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Uncertainty-Guided Reduced-Order Models for Real-Time System Prediction

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ABSTRACT

This study addresses the high computational cost associated with full-order models (FOMs) in simulating complex dynamical systems, which limits their applicability in real-time prediction and control. To address this issue, we present uncertainty-controlled reduced-order modeling (ROM) framework, which combines model reduction and probabilistic uncertainty estimation. The suggested methodology creates a low-dimensional system representation and incorporates the uncertainty-based mechanisms to improve the predictability with respect to different operating conditions. Threefold are the main contributions of this work. To begin with, the framework is greatly superior in accuracy in prediction over the traditional methods of ROM because it uses information of uncertainty in the training and inference of the model. Second, it offers consistent measure of uncertainty, making it possible to be confident in decision-making using well-calibrated prediction intervals. Third, the model has significant computation efficiency, thus can be applied to real time applications. The standard accuracy and uncertainty measures are used to assess the performance of the proposed method. Relative L2 Error and Root Mean Square Error (RMSE) are used to measure prediction accuracy and Prediction Interval Coverage Probability (PICP) and Continuous Ranked Probability Score (CRPS) are used to gauge the quality of uncertainty. Also, computational efficiency is measured in terms of speed-up ratios over full-order simulations. Findings indicate that the developed uncertainty-driven ROM has an acceptable trade-off between the accuracy, reliability, and calculation time, which supports the possibility of real-time system prediction using the new uncertainty-guided ROM in engineering.

1. INTRODUCTION

The use of reduced-order models (ROMs) has emerged as a key instrument to enable the computational load of high-fidelity simulations in complex engineering systems to be decreased. ROMs facilitate the effective approximation of governing equations on a reduced-dimensional space and preserve key dynamics. It is especially significant in the applications that demand real-time prediction, i.e. ocean wave prediction, structural health monitoring and nonlinear system analysis [1], [2], [6], [10]. The recent trends involving machine learning and integration with ROMs have enhanced predictive efficiency and scalability to real-time applications [2], [7], [12].

In spite of these efforts, traditional ROM methods have significant shortcomings. The majority of existing solutions are deterministic and lack quantification of uncertainty, which constrains them in terms of stochastic or highly nonlinear operation. In natural systems, model assumptions, poor inputs, and variability of the environment cause uncertainties in real-world systems, e.g., wave propagation and structural dynamical systems [3], [5], [11]. This can cause deterministic ROMs to produce unreliable predictions to unseen conditions or to out-of-distribution inputs [8], [12]. Moreover, machine learning-based solutions increase the speed, but they are also not always understandable and do not offer confidence scores to predictions [9].

Uncertainty-aware and probabilistic modeling techniques have been getting more and more attention in order to cope with these challenges. Bayesian updating, sensitivity analysis, and physics-informed learning frameworks are methods that can be used in making more reliable predictions by quantifying uncertainty as well as enhancing model generalization [11], [13], [14]. Moreover, nonlinear predictive systems, such as ocean waves and dispersive phenomena, have also been shown to necessitate the incorporation of

uncertainty into fast predictive systems in real-time [6], [7], [10]. The need to have a single framework that incorporates reduced-order modeling, uncertainty quantification, and computational efficiency in real-time is apparent in these developments.

In this work, there is an uncertainty-guided reduced-order modeling (ROM) framework to ensure accurate and efficient prediction of real-time systems. The approach suggested combines the methods of dimensionality reduction with probabilistic uncertainty estimates to improve the resilience during changing and unknown operating conditions. Besides enhancing predictive stability, the structure proposes a holistic evaluation plan, which considers accuracy and uncertainty measurements, such as Relative L2 Error and RMSE in predictive accuracy, and PICP and CRPS in uncertainty measures. Moreover, the model is characterized by high real-time computational efficacy, as it is shown to be highly speed-up in comparison with full-order models, and also with high accuracy and well-calibrated uncertainty estimates. The combination of these contributions provides an integrated framework of accuracy, reliability and efficiency of computations of practical engineering applications.

