14th International Conference on Structural Safety and Reliability - ICOSSAR'25
1-6 June, 2025 - Los Angeles California, USA
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METAMODELING OF NONLINEAR STOCHASTIC DYNAMIC SYSTEMS WITH HYBRID NEURAL OPERATOR SCHEMES

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Key words: Numerical simulations, Deep learning, Metamodeling

Abstract. In evaluating high-dimensional, nonlinear, and dynamic structural systems subjected to extreme natural hazards, incorporating uncertainty remains a challenging computational task. Recent advancements in neural networks as metamodeling techniques have shown promise in addressing this issue, yet significant hurdles persist. First, traditional neural networks are fundamentally designed to map finite-dimensional vector spaces, while dynamic structural systems inherently exist in infinite-dimensional function spaces characterized by continuous temporal and spatial variations. Consequently, conventional architectures often struggle to capture the complex behaviors of such systems over time histories and exhibit limited generalization outside their training distribution. Second, many existing approaches, including physics-informed machine learning frameworks, fail to guarantee that predicted solutions during inference strictly adhere to essential physical constraints, reducing their reliability for practical applications. This study presents a novel framework that integrates neural operators—an emerging machine learning paradigm designed to learn mappings between infinite-dimensional function spaces—with traditional numerical methods such as the Newmark-beta scheme. The framework's effectiveness is validated through its application to a steel moment-resisting frame subjected to stochastic seismic loads. Results demonstrate that the proposed approach achieves high accuracy and considerable computational speed-up compared to traditional numerical methods.

1 INTRODUCTION

In structural engineering, the dynamic behavior of structural systems is governed by ordinary differential equations (ODEs), namely the equations of motion. While analytical solutions can be derived for linear systems subjected to general excitations, real-world structures typically exhibit high dimensionality—with hundreds of degrees of freedom (DOFs)—and nonlinear behavior due to extreme loads that are stochastic and model the effects of natural hazards, such as earthquakes. Solving these complex, nonlinear ODEs necessitates numerical integration schemes. However, for large-scale structural systems with complex nonlinear behaviors, numerical simulations become computationally intensive, particularly for tasks requiring repeated evaluations, such as uncertainty quantification [1] and design optimization [2].

With recent advancements in machine learning, neural network architectures—such as Long Short-Term Memory (LSTM) networks, Transformers, and Convolutional Neural Networks (CNNs)—have been increasingly explored for metamodeling dynamic responses of structural systems under stochastic excitations [3, 4, 5, 6]. These methods were preceded by approaches based on system identification, which provided the initial motivation [7, 8]. In addition, physics-informed machine learning (PIML) approaches have been introduced to directly embed physical laws, particularly the equation of motion, into the learning process, thereby enhancing model interpretability, improving predictive accuracy, and reducing the need for extensive training datasets ([9, 10, 11, 12]). These methods typically incorporate the residuals of the equation of motion into the loss function, providing weak supervision that encourages adherence to known physical principles during training.

The present study addresses a key limitation of traditional physics-informed frameworks, where physical constraints are only enforced during training, leading to neural networks that operate without adherence to governing equations during inference. To overcome this, a novel hybrid framework has been developed, integrating classical numerical methods with modern neural operators to maintain consistency with underlying equations even during inference.

This approach specifically combines the implicit time-stepping algorithm of the Newmark-β method with DeepONet to quickly approximate nonlinear restoring forces, accelerating dynamic response simulations while preserving physical fidelity. This results in a computationally efficient method for modeling complex, nonlinear structural systems subjected to stochastic loading. To enhance efficiency, the neural operators expedite the computation of restoring forces, addressing the computational burden of traditional schemes, even of recent development [13]. Periodically, the proposed framework reverts to the classical Newmark-β method to ensure continued adherence to physical constraints.

The framework's effectiveness is demonstrated through its application to a fiber-discretized nonlinear steel moment-resisting frame under stochastic seismic excitation. Results highlight that this physics-informed LSTM network achieves high accuracy and significant computational speed-up compared to traditional methods, offering a robust solution for simulating structural responses under uncertainty.

