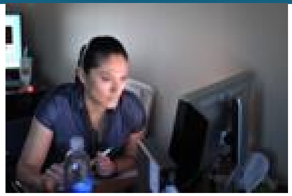
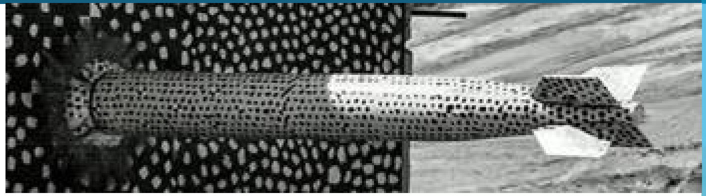
SAND2022-6837C

Sandia National Laboratories

Reduced order modeling with Barlow Twins self-supervised learning: Navigating the space between linear and nonlinear solution manifolds





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Interpore 2022

This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories and also DOE Office of Fossil Energy project -Science-informed Machine Learning to Accelerate Real

U.S. DEPARTMENT OF ENERGY NNSA

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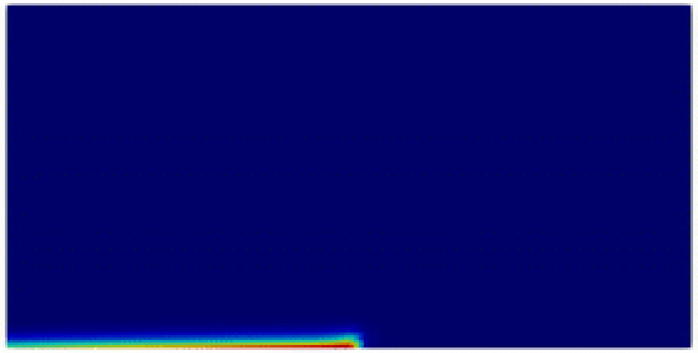
Why reduced order model?

Full order model (FOM) is computationally demanding



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

Imagine if you do 100,000 times of this

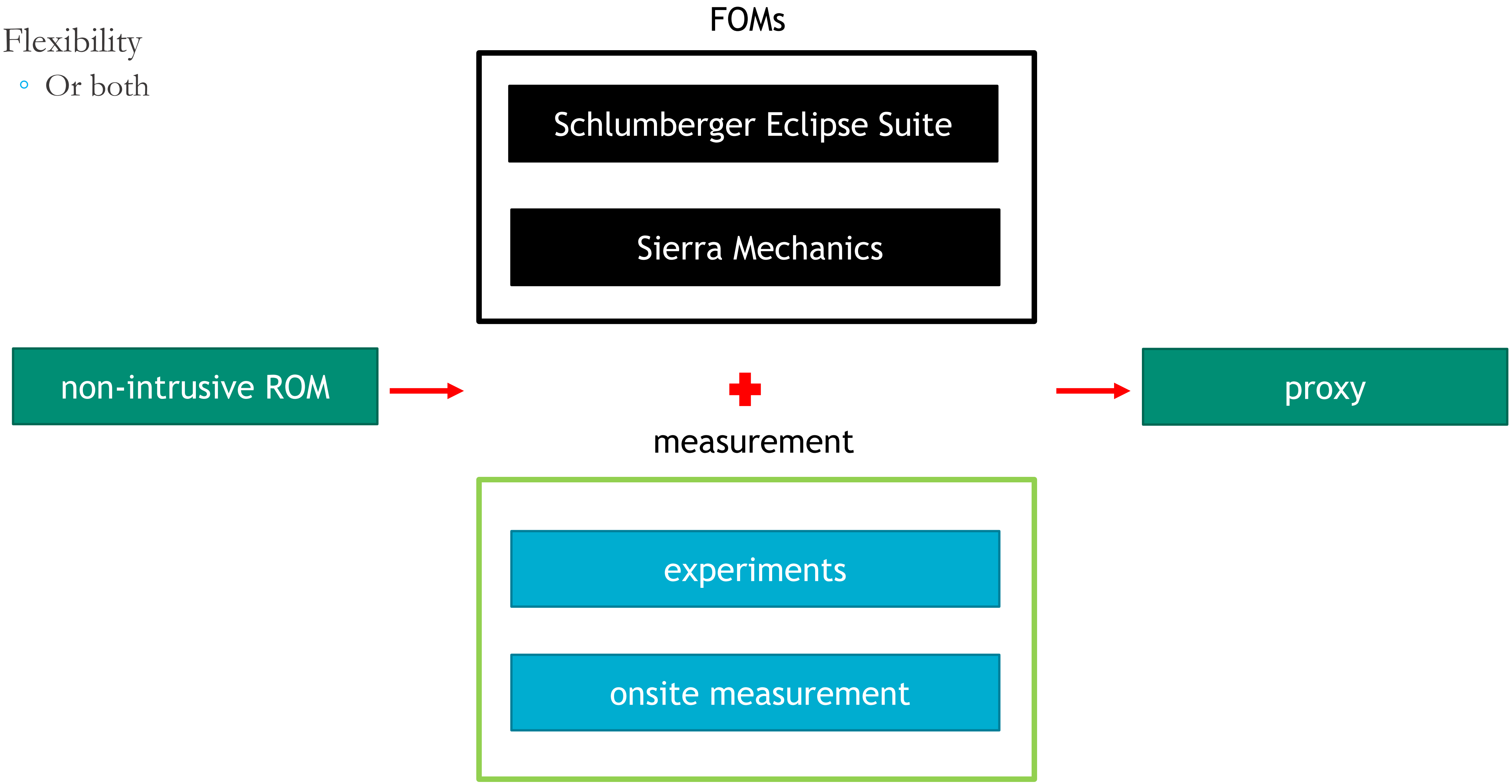
FOM is computationally very expensive for large-scale uncertainty quantification, optimization, or inverse modeling

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

Why non-intrusive approach?