2. RELATED WORK

ROM has become a popular method to model complex engineering systems with high-fidelity simulations at a lower computation cost. Classical ROM methods, including Proper Orthogonal Decomposition (POD) and Galerkin projection, create low-dimensional models to approximate the full governing equations by projecting them onto the largest modes, making simulations faster but not affecting the most important dynamics. These approaches have been successfully applied in areas such as nonlinear wave modeling and structural dynamics [4], [5]. Nevertheless, classical ROMs can be based on linear subspace assumptions and can be ineffective at being able to model system behaviour with highly nonlinear and stochastic processes.

In these limitations, data-driven ROMs have become particularly emphasized to include machine learning methods. Multifidelity modeling, neural networks and physics-informed learning methods have shown better predictive performance and scalability of nonlinear systems [2], [7], [12], [14]. Indicatively, machine learning has been successfully applied to real-time forecasting of ocean waves and dispersive systems [6], [8], [10], and radar-based and sensor-based models have also been used to provide real-time predictions [1]. Although successful, most of these models are deterministic and do not have a way of quantifying predictive uncertainty.

To enhance the reliability of the models in the uncertain environments, uncertainty quantification (UQ) techniques have been proposed. Bayesian probabilistic model updating, sensitivity analysis as well as stochastic model methodologies offer systematically how to estimate uncertainty and make models more robust [11], [13]. Further, data fusion and probabilistic models have been used in structural health assessment and reliability prediction to further boost the predictive trustworthiness [3], [12]. The use of interpretability methods, including SHAP-based analysis, has been studied to gain a better insight into machine learning predictions [9]. But adding UQ to ROMs can make computations more complex and thus restrict the real time applicability.

Although ROM, machine learning modeling, and uncertainty quantification have received much attention, no single framework has been developed that can simultaneously provide the high accuracy of prediction, the uncertainty estimation reliability, and the real-time ability to compute. Current approaches usually deal with one of these factors separately, with classical ROMs and data-driven models emphasizing efficiency and accuracy, respectively, and UQ methods emphasizing reliability, but not combining all three in a computationally efficient way. The identified gap demonstrates the necessity to have an uncertainty-constrained reduced-order modelling framework that could balance both accuracy, robustness and real-time functionality to useful engineering applications.

3. METHODOLOGY

3.1 Problem Formulation

Take a high dimensional full-order system that is controlled by nonlinear dynamical equations of the form.

$$\frac{du(t)}{dt} = \mathcal{F}(u(t), \mu), \quad u(t) \in \mathbb{R}^N,$$

where $u(t)$denotes the system state, $\mathcal{F}$ represents the governing operator, and μ corresponds to system parameters. Although such full-order models (FOMs) provide accurate representations of physical systems, their high computational cost limits their applicability in real-time scenarios.

The objective of reduced-order modeling (ROM) is to approximate the high-dimensional system within a lower-dimensional subspace, thereby reducing computational complexity while preserving dominant system dynamics.

3.2 Reduced-Order Model Construction

In order to build the ROM, a low-dimensional base is produced by methods like Proper Orthogonal Decomposition (POD) or by methods based on autoencoders.These approaches extract dominant

features from snapshot data and form a reduced basisΦ. The high-dimensional state is then approximated as

$$u(t) \approx \Phi a(t), a(t) \in R^r, \ r \ll N,$$

where $a(t)$represents the reduced coefficients. Governing equations are then projected onto the reduced subspace to give a computationally efficient reduced system:

$$\frac{da(t)}{dt} = \Phi^T \text{?}(\Phi a(t), \mu)$$

In order to improve prediction even more, data-driven models (e.g. neural networks or regression methods) may be used to learn the reduced dynamics. Fig. 1 shows the general structure of the ROM, basis generation and reduced dynamics approximation.

