Epistemic uncertainty-aware Barlow twins reduced order modeling for nonlinear contact problems

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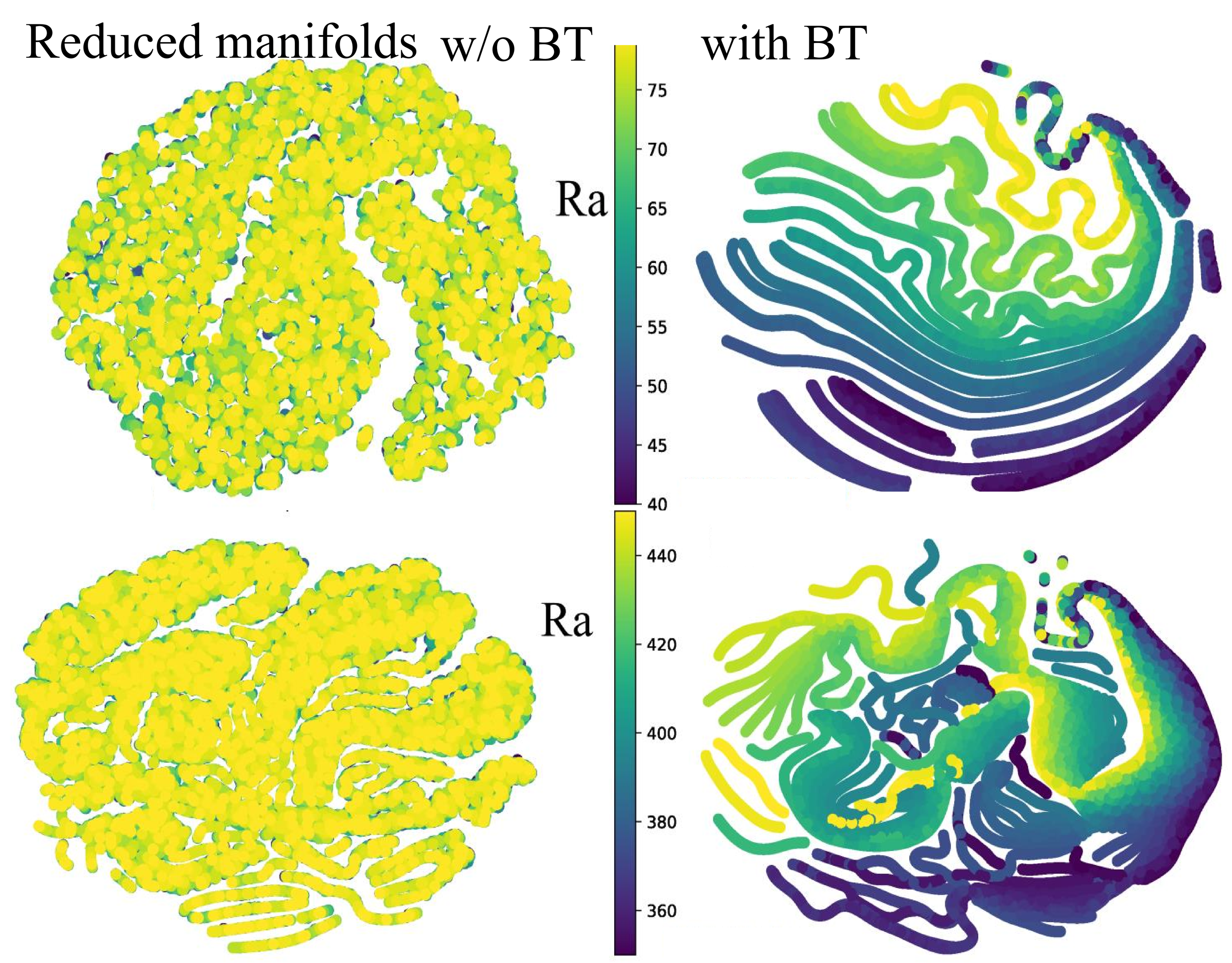
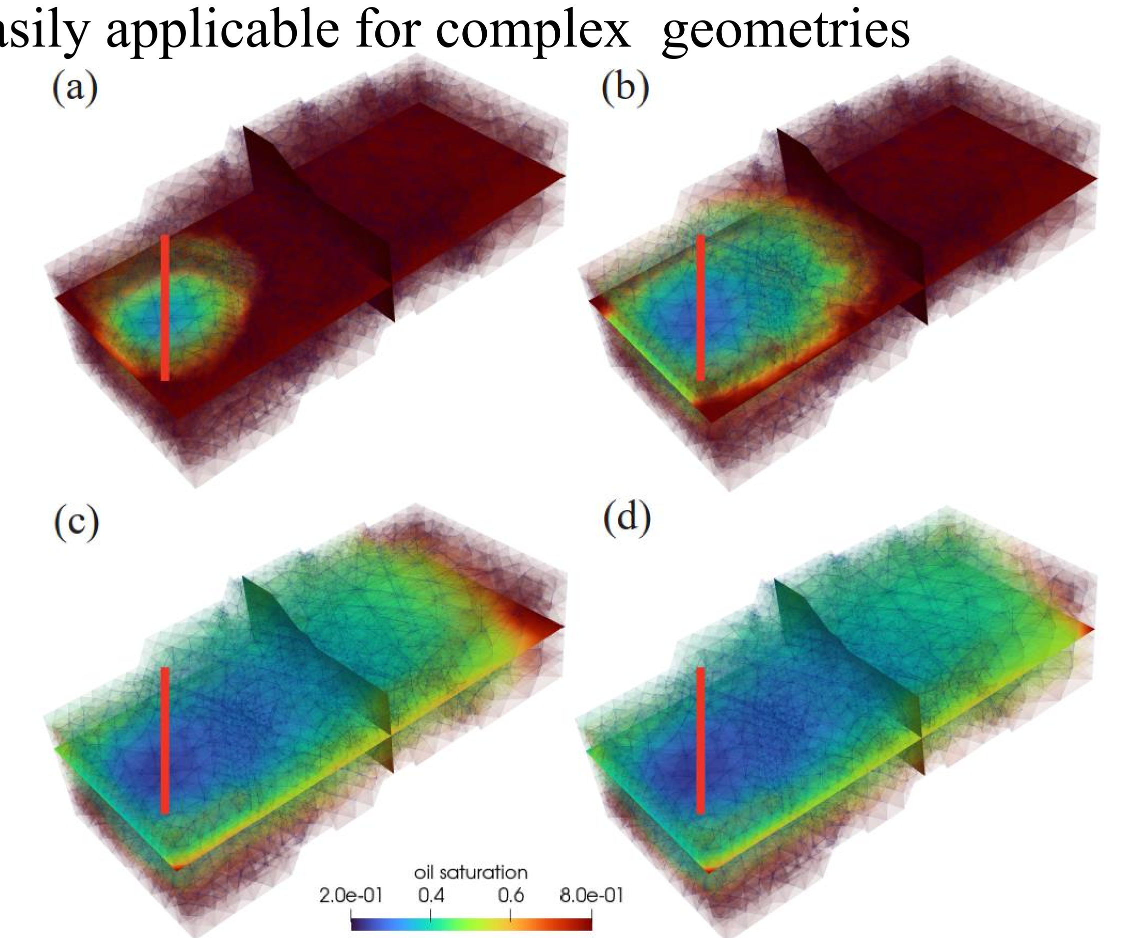
Barlow Twins reduced order modeling (BT-ROM)

