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Variational AutoEncoder (VAE) Boosted Parametric Reduced Order Modelling (pROM)

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Approach conceptualization

Physics-based pROM framework components

High Fidelity Model
(finite element model)

\+

Parametric dependencies
(structural properties & excitation traits)

→ *Vector of parameters* **p**

Sample parametric realizations
=> Full-order HFM evaluations

→ *Latin Hypercube Sampling design on realizations of vector* **p**

Projection-based reduction via POD

→ *Projection on governing equations of motion:*

$$\mathbf{M}(\mathbf{p})\ddot{\mathbf{u}}(t) + \mathbf{g}\left(\mathbf{u}(t), \dot{\mathbf{u}}(t), \mathbf{p}\right) = \mathbf{f}(t, \mathbf{p})$$

$$\mathbf{u}(t) \in \mathbb{R}^n, \mathbf{M}(\mathbf{p}) \in \mathbb{R}^{n \times n}, \mathbf{f}(t, \mathbf{p}) \in \mathbb{R}^n, \mathbf{g}\left(\mathbf{u}(t), \dot{\mathbf{u}}(t)\right) \in \mathbb{R}^n$$

- $\mathbf{u}(t)$: Response time history
- $\mathbf{M}(\mathbf{p})$: Mass matrix
- $\mathbf{f}(t, \mathbf{p})$: External excitation
- $\mathbf{g}$: Internal forces (nonlinear)

Reference system
(real-life)

Approach conceptualization

Physics-based pROM framework components

Reference system (real-life)

High Fidelity Model *(finite element model)* ✚ Parametric dependencies *(structural properties & excitation traits)* → *Vector of parameters* **p**

Sample parametric realizations => Full-order HFM evaluations → *Latin Hypercube Sampling design on realizations of vector* **p**

Projection-based reduction via POD → *Projection on governing equations of motion:*

$$\mathbf{M}_{\mathrm{r}}(\mathbf{p}_j)\ddot{\mathbf{u}}_{\mathrm{r}}(t) + \mathbf{g}_{\mathrm{r}}\left(\mathbf{u}(t), \dot{\mathbf{u}}(t), \mathbf{p}_j\right) = \mathbf{f}_{\mathrm{r}}(t, \mathbf{p}_j)$$

$$\mathbf{M}_{\mathrm{r}}(\mathbf{p}_j) \in \mathbb{R}^{r\times r}, \mathbf{g}_{\mathrm{r}}\left(\mathbf{u}(t), \dot{\mathbf{u}}(t), \mathbf{p}_j\right) \in \mathbb{R}^r, \mathbf{f}_{\mathrm{r}}(t, \mathbf{p}_j) \in \mathbb{R}^r$$

$$r \ll n$$

$$\mathbf{u}(t) = \mathbf{V}(\mathbf{p}_j)\mathbf{u}_{\mathrm{r}}(t) \quad \mathbf{M}_{\mathrm{r}}(\mathbf{p}_j) = \mathbf{V}(\mathbf{p}_j)^T\mathbf{M}(\mathbf{p}_j)\mathbf{V}(\mathbf{p}_j)$$

$$\mathbf{g}_r(\mathbf{p}_j) = \mathbf{V}(\mathbf{p}_j)^T\mathbf{g}\left(\mathbf{u}(t), \dot{\mathbf{u}}(t), \mathbf{p}_j\right)$$

Projection (Reduced-Order) Basis

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Approach conceptualization

Physics-based pROM framework components

High Fidelity Model *(finite element model)* + **Parametric dependencies** *(structural properties & excitation traits)* → *Vector of parameters* **p**

Sample parametric realizations => Full-order HFM evaluations → *Latin Hypercube Sampling design on realizations of vector* **p**

Projection-based reduction via *POD* → *Approximate reduced subspace via the Proper Orthogonal Decomposition* on response data*

Reference system (real-life)

*Proper Orthogonal Decomposition

$$\mathbf{U} \equiv [\mathbf{u}(t_1)...\mathbf{u}(t_N)] = \mathbf{W\Sigma R}^T$$

$$\mathbf{u}(t) = \mathbf{V}(\mathbf{p})\mathbf{u}_r(t) \quad \mathbf{V} \equiv \mathbf{W}_k = \mathbf{W}(:, 1:k)$$

POD modes

Approach conceptualization

Physics-based pROM framework components

Reference system (real-life)

High Fidelity Model
(finite element model)

+

Parametric dependencies
(structural properties & excitation traits)

Sample parametric realizations
=> Full-order HFM evaluations

Projection-based reduction via POD

*Approximate reduced subspace via the **P**roper **O**rthogonal **D**ecomposition* on response data*

Local ROMs

For ***each sample***, a ***POD subspace*** that captures local dynamic behavior is assembled

Clustering or Interpolation

- ***Clustering*** of local ROMs based on similarity measure & ***kNN*** for validation sample
- ***Interpolation techniques*** between local ROM subspaces to ***approximate validation basis***

Approach conceptualization

Physics-based pROM framework components

Reference system
(real-life)

High Fidelity Model
(finite element model)

+

Parametric dependencies
(structural properties & excitation traits)

Sample parametric realizations
=> Full-order HFM evaluations

Projection-based reduction via POD

*Approximate reduced subspace via the **P**roper **O**rthogonal **D**ecomposition* on response data*

Local ROMs

For ***each sample***, a ***POD subspace*** that captures local dynamic behavior is assembled

Previous work:
MAC-based clustering

- ***M**odal **A**ssurance **C**riterion* indirectly *relates POD modes* that capture local effects
- Enables ***dynamics-based clustering & adaptive sampling***

Approach conceptualization

Physics-based pROM framework components

High Fidelity Model *(finite element model)* + **Parametric dependencies** *(structural properties & excitation traits)*

Reference system (real-life)

Sample parametric realizations => Full-order HFM evaluations

Projection-based reduction via POD

Local ROMs

(MAC-based) Clustering

Physics-based parametric Reduced Order Model

- *A subspace for each sample via **P**roper **O**rthogonal **D**ecomposition* on response data*
- *Form clusters on parametric domain based on local dynamics => Similarity of POD subspaces*
- *Validation sample uses kNN and POD basis of assigned cluster for projection & ROM integration*

Approach conceptualization

Physics-based pROM framework components

Reference system (real-life)

High Fidelity Model *(finite element model)*

\+

Parametric dependencies *(structural properties & excitation traits)*

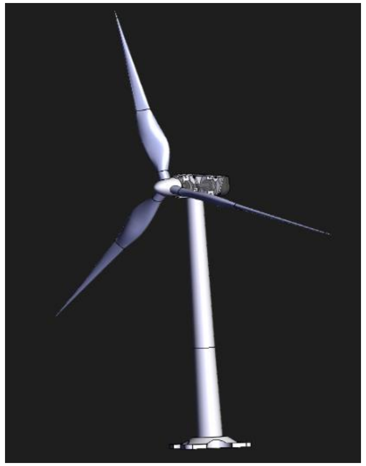
Sample parametric realizations => Full-order HFM evaluations

Projection-based reduction via POD

Local ROMs

MAC-based clustering

Physics-based parametric Reduced Order Model



Virtual representation (***Digital-Twin***)

