AI-Based Modeling Approaches for Multi-Physics Simulations of Rotary Mechanisms

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Abstract-- This study examines AI-based modeling for multi-physics simulations of rotary mechanisms, focusing on the complex interactions between mechanical, thermal, and fluid domains. While conventional simulation methods are often limited by high computational costs and long processing times, this study evaluates data-driven and physics-aware alternatives—specifically Artificial Neural Networks (ANN), Physics-Informed Neural Networks (PINN), and Graph Neural Networks (GNN). Due to hardware and time constraints, rather than large-scale data generation, the research establishes a conceptual and methodological framework for integrating simulation-aware AI into rotary systems. To assess practical implementation challenges, a Monte Carlo-based feasibility analysis was developed in Python; this analysis estimated a success probability of approximately 0.77% for training these models under current resource limitations. Ultimately, this study contributes to the literature by providing a structured roadmap for AI-supported multi-physics modeling and offering practical guidance for engineering applications operating under significant computational constraints.

Keywords-- Rotary mechanisms, multi-physics simulation, artificial intelligence, PINN, data-driven modeling, surrogate models**.**

1. INTRODUCTION

Modern engineering systems are becoming increasingly complex, which in turn amplifies the need for high-fidelity and multi-faceted simulation tools in both design and analysis phases. Rotary mechanisms, in particular, are characterized by intricate dynamic behaviors and operate under diverse loading and environmental conditions. As such, they inherently involve the interaction of multiple physical domains such as structural mechanics, thermal conduction, and fluid dynamics. While multi-physics simulations provide high-resolution insights into these interactions, their application is often limited by intensive computational cost and long processing times.

This study aims to develop an artificial intelligence (AI)-supported modeling approach to predict the performance of rotary mechanisms in a faster and more computationally efficient manner. Instead of relying solely on traditional simulation tools, the proposed method involves building data-driven surrogate models and physics-informed neural networks (PINNs) capable of approximating the complex interrelations of multi-physics phenomena. These models are expected to deliver rapid and accurate predictions of system behavior under varying operating conditions and design configurations, thereby accelerating the design process and enabling real-time decision support.

AI-based modeling techniques have recently gained significant traction in engineering due to their ability to enhance simulation speed and support optimization workflows. Deep learning architectures, in particular, are proficient in capturing nonlinear relationships in high-dimensional datasets and approximating system dynamics with high accuracy. The envisioned models in this study are designed to emulate the fidelity of multi-physics solvers while drastically reducing computational demands.

To this end, a simulation dataset will be constructed based on rotary mechanism designs with varying geometries and operational conditions using tools such as Autodesk Fusion 360. This dataset will serve as the foundation for training one or more AI-based models, whose predictive accuracy, computational efficiency, and ability to represent cross-physical interactions will be thoroughly evaluated. Through this, the feasibility of AI-enhanced simulation techniques specifically tailored to rotary systems will be demonstrated.

Key Contributions:

- Unlike most existing studies that focus on a single physical domain (e.g., structural analysis) or simplified scenarios, this research targets the integrated modeling of coupled multi-physics behaviors.

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- The effectiveness of advanced AI methods—such as Graph Neural Networks (GNN) and Fourier Neural Operators (FNO)—in learning spatio-temporal patterns from multi-physics data will be investigated.
- The study aims to contribute to the literature by introducing an open-source benchmark dataset for industrial rotary systems and developing a hybrid (physics + data-driven) AI model architecture.

2. LITERATURE REVIEW

Rotating mechanisms play a critical role in energy, manufacturing, and transportation systems, where system performance and reliability are governed by strongly coupled mechanical, thermal, and fluid-dynamic effects. High rotational speeds and complex loading conditions make single-physics analyses insufficient for accurately capturing system behavior. Previous studies have shown that neglecting thermo-mechanical coupling in gas turbine rotors can lead to severe underestimation of fatigue risks, while fluid-induced pressure fluctuations have been identified as a major source of vibration and efficiency loss in rotating machinery under transient conditions [30]. These findings highlight the necessity of integrated multi-physics modeling for ensuring the safe and reliable operation of rotary systems.