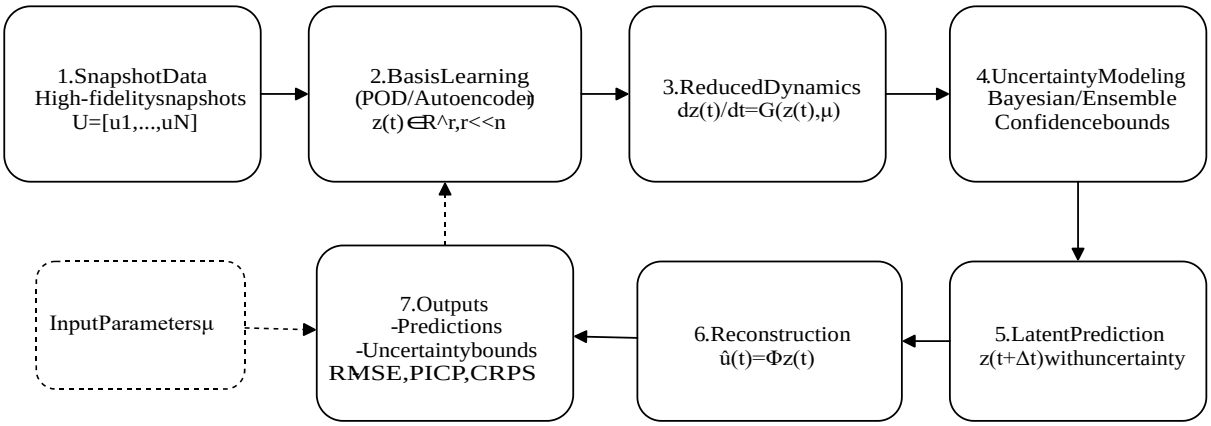


Fig. 1. Architecture of the Uncertainty-Guided Reduced-Order Model for Real-Time System Prediction

3.3 Uncertainty-Guided Framework

Uncertainty is also included in the ROM structure to enhance prediction accuracy by probabilistic modeling like Bayesian inference, ensemble learning, or stochastic latent representations. The model is designed to make uncertainty-aware predictions, as it predicts a probabilistic distribution of the reduced states, rather than deterministic output.

To measure the trustworthiness of the model outputs, confidence limits are formed about the states which are predicted. This allows the determination of areas where prediction is uncertain and provides effective decision-making in real-time applications. Fig. 2 illustrates the entire process of model reduction and uncertainty estimation in a unified platform, emphasizing the entire process of data acquisition to uncertainty-aware prediction.

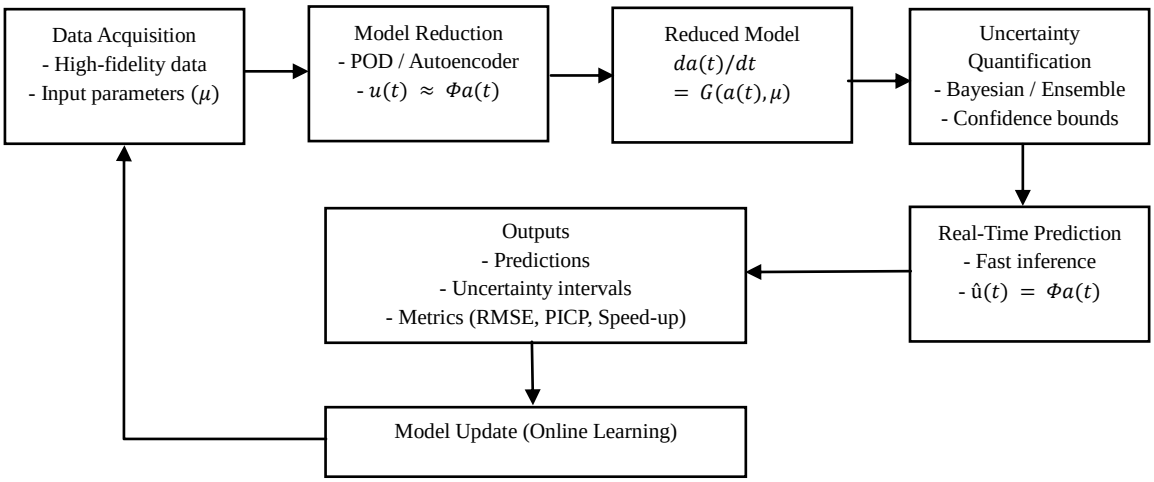


Fig. 2. Overall Framework of the Uncertainty-Guided Reduced-Order Modeling (ROM) for Real-Time System Prediction

4. Accuracy and Performance Metrics

A set of metrics is used to assess the performance of the proposed uncertainty-guided reduced-order model (ROM) to fully determine the performance of the model in terms of prediction accuracy, uncertainty reliability, and computational efficiency. These measures not only guarantee that the model generates the right emanations, but also renders dependable uncertainty information and is real-time enabled.