Throughout this work, we are developing a proxy of a high-fidelity model (FOM) that represents contact problems with finite deformation. Kadeethum et al. [1] illustrate two essential issues associated with the nonlinear compression framework: (1) the nonlinear compression could not exceed the level of its linear counterpart's accuracy for problems that naturally lie within linear manifolds, and (2) although the nonlinear approach excels in highly nonlinear problems, it relies on convolutional operators, hindering its application for unstructured meshes and limiting this approach to less practical problems. Very recently, Kadeethum et al. [2] developed Barlow Twins ROM (BT-ROM) that possess either linear or nonlinear low-dimensional manifolds. This outstanding result derives from the use of BT self-supervised learning [3], which maximizes the information content of the embedding with the latent space through a joint embedding architecture, resulting in an improved information structure of reduced manifolds; consequently, a better prediction capability.

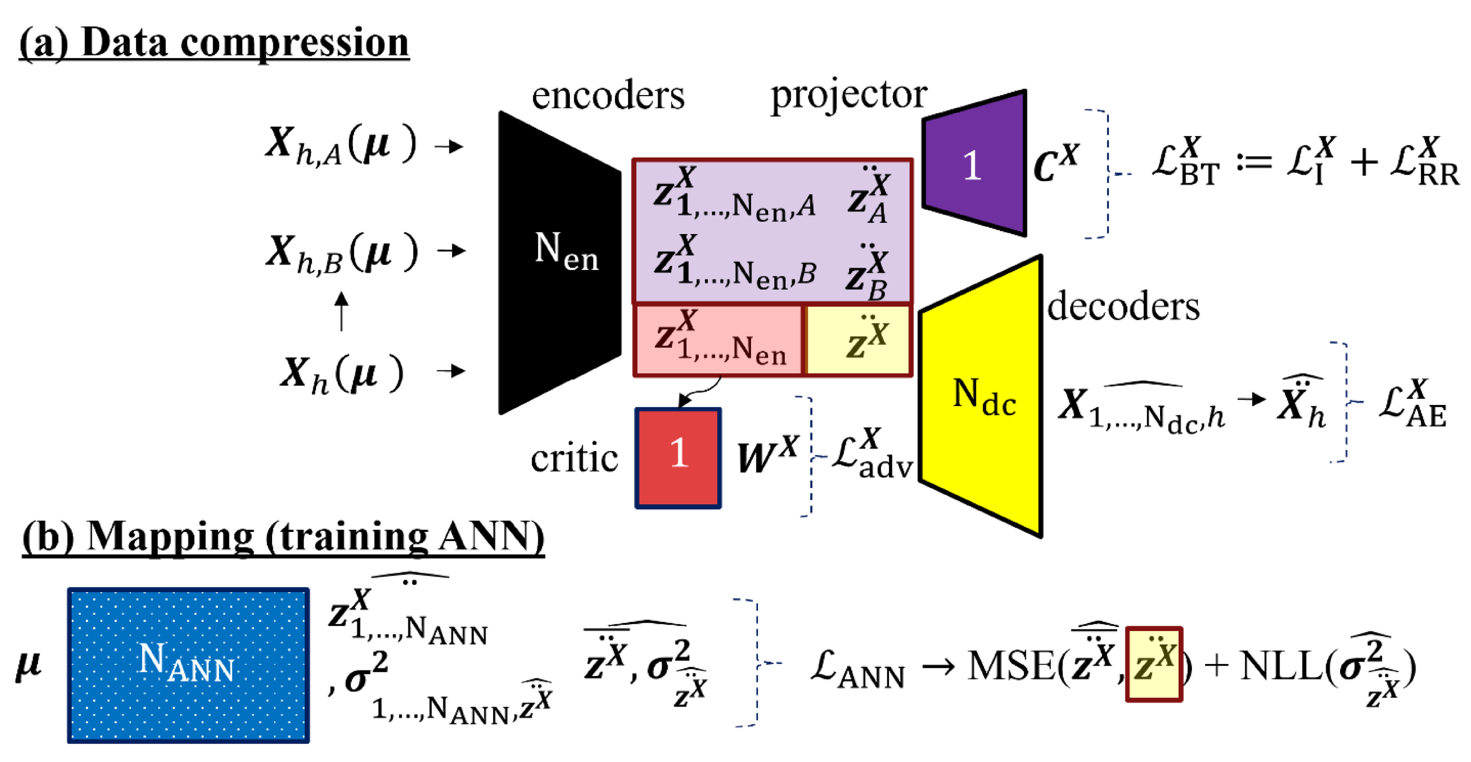


Easily applicable for complex geometries



Epistemic uncertainty quantification (UQ-BT-ROM)

ROMs are often utilized for design and quantifying the impact of uncertainty in parameter space on model predictions [4]. However, little attention has been given to quantifying the epistemic uncertainty in model predictions introduced by using ROMs in place of FOM. Methods that quantify the amount of training data (knowledge) on the accuracy and uncertainty in ROM predictions are needed [5]. Estimates of epistemic uncertainty are needed to engender trust in ROMs (trustworthy AI) and can be used for active learning strategies to improve ROM robustness and accuracy for a fixed budget [6].



