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A Physics-based Reduced Order Model with Machine Learning Boosted Hyper-Reduction

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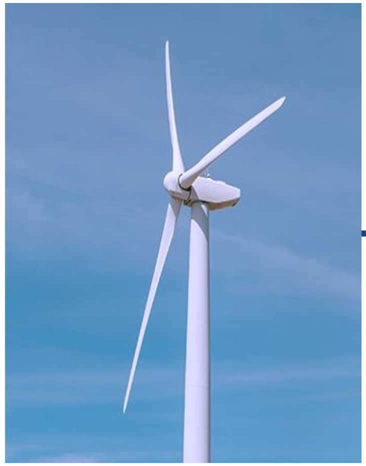
Problem Statement

Virtualization of nonlinear dynamical systems



Reference system (real-life)

High Fidelity Model
(finite element model)

HFM features:

Complex dynamics

Nonlinear behaviour

Parametric dependencies on:

- *Geometric features*
- *Material properties*
- *EOPs:*
  - *Environmental conditions*
  - *Operational conditions*
- *Excitation*

Low-order representation that:

Captures underlying dynamics

Reproduces physical behaviour

Retains parametric dependencies

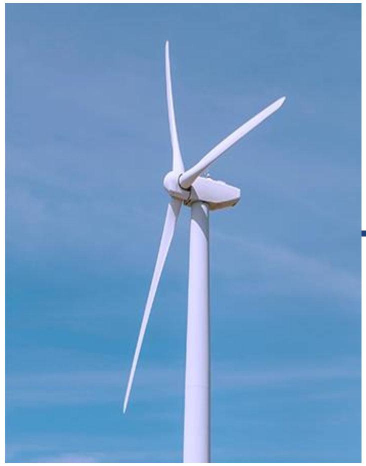
Computationally efficient

physics-based
parametric Reduced Order Model
(low-order, equivalent model)

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

Problem Statement

Virtualization of nonlinear dynamical systems



Reference system
(real-life)

High Fidelity Model
(finite element model)

Low-order representation that:

Captures underlying dynamics

Reproduces physical behaviour

Retains parametric dependencies

Computationally efficient

Projection-based reduction enables:

- Representation of the ***full response of the HFM*** (displacements, velocities, accelerations, stresses).
- the use of the ROM for ***making predictions***, thus creating the potential for a ***higher level SHM*** system.

physics-based
parametric **R**educed **O**rder **M**odel
(low-order, equivalent model)

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

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Approach conceptualization

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:*

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

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

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

Approach conceptualization

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

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

→ *Approximate reduced subspace via the Proper Orthogonal Decomposition* on response data*

*Proper Orthogonal Decomposition

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

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

POD modes

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Approach conceptualization

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*

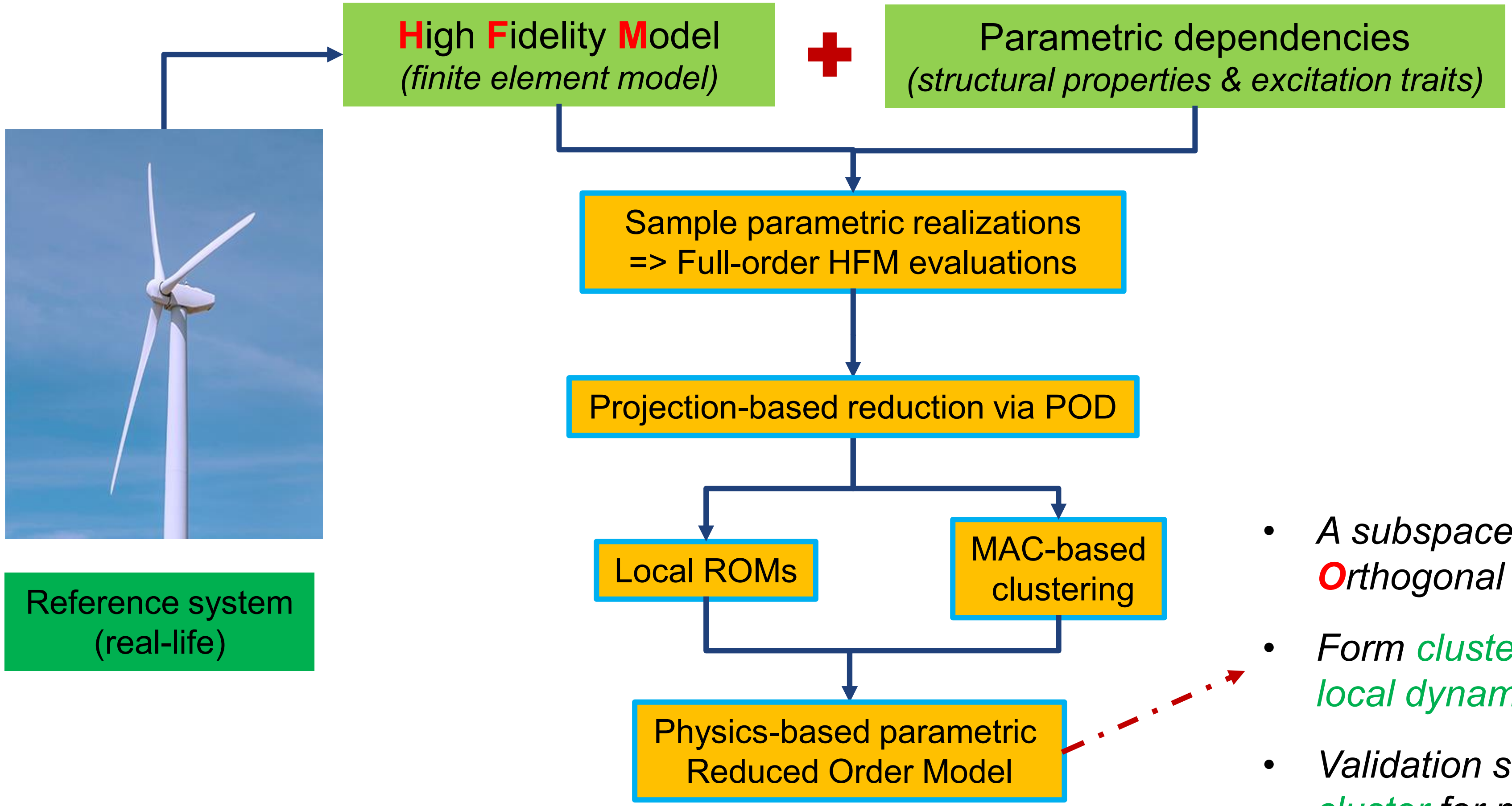
Local ROMs

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

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
Framework components



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

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Approach conceptualization

Framework components

Reference system (real-life)

