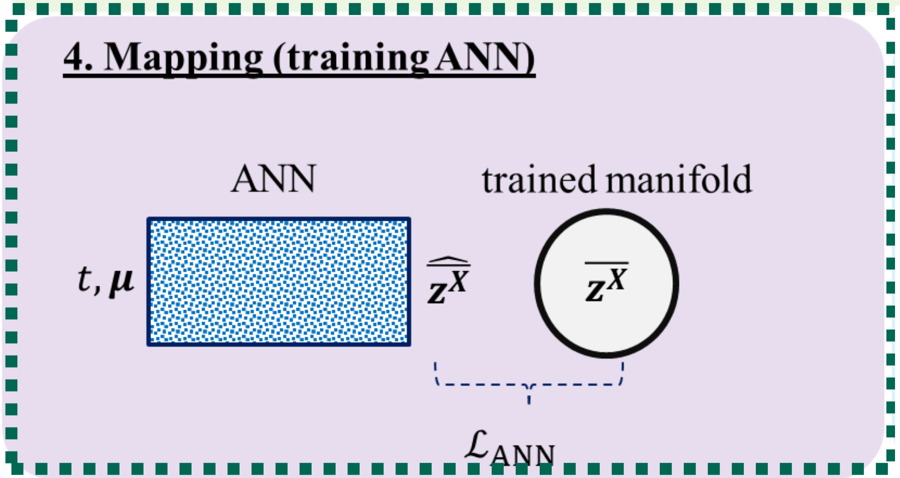
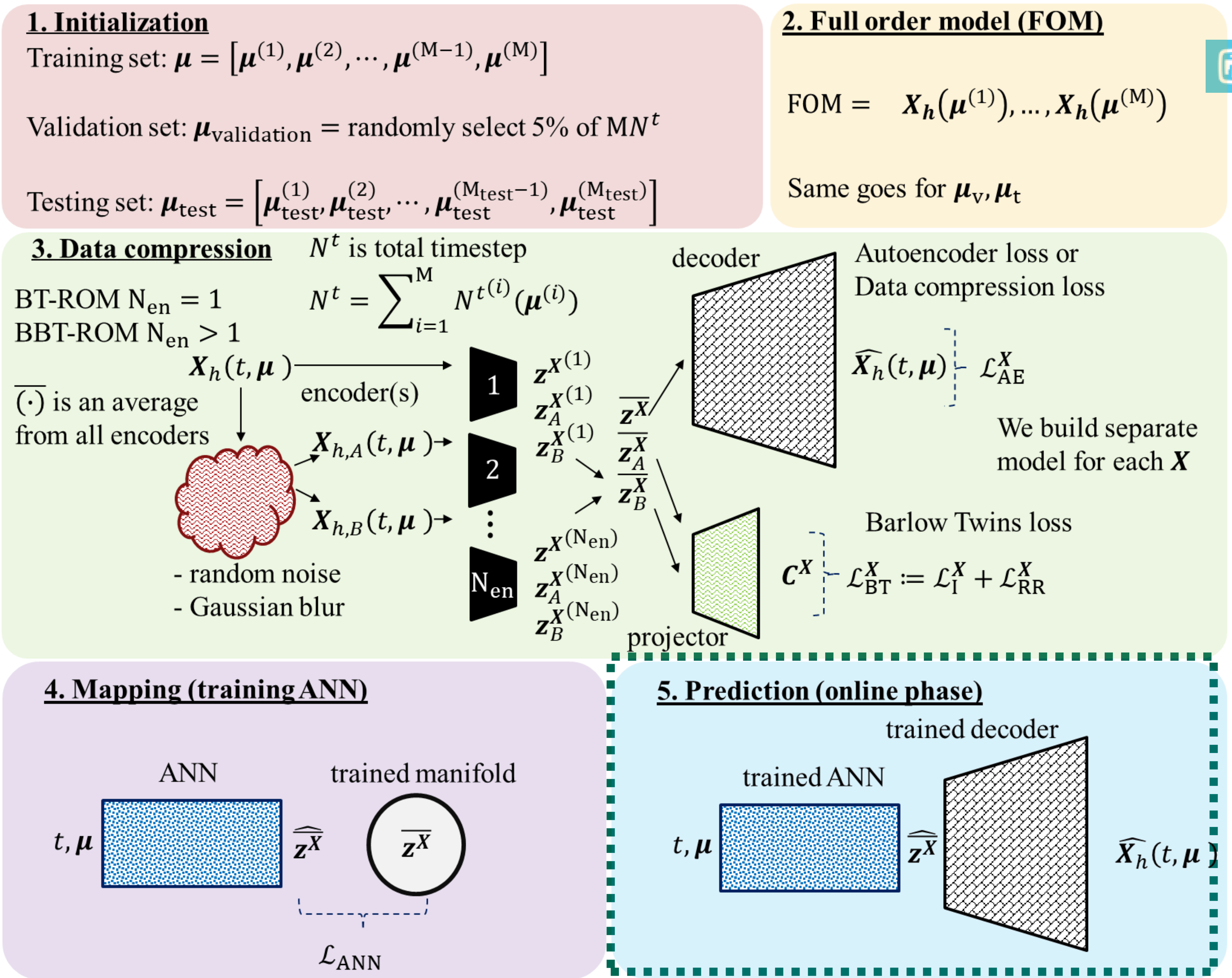