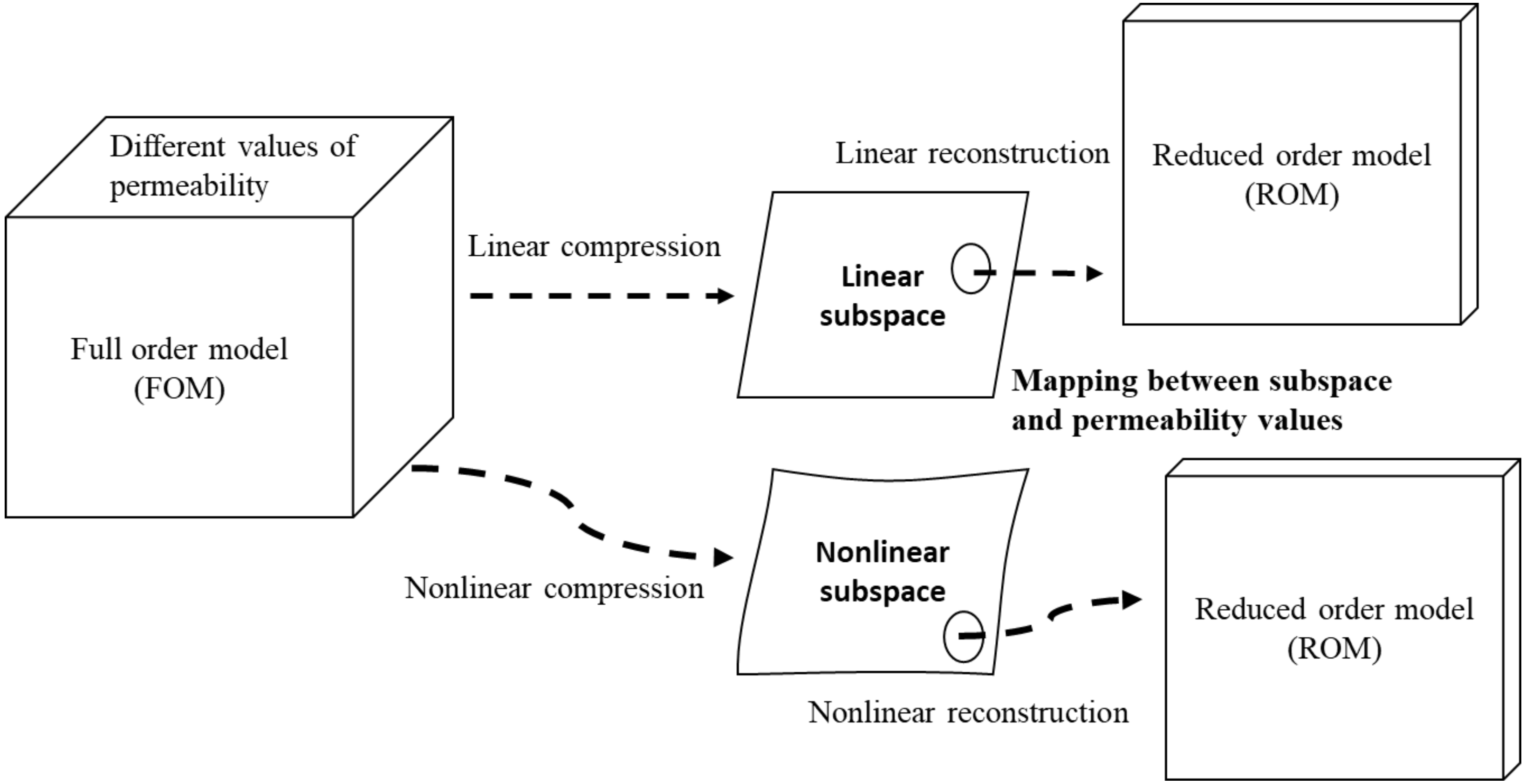
Flexibility

- Or both



Motivation

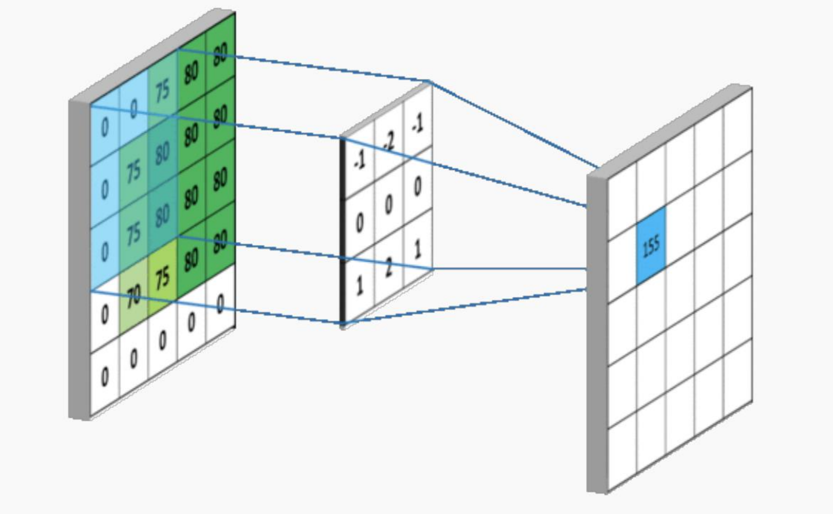
ROM typically works on ‘parameterized PDEs’ and ‘reduced subspace’



Motivation - continue

1. Unified framework that works well for both problems that lie within **linear** and **nonlinear** manifolds (proper orthogonal decomposition (pod) yields optimal data compression for linear manifolds) [1]

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



[3]

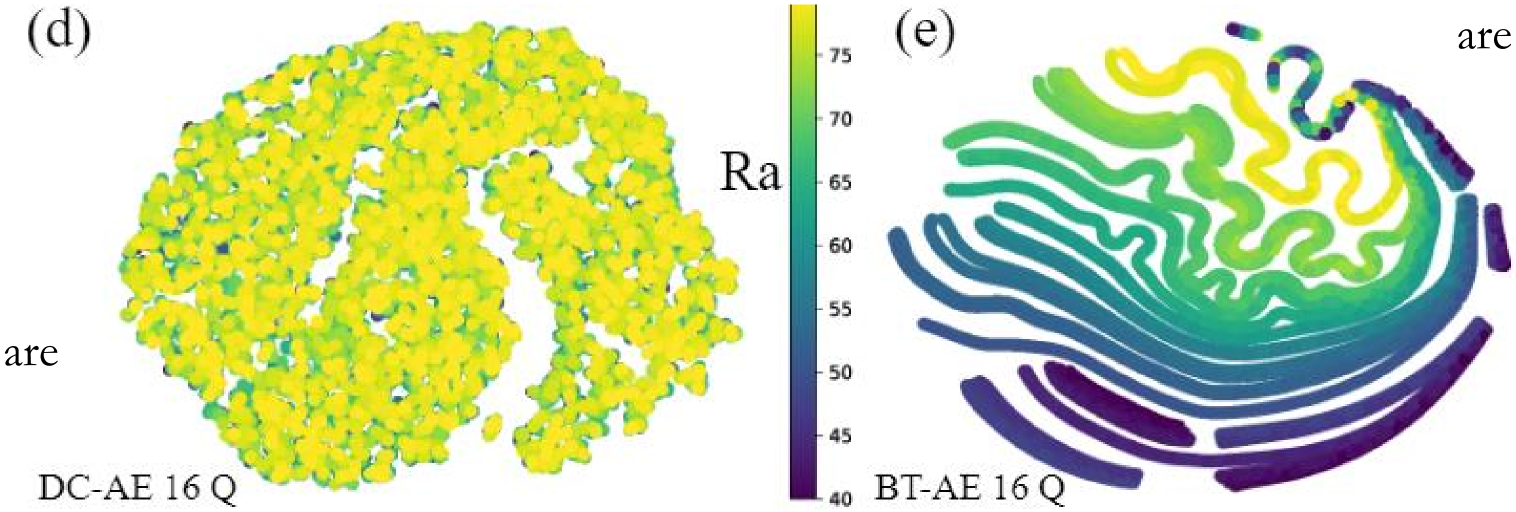
[1]Kadeethum et al. (2022, Advances in Water Resources)
[2]Kadeethum et al. (2021, Nature Computational Science)
[3]https://towardsdatascience.com/simple-introduction-to-convolutional-neural-networks-cdf8d3077bac

