Internship Report

Potential Applications of Machine Learning in Computational Fluid Dynamics

Gas Turbine Auxilliaries

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Abstract

This report explores the integration of machine learning (ML), particularly Physics-Informed Neural Networks (PINNs), into Computational Fluid Dynamics (CFD) applications, with a focus on gas turbines and their auxiliaries. It provides a comprehensive overview of gas and steam turbine technologies, detailing their components, working principles, applications, and challenges. The study emphasizes the transformative potential of PINNs in CFD, specifically for the lube oil degasification problem. By embedding physical laws into ML models, PINNs offer a cost-effective and computationally efficient alternative to traditional solvers. The findings demonstrate how PINNs enhance simulation accuracy, reduce computational costs, and pave the way for scalable applications in turbine-related processes, marking a significant advancement in engineering and fluid dynamics.

Contents

Acknowledgment

I am sincerely thankful to Siemens Energy, Gurugram, for offering me an internship opportunity in the Winter of 2024, that greatly contributed to my learning and professional growth. I am a Junior at IIT Delhi with a major in Engineering and Computational Mechanics. I have developed keen interest in my subjects and this internship was my first opportunity to explore the application of them in the industry.

This internship also allowed me to interact with and learn from an array of talented professionals who guided and supported me throughout this period. I would like to especially thank Mr. Arun Gupta, Mr. Danish Khan, Mr. Karambir Singh and Mr. Antony Dinto. They were always eager to share their expertise, patiently answering my queries and helping me gain a deeper understanding of the company's operations and the industry as a whole.

About Siemens Energy

Siemens Energy is a global leader in the energy sector, dedicated to shaping the future of energy through innovative solutions and technologies. The company provides a comprehensive portfolio ranging from gas turbines, steam turbines, and power plants to sustainable energy solutions, including renewable energy integration and power transmission.

With a strong commitment to sustainability, Siemens Energy focuses on decarbonizing energy systems, enhancing energy efficiency, and fostering technological advancements to address the growing global energy demand. Its mission is to empower societies with reliable, affordable, and environmentally friendly energy solutions.

Operating in over 90 countries, Siemens Energy has a diverse workforce of highly skilled professionals who drive innovation and excellence. The Gurugram office serves as a hub for R&D, project management, and customer operations, contributing significantly to the company's success and global presence.

Objective

This report is to be a summary of the knowledge I gained about gas turbines, steam turbines, gas turbine auxiliaries, and Physics-Informed Neural Networks (PINNs) during my internship at Siemens Energy.

Building on that foundation, I aim to develop a comprehensive study on the potential **integration of PINNs into CFD applications** within Siemens Energy. The study will specifically focus on the *Lube Oil Degasification* problem as a case study, emphasizing how PINNs can significantly enhance efficiency and reduce computational costs in addressing such challenges.

Chapter 1

Turbines and Auxiliaries

1.1 Gas Turbines

1.1.1 Introduction

Gas turbines are internal combustion engines that convert natural gas or other liquid fuels into mechanical energy. This energy then drives a generator, producing electrical energy. They are widely used in various applications, including power generation, aviation, and industrial processes, due to their high efficiency and reliability.

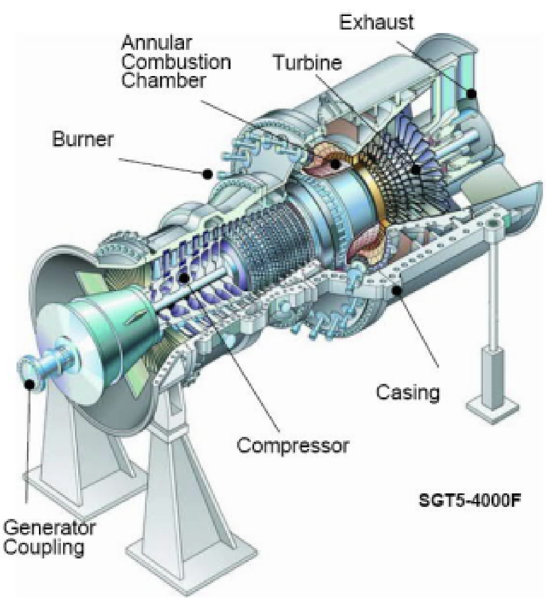
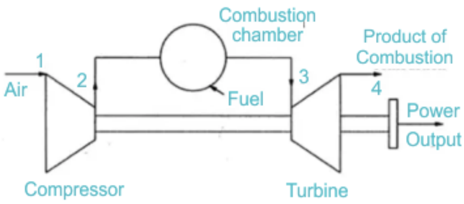


Figure 1.1: Siemens Gas Turbine - SGT5-4000F

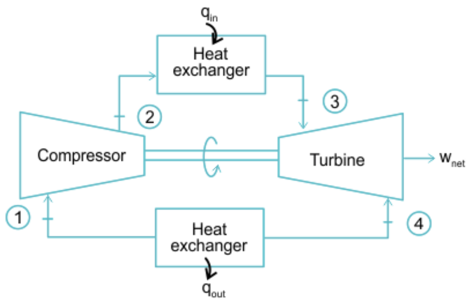
1.1.2 Components of a Gas Turbine

A typical gas turbine consists of three main components:

- **Compressor:** Draws in and compresses ambient air, increasing its pressure.
- **Combustion Chamber:** Mixes the compressed air with fuel and ignites the mixture, producing high-temperature and high-pressure gases.
- **Turbine:** Extracts energy from the high-pressure gases to drive the compressor and generate mechanical output.



(a) Open Cycle



(b) Closed Cycle

Figure 1.2: Thermodynamic GT Cycles

1.1.3 Working Principle

The operation of a gas turbine involves the following steps:

1. **Air Compression:** Ambient air is drawn into the compressor, where its pressure and temperature are increased.
2. **Fuel Injection and Combustion:** The compressed air enters the combustion chamber, where fuel is injected and ignited, resulting in high-energy exhaust gases.
3. **Expansion and Power Extraction:** The high-energy gases expand through the turbine stages, causing the turbine blades to spin and produce mechanical energy.
4. **Exhaust:** The spent gases are expelled through the exhaust, and in some configurations, heat recovery systems are used to improve efficiency.