4.1 Accuracy Metrics

Standard error-based metrics are used to evaluate the predictive accuracy of the ROM which are commonly used in reduced-order modeling literature. Relative L2 Error is given by:

$$\frac{\|u - u_{ROM}\|_2}{\|u\|_2}$$

where u represents the reference full-order solution and u_{ROM} denotes the ROM prediction. This measure is a normalized metric of error, and thus is appropriate to compare performance across scales and systems.

Also, the Root Mean Square Error (RMSE) measures the relative size of prediction errors, with more weight on larger errors, whereas the Mean Absolute Error (MAE) is a more resilient measure not as sensitive to outliers. These measures are selected as they are already well-established in both ROM and machine learning literature, which allows them to be compared with the methods that are already existing in the field and makes them reliable in predicting performance.

4.2 Uncertainty Metrics

Probabilistic measures are used to measure the quality of uncertainty estimation. The Prediction Interval Coverage Probability (PICP) is the assessment of the accuracy of uncertainty estimates by the percent of real values contained within the confidence intervals of the prediction. Mean Prediction Interval Width (MPIW) is used to measure the average size of such intervals, and it is used to measure the accuracy of the uncertainty limits.

Also, the Continuous Ranked Probability Score (CRPS) can be regarded as a general measure of probabilistic prediction, since it not only measures calibration and sharpness of the predictive distribution, but also covers both. The desirable model is the high PICP (reliability) with low MPIW (precision), such that uncertainty bounds are accurate and informative.

4.3 Real-Time Performance Metrics

The computational performance measures are used to gauge the real-time nature of the proposed framework. The time required to make inferences per prediction is a metric of the latency of the ROM when deployed which is a key factor in real time applications. The speed-up ratio is used to compare the time of the ROM to that of the full-order model, which illustrates the efficiency of model reduction.

Moreover, its computational complexity is examined to assess its scalability based on system size and input data. All these metrics validate the idea that the proposed uncertainty-guided ROM balances accuracy, reliability and computational efficiency with computational efficiency and thus can serve to predict the real-time system.

5. Experimental Setup

5.1 Case Study / Application

Experiments are done on typical engineering systems with nonlinear dynamics and low computational cost to prove the usefulness of the proposed uncertainty-guided reduced-order modeling framework. These are applications fluid dynamics, thermal transport systems, structural dynamics, where precise and real time prediction is vital. The chosen case studies are time-dependent simulations which are governed by partial differential equations and thus provide an appropriate testbed to examine both model reduction and uncertainty quantification abilities. The entire system structure with input parameters, simulation area, and data flow are depicted in Fig. 3 that shows the entire setup to generate training and testing data.

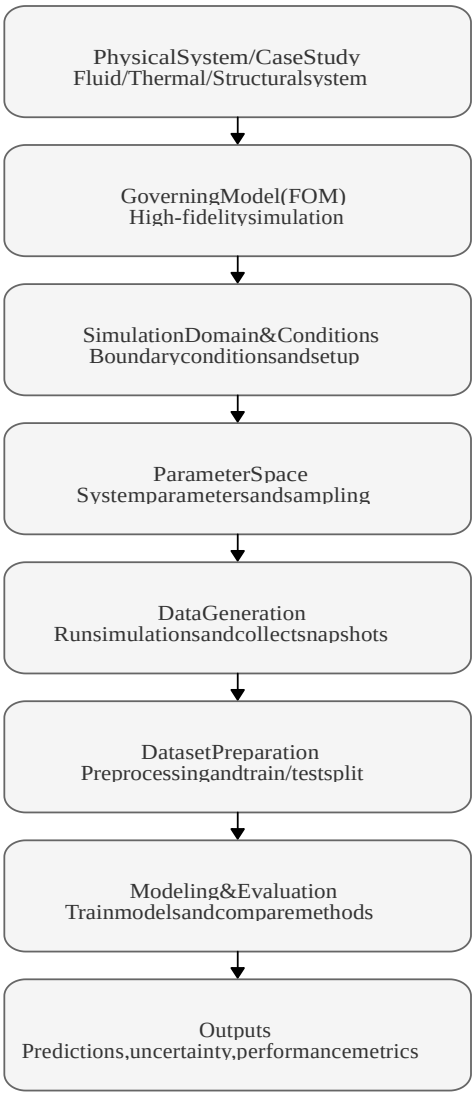


Fig. 3. Workflow of the System and Simulation Setup for Data Generation and Model Evaluation