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

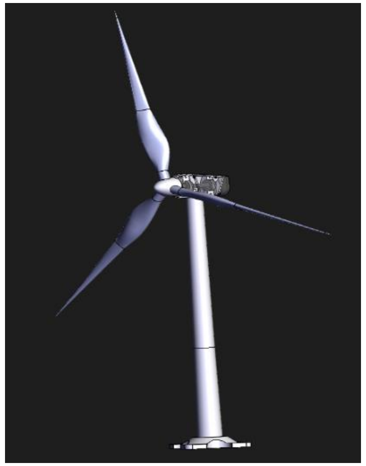
Sample parametric realizations => Full-order HFM evaluations

Projection-based reduction via POD

Local ROMs

MAC-based clustering

Physics-based parametric Reduced Order Model



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

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Framework Components - Explanation

Modal Assurance Criterion-guided clustering/sampling

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 modes**
  => *Relate subspace eigenvectors*
  => Dynamics-based clustering
  => Define sampling rate adaptively

Framework Components - Explanation

Modal Assurance Criterion-guided clustering/sampling

Modal Assurance Criterion

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

Advantages / Implications

- **MAC assumes functionality of error indicator**
- ***Enables adaptive sampling (coarse rate to finer)***
  => Reduces training cost/resources
- ***Physics-based interpretability***
  => MAC relates local dynamics

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Framework Components – Limitations
Projection-based parametric ROM bottleneck

POD - Projection-based Reduction

Assemble POD Basis

Proper Orthogonal Decomposition

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

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

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*

Ongoing research
Not addressed in this contribution

Framework Components – Limitations

Projection-based parametric ROM bottleneck

Training / Offline Phase

Step 1: Parametric input states

$$\forall \mathbf{p}_k, k \in [1, N_s]$$

Step 2: Time Integration of Full Model

$$\forall t_i, i \in [0, N_t]$$

For each parametric state:

- Assemble **system matrices**
  (stiffness K / mass M / damping C / *Excitation f*
- Evaluate the **time domain response** (integration)

The full-order, high fidelity finite element model **depends on a parametric input state.**

The parametric states are first sampled. The respective **parameters may represent**:

- ***system properties:*** *yield stress, hysteretic damping coeffs.*
- ***excitation traits:*** *amplitude of ground motion, frequency content*

Notation:
n : Full-order dimension
N_s : Number of training samples
N_t : Number of simulated timesteps
$\mathbf{M}$: Mass matrix
$\mathbf{f}$: External forcing
$\mathbf{u}$: Response solution

Framework Components – Limitations

Projection-based parametric ROM bottleneck

Training / Offline Phase

Step 1: Parametric input states

$$\forall \mathbf{p}_k, k \in [1, N_s]$$

Step 2: Time Integration of Full Model

$$\forall t_i, i \in [0, N_t]$$

Step 3: Assemble matrices and evaluate Equations of Motion

$$\mathbf{M}(\mathbf{p})\ddot{\mathbf{u}}(t_i) + \mathbf{g}_i(\mathbf{u}(t_i), \dot{\mathbf{u}}(t_i), \mathbf{p}) - \mathbf{f}(\mathbf{t_i}, \mathbf{p}) = \mathbf{0}$$

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

Nonlinear terms

Step 4: Compute Residual and “predict” correction

$$if \quad \mathbf{R}_i(\mathbf{u}_r(t_i)) > tol => \tilde{\mathbf{u}}(t_i)$$

Step 5: Employ updated solution to re-assemble nonlinear terms & matrices

$$\tilde{\mathbf{u}}(t_i) => \mathbf{g}_i(\tilde{\mathbf{u}}(t_i), \dot{\tilde{\mathbf{u}}}(t_i), \mathbf{p})$$

Notation:
- N_s: Full-order dimension
- n : Number of training samples
- N_t : Number of simulated timesteps
- $\mathbf{M}$: Mass matrix
- $\mathbf{f}$: External forcing
- $\mathbf{u}$: Response solution

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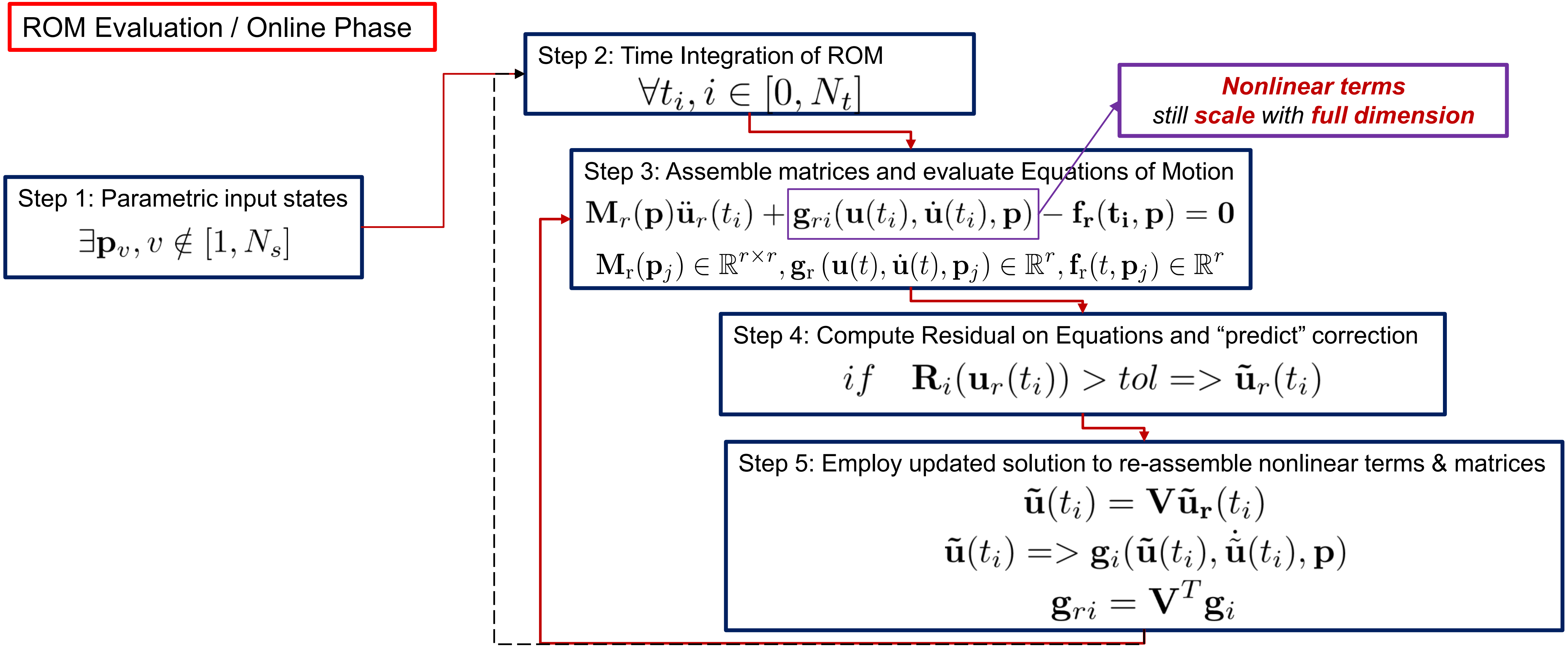
Framework Components – Limitations