1.1.4 Types of Gas Turbines

Gas turbines can be classified based on their applications:

- **Aero-Derivative Gas Turbines:** Adapted from aircraft jet engines for power generation and mechanical drive applications.

Figure 1.3: Siemens 44 mega-watt GT - SGT-A45 TR

- **Heavy-Duty Industrial Gas Turbines:** Designed specifically for stationary power generation and industrial applications.

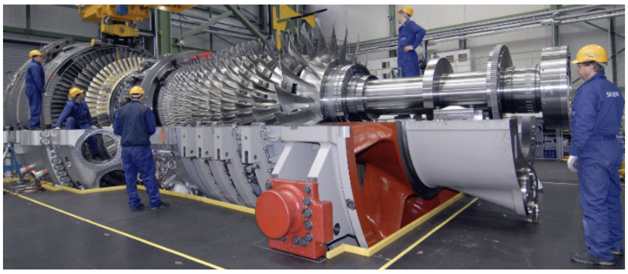


Figure 1.4: Siemens H-Class GT - SGT5-8000H

1.1.5 Applications

Gas turbines are utilized in various sectors:

- **Power Generation:** Used in both simple and combined cycle power plants to produce electricity.
- **Aviation:** Serve as jet engines for aircraft propulsion.
- **Industrial Processes:** Provide mechanical drive for compressors and pumps in industries like oil and gas.

1.1.6 Advantages

The benefits of gas turbines include:

- **High Efficiency:** Especially in combined cycle configurations.
- **Low Emissions:** Advanced combustion technologies reduce pollutant emissions.
- **Fuel Flexibility:** Capable of operating on a variety of fuels, including natural gas and liquid fuels.
- **Reliability and Durability:** Designed for continuous operation with minimal maintenance.

1.1.7 Challenges

Despite their advantages, gas turbines face certain challenges:

- **High Initial Costs:** Significant capital investment is required for installation.
- **Complex Maintenance:** Requires specialized knowledge and equipment.
- **Efficiency Reduction at Partial Loads:** Performance can decrease when not operating at full capacity.

1.2 Steam Turbines

1.2.1 Introduction

Steam turbines are mechanical devices that convert the thermal energy of pressurized steam into mechanical work, which is then used to generate electricity or perform other mechanical tasks. Invented by Charles Parsons in 1884, steam turbines have become integral components in power plants, industrial processes, and marine propulsion systems. They operate on the principle of the Rankine cycle, efficiently transforming heat energy into mechanical energy through phase transitions.

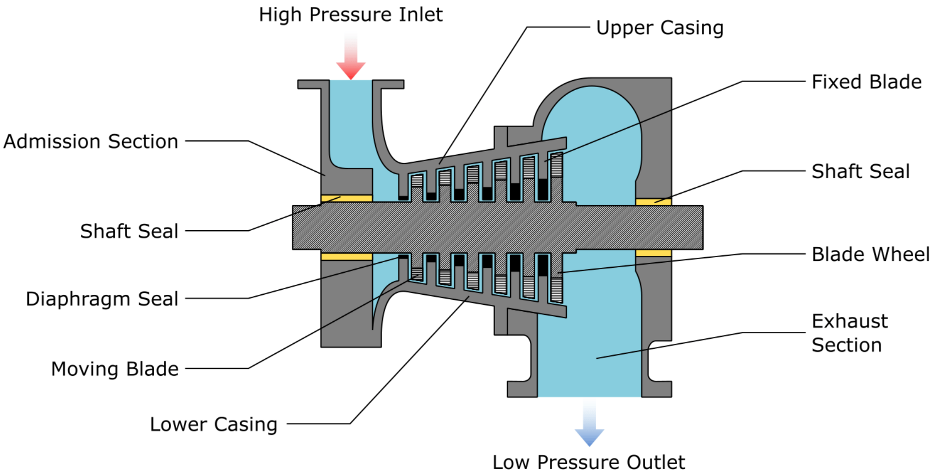


Figure 1.5: Labelled Steam Turbine

1.2.2 Components of a Steam Turbine

A typical steam turbine comprises several key components:

- **Rotor:** The rotating part that carries the turbine blades and converts steam energy into mechanical work.
- **Stator:** The stationary part that directs the flow of steam onto the rotor blades.
- **Blades:** Attached to the rotor, these are designed to efficiently extract energy from the steam.
- **Casing:** Encloses the turbine components and contains the steam pressure.
- **Nozzles:** Accelerate and direct the steam flow onto the turbine blades.
- **Bearings:** Support the rotor and allow smooth rotation.

1.2.3 Working Principle

The operation of a steam turbine involves the following steps:

1. **Steam Generation:** Water is heated in a boiler to produce high-pressure, high-temperature steam.
2. **Expansion:** The steam expands through nozzles, converting thermal energy into kinetic energy.

3. **Energy Extraction:** The high-velocity steam impinges on the turbine blades, causing the rotor to spin and produce mechanical work.

4. **Condensation:** After passing through the turbine, the steam is condensed back into water in a condenser for reuse.

1.2.4 Types of Steam Turbines

Steam turbines can be classified based on various criteria:

- **Based on Pressure Stages:**
  - **Single-Stage Turbines:** Steam expands in a single set of nozzles and blades.
  - **Multi-Stage Turbines:** Steam expands through multiple sets of nozzles and blades for higher efficiency.

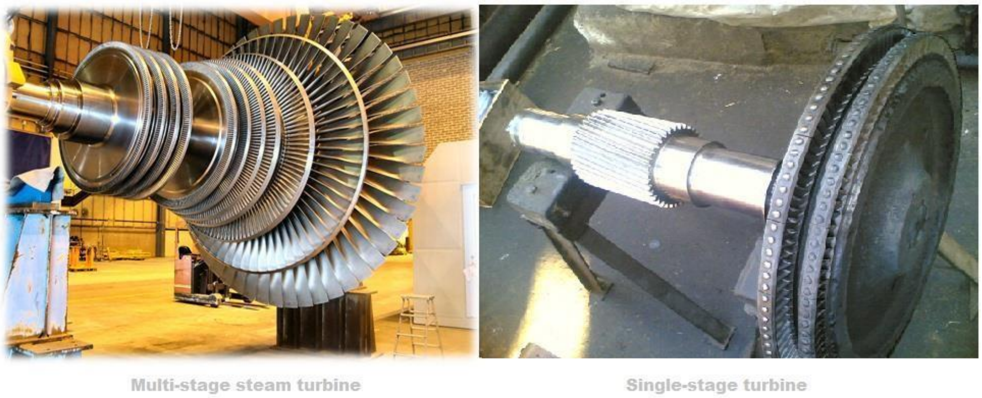


Figure 1.6: New age Turbine Technology

- **Based on Exhaust Conditions:**
  - **Condensing Turbines:** Exhaust steam is condensed in a condenser, allowing for maximum energy extraction.
  - **Non-Condensing Turbines:** Exhaust steam is utilized for industrial processes or heating, not condensed.

