**Physics-Based Modeling of Industrial Systems: A Multi-Scale Framework for Predictive Digital Twins**

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**Abstract.** This paper presents a comprehensive physics-based modeling framework for developing predictive digital twins of industrial systems, integrating multi-scale physical principles with machine learning for enhanced accuracy in prognostic health management. The research develops and validates hierarchical models spanning quantum-scale material behavior to system-level dynamics, with particular focus on rotating machinery, heat exchangers, and chemical reactors as representative industrial systems. For rotating equipment, we integrate rotor dynamics (Timoshenko beam theory with shear deformation effects), hydrodynamic bearing physics (solutions to Reynolds equation incorporating thermal effects), and gear tribology (time-varying stiffness models with elasto-hydrodynamic lubrication analysis). The thermal systems model employs conjugate heat transfer simulations with turbulence modeling (k-ω SST) and fouling resistance algorithms based on crystallization kinetics. Chemical process modeling incorporates computational fluid dynamics (CFD) with species transport and reaction kinetics based on transition state theory. A novel hybrid validation approach combines finite element analysis (FEA), computational fluid dynamics (CFD), and experimental data from industrial-scale test rigs, including a 2.5 MW compressor station operating continuously for 14 months with comprehensive sensor arrays. The framework demonstrates capability to predict remaining useful life (RUL) with mean absolute error of 7.8% across different failure modes, representing 41% improvement over purely data-driven approaches. Implementation in three industrial case studies shows annual maintenance cost reduction of 32-46% while improving system availability by 18-27%. The twin model architecture allows optimization in real-time at best-in-class energy savings of 8-15% based on adaptive control and the insights from physics-based predictions.

**Keywords:** hysics-based modeling, digital twin, predictive maintenance, multi-scale simulation, industrial system(s), hybrid modelling.

**INTRODUCTION**

Industry 4.0 has revolutionized industrial landscapes and opened doors to new opportunities for digitalization in manufacturing, prompting the global digital twin solutions market size to exceed $48.2 billion by 2026, according to a recent report. Although data-driven approaches have tended to prevail as early implementations, since they do not readily extrapolate beyond training data and require large amounts of failure histories, physics-based modeling (PBM) has emerged with growing interest. PBM provides basic benefits when it is necessary to find out the distortion of system behaviour without data on malfunctions (for novel operating regimes) and in the early stages of its life cycle. But the current performing PBMs are usually computational intensive, hard to model intricate multi-physics synergistic system and lack real industrial data validation [1-3].

In this work, we overcome these limitations and develop a multi-scale physics-based modelling framework tailored for industrial digital twins. It combines idfamodels of various transciplevels like quantum mechanical simulations of material degradation/ systemlevel performance prediction and machine learning methods for parameter calibration/ uncertainty quantification. The study considers three example industrial systems that between them cover the main relevant physical phenomena such as rotating machinery (mechanical dynamics, tribology), heat exchangers (thermofluid dynamics, fouling) or chemical reactors (reaction kinetics, transport phenomena). Validation against large scale industrial data gives an assurance on the capabilities of model predictivesystems in the real application [4].

**THEORETICAL FRAMEWORK AND METHODOLOGY**

The developed hierarchical modeling has been performed with four levels of scale but interconnected from material level to system level, for the simulation and prediction of basic materials phenomena that link the underlying or elementary constitutive laws to overall performance. In the quantum atomistic level DFT calculations offer fundamental understanding of material properties and degradation mechanisms. For example, DFT simulations predict fatigue crack nucleation at grain boundaries in bearing materials and provide critical input parameters such as interface energies and dislocation barriers for higher-level models. Starting from molecular data, the CPFE approach uses this atomic scale information to predict the behavior of a polycrystalline microstructure under cyclic loading. This scale encompasses the localization of plastic strain and defect nucleation so that the initial damage site can be predicted for critical components such as gear teeth and compressor blades [5-8].

At the component level, the framework would lead to continuum-based models – using FEA/CFD to predict behavior of complete components under operational and environmental loads. Based on the defect initiation data at the microscale, these models provide stress distributions, thermal gradients, and fluid-structure interactions for assessing component integrity and performance limits. Ultimately, computationally efficient Reduced-Order Models (ROMs) at the system-level are developed starting from the high-fidelity component-scale simulations. These ROMs capture the key physics in a reduced formfactor that can be used for online model-based performance prediction, prognostic health management and situational awareness within a living digital twin of the full industrial system. This coarsening of scales allows for fundamental physics and principles to be used in model predictions but for the resulting models to still be operationally usable.

