REDUCED-ORDER MODEL AND NEURAL OPERATORS FOR STOCHASTIC MECHANICS PROBLEMS UNDER PARAMETRIC UNCERTAINTY

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by

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Certificate

This is to certify that the thesis titled **Reduced-Order Model and Neural Operators for Stochastic Mechanics Problems Under Parametric Uncertainty**, submitted by **Mr. Navaneeth**, to the Indian Institute of Technology, Delhi, for the award of the degree of **Doctor of Philosophy**, is a bonafide record of the research work done by him under our supervision and guidance. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

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Abstract

Practical engineering systems inherently exhibit uncertainties arising from factors such as random variations in geometry, material properties, boundary conditions, and loading scenarios. Despite these uncertainties, ensuring that systems consistently meet desired performance standards during operation remains a critical requirement. Consequently, the quantitative assessment of these uncertainties is indispensable, necessitating their systematic incorporation into analysis and design frameworks. Achieving this demands robust methodologies that integrate probability, statistics, and the principles of mathematical and physical sciences for uncertainty quantification and reliability analysis. However, such frameworks often encounter computational bottlenecks, particularly due to the reliance on expensive numerical solvers. On the other hand, analytical approximation methods may yield unreliable solutions or fail to handle irregular domains and high-dimensional input spaces effectively.

Traditional surrogate-based approaches offer partial relief from these challenges but are not without their own limitations. They often struggle with high input dimensionality, require extensive training data, exhibit limited generalizability beyond the training domain, and face difficulties in addressing long-term, time-dependent problems. These shortcomings underscore the need for innovative modeling methodologies that are computationally efficient and scalable. This thesis addresses these gaps by developing a suite of advanced machine-learning methods tailored to solve stochastic mechanics problems under parametric uncertainty, providing a foundation for accurate, reliable, and scalable uncertainty quantification in complex engineering systems

Dealing with high dimensional inputs is one of the persisting problems in uncertainty quantification and reliability analysis. Traditional approaches often rely on dimensionality reduction techniques to identify a low-dimensional manifold, enabling surrogate models to be trained in this reduced space. Unsupervised dimensionality reduction methods, such as Principal Component Analysis (PCA), are widely used to approximate lower-dimensional representations based solely on input variable information. However, these methods disregard the target data (i.e., the quantity of interest) and often fail to effectively reduce dimensionality, particularly when all input variables contribute nearly equally to the output. To overcome these limitations, this thesis proposes a novel approach for solving high-dimensional reliability analysis problems. The proposed method employs the active sub-

space algorithm to learn a low-dimensional manifold by leveraging the gradient information of the response variable. Recognizing the challenges in gradient estimation, the framework integrates a sparse learning algorithm with the active subspace method, resulting in the Sparse Active Subspace (SAS) algorithm. This approach projects high-dimensional inputs onto a reduced-dimensional space identified by SAS, where a more accurate surrogate model, the Hybrid Polynomial Correlated Function Expansion (HPCFE), maps the inputs to the output response. The resulting framework proves highly efficient for time-independent reliability analysis in high-dimensional systems. However, direct application to dynamic systems remains a limitation, necessitating further advancements.

Modeling the reliability of complex and nonlinear dynamical systems remains a significant challenge in structural reliability and uncertainty quantification, as most traditional methods are constrained to time-independent systems. To address this limitation, this thesis introduces a Koopman operator-based approach for time-dependent reliability analysis. Koopman theory enables the transformation of nonlinear dynamical systems into linear ones by identifying intrinsic coordinates, allowing the seamless computation of time evolution even for systems exhibiting nonlinear or chaotic behavior. However, determining these intrinsic coordinates has traditionally been a challenging task.

To overcome this, a novel deep learning framework is developed that learns Koopman observables in an end-to-end manner, subsequently using these observables for time marching the systems dynamic response. Two distinct architectures are proposed: one tailored for systems with uncertainties in initial conditions and the other designed for systems with uncertainties in underlying parameters. These frameworks demonstrate robustness and the ability to generalize to unseen environments, effectively handling out-of-distribution predictions. However, despite its strengths, the direct application of the Koopman-based approach to long-term response prediction does not yield satisfactory results. This necessitates extending the frameworks capabilities to address such scenarios. To this end, a novel operator learning approach, referred to as the “Waveformer”, is proposed to model dynamical systems with enhanced accuracy and scalability. The Waveformer integrates wavelet transforms for capturing the spatial multi-scale behavior of the solution field with transformers for modeling long-horizon temporal dynamics. Numerical evaluations highlight the Waveformers exceptional performance in learning solution operators, significantly surpassing existing state-of-the-art operator learning methods, particularly in extrapolation tasks. Furthermore, waveformer performs exceedingly well in solving uncertainty quantification and time-dependent reliability analysis problems. This advancement paves the way for more reliable and efficient modeling of dynamical systems under uncertainty.