Problem Statement

Treatment of parametric dependencies in ROMs

POD - Projection-based Reduction

Proper Orthogonal Decomposition

$$\mathbf{u}(t) = \mathbf{V}(\mathbf{p})\mathbf{u}_{\mathrm{r}}(t) \qquad \mathbf{U} \equiv [\mathbf{u}(t_1)...\mathbf{u}(t_N)] = \mathbf{W\Sigma R}^T$$

$$\mathbf{V} \equiv \mathbf{W}_k = \mathbf{W}(:, 1:\mathrm{k})$$

Limitations:

- **POD is a linear operator**
  Linearization *in neighbourhood of stable points is assumed to address nonlinearities*
- **Accuracy** for new parametric states *relies on* ***clustering or interpolation*** *between POD bases*

Interpolation-based approaches

- ROM matrices interpolation (linear ROMs)
- POD bases interpolation in proper space

Clustering-based approaches

- Clustering of POD bases with proper metric
- k-NN schemes for validation samples

However:

- Multi-parametric dimensionality
- Linearization limitations

Approach conceptualization

VAE-scheme for parametric ROM treatment

Idea: Employ VAE scheme to estimate validation POD basis

Argumentation:
ROM performance relies on ***approximating validation POD bases*** based on ***interpolation*** or ***kNN-based clustering*** between training POD bases

→ **Insert dependencies on VAE bases to substitute interpolation/clustering**

- *VAE provides **nonlinear** and potentially more **accurate mapping between POD bases** across parameter space*
- *VAE scheme provides **uncertainty quantification** assessment*
- ***Utility by multi-parametric** dependencies*
- *Potential of parametric treatment on the latent space / Inject dependencies on latent space*

Approach conceptualization

Additional projection level to retain basis properties

$$\mathbf{V}^{rg}_{global} = \left[\mathbf{V}^{rg}_{local,1}, \mathbf{V}^{rg}_{local,2}, \ldots, \mathbf{V}^{rg}_{local,N}\right]$$

→

$$\mathbf{V}^{\mathrm{rg}}_{\mathrm{local},i} = \mathbf{V}^{\mathrm{rg}}_{\mathrm{global}} \mathbf{\Xi}_i$$

✓ ***Relate global dynamics (or region dynamics) with single realization***

To achieve this, we formulate:

- a global projection basis → $\mathbf{V}^{\mathbf{rg}}_{\mathbf{global}} \in \mathbb{R}^{N_{dof} \times N_{modes,global}}$
- a coefficient matrix projecting the single realization dynamics to the cluster global basis → $\mathbf{\Xi_i} \in \mathbb{R}^{N_{modes,global} \times N_{modes,local}}$

Then, ***the VAE is trained on the coefficient matrices!***

- ***Uncoupled*** *of high fidelity,* ***full order dimension*** => ***Efficiency***
- ***Reduced dimensionality*** *that* ***captures dynamics*** *due to additional projection*
- ***Orthogonality*** *properties and symmetries* ***retained*** *in mapping*

$N_{modes,global}$:

- Controls dimensionality
- Defines training complexity and cost
- Can be a large number to capture effects

VAE-scheme for parametric ROM treatment

Implementation details

- ***High dimensional data*** → Generative model → ***Deep latent variable model***

- This problem involves ***maximising*** the following ***likelihood for the chosen prior over the latent variables*** $p_{\phi}(X) = \int p_{\phi}(X|Z)p(Z)$

- VAE's give an efficient model by ***parameterizing***:
(a) an ***encoding to the latent space*** and (b) a ***decoding from the latent space*** using deep NNs
(Widely used for deep latent variable modelling for many purposes e.g., NLP and computer vision)

- Interesting in our case as a ***flexible generative model*** capable of learning ***nonlinear dependencies*** with ***relatively high dimensionality.***

VAE-scheme for parametric ROM treatment

Implementation details

Traditional autoencoder + ***'regularisation'***

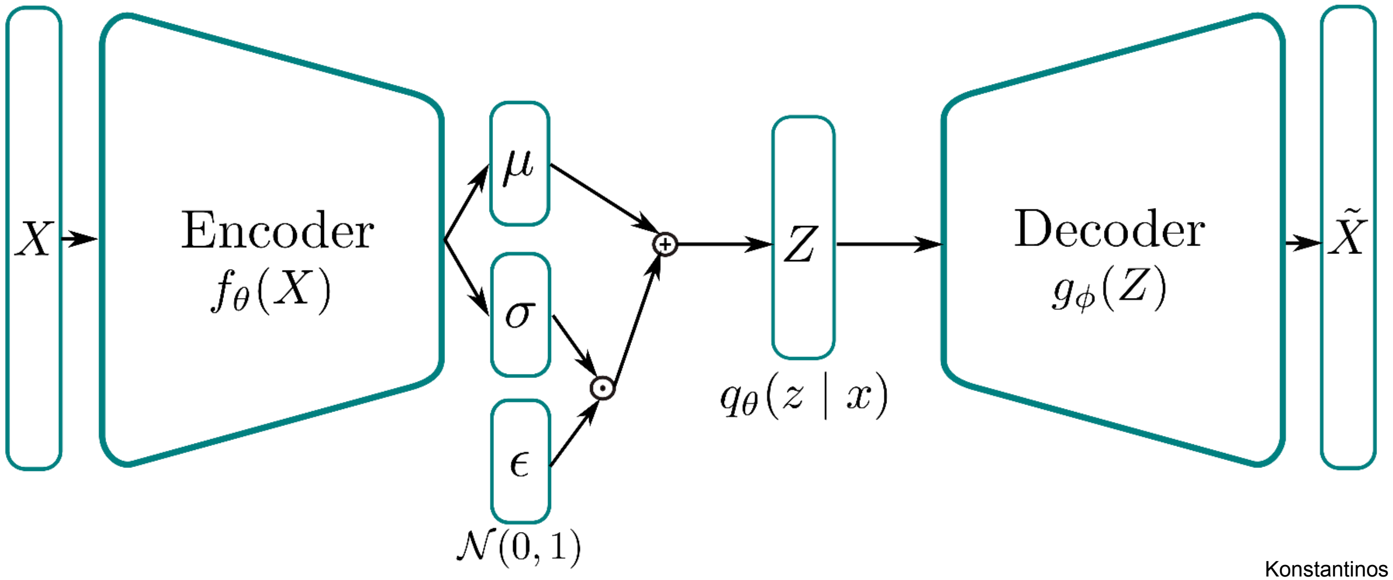
*(in the form of **encouraging the latent space** to **resemble a prior distribution**)*

Cost Function

The ***first term*** is the ***reconstruction*** error

The ***second term*** is the ***KL divergence*** between the true and approximate posterior on the latent space.

$$\mathcal{L}(\theta,\phi,X) = \mathbb{E}_{q_\theta(Z|X)}\left[\log\left(p_\phi(X|Z)\right] - \mathcal{D}_{KL}(q_\theta(Z|X)||p(Z))\right)$$