- **Based on Steam Flow Direction:**
  - **Axial Flow Turbines:** Steam flows parallel to the axis of the rotor.

- **Radial Flow Turbines:** Steam flows perpendicular to the axis of the rotor.

1.2.5 Applications

Steam turbines are utilized in various sectors:

- **Power Generation:** Serve as prime movers in thermal power plants, converting steam energy into electrical energy.
- **Industrial Processes:** Provide mechanical drive for equipment like compressors and pumps.
- **Marine Propulsion:** Used in ships for propulsion systems.
- **Combined Heat and Power (CHP) Systems:** Simultaneously generate electricity and useful heat for industrial processes or district heating.

1.2.6 Advantages

The benefits of steam turbines include:

- **High Efficiency:** Particularly in large-scale power generation.
- **Reliability:** Capable of continuous operation with minimal maintenance.
- **Fuel Flexibility:** Can utilize various heat sources, including fossil fuels, nuclear, and renewable energy.
- **Scalability:** Suitable for a wide range of power outputs.

1.2.7 Challenges

Despite their advantages, steam turbines face certain challenges:

- **High Initial Costs:** Significant capital investment required for installation.
- **Complex Maintenance:** Requires specialized knowledge and equipment.
- **Water Usage:** Dependence on water for steam generation and cooling can be a limitation in arid regions.

1.3 Recent Developments in Turbine Technology

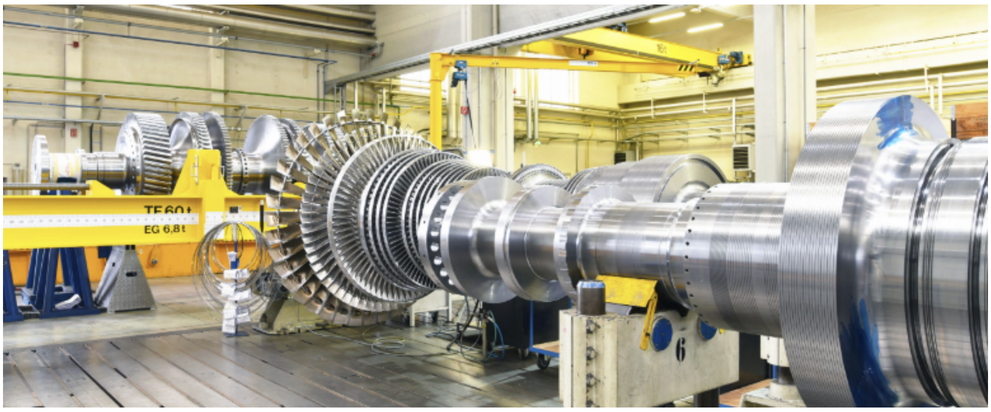


Figure 1.7: New age Turbine Technology

Advancements in both gas and steam turbine technologies focus on:

- **Improved Materials:** Development of high-temperature-resistant materials and advanced alloys to enhance efficiency and durability in both turbine types.
- **Advanced Design Techniques:**
  - Gas turbines: Implementation of innovative cooling techniques to allow higher operating temperatures
  - Steam turbines: Optimization of blade design to reduce aerodynamic losses and improve performance
- **Integration with Renewable Energy:** Development of hybrid systems combining both turbine types with renewable energy sources for improved sustainability and operational flexibility.
- **Digital Technologies:** Implementation of advanced monitoring, diagnostics, and control systems to optimize performance and maintenance schedules.

1.3.1 Conclusion

Gas and steam turbines remain fundamental technologies in modern energy production and industrial processes. While each type has its specific applications - gas turbines excelling in quick response and power density, and steam turbines in large-scale power generation - both share common developmental goals. These include improving efficiency, reducing environmental impact, and enhancing reliability through technological advancement. Ongoing research and development continue to address existing challenges while adapting these technologies to meet evolving energy needs and environmental standards. The integration of digital technologies and renewable energy systems represents the next frontier in turbine evolution, ensuring their relevance in the transition to a more sustainable energy future.

1.4 Gas Turbine Auxiliaries

1.4.1 Introduction

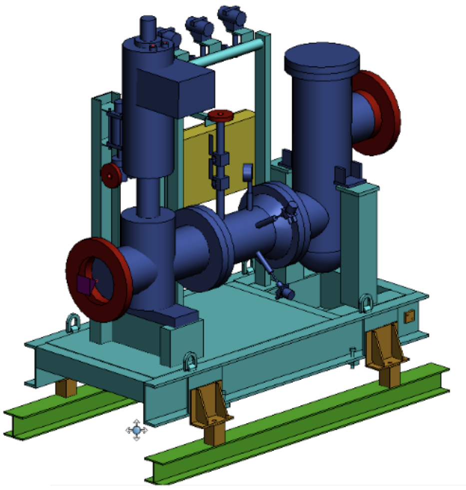
Gas turbine auxiliaries are critical systems designed to ensure the efficient operation, reliability, and safety of gas turbines. These systems are modular, integrated units that incorporate mechanical equipment, valves, controls, piping, and wiring onto a single structural base. While the main components of a gas turbine include the rotor, casing, and bearings, auxiliaries enhance functionality, improve efficiency, and support essential operations.