Projection-based parametric ROM bottleneck



Framework Components – Limitations

Projection-based parametric ROM bottleneck

Step 2: Time Integration of ROM

$$\forall t_i, i \in [0, N_t]$$

Step 3: Assemble matrices and evaluate Equations of Motion

$$\mathbf{M}_r(\mathbf{p})\ddot{\mathbf{u}}_r(t_i) + \mathbf{g}_{ri}(\mathbf{u}(t_i), \dot{\mathbf{u}}(t_i), \mathbf{p}) - \mathbf{f}_\mathrm{r}(\mathbf{t_i}, \mathbf{p}) = \mathbf{0}$$

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

Nonlinear terms
*still **scale** with **full dimension***

Step 4: Compute Residual on Equations and "predict" correction

$$if \quad \mathbf{R}_i(\mathbf{u}_r(t_i)) > tol => \tilde{\mathbf{u}}_r(t_i)$$

Step 5: Employ updated solution to re-assemble nonlinear terms & matrices

$$\tilde{\mathbf{u}}(t_i) = \mathbf{V}\tilde{\mathbf{u}}_\mathbf{r}(t_i)$$

$$\tilde{\mathbf{u}}(t_i) => \mathbf{g}_i(\tilde{\mathbf{u}}(t_i), \dot{\tilde{\mathbf{u}}}(t_i), \mathbf{p})$$

$$\mathbf{g}_{ri} = \mathbf{V}^T\mathbf{g}_i$$

- The evaluation of the nonlinear terms still ***scales with the full order dimension.***
- For every solution increment we need to:
  - ***Project*** displ./vel. ***back to full-order***
  - Evaluate nonlinear terms
  - ***Update*** forces and stiffness matrix
  - ***Project*** updated matrices ***back to reduced-order*** coordinates.

*This **back-and-forth projection is a major computational bottleneck**.*

Especially in large scale systems
where time integration savings cannot outweigh
the projection & evaluation.

*To address this, we rely on **hyper-reduction:***
A second-tier approximation of the nonlinear contributions.

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Machine Learning Boosted pROM

Hyper-Reduction surrogate through ML

- **Back & forth projection** to update nonlinear terms **compromises efficiency**
- Hyper-reduction is introduced
  - *Several alternatives available (ECSW, DEIM, GNAT, EQM)*
  - ✓ Hyper-reduction **is essential for efficiency**
    - ❖ Introduces an ***additional source of error*** that outweighs the POD reconstruction error

=> Bottleneck for the parametric ROM

Step 5: Employ updated solution to re-assemble nonlinear terms & matrices

$$\tilde{\mathbf{u}}(t_i) = \mathbf{V}\tilde{\mathbf{u}}_{\mathbf{r}}(t_i)$$

$$\tilde{\mathbf{u}}(t_i) => \mathbf{g}_i(\tilde{\mathbf{u}}(t_i), \dot{\tilde{\mathbf{u}}}(t_i), \mathbf{p})$$

$$\mathbf{g}_{ri} = \mathbf{V}^T\mathbf{g}_i$$

✓ ***N3-PROM***

- ***Replaces hyper-reduction*** with NARX-NN surrogate
- Learns ***nonlinear mapping directly in ROM coordinates***
- Every iteration contributes nonlinear mapping training data
  => A single training realization has thousands of datapoints
- Potential ***superiority in efficiency*** => ***Real-time evaluations***

Nonlinear force terms ←

$$f_g(\mathbf{u}_r^{t_{k-w}:t_k}, \mathbf{g}_r^{t_{k-w}:t_k}) \rightarrow \mathbf{g}_r^{t_k}$$

Nonlinear stiffness terms ←

$$f_K(\mathbf{u}_r^{t_{k-w}:t_k}, \mathbf{K}_r^{t_{k-w}:t_k}) \rightarrow \mathbf{K}_r^{t_k}$$

Machine Learning Boosted pROM

Network implementation details

Neural Network Details

Hyperparameter	Value
Time lag parameter	$\{4\}$
Number of hidden layers	$\{10\}$
Size of hidden layers	$\{16\}$
Activation of layers	Hyperbolic tangent functions $tanh(\cdot)$
Activation of output neuron	Linear
Input/Output data scaling	Min-Max in $[0, 1]$
Batch size	$\{64\}$
Optimizer	Adam
Initial learning rate	$\{0.001\}$
Loss function	MSE loss

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- Potential ***superiority in efficiency*** => ***Real-time evaluations***

✓ ***NARX-NN training process***

- *High fidelity simulations on training samples*
- *Local ROMs assembly and MAC-guided clustering*
- ***For every cluster train a separate NN mapping***
- *The **mapping data on the ROM coordinates** are produced for each sample **based on the cluster's projection basis***
- *90% of samples are used for NN training, 10% for testing*
- ***All datapoints of the time history response are used** for training/testing respectively*