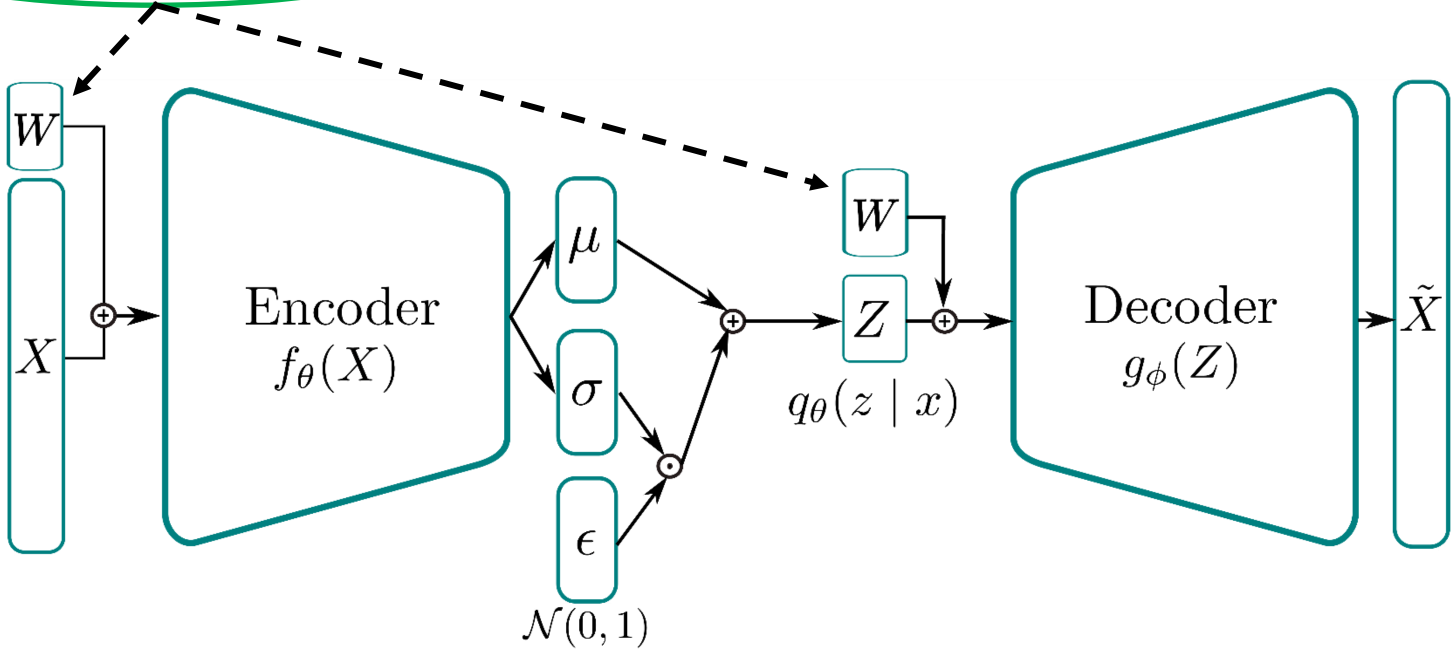


VAE-scheme for parametric ROM treatment

Conditional Variational AutoEncoder

In our case → ***Explicitly*** treat parametric ***dependencies*** → **Conditional VAE**

(The ***parametric dependencies*** are ***injected both at the input and at the latent space*** during training)



VAE-scheme for parametric ROM treatment

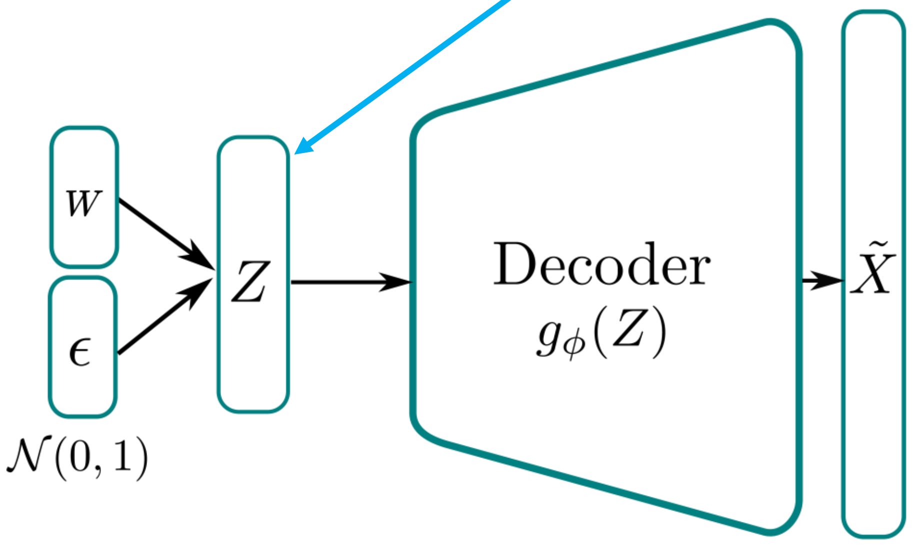
Generating from the conditional VAE

Generating new bases

VAE is simplified to just the ***prior distribution*** of the latent space ***and the decoder***

- ➢ Samples are drawn from the prior
- ➢ They are concatenated with the parameter vector

=> New bases are generated by passing this concatenated vector through the decoder.



Approach conceptualization

Variational AutoEncoder (VAE) boosted pROM

High **F**idelity **M**odel
(finite element model)

+

Parametric dependencies
(structural properties & excitation traits)

Reference system
(real-life)

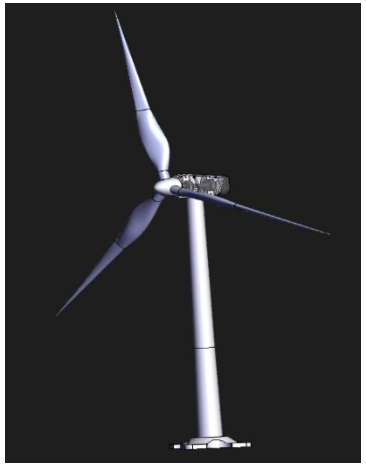
Sample parametric realizations
=> Full-order HFM evaluations

Projection-based reduction via POD

Local ROMs

VAE scheme

Physics-based VAE-boosted pROM



Virtual representation
(***Digital-Twin***)

Numerical Validation Benchmark

Two-Story Frame with Hysteretic Links

Earthquake ground motion excitation

Parametric dependencies: Angle of ground motion & Amplitude factor

Hysteretic links response model

- *Total restoring force:*

$$\mathbf{R} = \mathbf{R}_{linear} + \mathbf{R}_{hysteretic} = \alpha k \mathbf{u} + (1-\alpha) k \mathbf{z}$$

- *Bouc-Wen equation with degradation/deterioration effects:*

$$\dot{\mathbf{z}} = \frac{A\dot{\mathbf{u}} - \nu(t)(\beta|\dot{\mathbf{u}}|\mathbf{z}|\mathbf{z}|^{w-1} - \gamma\dot{\mathbf{u}}|\mathbf{z}|^{w})}{\eta(t)}$$