2 PROPOSED FRAMEWORK

2.1 Background solver

The response trajectories of nonlinear dynamic systems driven by general stochastic excitation can be estimated by solving the following set of nonlinear ordinary differential equations:

$$\mathbf{M}\,\ddot{\mathbf{u}}(t) + \mathbf{C}\,\dot{\mathbf{u}}(t) + f_{\mathrm{nl}}\big(t;\, \mathbf{u}(t)\big) = \mathbf{F}(t). \tag{1}$$

where $\mathbf{u}(t)$, $\dot{\mathbf{u}}(t)$, and $\ddot{\mathbf{u}}(t)$ are the vectors collecting the displacement, velocity, and acceleration trajectories of the system; $\mathbf{M}$ and $\mathbf{C}$ are the mass and damping matrices of the system; $f_{\mathrm{nl}}(t;\, \mathbf{u}(t))$ is the nonlinear restoring force that generally depends on the displacement and velocity response of the system; and $\mathbf{F}(t)$ is the vector of external stochastic excitation. After discretizing Eq.(1), the proposed framework uses an implicit Newmark-β time-integration scheme to solve the nonlinear ordinary differential equation. Specifically, give the solution at i $(\mathbf{u}_i, \dot{\mathbf{u}}_i, \ddot{\mathbf{u}}_i)$ the time-integration scheme aims to obtain the solution at $i+1$ $(\mathbf{u}_{i+1}, \dot{\mathbf{u}}_{i+1}, \ddot{\mathbf{u}}_{i+1})$ with a pre-determined change in time-step, Δt.

In more detail, given the solution of the displacement response at time-step $i+1$ and the previous state of the structure at i, the Newmark-β scheme approximates the acceleration and velocity response as follows:

$$\dot{\mathbf{u}}_{\mathbf{i+1}} = \frac{\gamma}{\beta\,\Delta t}\left(\mathbf{u}_{\mathbf{i+1}} - \mathbf{u}_{\mathbf{i}}\right) + \Big(1 - \tfrac{\gamma}{\beta}\Big)\dot{\mathbf{u}}_{\mathbf{i}} + \Delta t\,\Big(1 - \tfrac{\gamma}{2\beta}\Big)\ddot{\mathbf{u}}_{\mathbf{i}}, \tag{2}$$

$$\ddot{\mathbf{u}}_{\mathbf{i+1}} = \frac{1}{\beta\,\Delta t^2}\left(\mathbf{u}_{\mathbf{i+1}} - \mathbf{u}_{\mathbf{i}}\right) - \frac{1}{\beta\,\Delta t}\,\dot{u}_i - \Big(\frac{1}{2\beta} - 1\Big)\ddot{\mathbf{u}}_{\mathbf{i}}. \tag{3}$$

where β and γ are the parameters for the Newmark scheme that govern whether the approximation is obtained through the assumption of linear or constant acceleration method between the time-steps. To enforce the equilibrium at $i+1$ while solving for the displacement response, the discretized version of Eq. (1) at time-step $i+1$ needs to be obtained, and the residual of the equation is written as follows:

$$\mathbf{R}(\mathbf{u}_{i+1}) = \mathbf{M}\,\ddot{\mathbf{u}}_{i+1} + \mathbf{C}\,\dot{\mathbf{u}}_{i+1} + f_{\mathrm{nl}}\big(\mathbf{u}_{i+1}\big) - \mathbf{F}_{i+1} = \mathbf{0} \tag{4}$$

Since the formulation of $\mathbf{R}(\mathbf{u}_{i+1})$ is nonlinear due to the nonlinear restoring force, the root of $\mathbf{R}(\mathbf{u}_{i+1}) = \mathbf{0}$ is obtained by iteration through the Newton-Raphson method. More specifically, at iteration j:

$$\mathbf{R}^{(j)} = \mathbf{M}\,\ddot{\mathbf{u}}_{i+1}^{(j)} + \mathbf{C}\,\dot{\mathbf{u}}_{i+1}^{(j)} + \mathbf{f}_{nl}\big(\mathbf{u}_{i+1}^{(j)}\big) - \mathbf{F}_{i+1}, \tag{5}$$