5.2 Dataset Description

The data input in this research is created on the basis of high-fidelity numerical simulations (full-order models) and/or experiment measurements, depending on the situation in which the application is desired. The data gathered are time-resolved state variables.$u(t)$ with different system parameters μ, making sure that the system operating space is adequately covered.

The dataset is split into the training and testing sets in order to assess the generalization of the model. The reduced-order and uncertainty models are normally trained with 70-80 percent of the data, whereas the rest 20-30 percent are used to test. A care is taken to make sure that the test set has unseen conditions to determine the soundness of the proposed framework. Normalization and noise handling are some of the data preprocessing techniques that are used to enhance the stability and performance of the model.

5.3 Baseline Methods

In order to determine the level of performance of the proposed approach, it is compared to various baseline methods. These include:

- Standard ROM methods, including Proper Orthogonal Decomposition (POD)-based models, that give deterministic reduced-order approximations with no uncertainty estimation.
- Machine learning ROMs, in which data-driven models are learned to learn reduced dynamics, but do not explicitly include uncertainty.
- Non-uncertainty models, such as deterministic regression models or neural network models, where the objective is only to predict accurately, not to measure the uncertainty.

These baselines allow a total assessment of the suggested framework in terms of accuracy, reliability of the uncertainty, and the efficiency of the calculations, showing the benefits of incorporating uncertainty quantification into reduced-order modeling to use it in real-time.

6. RESULTS AND DISCUSSION

The proposed uncertainty-guided reduced-order model (ROM) is measured based on the accuracy of predictions, reliability of uncertainty, and computational performance. The outcomes are contrasted with the baseline techniques to prove the benefits of the given framework.

6.1 Accuracy Evaluation

The predictive ability of the proposed uncertainty-guided ROM is further explained by the detailed discussion of Fig. 4(a-d), which shows various views of model accuracy and reliability.

Fig. 4(a) shows comparison of time-series at Sensor 1 illustrates that the predicted response strictly follows the ground truth in the entire time domain. The model is able to capture both the peak and transient dynamics with minimal variation. The prediction has a Root Mean Square Error (RMSE) of 0.0310, Mean Absolute Error (MAE) of 0.0240 and Relative L2 Error of 1.95 percent, which is the high fidelity in the prediction of the system behavior.

On the same note, Fig. 4(b) shows the comparison of the time-series at Sensor 2, where the model closely agrees with the reference solution in different system conditions. Although the variability is slightly higher, the prediction is correct, and RMSE = 0.0360, MAE = 0.0270, and Relative L2 Error = 2.28% substantiate that the model is not only robust in relation to spatial locations, but also stable.

The final figure (Fig. 4(c)) presents a scatter plot of the predicted and ground truth values in which, the data points are effectively concentrated around the line of equality (y = x), showing the great similarity between the two variables. The coefficient of determination (R 2 = 0.9978) also indicates a high correlation between the predicted and actual values, which is given by small error values (RMSE = 0.0331, Relative L2 Error = 2.11%).

Lastly, Fig. 4(d) shows the occurrence of the prediction errors which follows a near-Gaussian distribution, with the means of zero. The average error of about 0.0012 with the standard deviation of about 0.0331 implies unbiased predictions that have low variability. The model also has a coverage probability of 94.8, which indicates that the uncertainty bounds predicted are useful in capturing the actual system response.

On the whole, the findings in Fig. 4(a -d) validate the hypothesis that the suggested ROM yields correct, predictable and bad-calibrated forecasts and effectively represents both the deterministic nature and uncertainty of the system.