Numerical Validation

Case study description

Two-story shear frame with hysteretic links

Sinusoidal 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:*

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

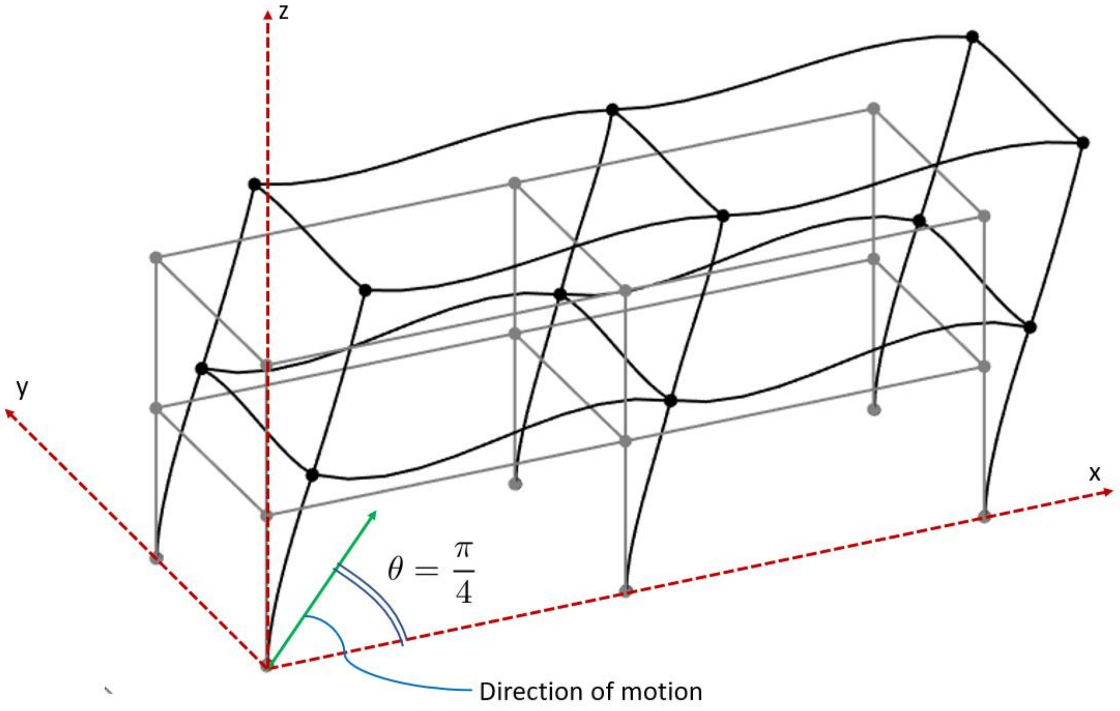
$$\nu(t) = 1.0 + \delta_\nu \epsilon(t), \quad \eta(t) = 1.0 + \delta_\eta \epsilon(t), \quad \epsilon(t) = \int_0^t \mathbf{z}\dot{\mathbf{u}}\delta t$$

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*

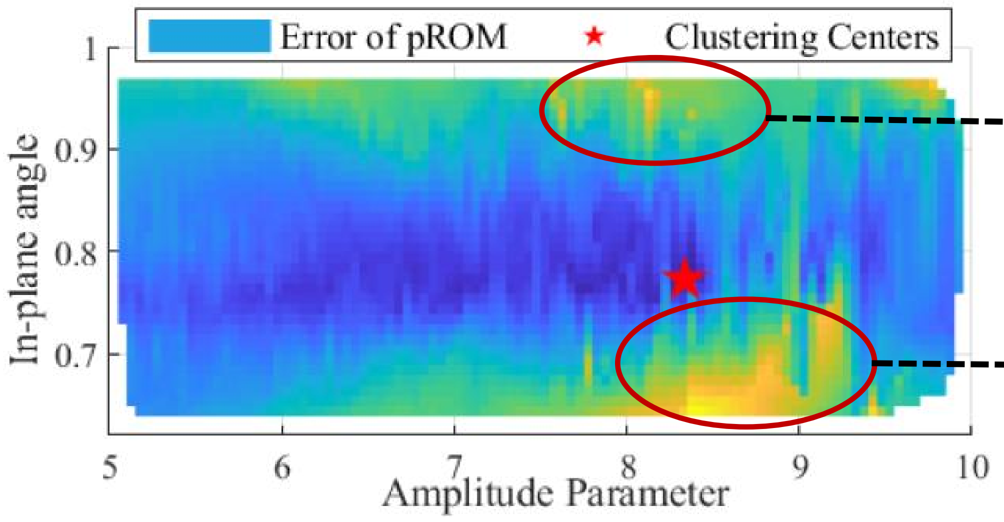


Benchmark example featured in:

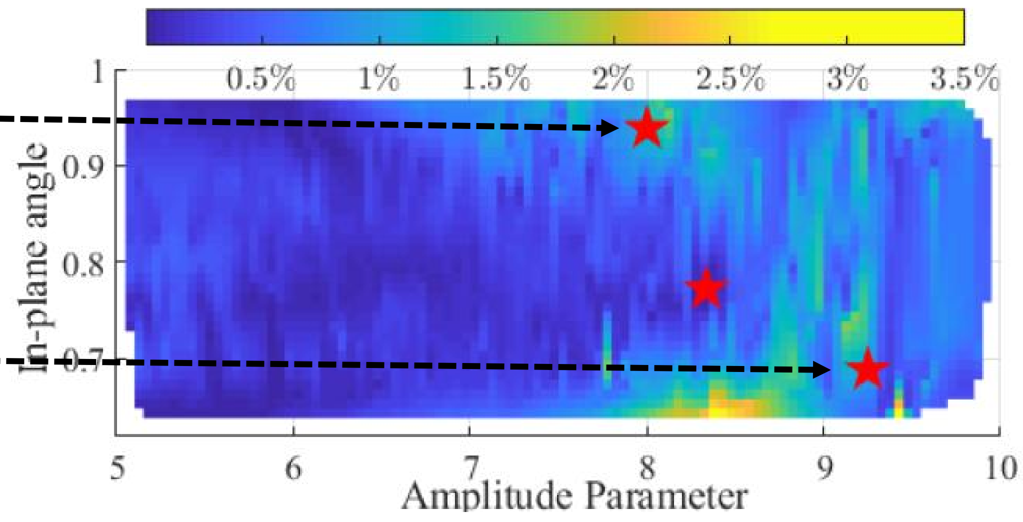
- Vlachas K. et al. "A local basis approximation approach for nonlinear parametric model order reduction." *Journal of Sound and Vibration* 502 (2021): 116055.
- Vlachas K. et al. " Two-story frame with Bouc-Wen hysteretic links as a multi-degree of freedom nonlinear response simulator." 5th edition of Workshop on Nonlinear System Identification Benchmarks, https://github.com/KosVla/NonlinearBoucWenFrameBenchmark.git, 2021.