Despite their accuracy, high-fidelity multi-physics simulations are associated with substantial computational cost and long execution times, limiting their applicability in design optimization and rapid prototyping. To address this limitation, surrogate modeling techniques have been introduced as computationally efficient alternatives. Data-driven surrogate models have demonstrated significant reductions in simulation time while preserving acceptable prediction accuracy for complex mechanical systems [10]. More recently, Physics-Informed Neural Networks have emerged as a promising approach by embedding governing physical equations directly into the learning process, enabling physically consistent predictions even under limited data availability [1], [5].

Advances in deep learning have further expanded the scope of surrogate modeling for rotating systems. Graph Neural Networks have been successfully applied to mechanical CAD representations, showing improved generalization across varying geometries through topology-aware learning [23]. In parallel, deep learning–based surrogate models for fluid flow prediction have achieved computational speedups of up to two orders of magnitude compared to conventional solvers, demonstrating the potential of AI-assisted simulation frameworks [11]. However, most existing studies remain focused on single-physics domains or static operating conditions, indicating a clear research gap in fully coupled, AI-based multi-physics modeling of rotating mechanisms under dynamic conditions. This study aims to address this gap by proposing a structured and scalable framework for AI-assisted multi-physics modeling of rotary systems.

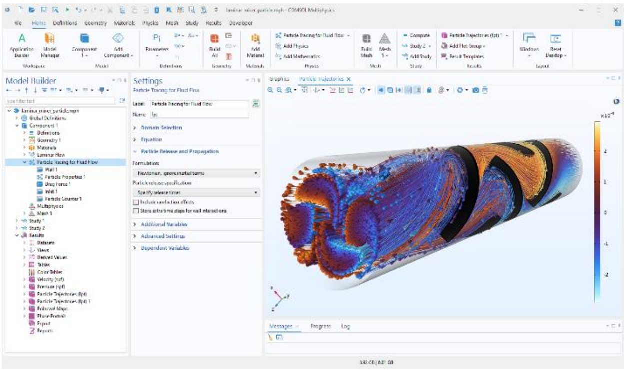

Figure 1 Computational fluid dynamics (CFD) visualization showing velocity and vortex structures in a rotating cylindrical geometry (generated using COMSOL Multiphysics software).

3. MATERIALS AND METHODS

In this study, a parametric rotary mechanism model inspired by a generic turbine rotor was developed using Autodesk Fusion 360. The geometry was defined in a flexible manner to allow systematic variation of key design parameters, including blade thickness, length, curvature, and hub diameter. This parametric setup enabled the generation of multiple design configurations representing different mechanical operating scenarios and formed the basis for subsequent simulation and data generation processes.

A coupled multi-physics simulation framework was employed to capture the interactions between structural, thermal, and fluid domains. Structural analyses were conducted to evaluate stress and deformation under centrifugal loading, thermal analyses were performed to assess temperature distribution, and computational fluid dynamics simulations were used to characterize airflow behavior and cooling performance. Each simulation was defined by a unique combination of geometric parameters and operating conditions such as rotational speed, material properties, and ambient temperature. Due to computational and hardware constraints, the target number of simulations was limited, and data augmentation strategies were considered to support initial model development.

Simulation outputs were organized into a structured dataset linking input parameters to physical response variables, including maximum stress, temperature, deformation, and airflow characteristics. The data were normalized using min–max scaling and divided into training and testing subsets. Several artificial intelligence models were explored, ranging from conventional artificial neural networks to physics-informed and graph-based architectures capable of incorporating physical constraints and spatial connectivity. Model performance was evaluated using standard regression metrics and computational efficiency indicators, with additional testing on unseen configurations to assess generalization capability.

Figure 2. Internal structure of a horizontal-axis wind turbine illustrating key rotary components such as the rotor hub, gearbox, and generator (adapted from Siemens)

4. METHODOLOGY

This study employs an artificial intelligence–based framework to model the multi-physics behavior of rotary mechanisms with reduced computational cost. A parametric turbine-inspired rotor geometry was generated to represent diverse operating scenarios. Key geometric, physical, and environmental parameters were systematically varied to ensure sufficient design diversity for data-driven learning.