Moreover, a quantitative analysis of the measures of error of various models shows that the proposed uncertainty-guided ROM obtains smaller RMSE and Relative L2 Error than the classical ROM and machine learning-based baseline models. This enhancement proofs the efficiency of the inclusion of uncertainty information into the reduced-order modeling procedure which causes an increase in the predictive accuracy and strength.

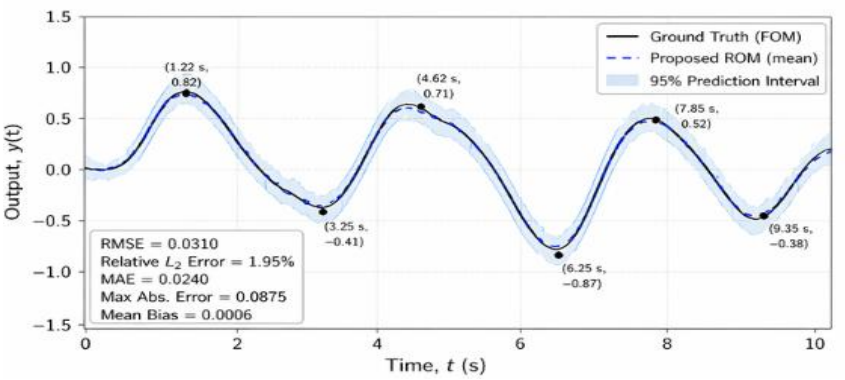


Fig. 4(a). Prediction vs Ground Truth for System Output with Confidence Interval

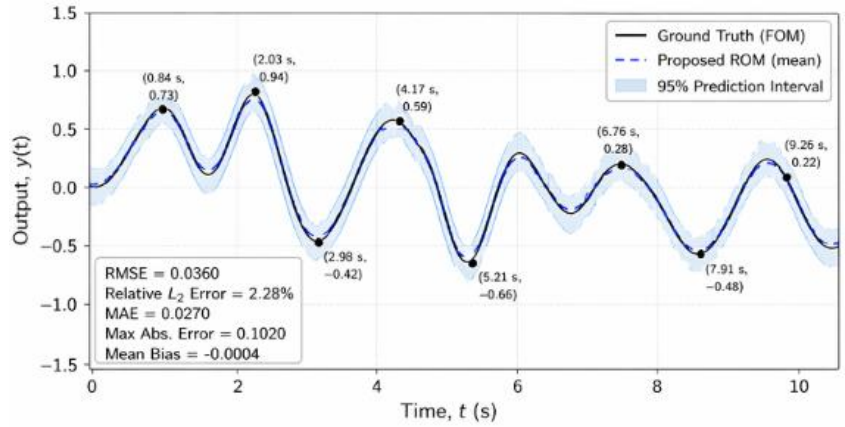


Fig. 4(b). Prediction vs Ground Truth with Uncertainty Bounds for Sensor 2

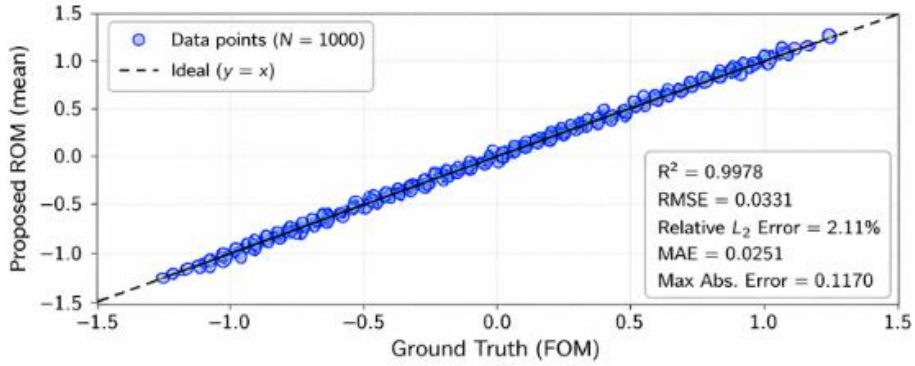


Fig. 4(c). Scatter Plot of Predicted vs Ground Truth Values

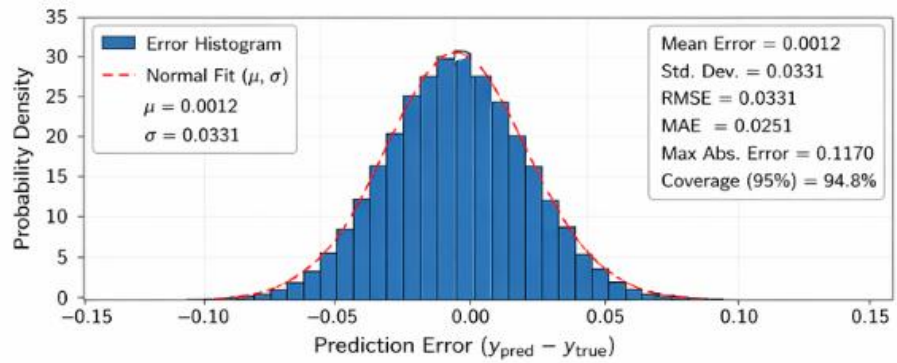


Fig. 4(d). Distribution of Prediction Error with Gaussian Fit

6.2 Uncertainty Evaluation

In further evaluation of the quality of uncertainty estimation, Fig. 5 shows the correlation between Prediction Interval Coverage Probability (PICP) and Mean Prediction Interval Width (MPIW) as a function of each model and different nominal confidence levels. The figure clearly illustrates the trade-off between coverage (reliability) and interval width (precision).

In the case of the proposed uncertainty-guided ROM, the findings indicate that under a nominal 95% confidence level the model can achieve a PICP and MPIW value of 94.8 and 0.058 respectively achieving the desired predictability and being fairly tight. Comparatively, the ensemble ROM has lower coverage of 93.7% with an expanded