Numerical Validation

Performance of MAC-guided clustering



Initial approximation error
(One single cluster)



Final approximation error
(Three clusters)

Numerical Validation

Network mapping example

✓ ***N3-PROM***

- ***Replaces hyper-reduction*** with NARX-NN surrogate
- Learns ***nonlinear mapping directly in ROM coordinates***
- Every iteration contributes nonlinear mapping training data
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- Potential ***superiority in efficiency*** => ***Real-time evaluations***

$$f_g(\mathbf{u}_r^{t_{k-w}:t_k}, \mathbf{g}_r^{t_{k-w}:t_k}) \rightarrow \mathbf{g}_r^{t_k}$$

$$f_K(\mathbf{u}_r^{t_{k-w}:t_k}, \mathbf{K}_r^{t_{k-w}:t_k}) \rightarrow \mathbf{K}_r^{t_k}$$

Example Detailed Task Formulation

Input:

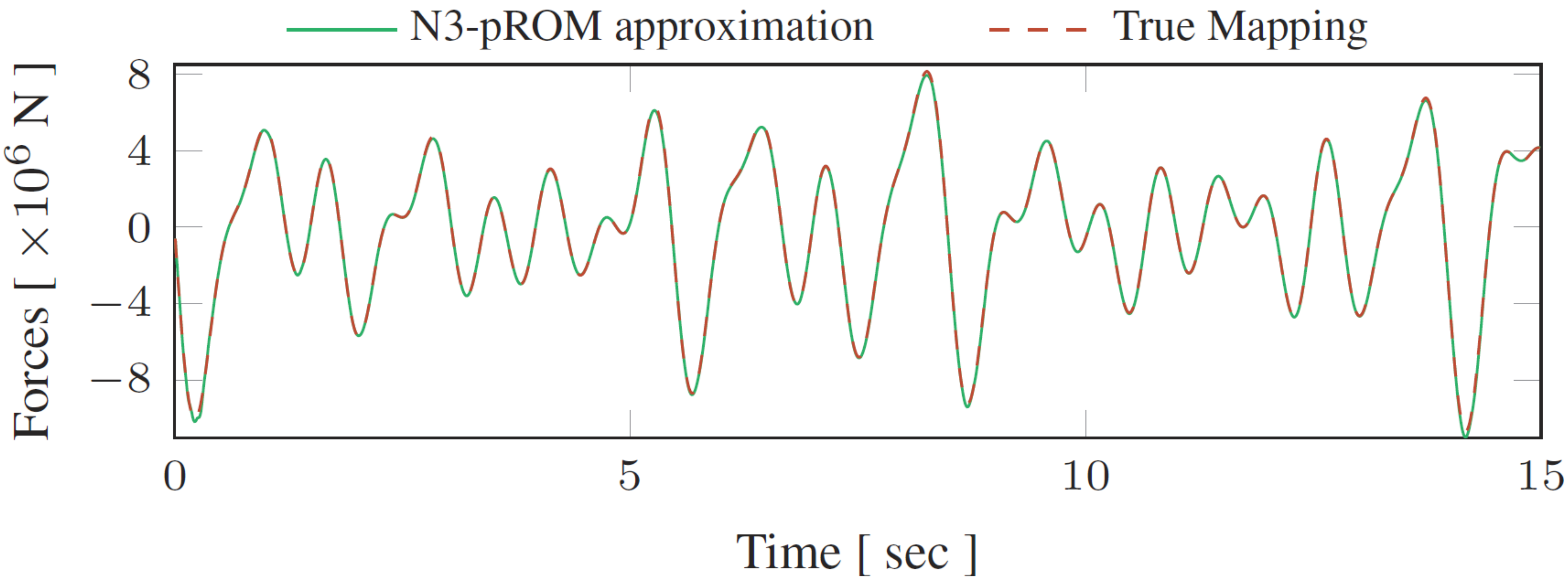
- *Reduced-Order Displacements in current iteration (and previous ones)* $\rightarrow \mathbf{U} \in \mathbb{R}^{4\times(t_{k-w}:t_k)}$
- *Reduced-Order Force terms in previous iteration(s)* $\rightarrow \mathbf{g} \in \mathbb{R}^{4\times(t_{k-w}:t_k)}$
- *Reduced-Order Stiffness terms in previous iteration(s)* $\rightarrow \mathbf{K} \in \mathbb{R}^{4\times4\times(t_{k-w}:t_k)}$

Output:

- *Reduced-Order Force terms in current iteration* $\rightarrow \mathbf{K} \in \mathbb{R}^{4\times4\times1}$
- *Reduced-Order Stiffness terms in current iteration* $\rightarrow \mathbf{g} \in \mathbb{R}^{4\times1}$

Numerical Validation

Accuracy performance of the NARX-NN surrogate



Reduced internal forces approximation
(***Coordinate d=1***)

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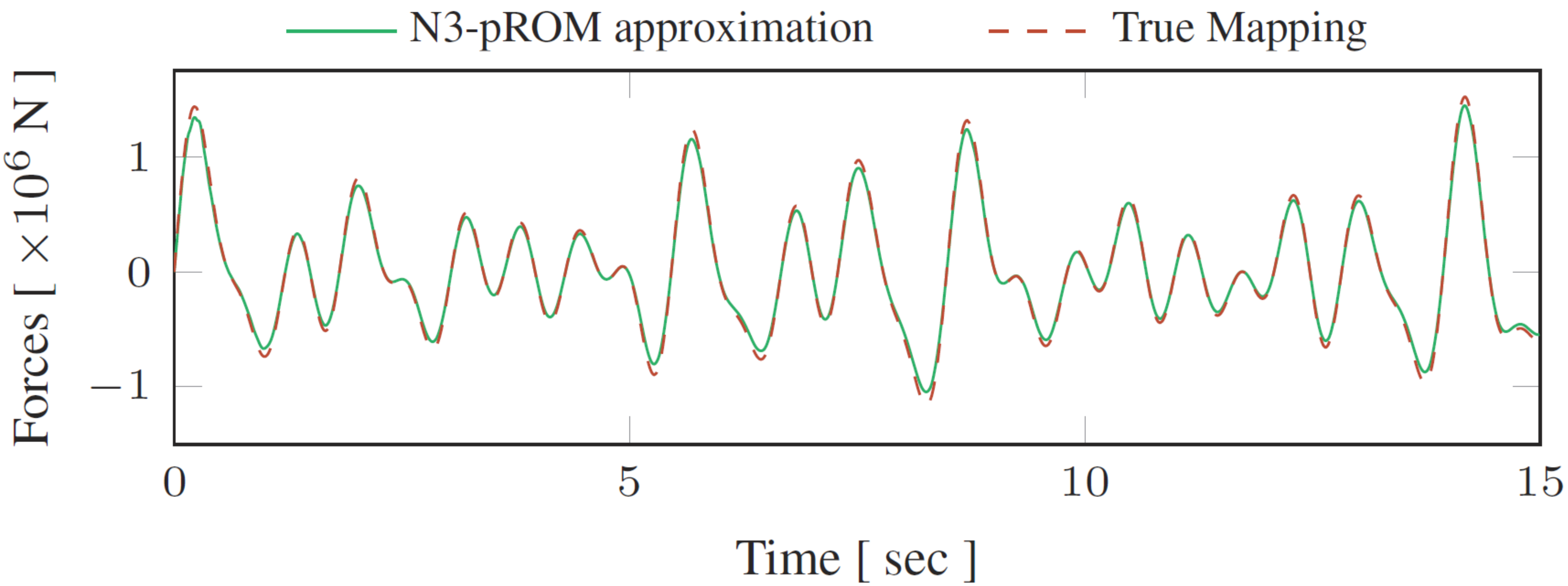
Numerical Validation