Motivation - continue

1. We believe the key to develop a good ROM is to produce **better reduced manifolds**.

2. We extend Barlow Twins (BT) self-supervised learning [1], 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 really well structure

[1]Zbontar et al. (2021, arXiv:2103.03230)

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 10% of MN^t

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

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

Validation set: $\boldsymbol{\mu}_{\mathrm{validation}}$ = randomly select 10% of MN^t

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

2. Full order model (FOM)

$$\mathrm{FOM} = \begin{matrix} \boldsymbol{u}_h(\boldsymbol{\mu}^{(1)}), p_h(\boldsymbol{\mu}^{(1)}), T_h(\boldsymbol{\mu}^{(1)}) \\ \vdots \\ \boldsymbol{u}_h(\boldsymbol{\mu}^{(\mathrm{M})}), p_h(\boldsymbol{\mu}^{(\mathrm{M})}), T_h(\boldsymbol{\mu}^{(\mathrm{M})}) \end{matrix}$$

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

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 BT-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**

1. Initialization

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

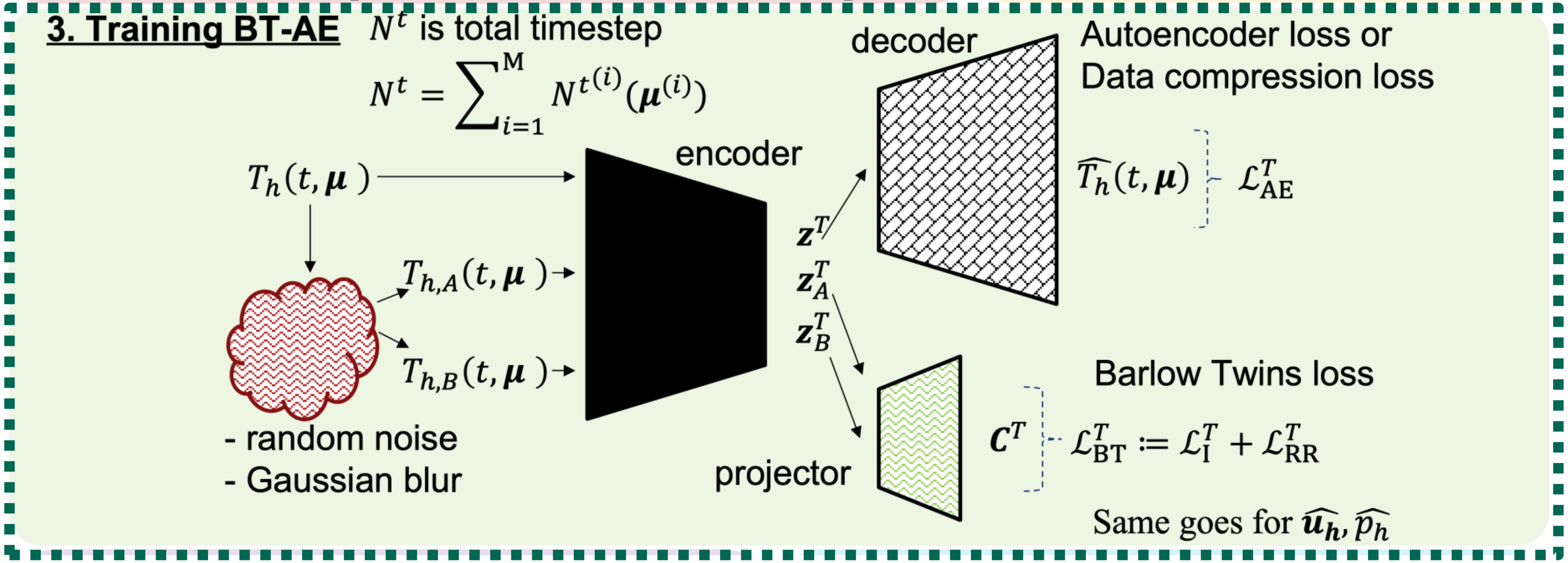
Validation set: $\boldsymbol{\mu}_{\text{validation}}$ = randomly select 10% of $\mathrm{M}N^t$

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

2. Full order model (FOM)

$$\text{FOM} = \begin{matrix} \boldsymbol{u_h}(\boldsymbol{\mu}^{(1)}), p_h(\boldsymbol{\mu}^{(1)}), T_h(\boldsymbol{\mu}^{(1)}) \\ \vdots \\ \boldsymbol{u_h}(\boldsymbol{\mu}^{(\mathrm{M})}), p_h(\boldsymbol{\mu}^{(\mathrm{M})}), T_h(\boldsymbol{\mu}^{(\mathrm{M})}) \end{matrix}$$