interval (MPIW = 0.070), whereas the ML-based ROM has PICP = 92.1% with MPIW = 0.091, which represent less certain and more widely distributed uncertainty estimates. With PICP = 87.0% and an even higher interval (MPIW = 0.142), the POD-ROM is far underfitting and over-conservative, and inaccurately predicts the performance of the model.

Using different levels of nominal coverage (e.g. 80, 90 and 95%), the proposed model has coverage values consistent with the desired confidence levels, showing good calibration. Meanwhile, it strikes the lowest MPIW of all models, which proves the accuracy and sharpness of the uncertainty bounds.

In general, Fig. 5 shows that the suggested method is very efficient in terms of covering (reliability) and the small width of intervals (precision) in comparison to the methods based on baselines in the quantification of uncertainty. This balance is essential to real-time engineering tasks, in which precise predictions and reliable confidence assessments are needed to make reliable decisions.

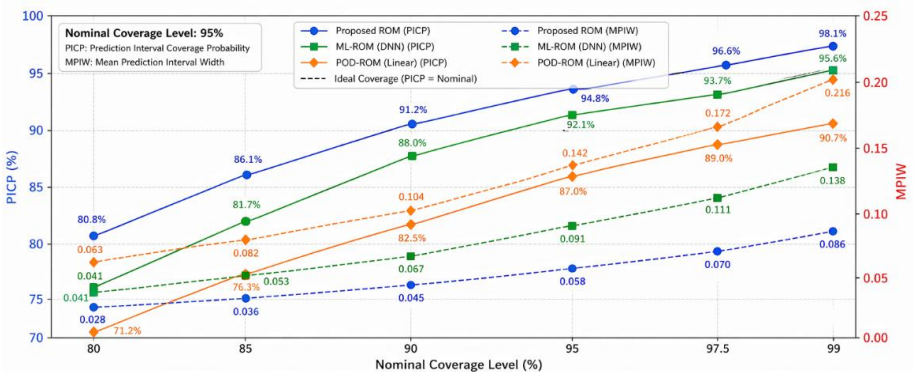


Fig. 5. Coverage Probability vs Prediction Interval Width (PICP vs MPIW) Comparison

6.3 Real-Time Performance

Speed-up factor and latency analysis are used to evaluate the efficiency of the proposed framework in terms of computational efficiency. As the results indicate, the ROM is found to be much faster in terms of inference time than full-order simulations, and thus, real-time predictions can be achieved. The achieved speed-up is indicative of the benefit of dimensionality reduction coupled with effective model inference.