While the developed frameworks demonstrate strong performance in uncertainty quantification for high-dimensional systems, they are notably data-intensive, relying on extensive training datasets that are typically generated using computationally expensive solvers. This reliance poses a significant challenge for scaling these methods to more complex systems. To address this, Physics-Informed Neural Networks (PINNs) have emerged as a promising alternative. By embedding governing physical laws directly into the training process, PINNs reduce the dependency on labeled data. However, standard PINNs encounter limitations when applied to problems with complex solution domains or discontinuities, as the reliance on automatic differentiation creates a computational bottleneck and impacts performance. To overcome this limitation, a novel Stochastic Projection-based Gradient-Free Physics-Informed Neural Network (SP-PINN) is proposed. This framework combines the

stochastic projection theory with the principles of PINNs, and is proven to be efficacious in problems involving the regular domain, complex domain, and complex response. Unlike traditional PINNs, SP-PINN avoids the reliance on automatic differentiation, allowing for the incorporation of non-differentiable neural network architectures, such as convolutional neural networks, into the training process. This flexibility makes SP-PINN particularly effective across a range of problems, including those with regular domains, irregular geometries, and intricate solution responses. However, despite its success in achieving high accuracy for fixed input conditions, SP-PINN requires retraining whenever boundary conditions, initial conditions, or source terms change, limiting its applicability to stochastic mechanics problems. To address this limitation, a physics-informed wavelet neural operator (PIWNO) is proposed in this thesis that can seamless solve both time-dependent and time-independent reliability analysis problems. By integrating physical principles directly into the learning process, PIWNO eliminates the need for labeled training data generated by conventional solvers, offering a robust and efficient framework for solving families of parametric PDEs across a variety of engineering and scientific domains.

The final part of this thesis extends the development of advanced operator learning frameworks to address two critical applications: reliability analysis using the PIWNO and cardiovascular modeling with the geometry-adaptive waveformer. For reliability analysis, PIWNO was employed to tackle high-dimensional engineering systems governed by parametric uncertainties, including diffusion-reaction systems and fluid flow through porous media. Both time-independent and time-dependent reliability analysis problems were tackled. By integrating physical laws directly into the learning process, PIWNO eliminates the dependency on labeled datasets, offering an efficient and scalable solution for quantifying uncertainties and reliability analysis in high-dimensional stochastic systems. For cardiovascular modeling, the waveformer was extended to handle irregular anatomical geometries and the time-dependent dynamics of cardiovascular systems. A geometry-adaptive approach was developed, transforming data from the irregular spatial domain into a regular latent space to efficiently learn patient-specific dynamics. The results obtained are found to be highly accurate, with a coefficient of determination over 0.9 in most cases. These advancements illustrate the potential of the developed frameworks to tackle diverse real-world problems, from engineering reliability to biomedical applications, while addressing computational challenges and enabling scalable, efficient solutions.

सारांश

व्यावहारिक इंजीनियरिंग प्रणालियाँ स्वाभाविक रूप से ज्यामिति में यादृच्छिक भिन्नताओं, भौतिक गुणों, सीमा स्थितियों और लोडिंग सिस्टम जैसे कारकों से उत्पन्न होने वाली अनिश्चितताओं को प्रदर्शित करती हैं। इन अनिश्चितताओं के बावजूद, यह सुनिश्चित करना कि संचालन के दौरान प्रणालियाँ लगातार वांछित उद्देश्य मानकों को पूरा करती हैं, एक महत्वपूर्ण आवश्यकता बनी हुई है। नतीजतन, इन अनिश्चितताओं का गुणात्मक मूल्यांकन अपरिहार्य है, जिससे विश्लेषण और डिजाइन ढांचे में उनके व्यवस्थित समावेश की आवश्यकता होती है। इसे प्राप्त करने के लिए मजबूत विधि की आवश्यकता होती है जो अनिश्चितता परिमाणीकरण और विश्वसनीयता विश्लेषण के लिए संभावना, सांख्यिकी और गणितीय और भौतिक विज्ञान के सिद्धांतों को एकीकृत करती है। हालांकि, इस तरह के ढांचे अक्सर कम्प्यूटेशनल बाधाओं का सामना करते हैं, विशेष रूप से महंगे संख्यात्मक सॉल्वर पर निर्भरता के कारण। दूसरी ओर, विश्लेषणात्मक सन्निकटन विधियाँ अविश्वसनीय समाधान दे सकती हैं या अनियमित डोमेन और उच्च-आयामी इनपुट स्पेस को प्रभावी ढंग से संभालने में विफल हो सकती हैं।