$$\mathbf{K}_T^{(j)} = \frac{\partial \mathbf{R}}{\partial \mathbf{u}_{i+1}}\Big|_{\mathbf{u}_{i+1}^{(j)}} = \frac{1}{\beta\Delta t^2}\,\mathbf{M} + \frac{\gamma}{\beta\Delta t}\,\mathbf{C} + \frac{\partial \mathbf{f}_{nl}}{\partial \mathbf{u}}\big(\mathbf{u}_{i+1}^{(j)}\big), \tag{6}$$

$$\Delta\mathbf{u}^{(j)} = -\big[\mathbf{K}_T^{(j)}\big]^{-1}\,\mathbf{R}^{(j)}, \tag{7}$$

$$\mathbf{u}_{i+1}^{(j+1)} = \mathbf{u}_{i+1}^{(j)} + \Delta\mathbf{u}^{(j)}. \tag{8}$$

The process is repeated until the pre-specified criterion of convergence is met. The exact steps of the algorithms are as follows:

1. Precompute coefficients

$$a_0 = \frac{1}{\beta\Delta t^2},\ a_1 = \frac{\gamma}{\beta\Delta t},\ a_2 = \frac{1}{\beta\Delta t},\ a_3 = \frac{1}{2\beta} - 1,\ a_4 = \frac{\gamma}{\beta} - 1,\ a_5 = \Delta t\Big(\frac{\gamma}{2\beta} - 1\Big).$$

2. Compute the *effective load*

$$\mathbf{p}^* = \mathbf{F}_{i+1} + \mathbf{M}\big(a_0\,\mathbf{u}_i + a_2\,\dot{\mathbf{u}}_i + a_3\,\ddot{\mathbf{u}}_i\big) + \mathbf{C}\big(a_4\,\dot{\mathbf{u}}_i + a_5\,\ddot{\mathbf{u}}_i\big).$$

3. Initialize Newton loop: $\mathbf{u}_{i+1}^{(0)} = \mathbf{u}_i$.

4. For $j = 0, 1, \ldots$ until convergence:

$$\begin{aligned}&\text{Assemble } \mathbf{R}^{(j)}, \quad \mathbf{K}_T^{(j)},\\ &\text{Solve } \mathbf{K}_T^{(j)}\,\Delta\mathbf{u}^{(j)} = \mathbf{R}^{(j)},\\ &\mathbf{u}_{i+1}^{(j+1)} = \mathbf{u}_{i+1}^{(j)} + \Delta\mathbf{u}^{(j)}.\end{aligned}$$

5. Upon convergence, set $\mathbf{u}_{i+1} = \mathbf{u}_{i+1}^{(j+1)}$ and calculate $\dot{\mathbf{u}}_{i+1}$ and $\ddot{\mathbf{u}}_{i+1}$ through Eq.2 and Eq.3

6. Advance $i \leftarrow i + 1$ and repeat.

Although it is possible to use the initial tangent stiffness at each iteration of the Newton-Raphson method to potentially alleviate computational costs (i.e, $\mathbf{K}_T^{(j)} = \mathbf{K}$), the estimation of the term $\mathbf{f}_{nl}\big(\mathbf{u}_{i+1}^{(j)}\big)$ is inevitable for the calculation of $\mathbf{R}^{(j)}$, and most expensive computations happens in calculating the term $\mathbf{f}_{nl}\big(\mathbf{u}_{i+1}^{(j)}\big)$. Therefore, this work proposes to use DeepOnet to surrogate the calculation of the restoring force.

2.2 Estimation of restoring forces with DeepONet and multi-layer perceptrons

DeepONet is a popular operator-learning architecture designed to approximate an operator $\mathcal{G} : \mathcal{X} \to \mathcal{Y}$,which maps an input function $w(x) \in \mathcal{X}$ to an output function $v(y) = \mathcal{G}(w)(y) \in \mathcal{Y}$. To achieve such as task, DeepONet uses into two sub-networks to a, the branch network and trunk network [14].