Coupled structural, thermal, and fluid simulations were conducted to capture the interactions governing system behavior. Simulation outputs were structured into an input–output dataset linking operating conditions and geometry to physical response variables. Due to computational constraints, the dataset size was limited, and data augmentation techniques were considered to support early-stage model development.

Several AI architectures were evaluated, ranging from conventional neural networks to physics-informed and graph-based models. Model performance was assessed using standard regression metrics and computational speedup indicators, with additional testing on unseen scenarios to evaluate generalization and feasibility for engineering applications(shown in Table 1).

Table 1. AI Models Considered

Model Type	***Purpose***	***Key Advantage***
ANN (MLP)	Baseline regression	Simple and fast training
PINN	Physics-aware learning	Reduced data dependency
GNN	Mesh-based representation	Captures spatial topology
Hybrid PINN–GNN	Advanced modeling	Physical consistency + geometry awareness

4.1. Data Generation And Implementation Constraints

The development of an AI-based model for predicting the multi-physics behavior of rotary mechanisms requires a sufficiently large and diverse simulation dataset. However, the planned large-scale data generation process could not be fully realized within the scope of this study due to practical limitations. Multi-physics simulations were found to be computationally expensive, with individual runs requiring several hours depending on model complexity, making extensive dataset generation infeasible on a single-machine setup.

Hardware instability further constrained the implementation process. Recurrent system-level failures involving memory, processing units, and graphics hardware prevented long-duration simulations from being executed reliably. As a result, generating a dataset on the order of 10,000 samples which is typically required for training robust deep learning models would have required multiple years of continuous computation under the available resources.

To mitigate these limitations, alternative modeling strategies were evaluated. Early-stage modeling using reduced datasets and physics-informed neural network architectures emerged as viable approaches for operating under limited data conditions. These findings highlight the importance of physics-aware learning and scalable computing infrastructures for AI-assisted multi-physics modeling. Future efforts will focus on small-data training strategies and physics-guided architectures to enable predictive modeling despite computational constraints.

4.2. Dataset And Training Plan

This section presents the dataset design strategy and training considerations for developing AI-based models to represent the multi-physics behavior of rotary mechanisms. The primary objective is to establish a predictive framework capable of estimating key engineering responses, including stress, temperature, deformation, and flow-related quantities, under varying geometric and environmental conditions.

The dataset structure is based on simulation-generated input–output pairs. Input features describe the operating conditions and geometric characteristics of the system, such as rotational speed, material type, key geometric parameters, ambient conditions, and cooling or airflow configuration. The corresponding outputs represent the physical response of the system, including maximum mechanical stress, surface temperature, total deformation, and representative flow velocity measures. This formulation enables the learning of coupled relationships between mechanical, thermal, and fluid domains.

The required dataset size strongly depends on the selected modeling approach. Conventional feedforward and deep neural networks typically require several thousand to tens of thousands of samples to achieve robust generalization, whereas Physics-Informed Neural Networks can operate effectively with significantly fewer samples due to embedded physical constraints. Based on this trade-off, a target dataset size of approximately 10,000 samples was identified as a reference benchmark for data-driven models (shown in Table 2 and Table 3).

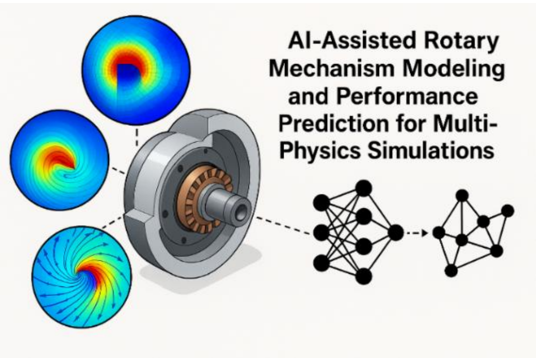

Figure-3 Conceptual representation of AI-assisted modeling for rotary mechanisms, illustrating the integration of multi-physics simulation outputs with neural network architectures (created by the author).