1.4.2 Major Gas Turbine Auxiliaries

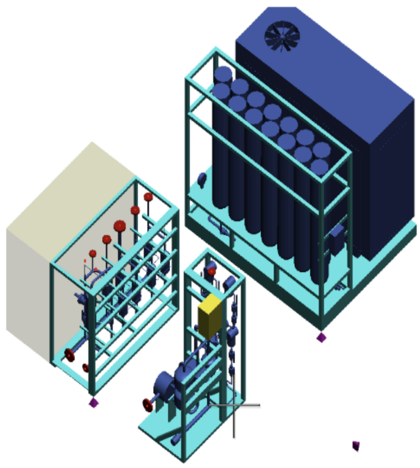
Gas turbine auxiliaries include a variety of essential systems, such as:

- **Fuel Gas Strainer Rack:** Filters and analyzes natural gas before combustion, preventing corrosion and erosion of components.
- **N_2 Purge Air Skid:** Cleans fuel gas piping using inert nitrogen gas, essential for safety during shutdown or trips.
- **Hydraulic Oil Skid:** Provides high-pressure hydraulic oil to control fuel and air valves.
- **Hydraulic Clearance Optimization Skid (HCO):** Reduces expansion losses by maintaining optimal clearance between turbine blades, enhancing power output and efficiency.
- **Lube Oil Skid:** Supplies lubricating oil to bearings, preventing wear and tear. Includes oil pumps, purifiers, and heat exchangers for efficient operation.
- **Base Module:** Consolidates multiple skids on a single frame to save space and reduce execution efforts.

- **Dual Fuel Module:** Handles both gas and liquid fuels, ensuring smooth fuel transition and system cleaning.
- **NOX Water Skid:** Reduces nitrogen oxide emissions during liquid fuel operation by injecting water into the fuel supply.
- **Purge Water Skid:** Cleans oil burners during fuel mode transitions to prevent residue buildup.
- **Compressor Cleaning Skid:** Cleans compressor blades to maintain performance by removing dirt and oily layers.
- **Instrument Air Skid:** Supplies high-pressure, dry air for operating pneumatic valves.
- **Wet Compression System:** Increases turbine power output by injecting atomized water into the inlet, enhancing air mass intake.



(a) Fuel Gas Strainer Rack



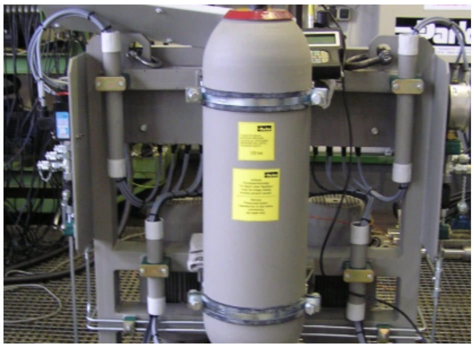
(b) N_2 Purge Air Skid

Figure 1.8: Gas Turbine Auxiliaries

1.4.3 Descriptions of Key Skids

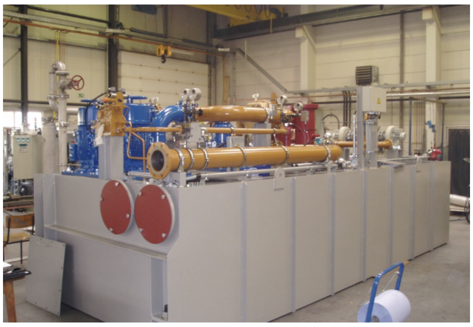
Fuel Gas Strainer Rack:
This skid filters and analyzes natural gas to ensure consistent quality and prevent damage to turbine components. It includes a strainer, flow meter, gas analyzer, and control valves.

(a) Hydraulic Oil Skid



(b) Hydraulic Clearance Optimization Skid (HCO)

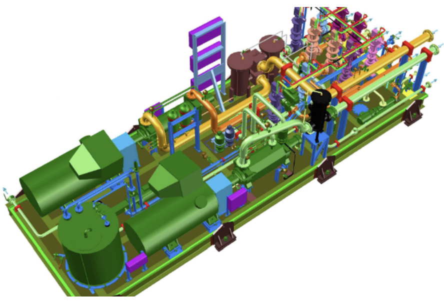
Figure 1.9: Gas Turbine Auxiliaries



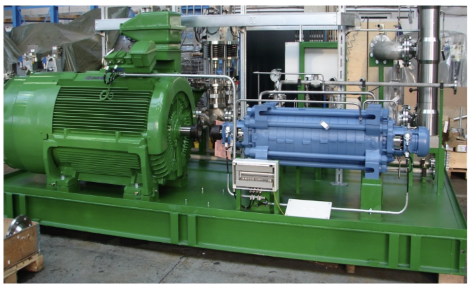
(a) Lube Oil Skid

(b) Base Module

Figure 1.10: Gas Turbine Auxiliaries



(a) Dual Fuel Module



(b) NOX Water Skid

Figure 1.11: Gas Turbine Auxiliaries

N_2 Purge Air Skid:
Utilized for cleaning fuel gas pipelines with nitrogen after shutdowns. Nitrogen is generated, stored, and distributed through a rack with flow control

(a) Purge Water Skid

(b) Compressor Cleaning Skid

Figure 1.12: Gas Turbine Auxiliaries

(a) Instrument Air Skid

(b) Wet Compression System

Figure 1.13: Gas Turbine Auxiliaries

and safety mechanisms.

Hydraulic Clearance Optimization Skid (HCO):
Designed to counteract expansion losses by maintaining optimal clearance between rotor and stationary blades. High-pressure hydraulic oil, up to 180 bar, exerts opposing forces to reduce gaps and enhance efficiency.

Lube Oil Skid:
Essential for lubricating journal bearings of the gas turbine and generator shafts. Features jacking oil pumps, oil purifiers, and heat exchangers to maintain optimal oil temperature and quality.

Compressor Cleaning Skid:
Removes dirt and moisture from compressor blades using pressurized water or a water-detergent mixture during offline or online cleaning. This prevents performance degradation caused by deposits.

Wet Compression System:
Boosts turbine output by injecting atomized water into the compressor inlet, increasing air mass intake. This system includes a strainer, injection pump, and flow meters to regulate water flow effectively.