Methodology

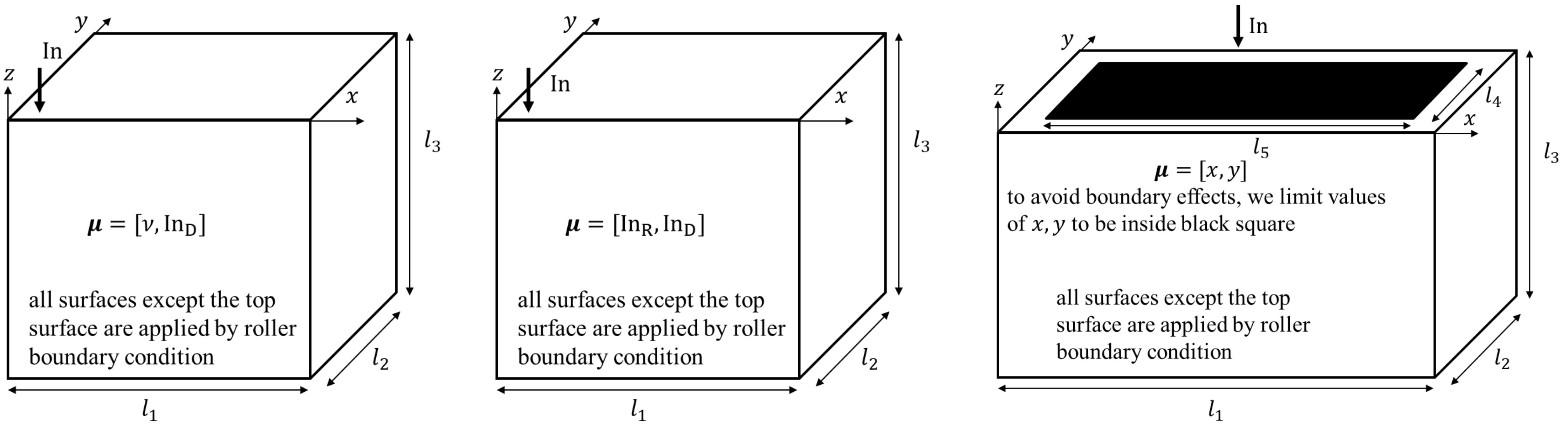
During the online or prediction phase, we approximate our quantities of interest through the **trained ANN** and **trained decoder**.