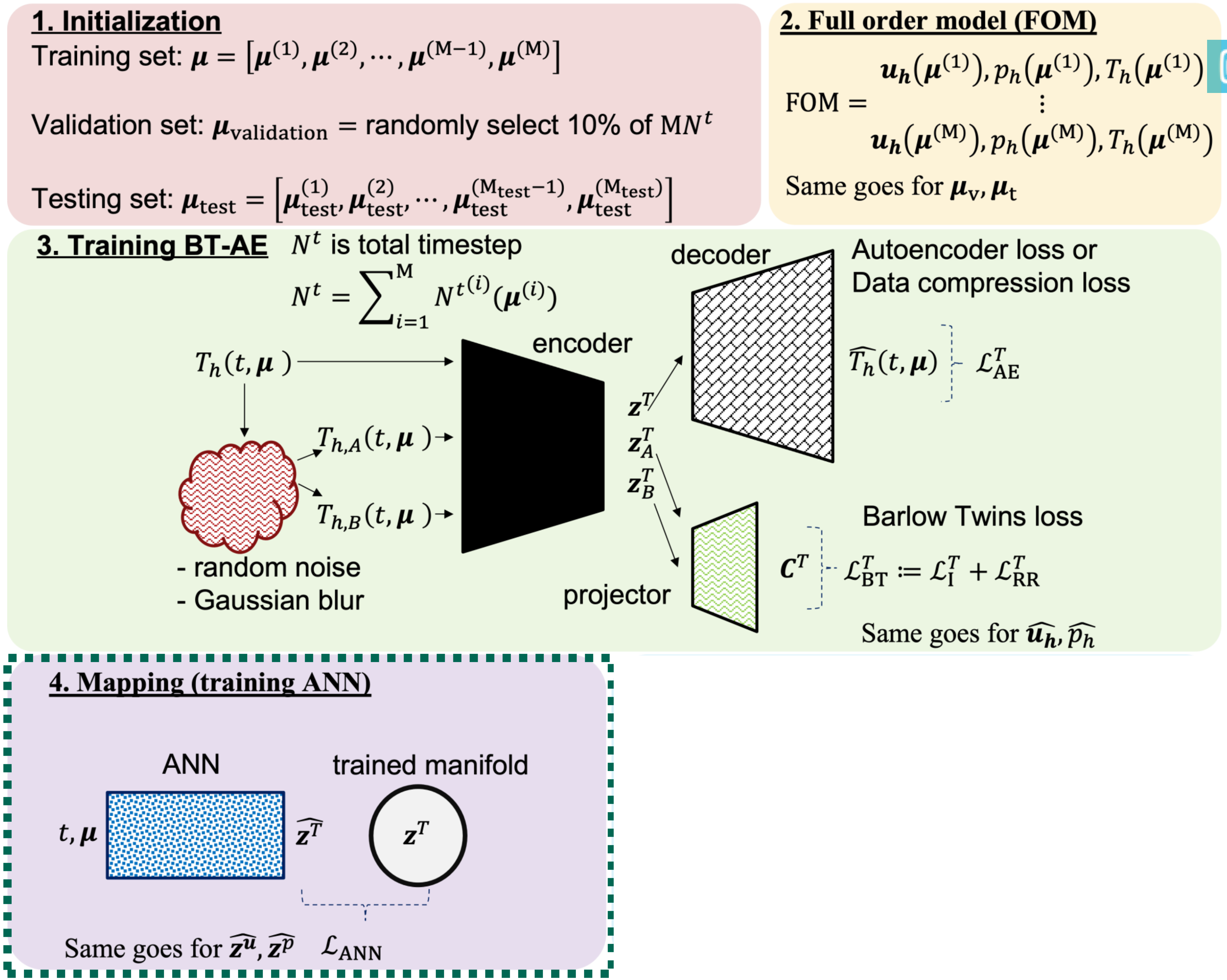
Same goes for $\boldsymbol{\mu}_{\mathrm{v}}, \boldsymbol{\mu}_{\mathrm{t}}$



Methodology

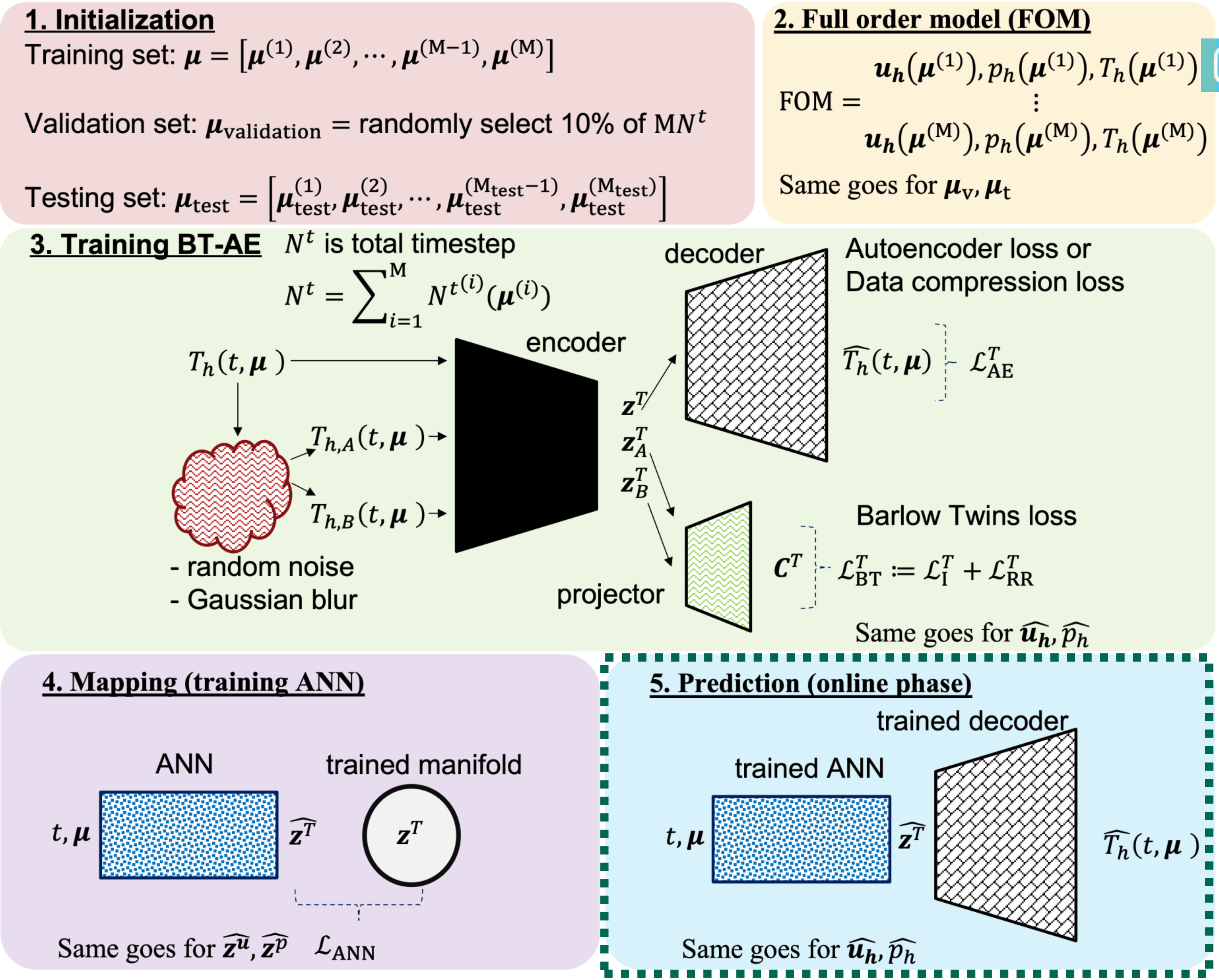
We then map our parameters to reduced manifolds using ANN.