Summary of UQ-BT-ROM: (a) data compression and (b) mapping. μ is a set of parameterized parameters, which is an input to our framework while $\widehat{X_h}$ ensemble version of $\widehat{X_h}$ is an output, which is an approximation of X_h, solutions of FOM. (a) Subscripts A and B represent BT-based images for training a part of BT in the upper part of the schematic.

Model summary

In a nutshell, the framework utilizes multiple encoders and decoders for two reasons; (1) by weighted sub-sampling and sequentially training process, we encourage the current encoder to learn a set of training samples that previous encoders fail to encode, and (2) by ensemble the approximation of decoders through a set of trainable weights, we can dynamically adapt the focus region of the material domain for each decoder. This is very important because the contact problem in material science has only a tiny area where the deformation occurs while most of the domain remains undeformed.

We use Barlow Twins loss to help encoders deliver a proficient construction of the latent space; subsequently, it enables us to map these latent spaces using regression models easily [2]. Besides, comparing specifically to [7] where the linear expansion coefficients of POD are generally not a normal distribution, our approach enforces the normality of the reduced manifolds through a critic. We want to emphasize that, throughout this work, we are developing a proxy of a high-fidelity model (FOM) that represents contact problems with finite deformation in a sense of deterministic nature. In the future, experimental results or field measurements can be utilized in a Bayesian framework to quantify aleatoric uncertainty in addition to epistemic uncertainty in this study.

Contact problems

Frictionless contact of a rigid indenter with hyperelastic substrate

The weak form of mechanical equilibrium equations in the reference configuration is