Physical problems that we test

- **Contact** between a **rigid** indenter and a **hyperelastic** substrate at **finite deformations**
- Goal: To improve ML training with **imbalanced** training data (i.e., only one point of contact)
- A **small area where the deformation occurs** while **most of the domain remains are undeformed**.
- Weak form of contact physics

$$\mathrm{k_{pen}} \int_{\partial\Omega_c} \langle -g_N \rangle \delta u_N \, dS + \int_{\Omega_0} \mathbf{P} : \nabla(\boldsymbol{\delta}\mathbf{u}) \, dV - \int_{\Omega_0} \mathbf{B} \cdot \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\partial\Omega_N} \mathbf{T} \cdot \boldsymbol{\delta}\mathbf{u} \, dS = 0$$



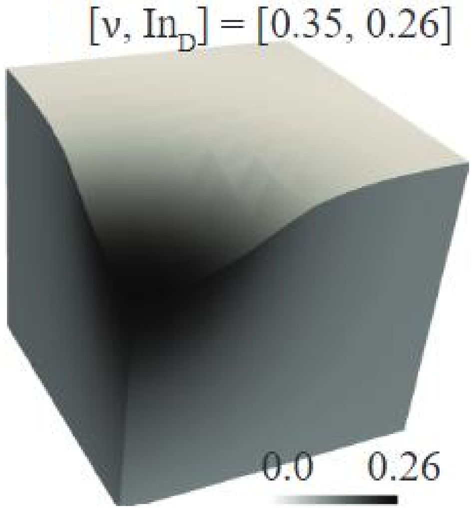
Results – Poisson's ratio and indentation depth as parameters

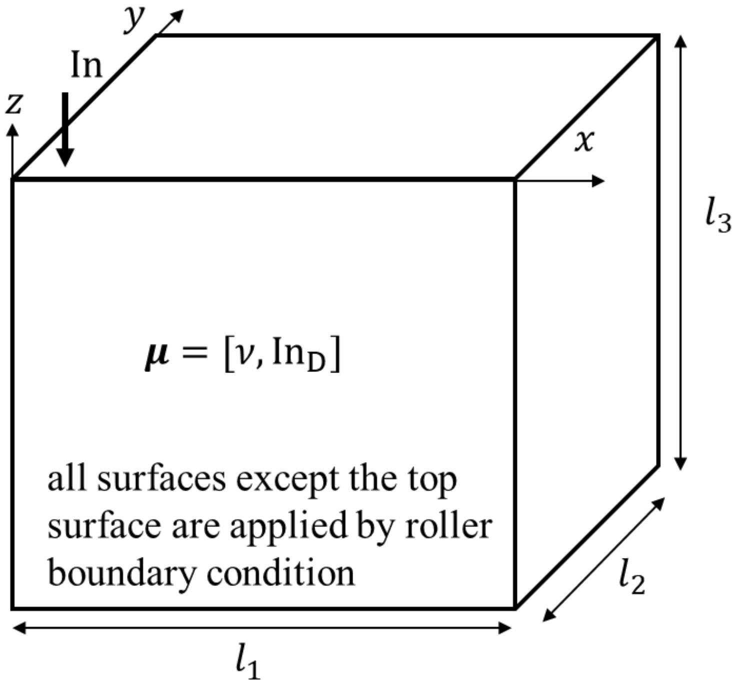
1. It is symmetric; so, we only model a quarter of the full domain (the contact point is in the middle of the material)