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



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

Fluid density is a function of its concentration and temperature, impacting fluid flow behavior

Examples: geothermal energy recovery, seawater intrusion, storage of nuclear and radioactive waste, contaminant transport among others.

Depending on system Rayleigh number and the formation heterogeneity, convective mixing can greatly accelerate CO2 dissolution during geologic carbon storage.

Physical problems that we test - continue

velocity (1st Brezzi-Douglas-Marini element)

pressure (piecewise constant)

locally mass conservative

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\boldsymbol{u} + \nabla p = \mathbf{z} T \mathrm{Ra}$$

$$\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \nabla T = \nabla^2 T,$$

$$\mathrm{Ra} = \frac{g \alpha k \Delta T^* H}{\mu \kappa}$$

temperature (1st enriched Galerkin)

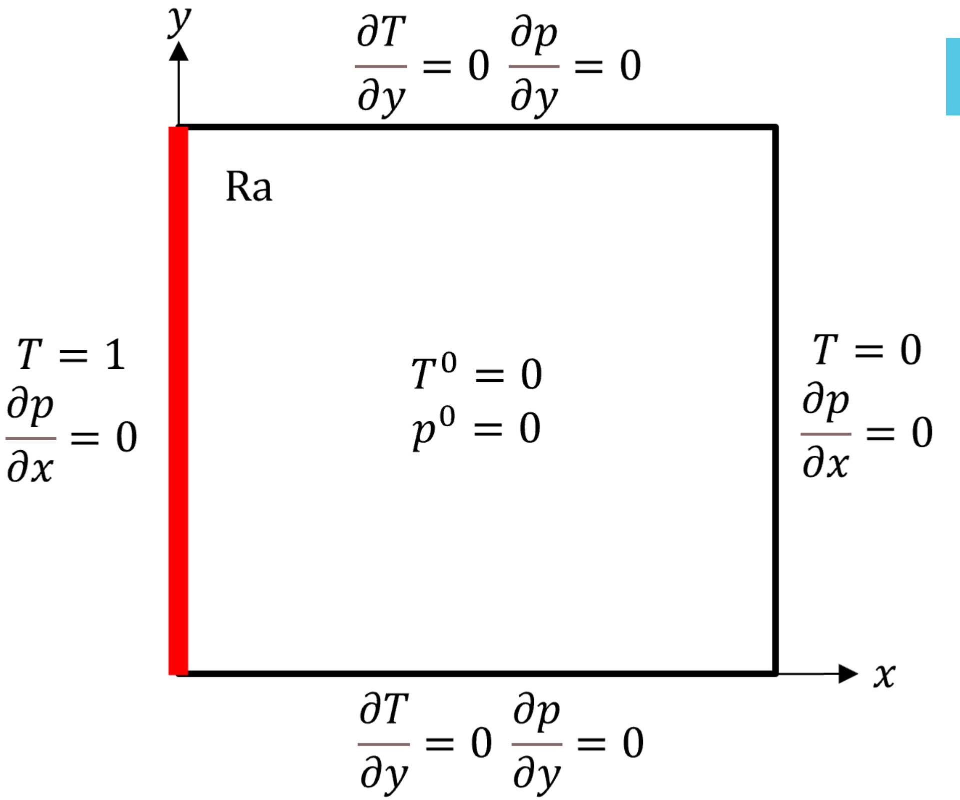
time (4th backward differentiation formula)

Kadeethum et al. (2021, Computers & Geosciences)

Results – Heated from side (HFS)

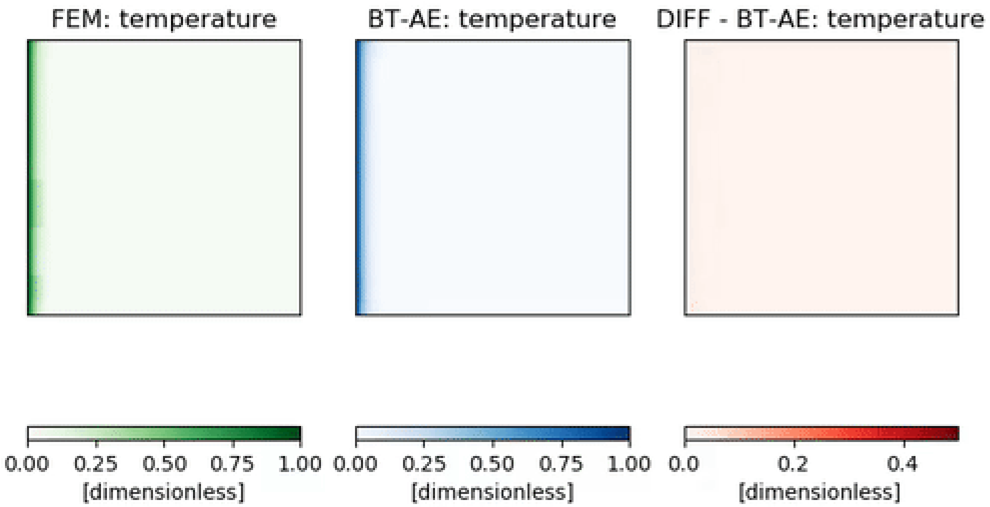
1. We test our model using heated from side problem [Zhang et al. (2016, Comput. & Geosci)]