पारंपरिक सरोगेट-आधारित दृष्टिकोण इन चुनौतियों से आंशिक राहत प्रदान करते हैं लेकिन उनकी अपनी सीमाओं के बिना नहीं हैं। वे अक्सर उच्च इनपुट आयाम के साथ संघर्ष करते हैं, व्यापक प्रशिक्षण डेटा की फिर से आवश्यकता होती है, प्रशिक्षण क्षेत्र से परे सीमित सामान्यता प्रदर्शित करते हैं, और दीर्घकालिक, समय-निर्भर समस्याओं को संबोधित करने में कठिनाइयों का सामना करते हैं। ये संक्षिप्त विवरण नवीन मॉडलिंग पद्धतियों की आवश्यकता को रेखांकित करते हैं जो कम्प्यूटेशनल रूप से कुशल और स्केलेबल हों। यह थीसिस जटिल इंजीनियरिंग प्रणालियों में सटीक, विश्वसनीय और स्केलेबल अनिश्चितता के लिए एक आधार प्रदान करते हुए पैमानों की अनिश्चितता के तहत यादृच्छिक यांत्रिकी समस्याओं को हल करने के लिए उन्नत मशीन-लर्निंग विधियों का एक समूह विकसित करके इन अंतरालों को संबोधित करता है।

उच्च आयामी निवेशों से निपटना अनिश्चितता और विश्वसनीयता विश्लेषण की निरंतर समस्याओं में से एक है। पारंपरिक दृष्टिकोण अक्सर कम आयामी मैनिफोल्ड की पहचान करने के लिए आयामी पुनर्वितरण तकनीकों पर निर्भर करते हैं, जिससे सरोगेट मॉडल को इस कम स्थान में प्रशिक्षित किया जा सकता है। प्रिंसिपल कंपोनेंट एनालिसिस (PCA) जैसी गैर-पर्यवेक्षित आयामी कमी विधियों का व्यापक रूप से केवल इनपुट परिवर्तनीय जानकारी के आधार पर निम्न-आयामी प्रतिनिधित्वों का अनुमान लगाने के लिए उपयोग किया जाता है। हालांकि, ये तरीके लक्ष्य डेटा (i.e., ब्याज की मात्रा) का सम्मान नहीं करते हैं और अक्सर आयाम को प्रभावी ढंग से कम करने में विफल रहते हैं, खासकर जब सभी इनपुट चर लगभग समान रूप से योगदान करते हैं। इन सीमाओं को दूर करने के लिए, यह शोध प्रबंध उच्च आयामी विश्वसनीयता विश्लेषण समस्याओं को हल करने के लिए एक नए दृष्टिकोण का प्रस्ताव करता है। प्रस्तावित विधि प्रतिक्रिया चर की ढाल जानकारी का लाभ उठाकर एक निम्न-आयामी मैनिफोल्ड सीखने के लिए ऐक्टिव सबस्पेस (AS) एल्गोरिथ्म को नियोजित करती है। ढाल आकलन में चुनौतियों को पहचानते हुए, फ्रेम-वर्क ऐक्टिव सबस्पेस विधि के साथ एक विरल शिक्षण एल्गोरिदम को एकीकृत करता है, जिसके परिणामस्वरूप स्पार्स ऐक्टिव सबस्पेस (SAS) एल्गोरिदम होता है। यह दृष्टिकोण SAS द्वारा पहचाने गए एक कम-आयामी स्थान पर उच्च-आयामी इन-पुट को प्रोजेक्ट करता है, जहां एक अधिक सटीक सरोगेट मॉडल, हाइब्रिड पॉलीनोमियल कोरिलेटेड फंक्शन एक्सपेंशन (HPCFE) आउटपुट प्रतिक्रिया