Parameters
Poisson's ratio = $[0.1, 0.4]$
indentation depth = $[0.1, 0.3]$

Training: 1600
Validation: 80 (5% of training set)
Testing: 100

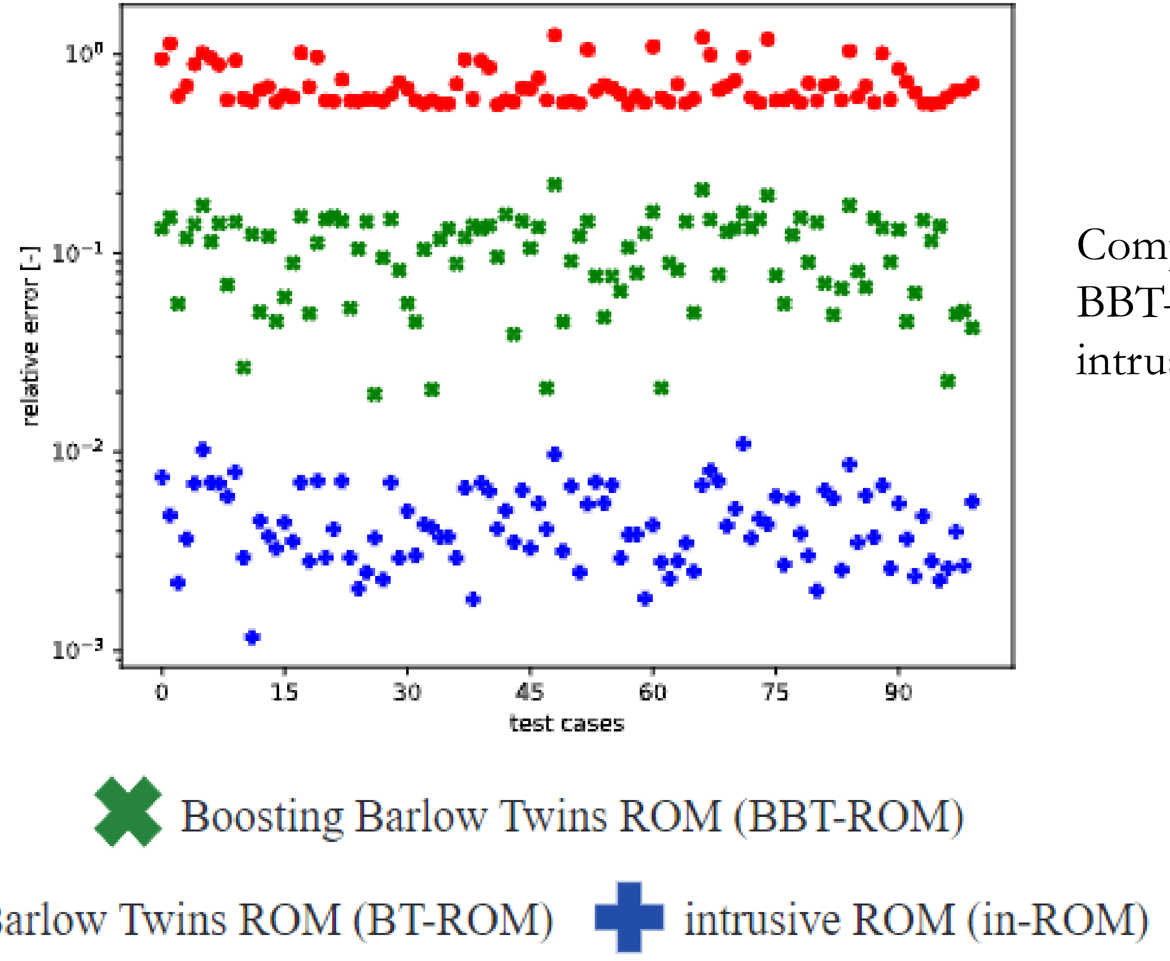
DOFs: 3993





Results – Poisson's ratio and indentation depth as parameters

1. We show here relative error results (compared to full order model)
2. We observe that the proposed model (BBT-ROM) has a better accuracy than our previous model (BT-ROM), but worse than intrusive-ROM.



Computational time:
BBT-ROM = **0.001** s
intrusive-ROM = **8.0** s

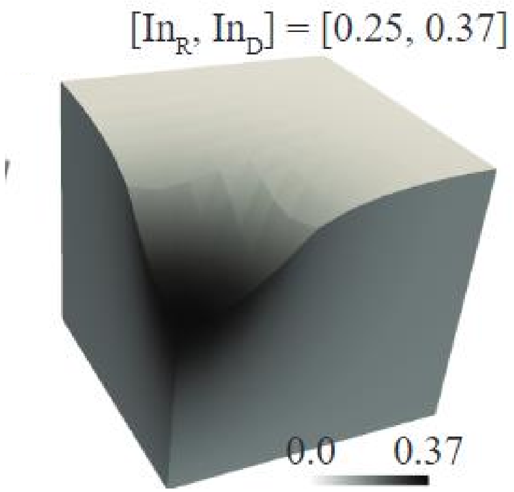
Results – indentation radius and depth as parameters