penalty term   Piola Kirchhoff stress tensor   body force

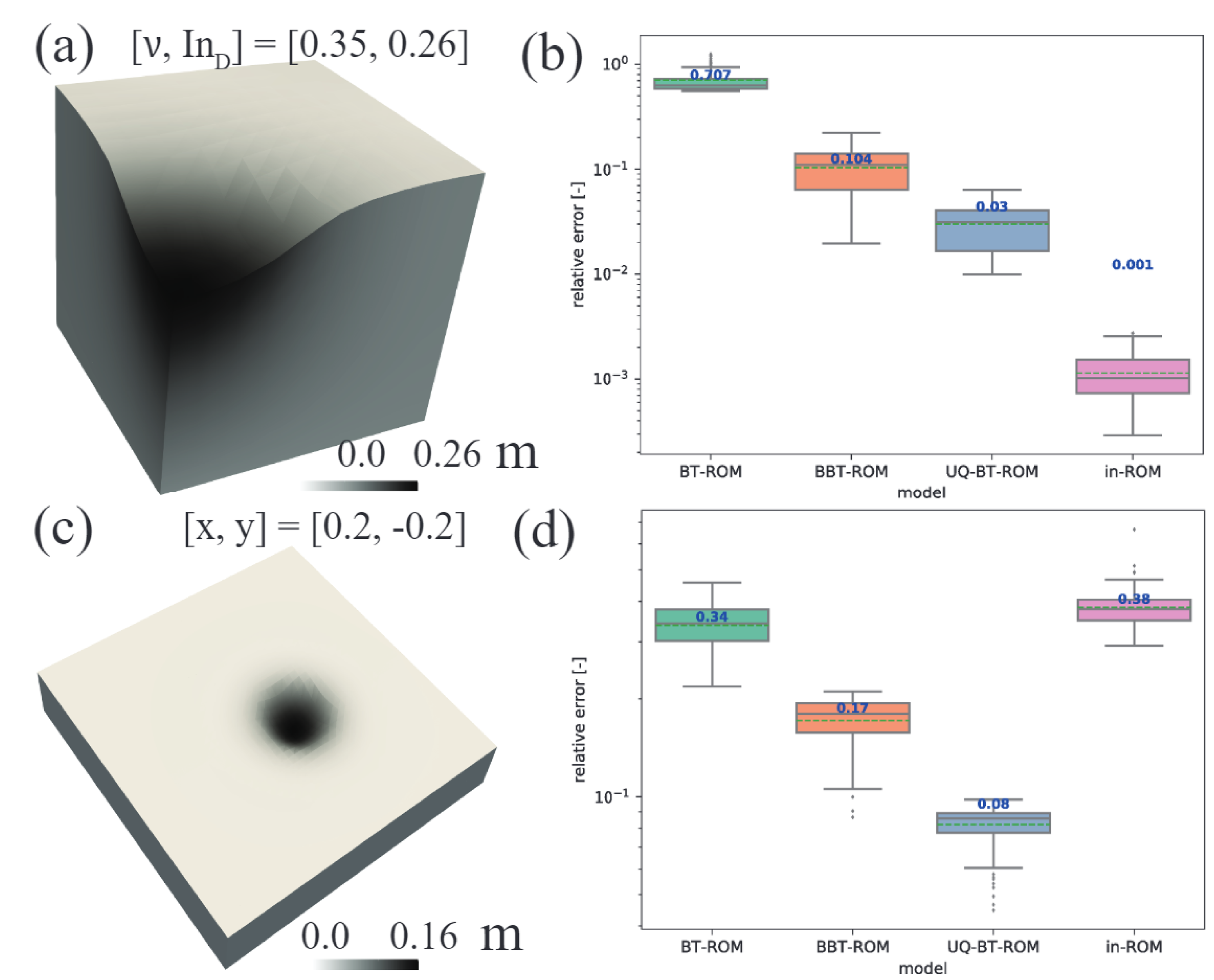
$$\mathrm{k}_{\mathrm{pen}} \int_{\partial\Omega_c} \langle -g_N \rangle \delta u_N \, dS + \int_{\Omega_0} \mathbf{P} : \nabla(\boldsymbol{\delta}\mathbf{u}) \, dV - \int_{\Omega_0} \mathbf{B} \cdot \boldsymbol{\delta}\mathbf{u} \, dV - \int_{\partial\Omega_N} \mathbf{T} \cdot \boldsymbol{\delta}\mathbf{u}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

normal displacement   displacement   traction force

To solve this system of equation, we use a continuous Galerkin approximation of the first order and PETSc SNES as a nonlinear solver and MUMPS as a linear solver

Results: Accuracy comparisons

We showcase our framework using (a) Example 1: Poisson's ratio and indentation depth parametrization and (c) Example 2: Indentation location parametrization.



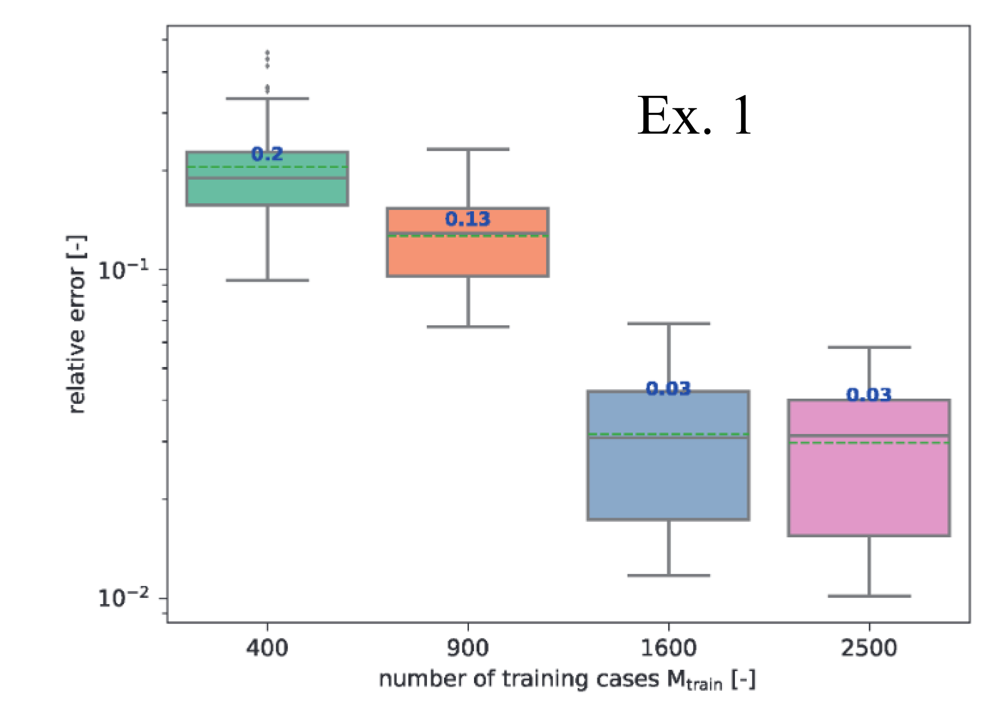
The proposed model, UQ-BT-ROM, provides a good accuracy and even outperforms an intrusive ROM with Galerkin projection (in-ROM) for Example 2 (b and d).