The branch network B takes the values of w at m discrete locations $\{x_1, \dots, x_m\}$ and produces a p-dimensional "basis" vector:

$$\mathbf{b} = B\big(w(x_1), \dots, w(x_m)\big) = (b_1, \dots, b_p)^\top \in \mathbb{R}^p. \tag{9}$$

The trunk network T takes the query coordinate $y \in \mathbb{R}^d$ and outputs another p-dimensional vector of basis functions:

$$\mathbf{t}(y) = T(y) = \big(t_1(y), \dots, t_p(y)\big)^\top \in \mathbb{R}^p. \tag{10}$$

Their outputs are combined via an inner product (plus bias b_0) to produce the DeepONet prediction:

$$\widehat{v}(y) = \sum_{i=1}^{p} b_i\, t_i(y) \; + \; b_0 = \mathbf{b}^\top\, \mathbf{t}(y) \; + \; b_0. \tag{11}$$

All weight matrices and biases in B and T are learned via standard back-propagation.

In the proposed approach, the branch network input is formed by concatenating the velocity vector $\dot{\mathbf{u}}_i$ and the nonlinear force vector $f_{\mathrm{nl}}\big(\mathbf{u}_{i+1}\big)$. The trunk network input is the incremental displacement $\Delta\mathbf{u}_i^{(j)} = \mathbf{u}_{i+1}^{(j)} - \mathbf{u}_i$. Hence, $\mathbf{b} = B\big(\mathbf{f}_{nl}(\mathbf{u}_i),\, \dot{\mathbf{u}}_i\big)$ and $\mathbf{t} = T\big(\Delta\mathbf{u}_i^{(j)}\big)$. Raw output of DeepONet is denoted by $\mathbf{z}_{i+1}^{j}$. Whenever the structure remains elastic, the restoring force update follows the exact linear relation:

$$\mathbf{f}_{nl}(\mathbf{u}_{i+1}^{(j)}) = \mathbf{K}\,\Delta\mathbf{u}_i^{(j)} + \mathbf{f}_{nl}(\mathbf{u}_i). \tag{12}$$

Instead of relying on DeepONet in those linear regimes, this work introduces a small gating MLP with sigmoid output:

$$\boldsymbol{\lambda}_{i+1}^{j} = \mathrm{MLP}\big(\mathbf{u}_i, \mathbf{f}_{nl}(\mathbf{u}_i),\; \mathbf{u}_{i+1}^{(j)}\big) \in [0,1]^n, \tag{13}$$

where n is the dimension of the restoring force vector. The proposed approach fuses the two prediction elements-wise as:

$$\hat{\mathbf{f}}_{nl}(\mathbf{u}_{i+1}^{(j)}) = \boldsymbol{\lambda}_{i+1}^{j} \odot \big(\mathbf{z}_{i+1}^{j} + \mathbf{f}_{nl}(\mathbf{u}_i)\big) + \big(\mathbf{1} - \boldsymbol{\lambda}_{i+1}^{j}\big) \odot \Big(\mathbf{K}\,\Delta\mathbf{u}_i^{(j)} + \mathbf{f}_{nl}(\mathbf{u}_i)\Big). \tag{14}$$

where $\hat{\mathbf{f}}_{nl}(\mathbf{u}_{i+1}^{(j)})$ is the predicted restoring force at time-step i and iteration j, $\odot$ denotes element-wise multiplication. If $\lambda_{i+1}^{j} = 0$ for a given component of the restoring force vector, then the component uses purely the linear update of Eq. (12). If $\lambda_{i+1}^j = 1$ for a given component of the restoring force vector, it relies entirely on the nonlinear DeepONet output (i.e, Eq. (11)). For intermediate values, the formulation blends the two predictions. This gating mechanism enables DeepONet to focus purely on nonlinear behaviors while defaulting to the exact linear update whenever appropriate.

To ensure the numerical stability of the neural networks during training and inference, the dimension of inputs and outputs of neural networks are reduced via principal component analysis. Furthermore, to prevent error accumulation during the inference, the structural system is periodically solved using the traditional Newmark-beta scheme.