2. The flow is driven by the change of temperature on the left side



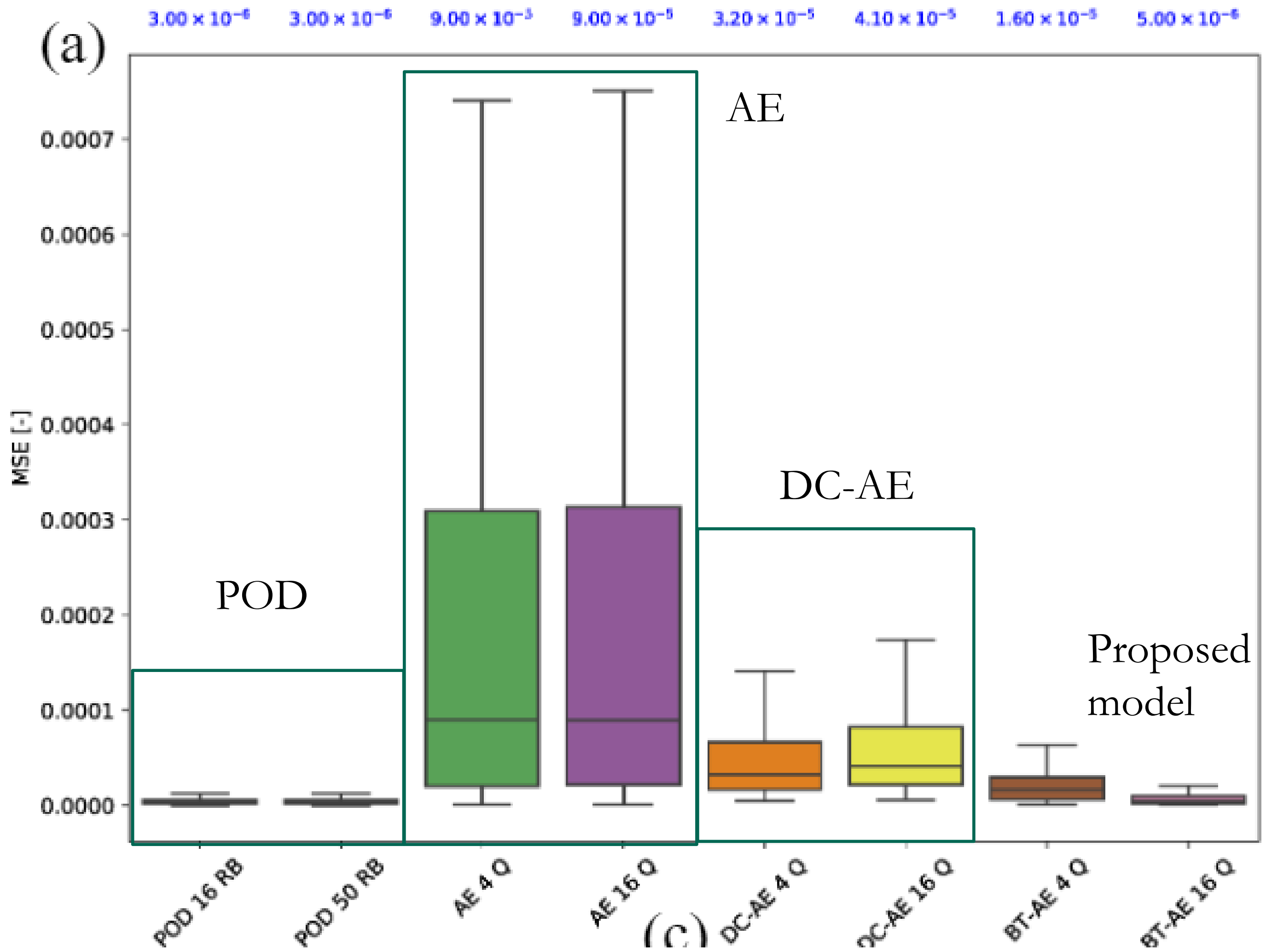
Parameters
$\mathrm{Ra}_1 = [40, 80]$

Training: 40
Testing: 10



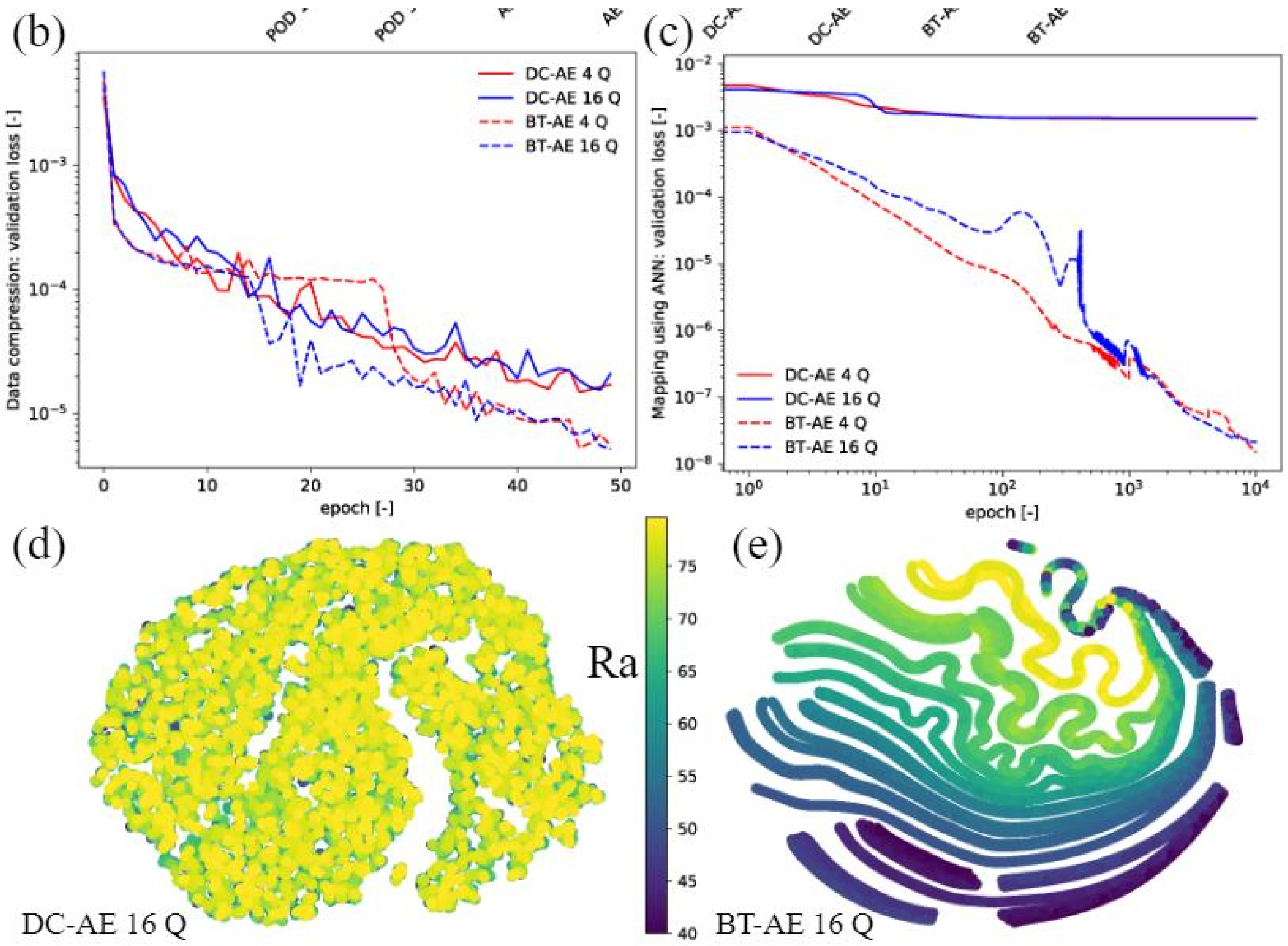
Results – HFS - continue

1. We can see that BT model provide almost similar performance as POD model, but much better than AE and deep convolutional AE (i.e., problem lies within linear manifolds)