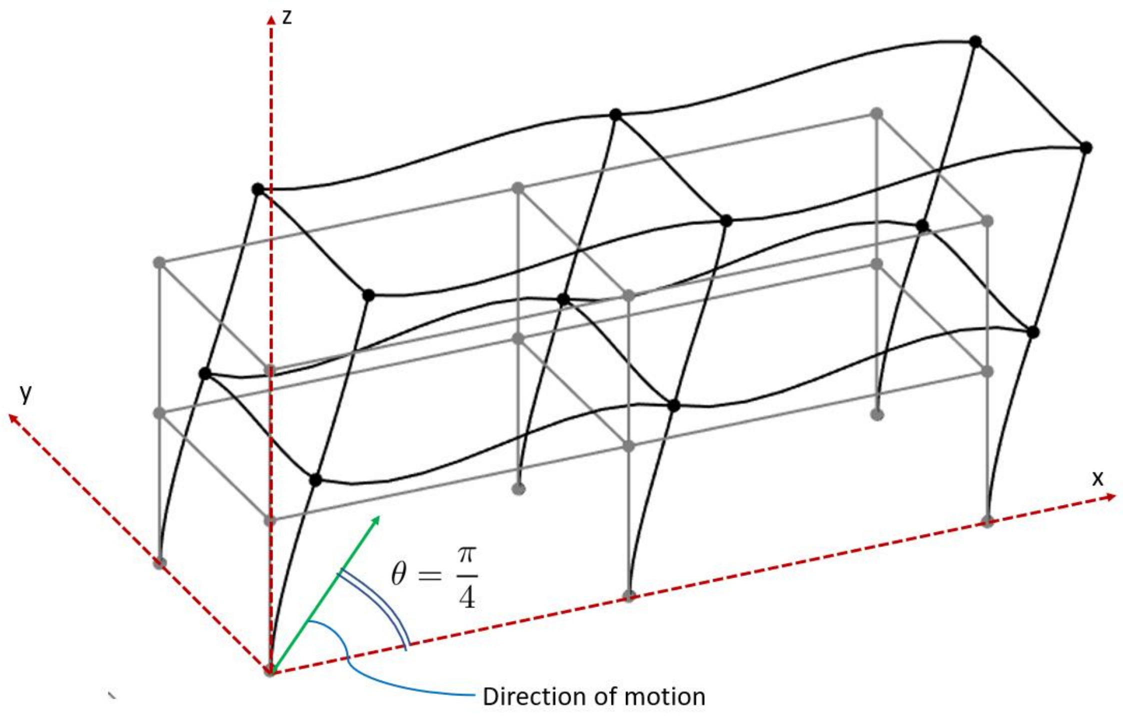
$$\nu(t) = 1.0 + \delta_\nu \epsilon(t), \quad \eta(t) = 1.0 + \delta_\eta \epsilon(t), \quad \epsilon(t) = \int_0^t \mathbf{z}\dot{\mathbf{u}}\delta t$$

Characteristics of the Bouc-Wen links:

β, γ, A, w : *Smoothness and shape of hysteresis curve*

δ_ν, δ_η : *Degradation/Deterioration effects*

a, k : *Linear/Hysteretic contribution weighting*



Benchmark example featured in:

- Vlachas K. et al. "A local basis approximation approach for nonlinear parametric model order reduction." *Journal of Sound and Vibration* 502 (2021): 116055.
- Simpson, Thomas, Nikolaos Dervilis, and Eleni Chatzi. "Machine learning approach to model order reduction of nonlinear systems via autoencoder and LSTM networks." *Journal of Engineering Mechanics* 147.10 (2021): 04021061.

Numerical Validation Benchmark

Two-Story Frame with Hysteretic Links

Earthquake ground motion excitation

Parametric dependencies: Angle of ground motion & Amplitude factor

Scenario A:

- ***Dependencies*** on ***excitation traits***
- Simplified case study (2 parameters) as ***proof-of-concept***

Scenario B:

- ***Multi-parametric dependency (7 parameters)*** on excitation characteristics, system traits and properties of the links
- ***White noise excitation*** passed through low-pass filter (ROM dependencies on ***Amplitude*** & ***Frequency*** content)
- ***Elastic Young's modulus*** as a material parameter with input uncertainty
- Additional weighting ***coefficient on linear spring*** to represent ***damage***
- Varying ***beta coefficient*** to induce ***bifurcation-like behavior***

Hysteretic Bouc-Wen links

➢ ***Total restoring force:***

$$\mathbf{R} = \mathbf{R}_{linear} + \mathbf{R}_{hysteretic} = \alpha k \mathbf{u} + (1-\alpha) k \mathbf{z}$$

➢ ***Bouc-Wen equation with degradation/deterioration effects:***

$$\dot{\mathbf{z}} = \frac{A\dot{\mathbf{u}} - \nu(t)\left(\beta|\dot{\mathbf{u}}|\mathbf{z}|\mathbf{z}|^{w-1} - \gamma\dot{\mathbf{u}}|\mathbf{z}|^{w}\right)}{\eta(t)}$$

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Characteristics of the Bouc-Wen links:

β, γ, A, w : Control smoothness and shape of *hysteresis*

δ_ν, δ_η : *Degradation/Deterioration effects*

a, k : *Linear/Hysteretic contribution weighting*

Numerical Validation Benchmark

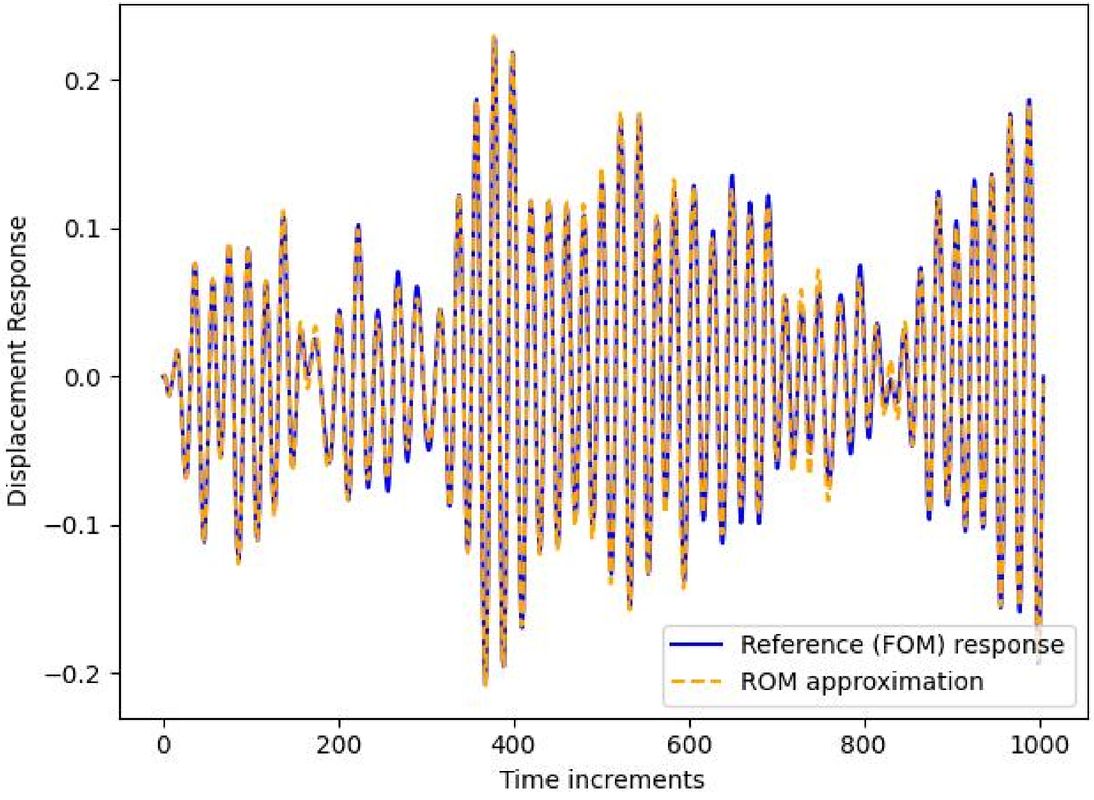
Accuracy performance of the framework (Scenario B)