Table 2 Estimated Total Time for large datasets on a system

System Type	Parallel Simulations	Estimated Total Time (10,000 samples)
1-Core PC	1	2.3 years
8-Core Workstation	4	~6 months
32-Core Server	16	~1.5 months
Amazon AWS (64 vCPU)	32	~3 weeks
128-CPU University Cluster	64	~10 days

Multi-physics simulations are computationally expensive, with an average execution time of approximately two hours per sample and longer runtimes for complex scenarios. Consequently, generating large datasets on a single-core system is impractical, motivating the use of parallel computing strategies. Parallel execution on multi-core workstations, servers, or cloud-based platforms can reduce total data generation time from years to weeks. In cases where such resources are unavailable, alternative strategies such as small-data modeling, data augmentation, transfer learning, and physics-informed neural architectures provide feasible pathways for early-stage model development.

Table 3 Estimated value and parameters

Criterion	Estimated Value
Dataset size	10,000 samples
Simulation time	2 hours/sample
Total time (no parallelism)	20,000 hours (~2.3 years)
With parallel computing	10 days – 6 months
Alternative options	PINN or small dataset modeling

4.3. Probabilistic Success Estimation Under Resource Constraints

This study includes a probabilistic analysis to assess the feasibility of successfully training an AI-based model for multi-physics modeling of rotary mechanisms under limited computational resources, time, and data availability. Success was defined as the completion of model training while achieving a minimum performance threshold of R^2>0.85 A Monte Carlo–based simulation framework was employed to estimate success likelihood by combining key contributing factors related to hardware reliability, data availability, simulation completion, and modeling proficiency.

The analysis indicates that, under the current project conditions, the probability of achieving a fully functional and accurate AI model is relatively low. This outcome is primarily driven by insufficient simulation data volume, instability in computational hardware, and long execution times associated with high-fidelity multi-physics simulations. These constraints significantly limit the ability to generate large datasets and maintain stable AI training workflows within the available timeframe.

Despite the low estimated success probability, the analysis provides valuable insight into potential mitigation strategies. Physics-informed learning approaches, small-data modeling supported by transfer learning, and access to parallel computing infrastructures emerge as effective pathways for improving feasibility. Rather than serving as a performance metric, this probabilistic assessment functions as a decision-support tool, highlighting the conditions under which AI-assisted multi-physics modeling of rotary mechanisms becomes practically achievable. Relative contribution of key factors influencing the probability of successful AI-based multi-physics model training under resource constraints (shown in Table 4). All values are normalized between 0 and 1. The weighted average is then compared to a success threshold (0.6).

Table 4 Relative contribution of key factors influencing the probability of successful

Factor	Description	Weight
Hardware Stability	System uptime and reliability	0.25
Normalized Data Volume	Proportion of data generated compared to target	0.30
Simulation Completion Rate	Percentage of simulations completed successfully	0.20
AI Expertise / Code Quality	Modeling and training proficiency	0.25

The outcomes of this study indicate that the primary limitations were not conceptual or methodological, but rather operational and resource-related. The proposed AI-based framework for multi-physics modeling of rotary mechanisms is theoretically sound; however, its practical realization was constrained by limited computational capacity, long simulation runtimes, and hardware instability. Addressing these constraints at earlier stages would have substantially increased the feasibility of achieving a fully trained and validated predictive model.

A critical factor affecting success was the data generation pipeline. Multi-physics simulations involving coupled structural, thermal, and fluid domains are inherently time-consuming. The study could have benefited from a staged simulation strategy, beginning with reduced-order or single-physics models to rapidly generate preliminary datasets. The use of simplified geometries and coarse meshes in early phases would have enabled faster iteration cycles, allowing model training to commence earlier and be progressively refined as higher-fidelity data became available. Access to parallel computing environments, such as institutional high-performance clusters or cloud-based infrastructures, would have further reduced simulation bottlenecks.