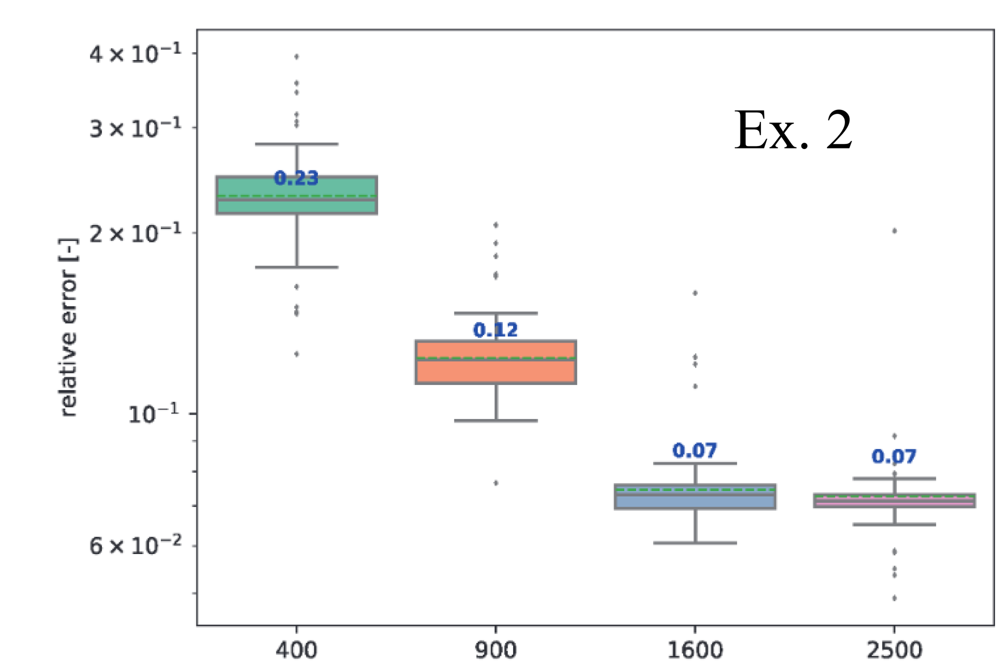
Take away:

1. Machine-learning-based reduced-order-model that can realize epistemic uncertainty
2. Through an ensemble approach this model provides a good accuracy and even outperforms intrusive ROM
3. The model can be used for active learning strategies to improve ROM robustness and accuracy for a fixed budget

Results: Epistemic UQ

Our UQ-BT-ROM illustrates that the error in the ROM decreases with increasing the training data, and so does the uncertainty estimate (variance of approximation). This framework helps us understand the effects of knowledge (amount of training data) for ROM construction on model performance (i.e., accuracy and confidence). From two contact examples, model accuracy sharply increases with increasing training data to 1600, followed by a small improvement from 1600 to 2500. Based on this, one could pick an optimal training set as 1600. While we only demonstrated our methodology on contact problems, the non-intrusive data-driven ROM approach proposed in this work applies to many other linear and nonlinear problems in computational mechanics and physics.





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