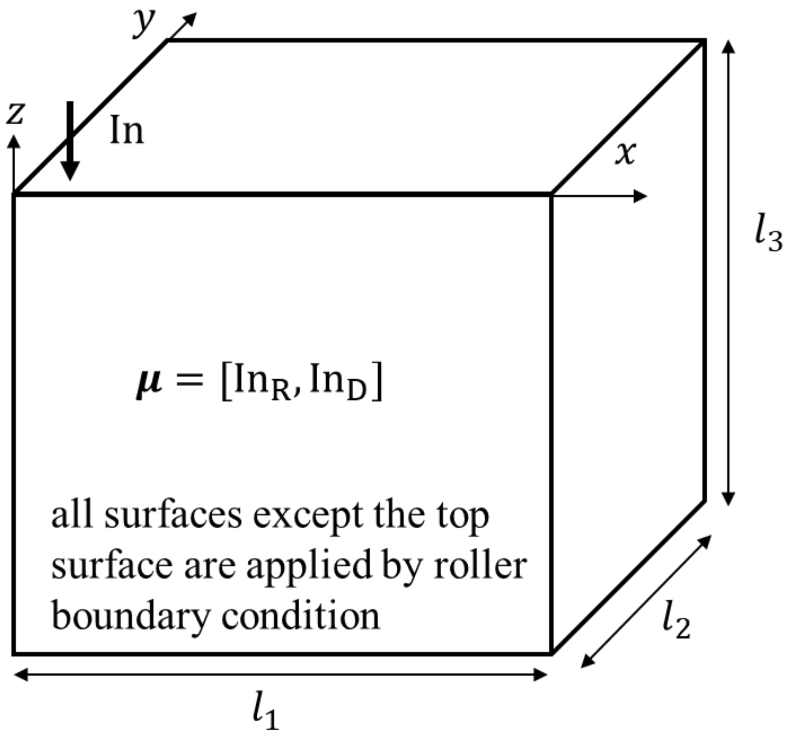
1. It is symmetric; so, we only model a quarter of the full domain (the contact point is in the middle of the material) (the same as in the first problem)