3 CASE STUDY

3.1 Setup

To demonstrate the effectiveness of the proposed hybrid scheme, the authors conducted a case studies on a multi-degree-of-freedom (MDOF) nonlinear fiber-discretized frame, a widely used method in high-fidelity structural modeling within structural engineering. The case studies focused on a 37-story, six-span steel frame depicted in Fig. 1. The design of the structure is based on the structure outlined in [15, 16]. The columns have square box sections, while the beams are AISC wide-flange standard W24 sections. All sections possess Young's modulus of 200 GPa and yield stress of 355 MPa. Calculations for structural mass included consideration of a building density of 100 kg/m^3 per floor, in addition to the self-weight of the members. The structure is considered to be subjected to stochastic seismic loading of 60 second duration. The structural model was developed in MATLAB and solved with Newmark-β method with initial stiffness matrix. All structural members were modeled using displacement-based fiber-discretized finite elements with five integration points along their length and a Gauss-Legendre integration scheme. Each fiber within the discretization was assumed to follow an elastic-perfectly-plastic constitutive relationship. Rayleigh damping was considered and calibrated to provide damping ratios of 2.5 % at the first two natural frequencies. To define the seismic hazard, a site-specific analysis was considered corresponding to a 10% probability of exceedance in 50 years for subsurface ground conditions classified as Site Class D [15]. Using this hazard description, stochastic ground motions were generated following the model described in Rezaeian and Der Kiureghian [17]. To increase the nonlinearity of the structure, the stochastic ground motion was artificially scaled by a factor of ten. The generated ground motions had a duration of 60 seconds and a time step of 0.005 seconds for a total of 12000 time-steps. To train the neural networks, a total of 150 training/validation samples were generated. Further, 15 samples were used for testing the proposed framework. The hidden unit of the neural network is 256. The inputs and outputs of neural networks are reduced via principal component analysis (PCA) from 555 to 23.

3.2 Results

To evaluate the performance of the proposed framework, the hybrid scheme was assessed using 15 independent test samples (different seismic sequences). Figure 2 presents a comparison between a representative time-series response predicted by the traditional Newmark-β scheme and that predicted by the proposed hybrid scheme. While the hybrid scheme is capable of predicting the structural response across all degrees of freedom (DOFs), for clarity, only the horizontal responses are presented, as the majority of the structural deformation occurs in the horizontal direction. As illustrated, the hybrid scheme achieves exceptional predictive accuracy, with errors on the order of 10^{-3} meters.

Given that accurate prediction of peak responses is critical for practical engineering applications,