pROM Notation	Explanation of setup
Reference Threshold	Reference accuracy performance obtained assuming the ***POD basis*** of each validation sample is ***approximated perfectly***.
EpROM	The pROM framework employs 3-NN ***clustering*** based on the ***Euler distance*** measure.
MACpROM	The pROM framework employs 3-NN ***clustering*** based on the ***Modal Assurance Criterion***.
VpROM	The pROM framework employs a ***Variational AutoEncoder*** scheme to estimate the POD basis coefficients.

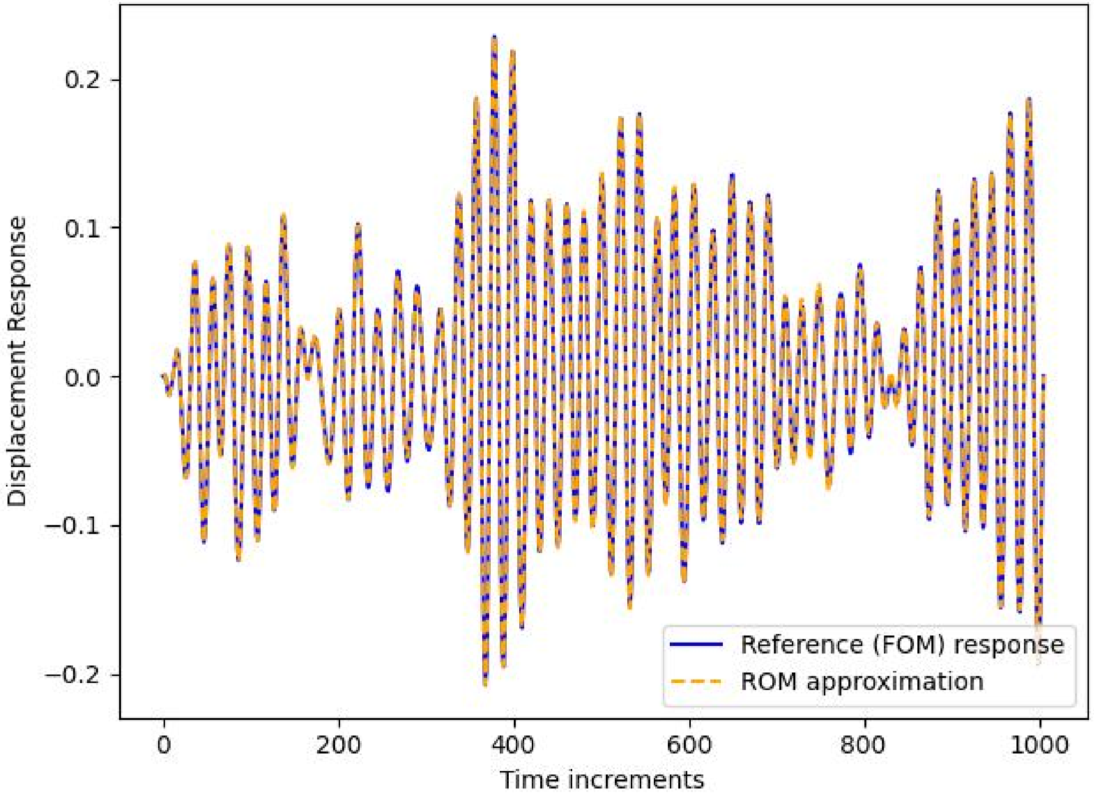
	Average Displacement Norm Error	99 % percentile	Average Restoring Forces Norm Error	99 % percentile
Reference Threshold	0.35 %	0.68%	1.14%	1.31%
EpROM	6.35 %	16.64%	2.62%	10.21%
MACpROM	6.29 %	16.17%	2.57%	9.19%
VpROM	4.29 %	10.01%	2.17%	7.60%

Numerical Validation Benchmark

Accuracy performance of the framework



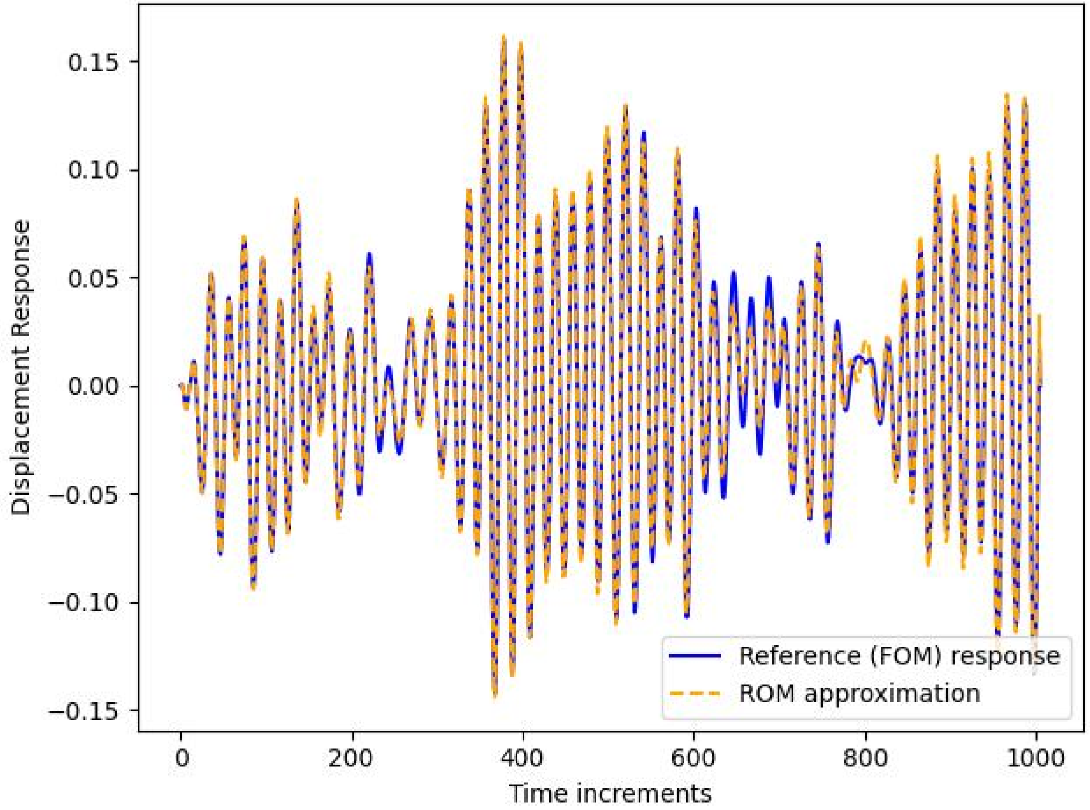
MACpROM approximation (Scenario A)