Parameters
indentation radius $= [0.15, 0.4]$
indentation depth $= [0.1, 0.4]$

Training: 1600
Validation: 80 (5% of training set)
Testing: 100

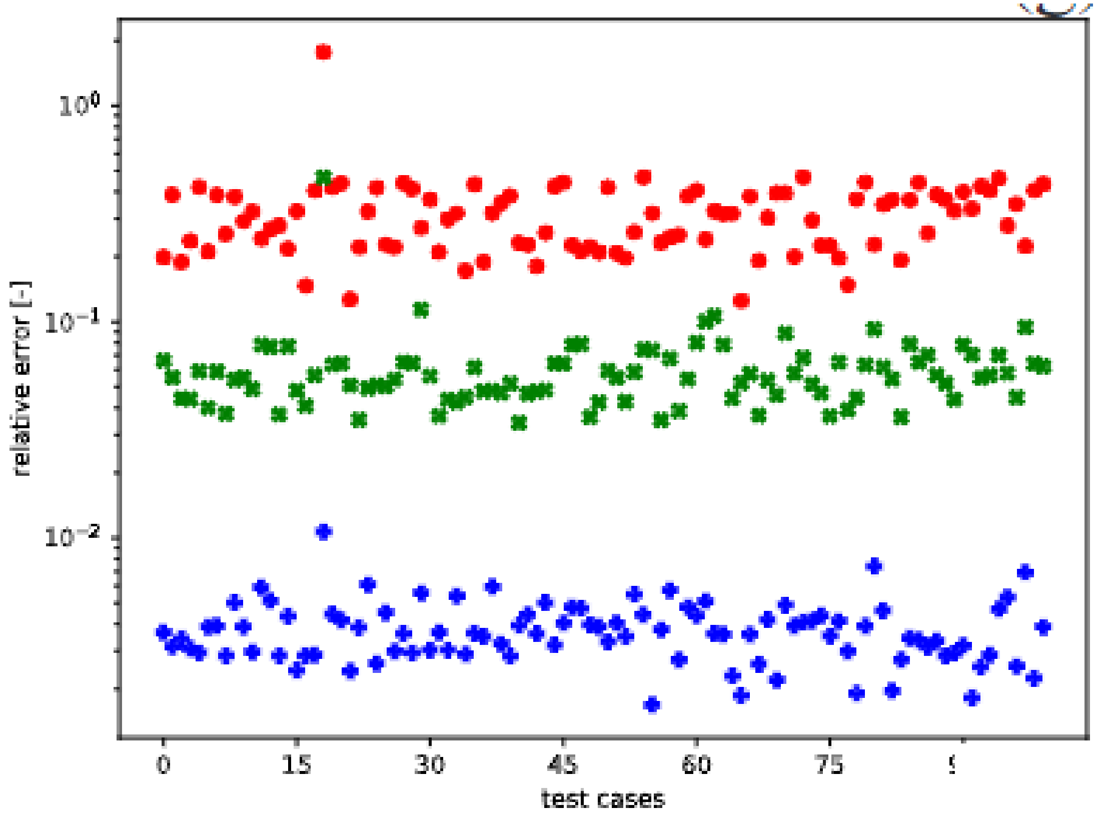
DOFs: 3993





Results – indentation radius and depth as parameters

1. We show here a relative error results (relative to full order model) – we observe that the proposed model (BBT-ROM) has a better accuracy than our previous model (BT-ROM), but worse than in-ROM.



Computational time:
BBT-ROM = **0.001** s
intrusive-ROM = **8.0** s

Boosting Barlow Twins ROM (BBT-ROM)

Barlow Twins ROM (BT-ROM) intrusive ROM (in-ROM)

Results – indentation locations as parameters

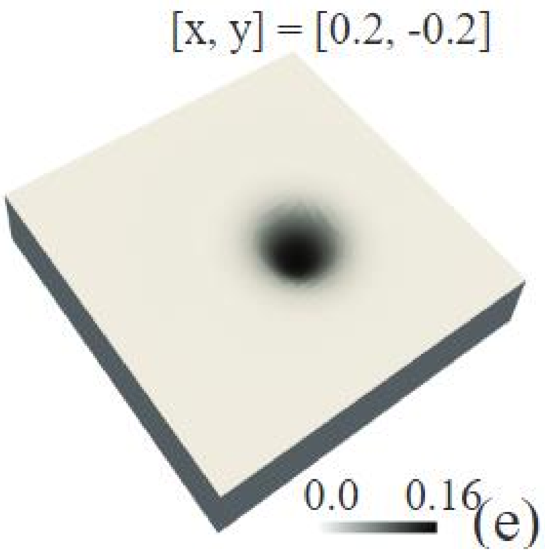
1. We model the whole domain and contact location could occur within the black square