1.4.4 Advantages of Gas Turbine Auxiliaries

- **Enhanced Efficiency:** Systems like the HCO and wet compression skids improve the overall performance of gas turbines.
- **Improved Reliability:** Proper lubrication and cleaning ensure consistent operation with minimal downtime.
- **Emission Reduction:** NOX water and purge systems minimize harmful emissions, making the operation environmentally friendly.
- **Flexibility:** Dual fuel modules allow turbines to operate on different fuel types, adapting to varying availability and cost.

1.4.5 Conclusion

Gas turbine auxiliaries are indispensable for the smooth operation and optimization of gas turbines. By addressing challenges like fuel quality, lubrication, emissions, and performance degradation, these systems ensure that gas turbines operate efficiently and reliably in various industrial and power generation contexts.

Chapter 2

Machine Learning in CFD

2.1 Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) is a branch of fluid mechanics that utilizes numerical analysis and algorithms to solve and analyze problems involving fluid flows. By employing computational resources, CFD predicts the behavior of liquids and gases within various engineering contexts, such as aerodynamics, hydrodynamics, and process engineering.

2.1.1 Governing Equations

The fundamental equations governing fluid dynamics are the Navier-Stokes equations, which represent the conservation laws of physics applied to fluid motion. These include:

Conservation of Mass (Continuity Equation):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

where: ρ is the fluid density, t is time, $\mathbf{u}$ is the velocity vector.

Conservation of Momentum:

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{f}$$

where: p is the pressure, $\boldsymbol{\tau}$ is the stress tensor, $\mathbf{f}$ represents body forces.

Conservation of Energy:

$$\frac{\partial(\rho e)}{\partial t} + \nabla \cdot (\rho e \mathbf{u}) = -\nabla \cdot \mathbf{q} + \boldsymbol{\tau} : \nabla \mathbf{u} + \rho s$$

where: e is the specific internal energy, $\mathbf{q}$ is the heat flux vector, s denotes energy sources (e.g., heat addition).

These partial differential equations are complex and often require numerical methods for solutions, especially in turbulent or compressible flow scenarios.

2.1.2 Numerical Methods in CFD

CFD employs various numerical methods to approximate solutions to the governing equations:

- **Finite Difference Method (FDM):** Approximates derivatives by differences between neighboring grid points.
- **Finite Volume Method (FVM):** Conserves quantities through control volumes, ensuring flux balance across cell faces.
- **Finite Element Method (FEM):** Utilizes variational methods to minimize errors in approximations, suitable for complex geometries.

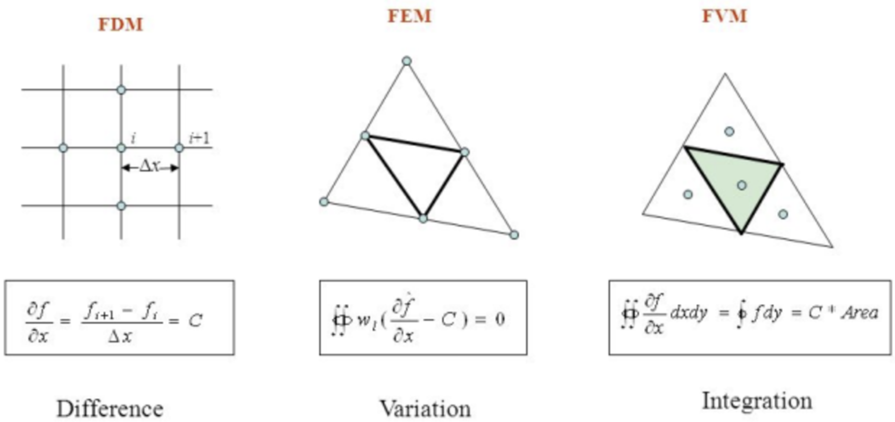


Figure 2.1: Types of Numerical Methods

2.1.3 Applications of CFD

CFD is instrumental in numerous fields:

- **Aerospace Engineering:** Designing aircraft and spacecraft by analyzing aerodynamic properties.
- **Automotive Industry:** Enhancing vehicle aerodynamics and cooling systems.
- **Civil Engineering:** Studying wind loads on structures and natural ventilation.
- **Environmental Engineering:** Modeling pollutant dispersion in air and water bodies.

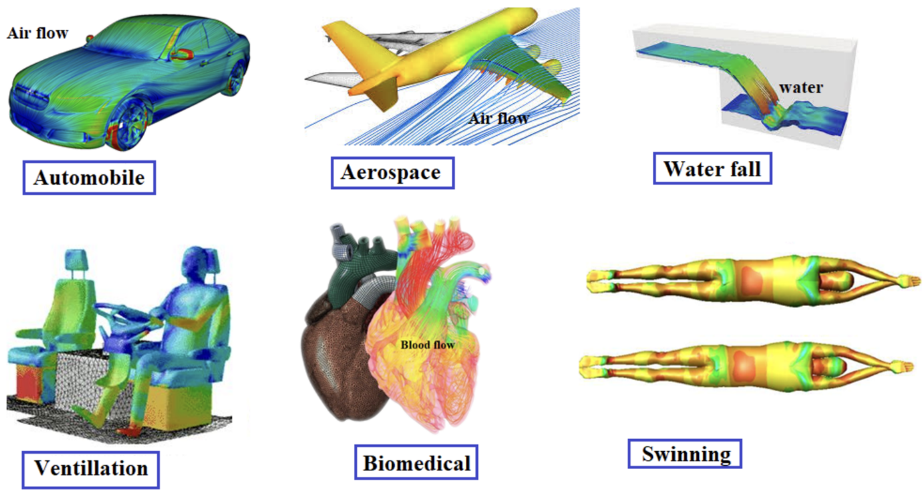


Figure 2.2: Applications

2.1.4 Advantages of CFD

- **Cost-Effective:** Reduces the need for expensive experimental setups.
- **Detailed Insights:** Provides comprehensive data on fluid behavior, including velocity fields, pressure distributions, and temperature gradients.
- **Flexibility:** Allows simulation of scenarios that may be impractical or hazardous to replicate physically.

2.1.5 Challenges in CFD

Despite its advantages, CFD faces challenges:

- **Computational Resources:** High-fidelity simulations can be resource-intensive.
- **Modeling Accuracy:** Requires precise modeling of physical phenomena; inaccuracies can lead to significant errors.
- **Turbulence Modeling:** Capturing turbulent flows accurately remains complex and often relies on empirical models.