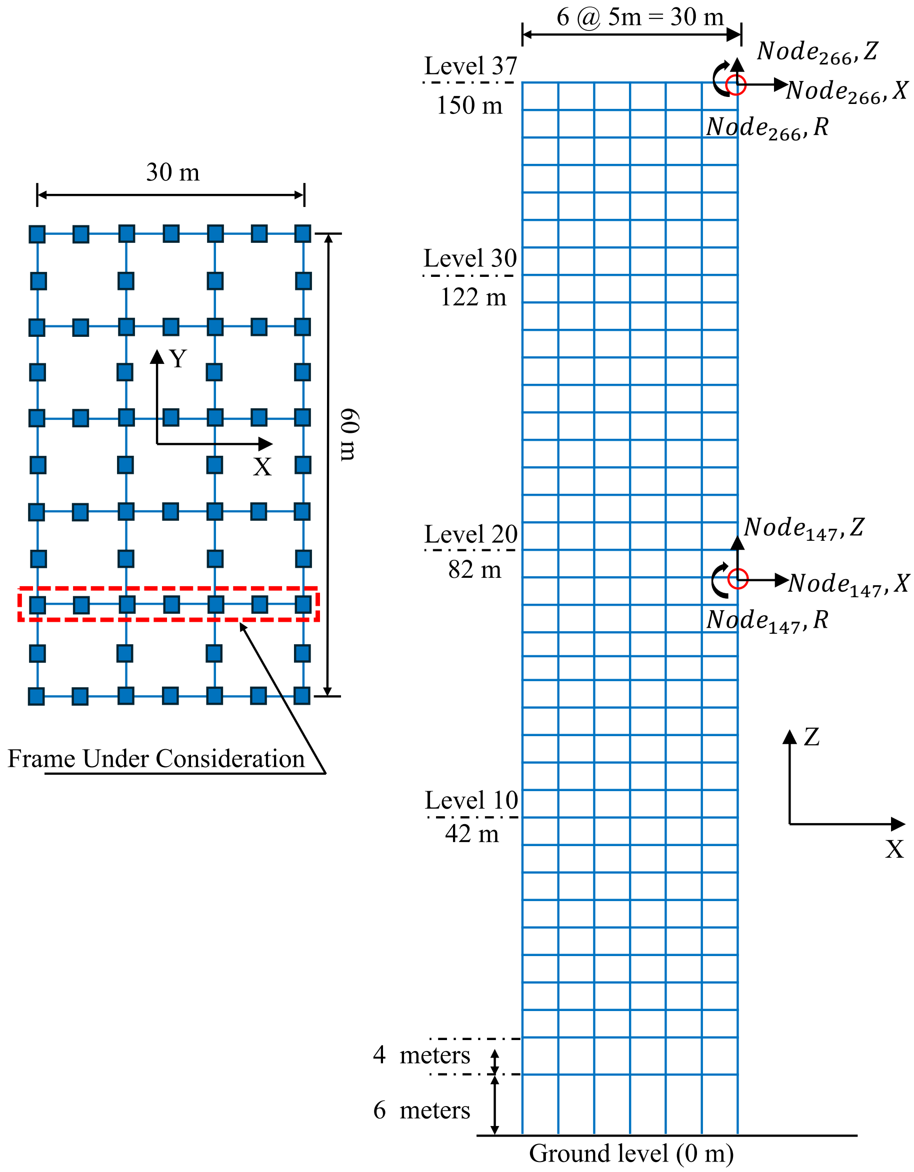

Figure 1: Layout of the 2D 37-story six-bay steel frame building.

Figure 3 examines the accuracy of peak horizontal response predictions by comparing the results of the proposed hybrid scheme with the ground truth obtained from the Newmark-β scheme. The proposed method demonstrates excellent correlation with the reference results.

In terms of computational efficiency, the hybrid scheme requires, on average, approximately 118.80 seconds to complete a single realization of the structural response, whereas the Newmark-β scheme requires approximately 206.80 seconds. In terms of estimation of restoring forces, the proposed approach requires approximately 0.001 seconds per evaluation of restoring forces, whereas the standard approach of calculating the restoring force requires approximate 0.01 seconds. Computational times were recorded using an Intel i7-14700KF CPU for both methods. Thus, the proposed hybrid scheme achieves nearly a twofold reduction in computational time while maintaining predictive accuracy comparable to that of the Newmark-β scheme.