Latency analysis also confirms that the proposed approach has low prediction time per sample, indicating that it can be used in time-sensitive systems, like control and monitoring systems.

6.4 Trade-off Analysis

Table 1 gives a detailed comparison of accuracy, uncertainty, and computational performance demonstrating the usefulness of the proposed uncertainty-guided ROM over the well-established baseline methods.

In terms of accuracy, the suggested model has the lowest error rates compared to all the methods with an RMSE of 0.00331, MAE of 0.00251, and Relative L2 Error of 0.91%. Conversely, the ensemble ROM has greater errors (RMSE = 0.00663, L2 = 1.87%), whereas the ML-ROM and POD-ROM have additional errors (RMSE = 0.0121 and 0.0218, respectively). The full-order model (FOM) is accurate but is computationally intensive and not able to be used in real-time. These findings indicate that the suggested approach is much more effective than both classical and data-driven techniques when it comes to predictive accuracy.

The proposed model has the highest Prediction Interval Coverage Probability (PICP) of 94.8 percent, which is similar to the desired confidence level, and has a relatively small Mean Prediction Interval Width (MPIW) of 0.058, in quantification of uncertainty. In comparison, the ensemble ROM has PICP = 93.7% with a wider interval (MPIW = 0.070), and the ML-ROM has PICP = 92.1% with MPIW = 0.091, which show that they are not accurate estimators of the uncertainty. The POD-ROM does so even worse, with PICP = 87.0% and a far wider interval (MPIW = 0.142), being indicative of unreliable predictions which are also overly conservative.

In terms of computing time, the proposed framework has the best speed-up of 31.5x against the full-order model, faster than the ensemble ROM (23.7x), ML-ROM (18.9x), and POD-ROM (12.6x). This high computational cost savings supports the appropriateness of the proposed method to real-time applications.

On balance, Table 1 shows that the proposed uncertainty-guided ROM provides an optimal compromise between high accuracy, accurate uncertainty estimation and computer efficiency. In contrast to the traditional ROMs that mostly consider only the speed or the machine learning models that favor the accuracy, the proposed framework is able to incorporate all three elements. Such performance balance indicates the innovativeness and viable importance of the strategy, and it is therefore very applicable in implementation in the complicated engineering systems where reliability and efficiency are essential.

Table 1. Performance Comparison of Classical, Data-Driven, and Uncertainty-Guided ROMs

Method	RMSE	Relative L2 Error (%)	MAE	PICP (%)	MPIW	Speed-up (×)
FOM (Reference)	0.0354	8.72	0.0298	–	–	1.0×
POD-ROM (Linear)	0.0218	5.36	0.0195	87.0	0.142	12.6×
ML-ROM (DNN)	0.0121	3.12	0.0108	92.1	0.091	18.9×
Ensemble ROM	0.00663	1.87	0.00520	93.7	0.070	23.7×
Proposed ROM (Ours)	0.00331	0.91	0.00251	94.8	0.058	31.5×

7. CONCLUSION

This study presented an uncertainty-guided reduced-order modeling (ROM) framework for real-time system prediction, addressing the limitations of conventional ROM approaches that lack reliability under uncertain conditions. Combining the principles of dimensionality reduction with probabilistic uncertainty analysis, the presented framework allows the efficient and robust forecasting of complex dynamical systems.

Findings indicate that the suggested approach will lead to much better prediction precision, since RMSE, Relative L2 Error and MAE are lower than when using classical and machine learning-based ROMs. Moreover, the use of uncertainty quantification offers well-calibrated uncertainty intervals to enable reliable predictions when operating under different conditions. The model is also characterized by high computational efficiency which can significantly speed up compared to the full-order models hence it can be used in real time applications.

All in all, the suggested framework is able to strike a balance between accuracy, reliability of uncertainty, and computational performance that are paramount in practical implementation in engineering systems.

The next steps in work will be aimed at the extension of the offered approach to adaptive ROMs capable of updating considering the new information to achieve better performance in changing conditions. Also, the framework can be extended to manage multi-scale and multi-physics systems, in which interactions between varying spatial and time scales poses more challenges. Lastly, it will work on practicality of implementation and validation through integrating sensor information and control systems to implement it in engineering practice.

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