प्रकार के इंजीनियरिंग और वैज्ञानिक क्षेत्रों में पैरामीट्रिक आंशिक अवकल समीकरणों (PDEs) के परिवारों को हल करने के लिए एक मजबूत और कुशल ढांचा प्रदान करता है।

इस थीसिस का अंतिम भाग दो महत्वपूर्ण अनुप्रयोगों को संबोधित करने के लिए उन्नत ऑपरेटर लर्निंग फ्रेमवर्क के विकास का विस्तार करता है: PIWNO का उपयोग करके विश्वसनीयता विश्लेषण और ज्यामिति-अनुकूली वेवफॉर्मर के साथ कार्डियोवैस्कुलर मॉडलिंग। विश्वसनीयता विश्लेषण के लिए, PIWNO को पैरामीट्रिक अनिश्चितताओं द्वारा नियंत्रित उच्च-आयामी इंजीनियरिंग प्रणालियों से निपटने के लिए नियोजित किया गया था, जिसमें प्रसार-प्रतिक्रिया प्रणाली और झरझरा मीडिया के माध्यम से द्रव प्रवाह शामिल थे। समय-स्वतंत्र और समय-निर्भर विश्वसनीयता विश्लेषण समस्याओं दोनों से निपटा गया। भौतिक नियमों को सीधे सीखने की प्रक्रिया में एकीकृत करके, PIWNO लेबल किए गए डेटासेट पर निर्भरता को समाप्त करता है, जो उच्च-आयामी यादृच्छिक प्रणालियों में अनिश्चितताओं और विश्वसनीयता विश्लेषण की मात्रा निर्धारित करने के लिए एक कुशल और स्केलेबल समाधान प्रदान करता है। कार्डियोवैस्कुलर मॉडलिंग के लिए, वेवफॉर्मर को अनियमित शारीरिक ज्यामिति और कार्डियोवैस्कुलर सिस्टम की समय-निर्भर गतिशीलता को संभालने के लिए विस्तारित किया गया था। एक ज्यामिति-अनुकूली दृष्टिकोण विकसित किया गया था, जो रोगी-विशिष्ट गतिशीलता को कुशलता से सीखने के लिए अनियमित स्थानिक क्षेत्र से डेटा को एक नियमित अव्यक्त स्थान में बदल देता था। अधिकांश मामलों में 0.9 से अधिक निर्धारण के गुणांक के साथ प्राप्त परिणाम अत्यधिक सटीक पाए जाते हैं। ये प्रगति कम्प्यूटेशनल चुनौतियों को संबोधित करते हुए और स्केलेबल, कुशल समाधान को सक्षम करते हुए, इंजीनियरिंग विश्वसनीयता से लेकर जैव चिकित्सा अनुप्रयोगों तक, विविध वास्तविक दुनिया की समस्याओं से निपटने के लिए विकसित ढांचे की क्षमता को दर्शाती हैं।

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Abbreviations

FD	**F**inite **D**ifference
FEM	**F**inite **E**lement **M**ethods
ODE	**O**rdinary **D**ifferential **E**quation
PDE	**P**artial **D**ifferential **E**quation
PCE	**P**olynomial **C**haos **E**xpansion
SAS	**S**parse **A**ctive **S**ubspace
GP	**G**aussian **P**rocess
SVM	**S**upport **V**ector **M**achine
SVR	**S**upport **V**ector **R**egression
PDF	**P**robability **D**ensity **F**unction
FORM	**F**irst **O**rder **R**eliability **M**ethod
SORM	**S**econd **O**rder **R**eliability **M**ethod
MCS	**M**onte **C**arlo **S**imulation
HPCFE	**H**ybrid **P**olynomial **C**orrelated **F**unction **E**xpansion
ML	**M**achine **L**earning
FNN	**F**ully connected **N**eural **N**etwork
PINN	**P**hysics **I**nformed **N**eural **N**etwork
SP-PINN	**S**tochastic **P**rojection based **P**hysics **I**nformed **N**eural **N**etwork
GNO	**G**raph **N**eural **O**perator
FNO	**F**ourier **N**eural **O**perator
WNO	**W**avelet **N**eural **O**perator
PIWNO	**P**hysics **I**nformed **W**avelet **N**eural **O**perator
ROM	**R**educed **O**rder **M**odelling