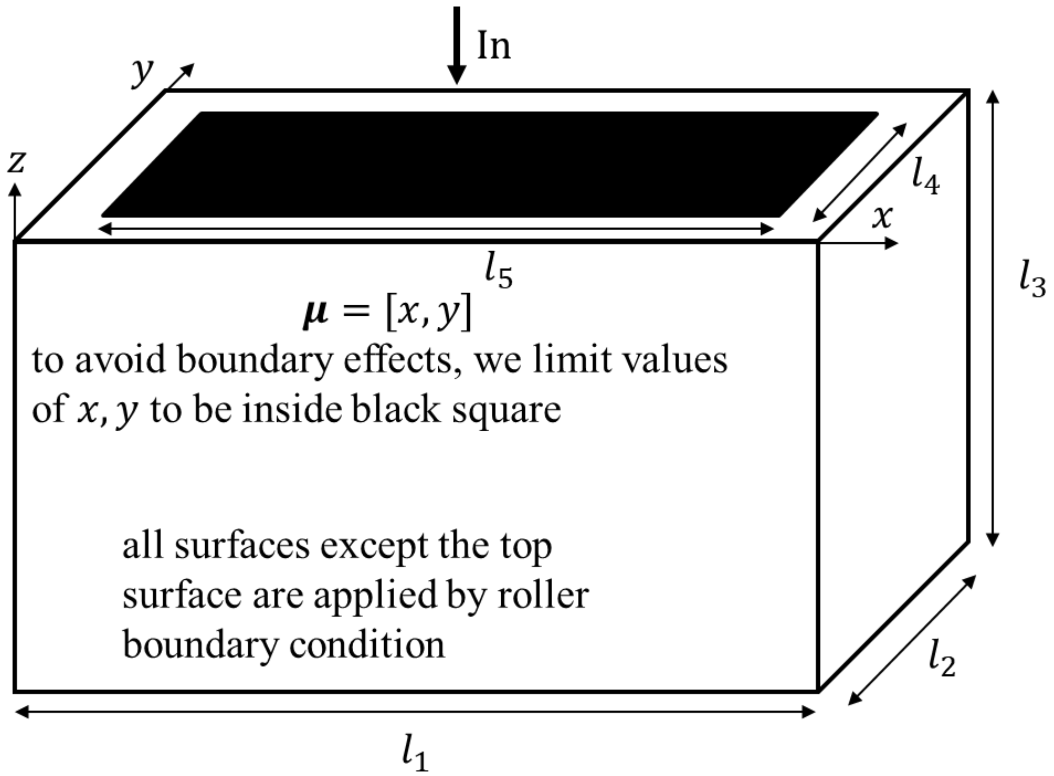
2. The indentation depth and radius are fixed