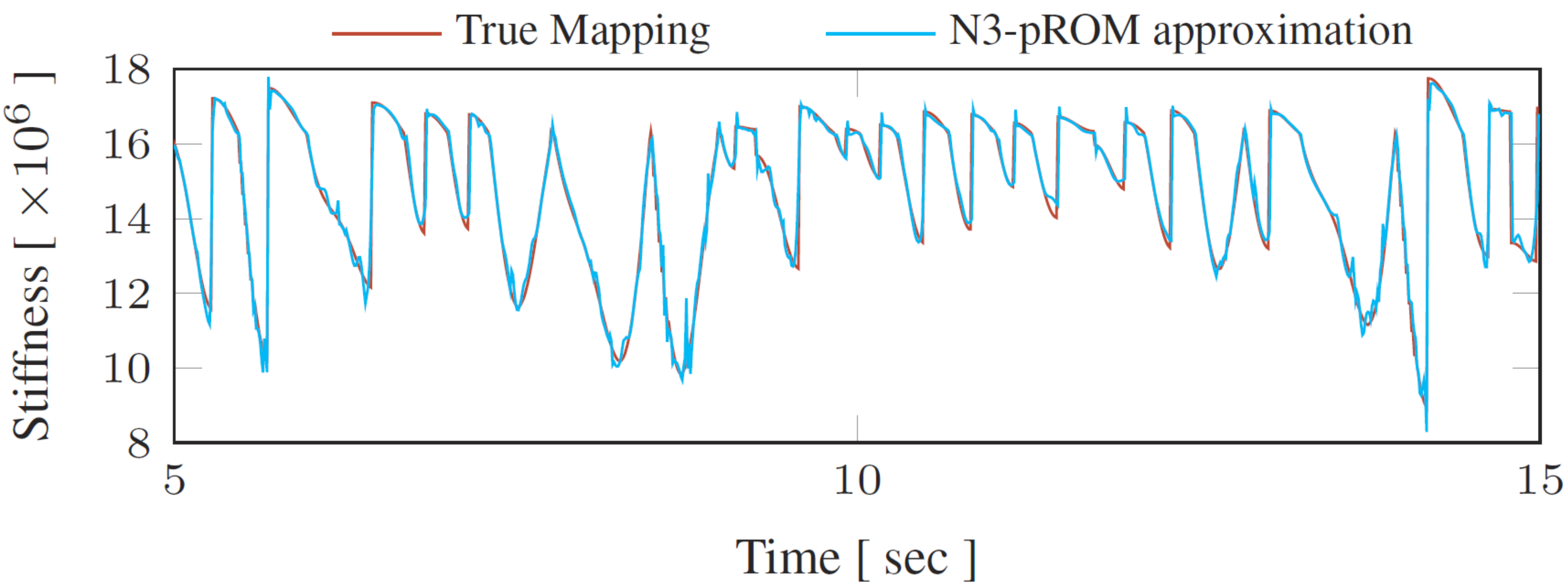
Accuracy performance of the NARX-NN surrogate



Reduced internal forces approximation
(***Coordinate d=4***)

Numerical Validation

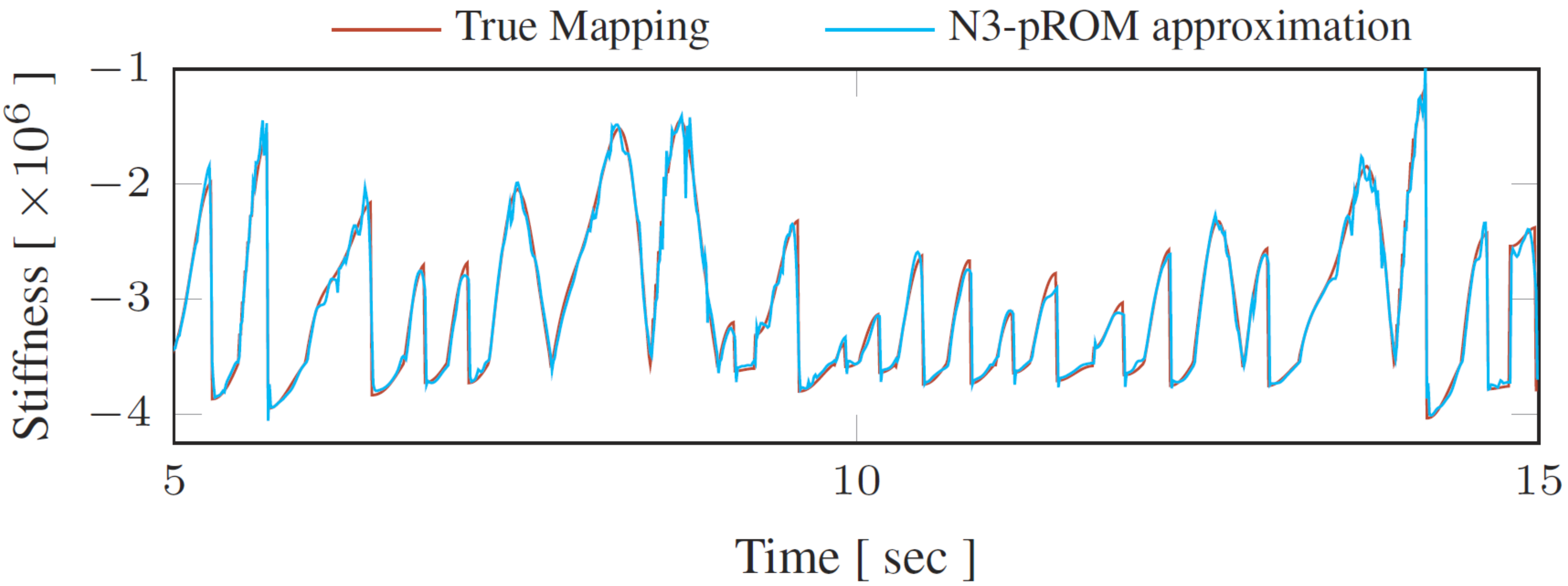
Accuracy performance of the NARX-NN surrogate