Results – HFS - continue

1. We can see that the BT model (dashed) has a **lower data compression loss** (step 3), and it has a much **lower mapping loss** (step 4)



The nonlinear manifolds are not really well structure

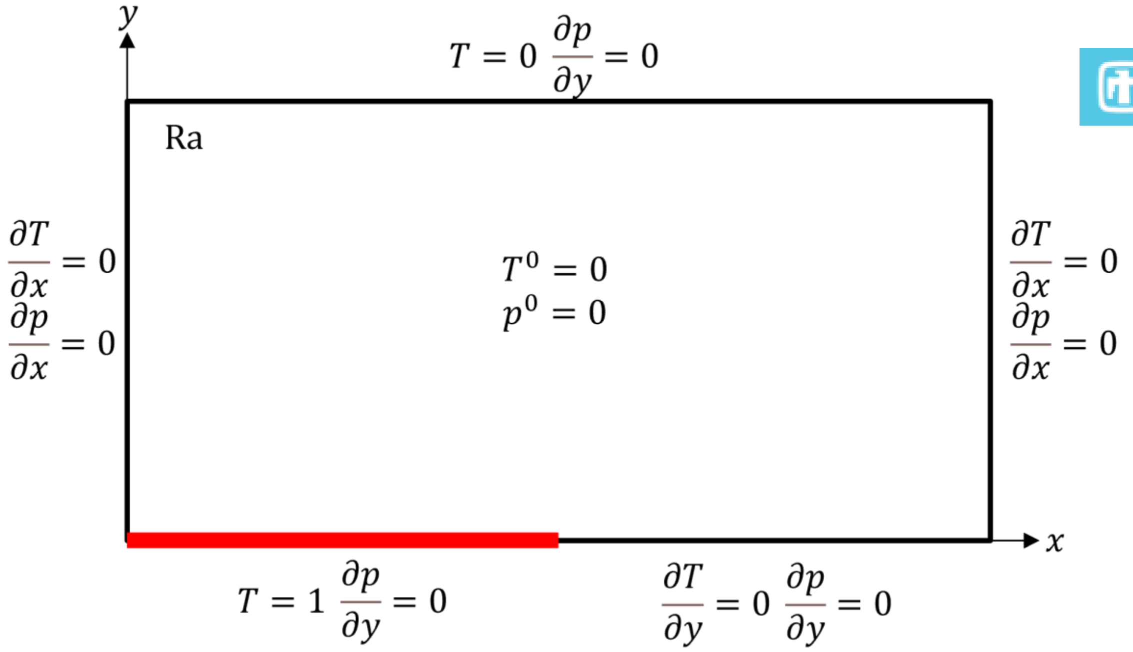
The nonlinear manifolds are well structure

Results - Elder

1. We test our model using Elder problem

   [Elder et al. (2017, Fluids)

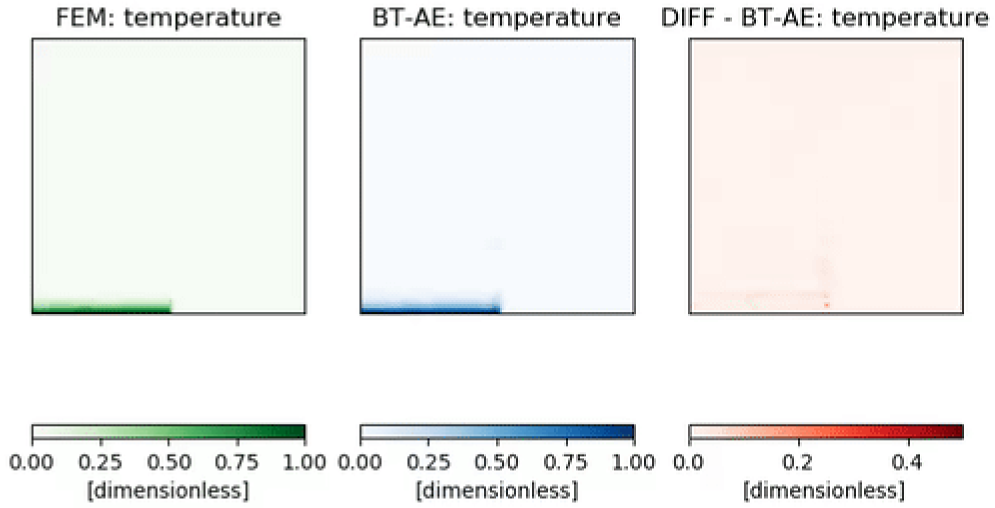
1. The flow is driven by the change of temperature at the bottom