The spinning assembly is modelled as per Timoshenko beam theory with shear deformation and rotary inertia:

(1)

Where *E* is Young’s modulus, I is area moment of inertia, ρ is density, A is cross-sectional area, κ is co-efficient of shear, G being the shear modulus and *q(x,t)* as distributed load.

Stiffness computation for the bearing stiffness modeling stiff) of variable radial andiginal arrangement is also considered in the critical speed analysis. Properly encouraged with varying rotational speeds can be done based on:

(2)

Here, Ω is the angular velocity, and G was the gyroscopic matrix that takes into account the rotational inertia effects.

Hydrodynamic journal bearings are modeled using the generalized Reynolds equation incorporating thermal effects:

(3)

The viscosity-temperature relationship follows the Vogel-Fulcher-Tammann equation:

(4)

Solutions provide stiffness (*Kxx*, *Kxy*, *Kyx*, *Kyy*) and damping (*Cxx*, *Cxy*, *Cyx*, *Cyy*) coefficients as functions of eccentricity ratio (*ϵ*) and Sommerfeld number , where *N* is rotational speed, *L* is bearing length, *D* is journal diameter, *W* is load, *R* is radius, and *C* is radial clearance.

Time-varying mesh stiffness accounts for changing contact ratio:

(5)

Where , are bending stiffnesses of mating teeth, and is Hertzian contact stiffness.

Elastohydrodynamic lubrication (EHL) film thickness is calculated using Dowson-Higginson equation:

(6)

Where *U* is speed parameter, *G* s material parameter, and *W* is load parameter.

Conjugate heat transfer simulations employ the k-ω SST turbulence model:

(7)

(8)

Fouling resistance prediction incorporates crystallization kinetics:

(9)

Where *Rf* is fouling resistance, *Cb* is bulk concentration, *Ea* is activation energy, *R* is gas constant, *T* is temperature, *τw* is wall shear stress, and *α*, *β*, *n* are empirical coefficients.

Species transport with reaction kinetics follows:

(10)

Where *Yi* is mass fraction of species *i*, is diffusion flux, and *Ri* is net production rate from chemical reactions.

Reaction rates based on transition state theory:

(11)

Where *kB* is Boltzmann constant, ℎis Planck constant, and Δ is Gibbs free energy of activation.

**DIGITAL TWIN IMPLEMENTATION AND VALIDATION**

The deployed digital twin architecture creates a closed-operation loop that has four interconnected components included in. The Physical Entity This is the tangible factory infrastructure that represents a real industrial equipment with rich sensor networks across all its components. This is then reflected by a Virtual Entity – high fidelity physics-based model, continuously adjusting based on the plant’s real time operation. A Bi-directional Digital Thread provides the means to continuously exchange data and keep physical/virtual objects synced, so as to ensure that their digital twins faithfully represent them. On top of this foundational layer is a Services Layer, providing enhanced analytics, live visualization and actionable decision support for operators and engineers.

A three-layered method was used to extensively test this framework. First, Component-Level Validation maintained model fidelity by validating predictions against laboratory test data for individual sub- components such as bearings, gears and the heat exchanger tubes. Second, System-Level Validation evaluated performance in a full instrumented test rigs in a controlled environment. Lastly, the industrial validation corresponded to the real-time monitoring of operational equipment under field conditions. This approach was tested on three important case studies. The authors reported that on a 2.5 MW natural gas compressor with 142 sensors over a period of 14 months, the digital twin predicted bearing degradation already around 68 days before standard vibration alarms would have issued an alert, so enabling predictive monthly maintenance scheduling having led to decrease in its annual unplanned downtime from 5.2% down to less than half of that value (1.8%). Application of the model to a 45 MW refinery heat exchanger confirmed that with distributed temperature sensing in place, optimal operating schedules designed by the model resulted in a mean deviation from actual fouling development of 12.3% over heat conversion coefficient reduction; this increase implied an improvement in annual thermal efficiency equal to +8.7%. In addition, for a Raman spectroscopy/tomography monitored 15 m³ polymerization reactor the model was able to predict variation in product quality 3-5 residency times ahead of time. This feature enabled feedforward control for preemptive corrections and reduced a key quality parameter's standard deviation by 47% in batch formation, leading to significant product consistency enhancements. Taken together, these industrial validations show the superior predictive quality and economic value of the digital twin over tradition in situ monitoring practices.

Implementation across three industrial sites demonstrated significant economic benefits.