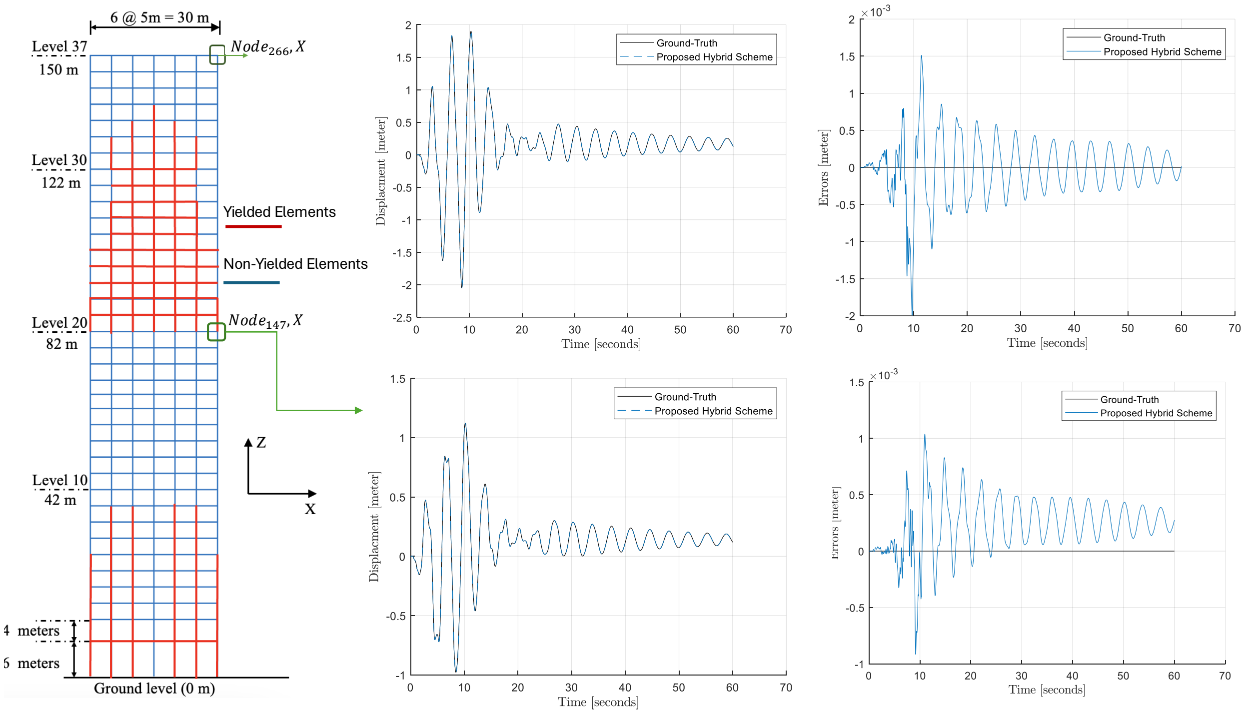

Figure 2: Comparison between the Newmark-β scheme (Ground-Truth) and proposed hybrid scheme for the displacement time-history in the horizontal direction.

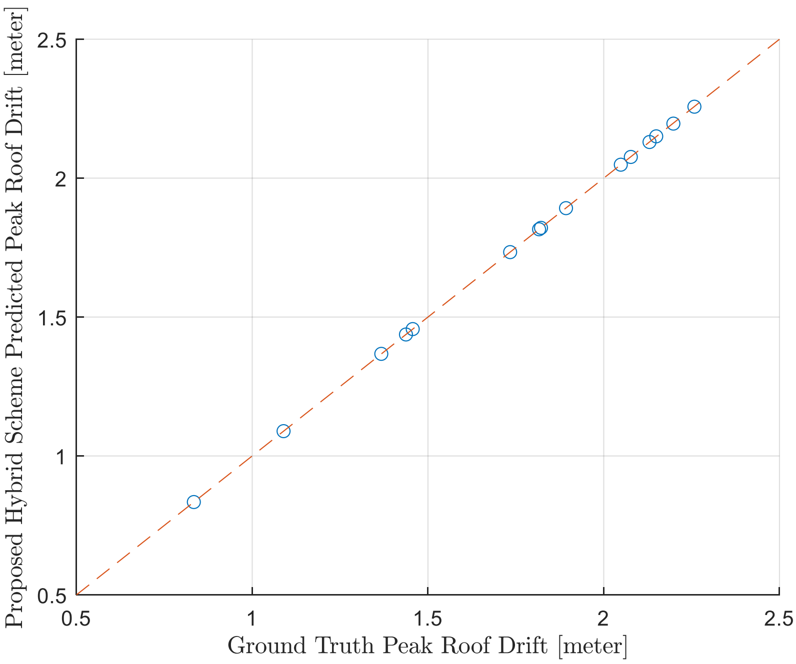

Figure 3: Performance of the proposed hybrid scheme in predicting peak roof drift.

4 CONCLUSIONS

This work proposed a hybrid framework that integrates neural operators with the Newmark-β scheme to efficiently and accurately model high-dimensional, nonlinear, and dynamic structural systems. By accelerating the computation of restoring forces while enforcing physical constraints through traditional numerical integration, the framework achieves substantial computational speed-up without sacrificing predictive accuracy. Validation on a steel moment-resisting frame subjected to stochastic seismic loads demonstrated the framework's effectiveness. The results suggest that the proposed approach offers a promising solution for fast and reliable simulation of complex structural responses.

ACKNOWLEDGMENTS

This research effort was supported in part by the National Science Foundation (NSF) under Grant Nos. TI-2140723 and CMMI-2118488. The opinions, findings, and conclusions or recommendations expressed in this paper are those of the authors only and do not necessarily reflect the views of the sponsors or affiliates.

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