In summary, CFD is a powerful tool that integrates principles of fluid mechanics with computational algorithms to analyze and predict fluid behavior in various engineering applications. Its effectiveness depends on the accurate representation of physical laws, numerical methods, and computational resources.

2.2 Machine Learning

2.2.1 Introduction to Machine Learning

Machine Learning (ML) is a branch of artificial intelligence (AI) that enables systems to learn patterns and make predictions or decisions without being explicitly programmed. At its core, ML involves the use of algorithms and statistical models to identify relationships within data and generalize these patterns to new, unseen scenarios.

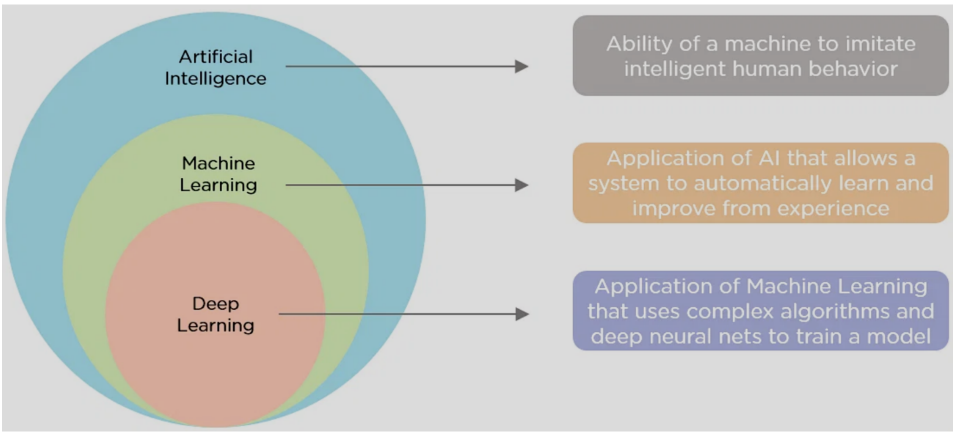


Figure 2.3: Artificial Intelligence

The process of ML typically involves three key steps:

- **Training:** Using historical data to train the model to recognize patterns.
- **Validation:** Evaluating the model's performance on unseen data to optimize parameters.
- **Testing:** Assessing the final model's ability to generalize to completely new data.

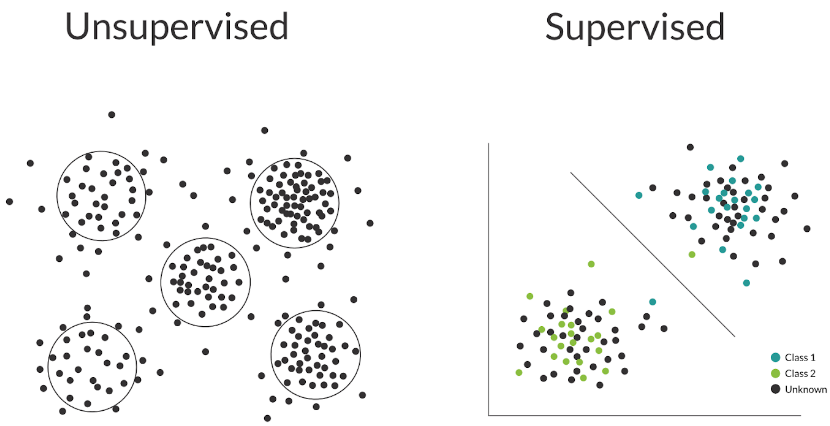


Figure 2.4: Supervised vs Unsupervised Learning

There are three primary types of machine learning:

- **Supervised Learning:** Involves labeled data where the input-output relationship is known. Example: Predicting airflow rates based on sensor data.
- **Unsupervised Learning:** Uses unlabeled data to find hidden patterns. Example: Clustering flow regimes in CFD simulations.
- **Reinforcement Learning:** Optimizes decisions through trial-and-error interactions with the environment. Example: Autonomous control of fluid systems.

2.2.2 Scientific Machine Learning (SciML)

Scientific Machine Learning (SciML) merges the principles of scientific computing and machine learning to address complex engineering and scientific problems. SciML goes beyond traditional ML by incorporating domain knowledge, such as physical laws, governing equations, and constraints, into the learning process.

Key features of SciML include:

- **Physics-Informed Neural Networks (PINNs):** Neural networks constrained by physical laws (e.g., Navier-Stokes equations).
- **Hybrid Models:** Combining data-driven models with first-principles-based simulations to enhance accuracy and efficiency.
- **Reduced-Order Models (ROMs):** Using ML to create simplified yet accurate representations of high-fidelity simulations.

2.2.3 Transforming Engineering Problems Through Machine Learning

Machine learning is revolutionizing engineering by enabling data-driven solutions to challenges that were previously computationally prohibitive or experimentally inaccessible. In engineering contexts, ML offers:

- **Optimization:** ML algorithms, such as genetic algorithms or neural networks, are being used to optimize designs, reducing iterations in product development.
- **Predictive Maintenance:** Models analyze sensor data to predict equipment failure, improving reliability and reducing downtime.
- **Material Science:** Accelerating the discovery of new materials with desired properties using ML-based predictive models.
- **Process Automation:** Autonomous control of engineering systems, such as chemical reactors or HVAC systems, through reinforcement learning techniques.

2.2.4 Enhancing Computational Fluid Dynamics with Machine Learning

CFD is computationally intensive, often requiring significant resources to solve large-scale problems with high fidelity. Machine learning has the potential to augment CFD in the following ways:

- **Data-Driven Turbulence Modeling:** ML-based turbulence models can replace traditional empirical models, providing more accurate predictions while reducing computational cost.
- **Accelerated Simulations:** ML techniques, such as neural networks, can create surrogate models to approximate the solutions of CFD problems, enabling rapid predictions without running full simulations.
- **Boundary Condition Estimation:** ML models can infer boundary conditions from sparse data, enhancing the usability of CFD in complex scenarios.
- **Error Correction:** ML can learn to correct discrepancies between numerical simulations and experimental results, improving accuracy without additional computational overhead.
- **Inverse Problems:** ML can assist in solving inverse problems in CFD, such as inferring flow characteristics from limited measurements.