Parameters

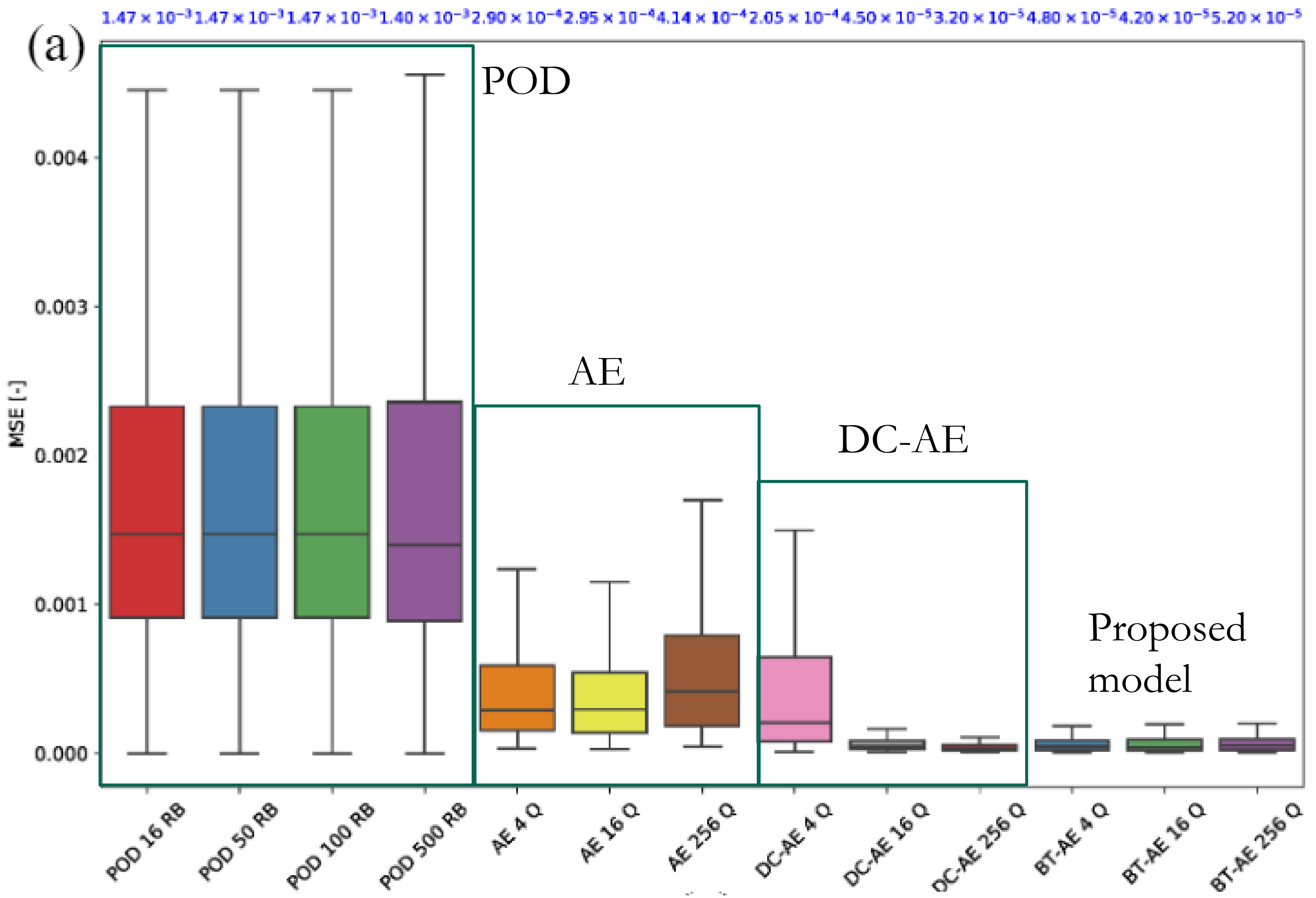
$\mathrm{Ra}_1 = [350, 450]$

Training: 40
Testing: 10



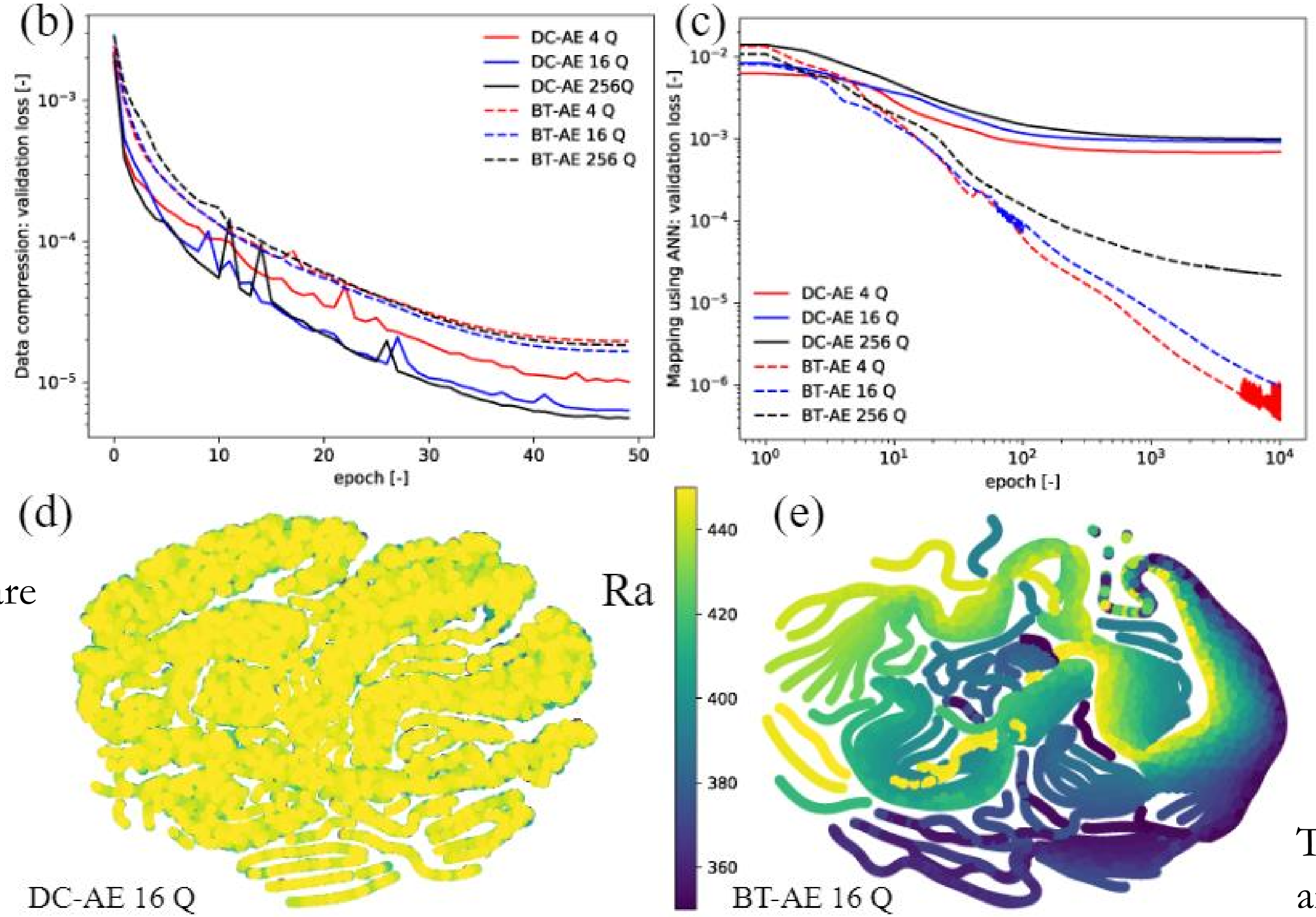
Results – Elder - continue

1. We can see that BT model provide almost similar performance as deep convolutional AE (as well as be able to achieve a very good accuracy with only **4 nonlinear manifolds**)



Results – Elder - continue

1. We can see that the BT model (dashed) has a **higher data compression loss** (step 3), but it has a much **lower mapping loss** (step 4)



The nonlinear manifolds are not really well structure

The nonlinear manifolds are well structure

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 to both **structured** and **unstructured** meshes

3. Uncertainty-aware BT-ROM is in progress to achieve uncertainty quantification.