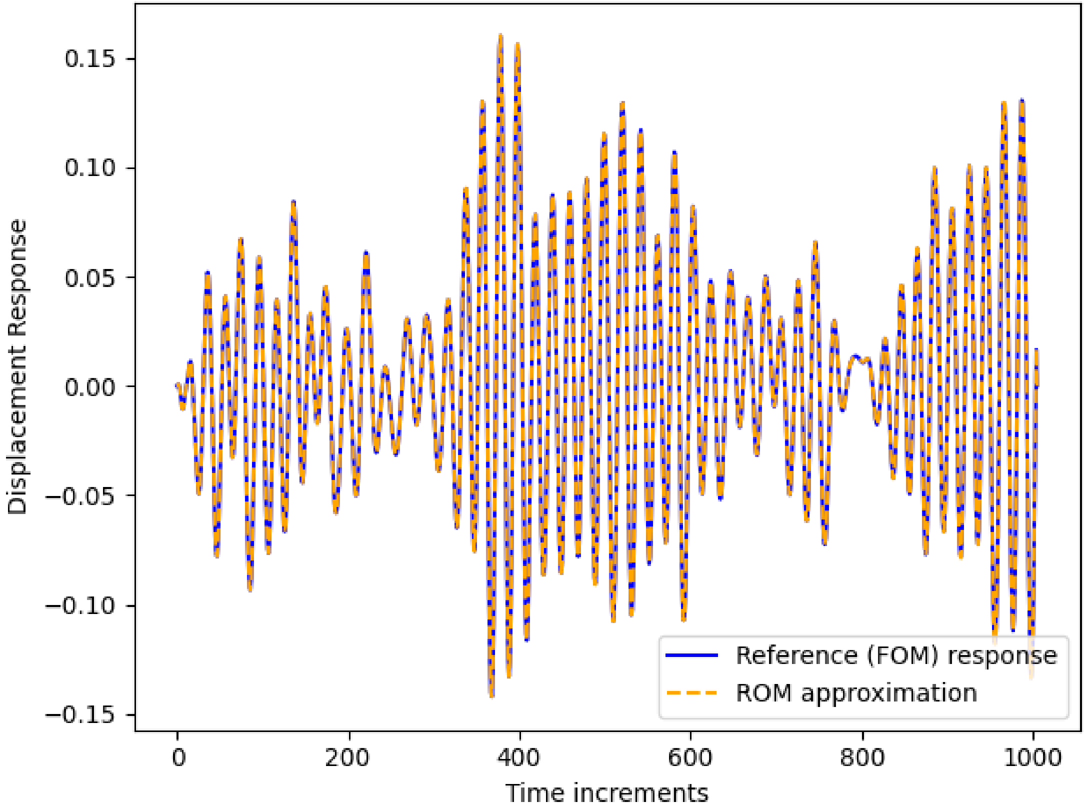
VpROM approximation (Scenario A)

Numerical Validation Benchmark

Accuracy performance of the framework



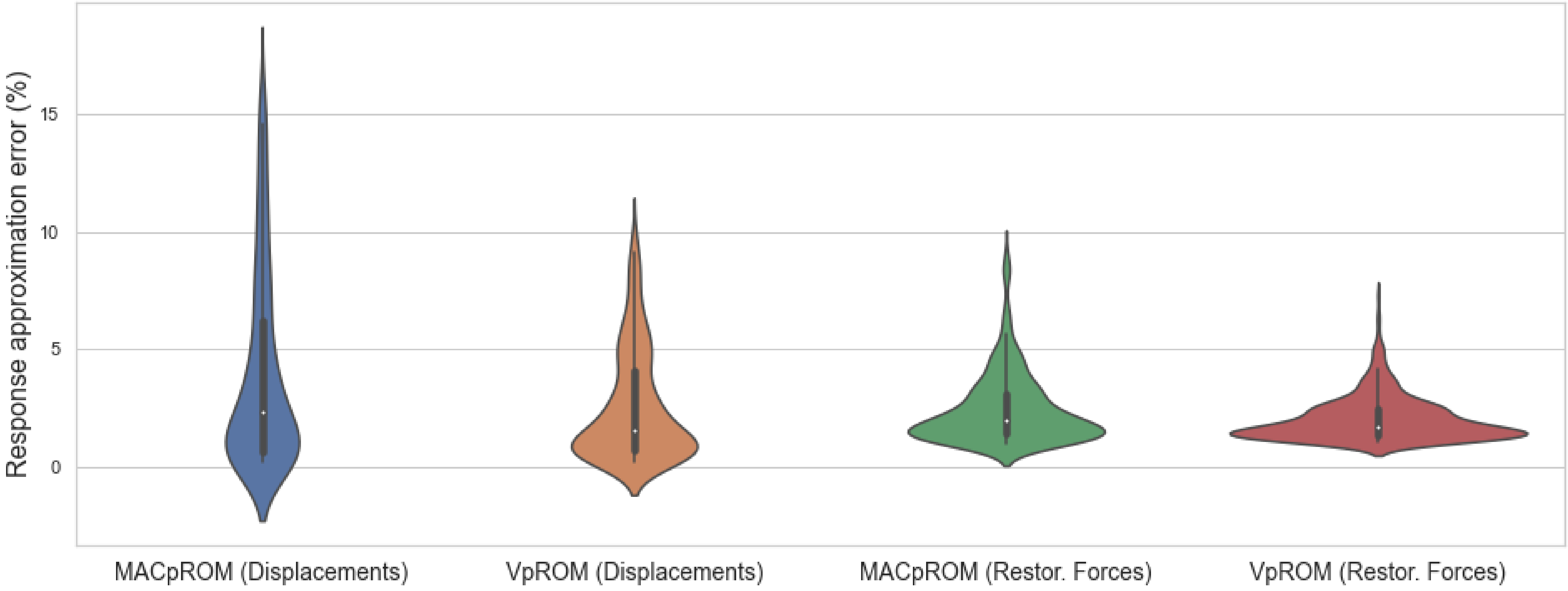
MACpROM approximation (Scenario B)



VpROM approximation (Scenario B)

Numerical Validation Benchmark

Accuracy performance of the framework (Scenario B)