**TABLE 1.** Comparison of Predictive Methods for RUL Estimation.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Method** | **Mean Absolute Error (%)** | **Early Detection Capability (days)** | **False Positive Rate (%)** | **Computational Cost (relative)** |
| **Physics-Based (this work)** | 7.8 | 42 ± 11 | 2.4 | 10.0 |
| **Traditional Vibration Analysis** | 24.3 | 18 ± 7 | 8.7 | 1.0 |
| **Machine Learning Only** | 13.2 | 31 ± 9 | 5.2 | 2.5 |
| **Hybrid Physics-ML (literature)** | 10.5 | 35 ± 10 | 3.8 | 6.5 |

**TABLE 2.** Economic Benefits of Physics-Based Digital Twin Implementation

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Metric** | **Compressor Station** | **Heat Exchanger Network** | **Chemical Reactor** | **Weighted Average** |
| **Maintenance Cost Reduction (%)** | 38.2 | 31.7 | 46.1 | 37.8 |
| **Energy Efficiency Improvement (%)** | 11.3 | 8.7 | 15.2 | 11.2 |
| **Availability Increase (%)** | 22.5 | 18.3 | 27.1 | 21.7 |
| **ROI Period (months)** | 8.5 | 10.2 | 6.8 | 8.3 |

Anchoring the use-cases of digital twin is its approach to multi-fidelity model; an approach combined with accuracy in predictive modeling along with efficiency in computation to render both deep analyses as well metric real-time operations. High-fidelity models using detailed finite element analysis and computational fluid dynamics, provide a full understanding but demand big computational power, on average it requires between 4 to 12 hours for one simulation. These models are crucial for offline design verification, root cause analysis and training data generation. These above-mentioned high-fidelity simulations can serve to generate computationally inexpensive Reduced-Order Models (ROMs) for real-time operation in the live digital twin. Running predictions at the 10-100 ms time scales possible with such ROMs, which capture the basic physics of the system, are then central to fully monitoring and predicting for a virtual entity. Interconnecting these two layers, an automatic calibration cycle updating every 30 to 60 min implicitly overwrites the real-time ROM parameters with current operational sensor measurements. Such an hierarchical structure allows the digital twin to provide timely decisions while its lower abstraction levels are dedicated to be anchored as much as possible on physically accurate representations and system’s current state (in contrast, say, with foreseers implemented into a static database).

**DISCUSSION**

Several key advantages of the physics-based DT framework over data-only driven approaches were highlighted, particularly its ability to extrapolate with confidence. Unlike statistical models, the model has capability to estimate system under the new operating conditions or fault scenarios which is not in its original training data. This functionality makes it useful in the initial life stage where reliable performance prediction and monitoring from date of commissioning can be difficult for data-driven methods without a significant operational history. Additionally, the overall physical interpretability is better thanks to predictions where actual phenomena (e.g. stress concentrations, thermal gradients) are basis for them which will make diagnosis much more transparent and effective. Multi-fault diagnosis is also supported by the framework, in which multiple interacting failure modes can be diagnosed simultaneously with disentanglement of each other, e.g., Compound unbalance and misalignment that combine to confound pattern recognition.

Yet the real application of such a paradigm also faced great challenges. The first is to cope with parameter uncertainty since exact material properties, boundary conditions and component geometries are frequently unknown or variable in an industrial context. This necessitates robust calibration routines. Moreover, control over model complexity involves a delicate and subjective balancing act between physical accuracy one wants to maintain and the practicability in terms of representing cost/benefit trade-offs. Another significant engineering challenge is the complexity involved in coupling different physics such as structural dynamics (SD), fluid flow (FF) and thermodynamics that work on widely separated time- and spatial scales. Finally, obtaining high-quality validation data from fully instrumented industrial systems operating to failure is both challenging and costly resulting in a bottleneck that must be overcome in order to conclusively prove long-term prognostic accuracy under true service environments.

The use of physics-based models coupled with machine learning for parameter calibration and uncertainty quantification was particularly successful. More specifically, machine learning / data-driven methods which are trained in terms of residual errors between model predictions and sensor measurements have been shown to enhance accuracy by learning unmodeled phenomena and system-specific features.

**CONCLUSION**

This research introduces and proves a robust physics-based modelling framework for industrial digital twins, with evident enhancements in prediction accuracy, maintenance efficiency optimization, and system operation efficiency over traditional methods. The multi-scale structure allows the suitable fidelty of modeling for different phases in the asset life, ranging from design optimization to predictive maintenance. By adopting a hybrid framework based on physics and data-driven calibration, we can utilize the advantages of both techniques to have physically explainable predictions with predictive power from the advantage of operational experiences.

Validation of the framework with large-scale industrial operational data confirms its relevance to practical systems. Results of implementation case studies show the concrete economic benefits resulting from maintenance cost savings, better energy efficiency or improved system availability. Future work will involve automatic model calibration methods, uncertainty quantification methodologies and extension to other types of industrial systems. The proposed method is a major step toward digital twins that are really predictive and can revolutionize industries through physics-based decision support.

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