Reduced stiffness terms approximation

(***Coordinate d=3***)

Numerical Validation
Accuracy performance of the NARX-NN surrogate



Reduced stiffness terms approximation
(***Coordinate d=15***)

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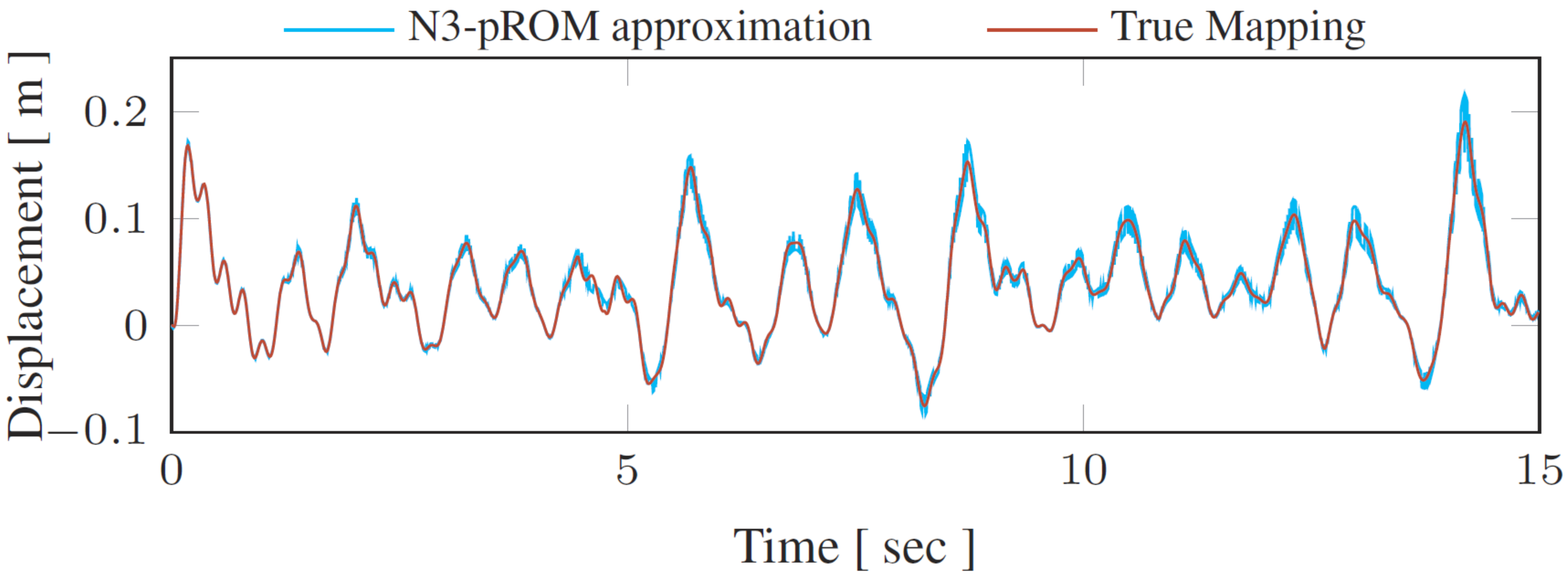
Numerical Validation

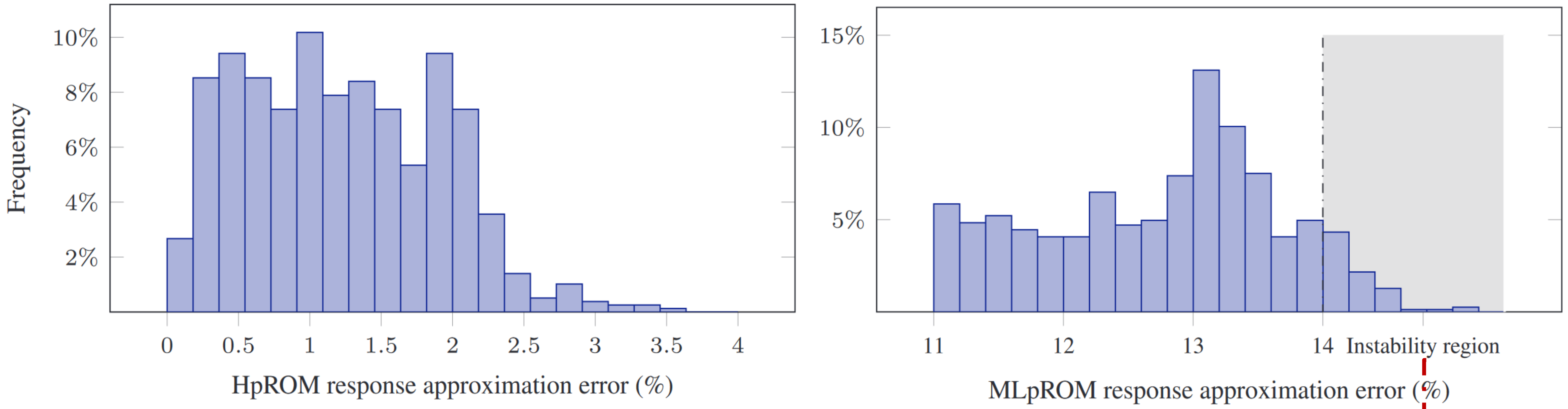
Accuracy performance of the ML-boosted pROM



Reduced stiffness terms approximation

(***Coordinate d=15***)