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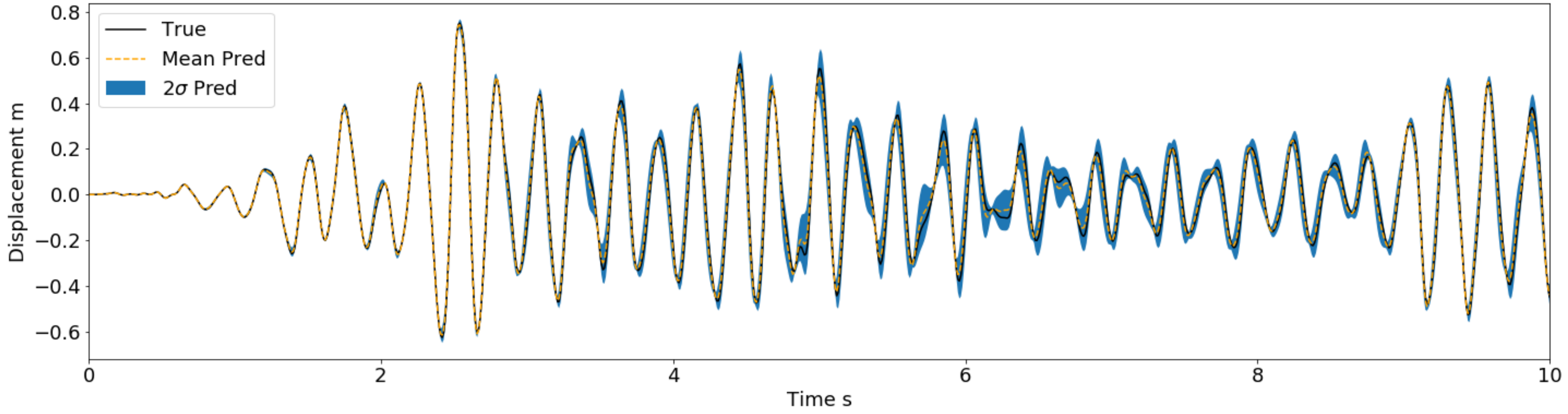
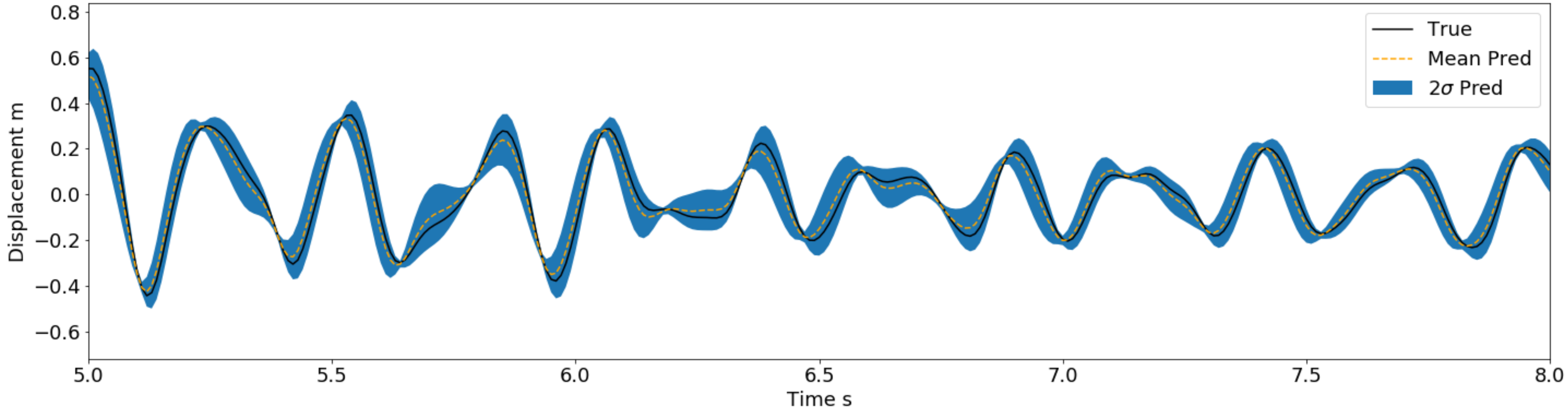
Uncertainty Quantification

Confidence bounds of inferred response (Scenario B)

Parametric ROM evaluated ***40 times using 40 VAE draws*** → Plot ***mean and SD*** at each time step





Concluding remarks
Limitations and outlook

The proposed Variational AutoEncoder (VAE) boosted-pROM

- ✓ Couples ***Variational AutoEncoders*** with ***ROMs*** to capture ***multi-parametric system dependencies*** or ***uncertainty on input*** features
- ✓ *Outperforms* and *extends performance range* of traditional projection-based pROMs
- ✓ Provides confidence bounds and uncertainty quantification for response estimation
- ✓ May be adapted as an ***approximative, online low-cost surrogate*** for *Structural Health Monitoring* applications

- ➢ Performance still ***bounded*** from ***ability of POD bases*** to capture dynamics
- ➢ Potential ***varying size of local POD bases*** needs additional treatment

Next steps - extensions:

- ❖ Generalize implementation – adjust scope:
  - Train pROM on PEER earthquake database => Estimate performance under any real-case scenario
  - Incorporate damage for condition monitoring applications
- ❖ Generalize implementation in ***large scale example with Hyper Reduced ROM***

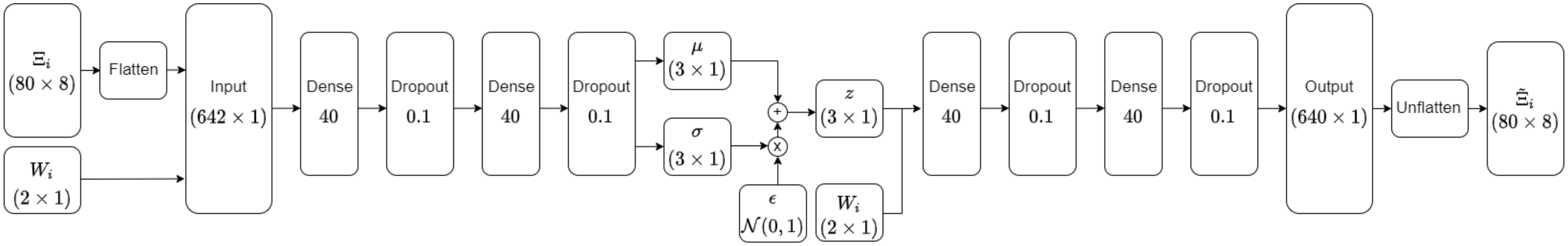
Questions

Appendix

Conditional VAE-scheme

Training scheme and implementation details

- We carry out 50 training simulations at 50 different points in the parameter space chosen by LHS.
- We train our VAE in Tensorflow optimising the cost function which balances reconstruction and Kullback-Leibler loss
- It is often important to use an "Annealing" scheme, starting by weighting the KL-divergence loss to zero and then increasing it during the training procedure.



Flow of pROM Framework

Overview of algorithmic implementation

POD - Projection-based Reduction

Assemble POD Basis

Proper Orthogonal Decomposition

$$\mathbf{u}(t) = \mathbf{V}(\mathbf{p})\mathbf{u}_r(t) \qquad \mathbf{U} \equiv [\mathbf{u}(t_1)...\mathbf{u}(t_N)] = \mathbf{W\Sigma R}^T$$

$$\mathbf{V} \equiv \mathbf{W}_k = \mathbf{W}(:, 1:\mathrm{k})$$

Limitations:

- **POD is a linear operator**
  Linearization *in neighbourhood of stable points is assumed to address nonlinearities*
- **Accuracy** for new parametric states *relies on* ***clustering or interpolation*** *between POD bases*

After training we end up with ***a pool of (training) local bases***. Each training snapshot leads to a single projection basis.