In conclusion, the integration of machine learning, particularly SciML, into engineering and CFD workflows has the potential to transform the field. By reducing computational demands, improving accuracy, and enabling new applications, ML is shaping the future of engineering and fluid dynamics. This synergy between traditional physics-based approaches and data-driven techniques offers a promising avenue for solving some of the most complex challenges in engineering.

2.3 Accelerated Simulations using Surrogate Models

2.3.1 Surrogate Modeling in Computational Fluid Dynamics

Surrogate modeling is an efficient approach that replaces expensive computational models with simpler approximations to enable faster simulations. In the context of Computational Fluid Dynamics (CFD), surrogate models use machine learning techniques to approximate the behavior of complex fluid dynamics, significantly reducing the computational cost associated with traditional solvers. These models are particularly valuable for iterative design optimization, uncertainty quantification, and real-time predictions.

Approach	Accuracy	What is needed?	Gives result...
experimental testing	Very High	Physical prototype Laboratory	in days
CFD	High / Very High	Physical models Skills (experience) HPC or cloud rental	in hours
human brain	Biased	Skills (experience)	in seconds
Machine (Deep) Learning	High / Very High	Data from CFD / experimental testing	in (milli)seconds

Figure 2.5: Comparison of various methods

The scope of this study focuses on the analysis of *Lube Oil Degasification*, with the goal of harmonizing the lube oil return designs for steam and gas turbines. A key objective is to **minimize computational costs and achieve faster results**. By leveraging Physics-Informed Neural Networks (PINNs), the study aims to efficiently model flow dynamics and the degasification process, delivering accurate predictions while significantly reducing reliance on computationally expensive CFD simulations. The application of surrogate models, particularly PINNs, provides a transformative solution to overcome the computational challenges associated with traditional CFD analysis.

2.3.2 Physics-Informed Neural Networks (PINNs)

Physics-Informed Neural Networks (PINNs) are a groundbreaking approach to surrogate modeling. Unlike purely data-driven methods, PINNs embed the governing physical laws, such as the Navier-Stokes equations, directly into the neural network's loss function. This ensures that the predictions adhere to the underlying physics, even in data-scarce scenarios.

- **Key Features of PINNs:**
  - Incorporate boundary conditions, initial conditions, and governing equations directly into the model.
  - Efficiently handle problems with limited or noisy data.
  - Provide robust and interpretable solutions for fluid flow, heat transfer, and multiphase problems.

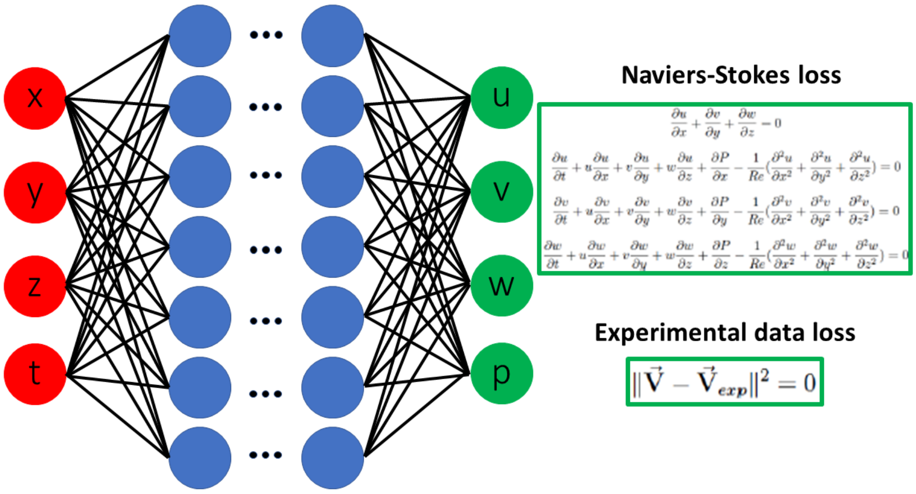


Figure 2.6: Physics Informed Neural Network

2.3.3 Data-Driven vs. PINN Approach

The traditional data-driven approach relies solely on training a model using large datasets without incorporating physical laws. While effective for problems with abundant data, this approach often struggles with generalization, especially in unseen scenarios or physics-driven problems.

- **Data-Driven Approach:**
  - Requires extensive, high-quality datasets for accurate predictions.
  - Lacks interpretability and adherence to governing physics.
- **PINN Approach:**
  - Requires fewer data points by leveraging physics-based priors.

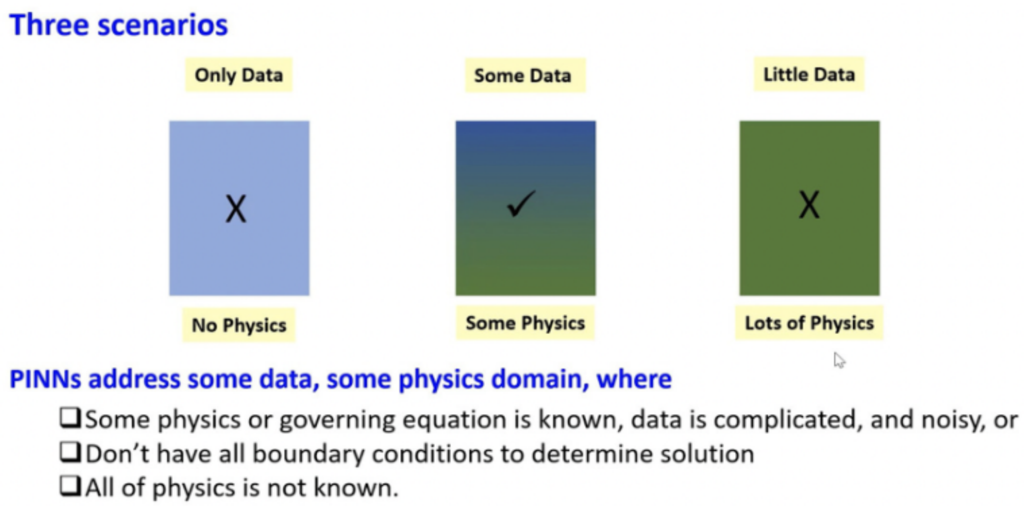


Figure 2.7: When to use a PINN

- Ensures physically consistent results across a wide range of scenarios.
- Efficiently models problems with complex geometries, boundary conditions, and physics.