Parameters
x-coordinate = $[-0.3, 0.3]$
y-coordinate = $[-0.3\ 0.3]$

Training: 1600
Validation: 80 (5% of training set)
Testing: 100

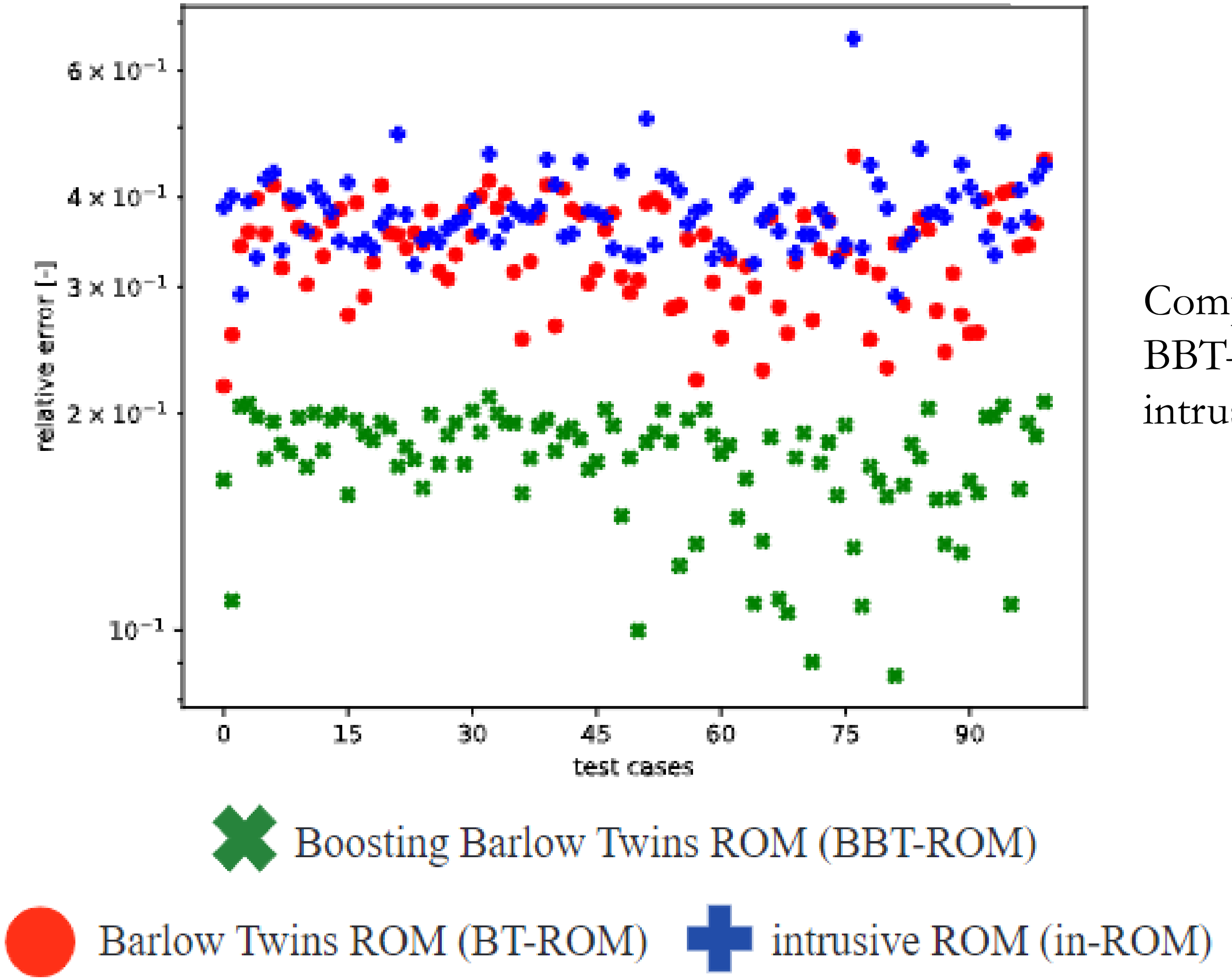
DOFs: 70602





Results – indentation locations as parameters

1. We show here a relative error results (relative to full order model) – we observe that the proposed model (BBT-ROM) has a **best** accuracy than our previous model (BT-ROM) and in-ROM.



Computational time:
BBT-ROM = **0.001** s
intrusive-ROM = ~**20.0** s

Conclusions

1. A ROM framework that works in an optimal way for both **linear** and **nonlinear** manifolds

2. A ROM framework that can be applied for both **structured** and **unstructured** meshes

3. A ROM framework that can handle **data imbalanced** problems

4. An uncertainty-aware BT-ROM is in progress to achieve uncertainty quantification (Neural IPS 2022, in review)

Physical problems that we test - continued

$$k_{pen}\int_{\partial\Omega_c}\langle -g_N\rangle \delta u_N\, dS + \int_{\Omega_0} \mathbf{P} : \nabla(\boldsymbol{\delta}\mathbf{u})\, dV - \int_{\Omega_0} \mathbf{B}\cdot\boldsymbol{\delta}\mathbf{u}\, dV - \int_{\partial\Omega_N} \mathbf{T}\cdot\boldsymbol{\delta}\mathbf{u}\, dS = 0$$

weak form

$$\begin{aligned} \nabla_X \cdot \mathbf{P} + \mathbf{B} &= 0 \quad \text{in } \Omega_0 \\ \mathbf{u} &= \bar{\mathbf{u}} \quad \text{on } \partial\Omega_D \\ \mathbf{P}\cdot\mathbf{N} &= \bar{\mathbf{T}} \quad \text{on } \partial\Omega_N \end{aligned}$$

$$\mathrm{In}(x,y) = -\mathrm{In}_D + \frac{1}{2\mathrm{In}_R}(x^2+y^2) \quad \text{about origin}$$

We approximate the contact profile with a parabolic function

We use PETSc SNES as a nonlinear solver and MUMPS as a linear solver with absolute and relative tolerances of 1×10^{-6} and 1×10^{-16}, respectively. We utilize a backtracking line search with slope descent parameter of 1×10^{-4}, initial step length of 1.0, and quadratic order of the approximation.

'Numerical Tours of Computational Mechanics with FEniCS