To address the linearization limitations, we need to decide how to ***approximate the projection basis for a new state*** prior to integrating in the reduced order domain. There are two alternatives:

✓ ***Interpolation***

-We perform ***elementwise or similar interpolation schemes between the bases in the training pool***. The weighting scheme may be simplified Lagrange polynomials or splines, RBFs, etc.
-A new basis is assembled for every unseen parametric state

✓ ***Clustering***

-We ***cluster the training samples with a suitable feature*** that relates local dynamics. E.g., we can use MAC or the subspace angle to relate POD bases of training samples and cluster them based on similar local dynamics.
-***Every cluster is represented by a single basis,*** the most suitable one. Using ***kNN and Euler distance we assign any new state to a cluster*** and use the representative basis.

Previous work

Clustering-based parametric ROM

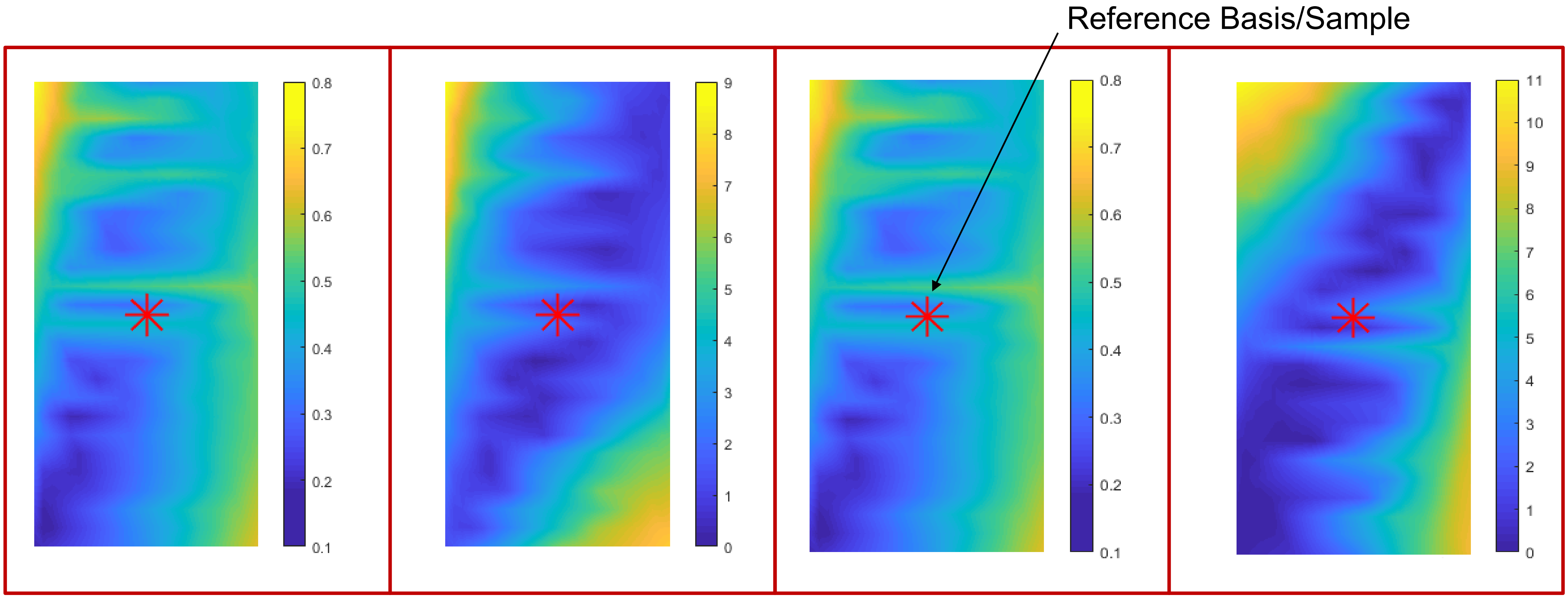
Modal Assurance Criterion

$$\mathrm{MAC}(\phi_r, \phi_s) = \frac{|{\phi_r}^T \phi_s|^2}{({\phi_r}^T \phi_r)({\phi_s}^T \phi_s)}$$

- Measure of **consistency between modeshapes Φ**
- System Identification:
  A form of confidence factor when evaluating modal vectors from different sources.
- Local POD projection bases
  => *POD modes capturing localized behavior*
- **MAC between POD bases**
  => *Relate manifold eigenvectors*
  => *Dynamics-based clustering*
  => *Define sampling rate adaptively*

Previous work

Limitations on employing MAC as error indicator



Approximation Error (%)

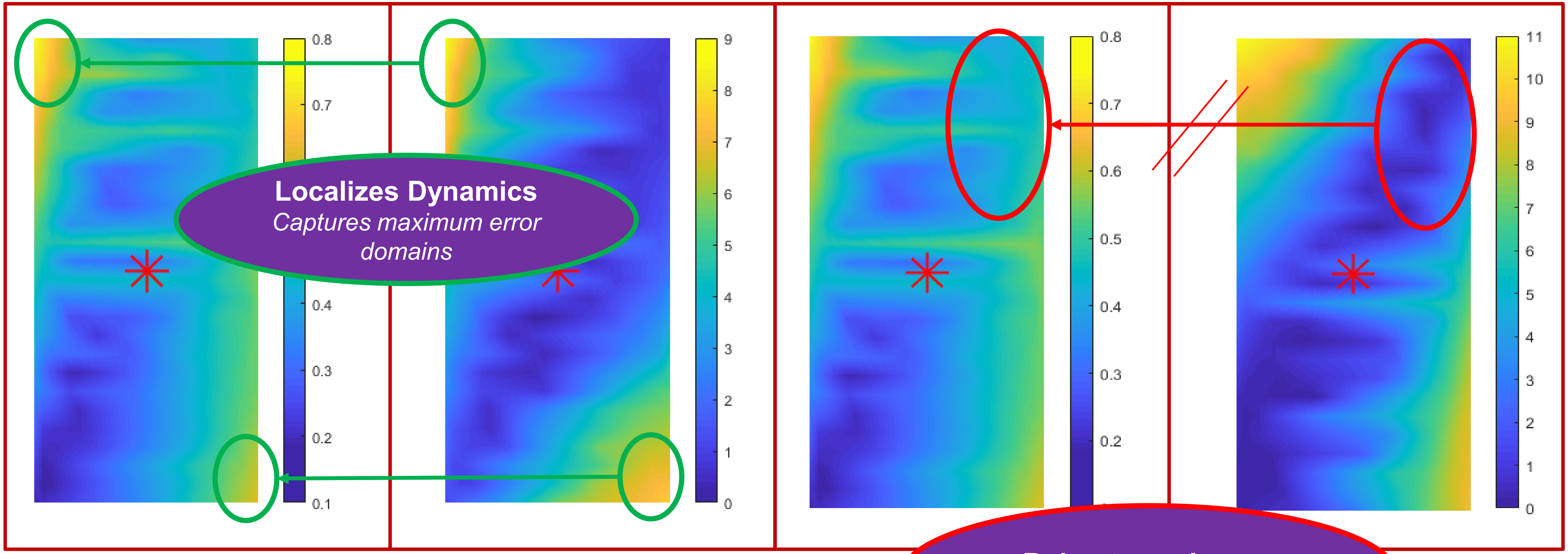
MAC values
(POD Bases – Sampling Seed A)

Approximation Error (%)

MAC values
(POD Bases – Sampling Seed B)

Previous work

Limitations on employing MAC as error indicator



Approximation Error (%)

MAC values (POD Bases – Seed A)

Approx

ues
s – Seed B)

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