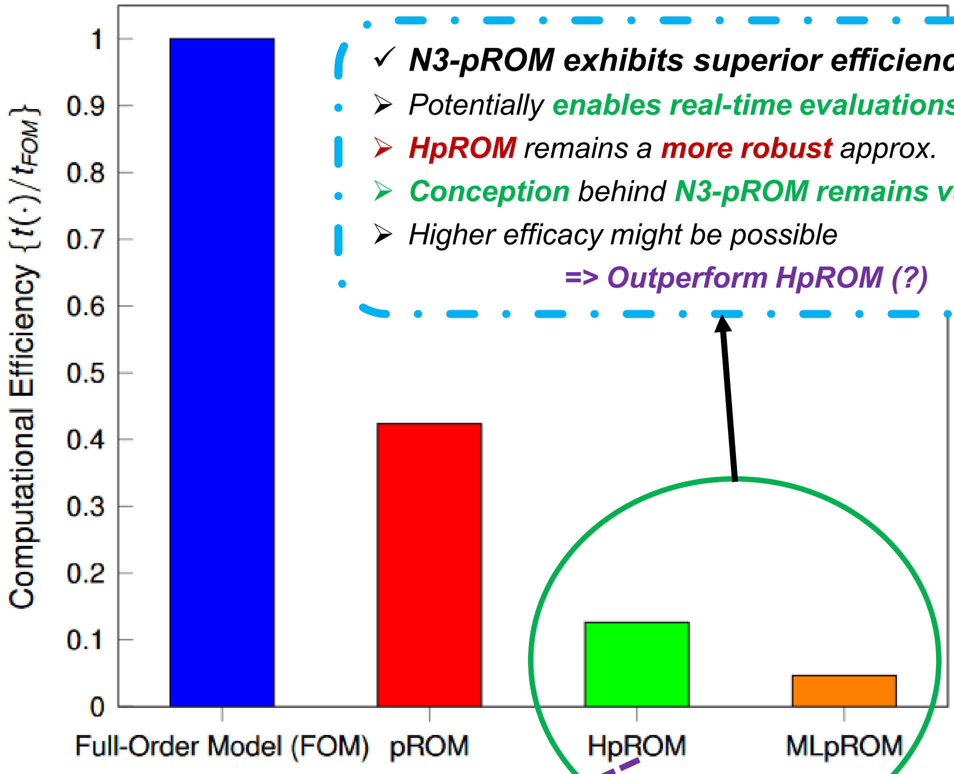
Numerical Validation
Performance Comparison



- ✓ ***Potential Improvements & Extensions***
  - ➢ ***Instabilities*** *due to error propagation*
    - ✓ *Use* ***only displacement as input***
    - ✓ *Don't feed in previous predictions in closed loop*
  - ➢ *Use* ***temporal CNNs*** *or other surrogates to* ***improve accuracy***

Numerical Validation

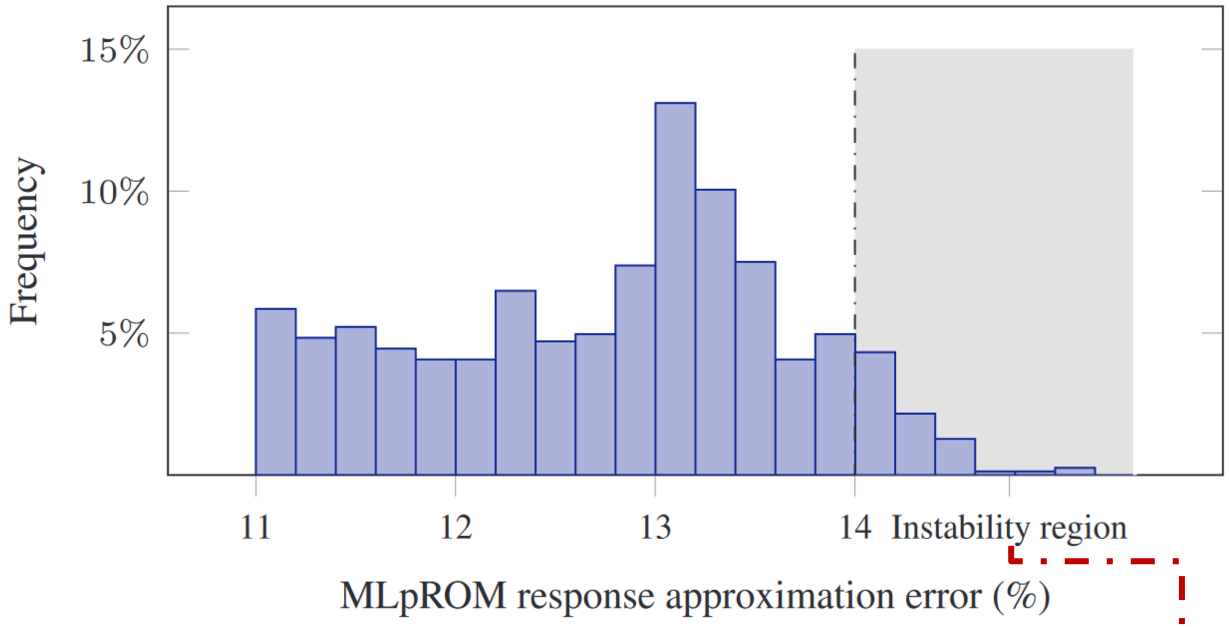
Performance Comparison



- ✓ ***N3-pROM exhibits superior efficiency***
  - ➢ *Potentially* ***enables real-time evaluations***
  - ➢ ***HpROM*** *remains a* ***more robust*** *approx.*
  - ➢ ***Conception*** *behind* ***N3-pROM remains valid***
  - ➢ *Higher efficacy might be possible*

  => Outperform HpROM (?)

Hyper-Reduction pROM



- ✓ ***Potential Improvements & Extensions***
  - ➢ ***Instabilities*** *due to error propagation*
    - ✓ *Use* ***only displacement as input***
    - ✓ *Don't feed in previous predictions in closed loop*
  - ➢ *Use* ***temporal CNNs*** *or other surrogates to* ***improve accuracy***

Concluding remarks

Limitations and outlook

The proposed machine-learning boosted N3-pROM

- ✓ Exhibits *superior efficiency* and potentially *enables (near) real-time ROM evaluations*
- ✓ *Captures underlying dynamics* and dependencies employing *dynamics-based clustering*
- ✓ Proposes a way to exploit machine learning tools to potentially *enhance the performance* of traditional projection-based ROMs to *deliver superior frameworks*
- ✓ May be adapted as an ***approximative, online low-cost surrogate*** for *Structural Health Monitoring* applications

- ➢ Proof-of-concept case study, generalization and implementation on large numerical case studies is needed
- ➢ Instabilities due to error propagation in closed loop formulation
- ➢ Parametric dependencies on the nonlinear mapping level need to be addressed
- ➢ Hyper-Reduction pROM remains a more robust approximation

Next short-term steps:

- ❖ *Treat instabilities* by modifying the surrogate so as not to rely on previous predictions
- ❖ *Generalize implementation*:
  - Improve surrogate accuracy by employing superior NN-based mappings
  - Treat dependencies on the nonlinear mapping level
  - Apply approach on large scale case studies
- ❖ Generalize machine-learning boosted pROM by *addressing the POD projection limitation*

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Question session

IMAC X IT'S NOT JUST MODAL ANYMORE IMAC XL