From a modeling perspective, reliance on data-intensive neural network architectures limited progress under small-data conditions. Greater emphasis on physics-aware and data-efficient approaches such as Physics-Informed Neural Networks, transfer learning from related mechanical systems, and structured data augmentation could have improved learning performance despite limited sample availability. These strategies are particularly well-suited to engineering problems where governing equations and physical constraints are well understood and can be explicitly embedded into the learning process.

Finally, project scope management played a decisive role. A more incremental research strategy focused on a narrowly defined proof of concept such as predicting a single performance metric under restricted operating conditions would have reduced complexity and facilitated earlier validation. By progressively expanding the model scope only after achieving stable intermediate results, the study could have maintained continuity despite hardware failures and time constraints. Overall, the lessons learned highlight the importance of adaptive planning, scalable computing resources, and physics-guided learning strategies for the successful deployment of AI-assisted multi-physics modeling under constrained research conditions.

5. RESULTS AND CONCLUSION

This study investigated the feasibility of applying artificial intelligence–based surrogate modeling to predict the multi-physics behavior of rotary mechanisms. Conventional numerical approaches such as finite element analysis and computational fluid dynamics provide high-fidelity results but suffer from excessive computational cost when mechanical, thermal, and fluid domains are simultaneously considered. In this context, the study proposed an AI-assisted modeling framework aimed at accelerating simulation-driven performance estimation while maintaining acceptable accuracy.

Although full-scale model training and validation could not be completed due to hardware instability, limited computational resources, and insufficient simulation data, the study achieved several meaningful outcomes. A comprehensive literature review, a structured methodological framework, dataset planning, and a probabilistic feasibility analysis were successfully developed. Together, these contributions clarify the technical requirements, constraints, and risks associated with AI-driven multi-physics modeling and provide a transparent assessment of what is realistically achievable under constrained research conditions.

Future research should prioritize data-efficient and physics-aware learning strategies to overcome the limitations identified in this work. Physics-Informed Neural Networks, small-scale proof-of-concept models, and parallel simulation pipelines represent promising directions for reducing data and computation demands.

With access to stable high-performance computing resources and a phased development strategy, the conceptual framework presented in this study can be extended toward practical AI-assisted tools for rotary mechanism analysis. Overall, the findings highlight both the potential and the prerequisites of integrating artificial intelligence into complex engineering simulation workflows.

5.1. Contributions, Gains, and Implications For Future Work

This study represents an exploratory investigation into the applicability of artificial intelligence–based modeling techniques for multi-physics engineering systems, with a particular focus on rotary mechanisms. Although a complete end-to-end implementation could not be achieved, the work delivers meaningful conceptual, technical, and methodological contributions that clarify both the opportunities and limitations of AI-assisted multi-physics modeling under constrained research conditions.

From an academic perspective, the study establishes a structured framework for integrating artificial intelligence with coupled mechanical, thermal, and fluid simulations. It systematically contrasts traditional high-fidelity simulation approaches with data-driven and physics-informed alternatives in terms of computational cost, scalability, and feasibility. Furthermore, the work identifies and contextualizes data-efficient strategies—such as Physics-Informed Neural Networks, transfer learning, and small-data modeling—as practical solutions for environments where large-scale simulation datasets and high-performance computing resources are unavailable.

Technically, the study defines a complete input–output parameterization scheme suitable for AI-based modeling of rotary systems and presents a probabilistic success estimation methodology implemented in Python. This feasibility-driven analysis provides a rarely documented but highly practical decision-support perspective, demonstrating how hardware reliability, data volume, and modeling expertise collectively influence project outcomes in AI-driven engineering workflows.

Beyond its technical scope, the study also yields significant methodological and experiential gains. It demonstrates how complex engineering problems can be decomposed into manageable analytical stages, even when implementation constraints prevent full execution. The insights gained regarding simulation planning, resource allocation, and adaptive modeling strategies are directly transferable to future research efforts in multi-physics systems.

Overall, this work serves as a foundational reference for future studies aiming to bridge physics-based simulations and artificial intelligence. By documenting not only successful methodologies but also realistic constraints and mitigation strategies, the study contributes a transparent and practical roadmap for advancing AI-assisted modeling of complex engineering systems in both academic and applied contexts.

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