2.3.4 Detailed Approach to the Lube Oil Degasification Problem

The analysis of the *Lube Oil Degasification* problem will utilize a combination of physics-based modeling and machine learning via PINNs. The following subsections elaborate on the specific methodologies for achieving each aspect of the study:

Flow Model

The turbulent flow behavior in the degasification process will be modeled using the ***k- realizable RANS model***, which is well-suited for high-Reynolds-number flows and provides improved accuracy for swirling and rotating flows. The key aspects of this approach include:

- **Turbulence Modeling:** The realizable k- *model* uses transport equations for turbulent kinetic energy (k) and its dissipation rate (ϵ):

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_i k)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + P_k - \rho\epsilon$$

$$\frac{\partial(\rho\epsilon)}{\partial t} + \frac{\partial(\rho u_i \epsilon)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_j}\right] + C_1\frac{\epsilon}{k}P_k - C_2\rho\frac{\epsilon^2}{k}$$

where P_k is the production of turbulent kinetic energy, μ_t is the turbulent viscosity, and σ_k and σ_ϵ are model constants.

- **Multiphase Interactions:** The Volume of Fluid (VOF) methodology will be employed to capture the interface between lube oil and air. The VOF method tracks the volume fraction α for each phase:

  $$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = 0$$

  Here, $\alpha = 1$ indicates a region filled with one fluid (e.g., lube oil), and $\alpha = 0$ indicates the other fluid (e.g., air). The slip velocity accounts for the relative velocity between phases, ensuring accurate multiphase interaction modeling.

Material Properties

The physical properties of lube oil and air, such as density and viscosity, are critical to accurate modeling. These properties will be parameterized based on the baseline configuration:

- **Lube Oil:** The density (ρ_{oil}) and viscosity (μ_{oil}) will be set according to standard industry specifications.
- **Air:** The density (ρ_{air}) and viscosity (μ_{air}) will be incorporated based on standard atmospheric conditions.
- **Property Interactions:** Multiphase dynamics will integrate the weighted properties of the two fluids for calculating the mixture density (ρ_m) and viscosity (μ_m):

  $$\rho_m = \alpha\rho_{\text{oil}} + (1-\alpha)\rho_{\text{air}}, \quad \mu_m = \alpha\mu_{\text{oil}} + (1-\alpha)\mu_{\text{air}}$$

Physics Integration Using PINNs

PINNs will embed the governing Navier-Stokes equations, boundary conditions, and porosity constraints into the neural network's loss function to simulate flow behavior with high accuracy. The following outlines the methodology:

- **Navier-Stokes Equations:** The flow dynamics are governed by the incompressible Navier-Stokes equations:

$$\nabla \cdot \mathbf{u} = 0, \quad \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f}$$

  Here, $\mathbf{u}$ is the velocity vector, p is the pressure, μ is the dynamic viscosity, and $\mathbf{f}$ represents body forces.

- **Boundary and Initial Conditions:** The PINN loss function includes terms that ensure adherence to boundary conditions (e.g., velocity at inlets and walls) and initial conditions for the flow field:

$$\mathcal{L}_{\text{BC}} = \|\mathbf{u} - \mathbf{u}_{\text{specified}}\|^2, \quad \mathcal{L}_{\text{IC}} = \|\mathbf{u}(t = 0) - \mathbf{u}_0\|^2$$

- **Loss Function for PINNs:** The overall loss function combines the residuals of the governing equations, boundary conditions, and data points:

$$\mathcal{L} = \mathcal{L}_{\text{NS}} + \mathcal{L}_{\text{BC}} + \mathcal{L}_{\text{IC}} + \mathcal{L}_{\text{data}}$$

  where:

$$\mathcal{L}_{\text{NS}} = \|\nabla \cdot \mathbf{u}\|^2 + \|\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) - \nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f}\|^2$$

- **Porosity Constraints:** The PINN will incorporate porosity constraints for regions with complex geometries, using Darcy's law where applicable:

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p$$

  where κ is the permeability.

Achieving Accurate Simulations

The PINN framework will be trained on historical CFD data, capturing the complex interaction of turbulent and multiphase flows while adhering to physical constraints. This ensures that the surrogate model provides accurate and computationally efficient predictions, enabling rapid design iterations and optimization for lube oil degasification systems.

2.3.5 Methodology

The following methodology will be adopted to implement PINNs for the lube oil degasification problem:

1. **Data Collection and Preprocessing:** Extract and preprocess CFD simulation data to train the PINN model. This includes data on velocity, pressure, and volume fraction fields.

2. **PINN Model Development:** Develop a PINN framework that incorporates the Navier-Stokes equations, boundary conditions, and multiphase interaction constraints.

3. **Model Training and Validation:** Train the PINN using historical CFD data and validate it on simplified cases to benchmark its accuracy and computational efficiency.

4. **Final Report and Recommendations:** Summarize findings, quantify computational cost savings, and propose scaling the solution to other turbine-related applications.

2.3.6 Benefits of PINNs for CFD

By replacing traditional CFD solvers with PINNs as surrogate models, significant benefits can be realized:

- **Reduced Computational Costs:** Drastically lower simulation time and computational resource requirements.

- **Improved Efficiency:** Enable real-time predictions and faster iterative design processes.

- **Scalability:** Extendable to other turbine-related applications beyond lube oil degasification.

In summary, leveraging PINNs for the lube oil degasification problem represents a transformative approach to CFD, offering a cost-efficient, physics-consistent, and scalable solution for complex fluid dynamics challenges.

Chapter 3

Conclusion

This internship underscored the transformative potential of integrating machine learning (ML) techniques with traditional engineering methods to address complex challenges in Computational Fluid Dynamics (CFD). Among the ML approaches explored, Scientific Machine Learning (SciML) stood out for its ability to blend domain-specific knowledge with advanced data-driven techniques. By embedding physical laws and constraints, such as the Navier-Stokes equations, into the learning process, SciML bridges the gap between empirical modeling and physics-based simulations.

The study on the lube oil degasification problem showcased how Physics-Informed Neural Networks (PINNs), a core component of SciML, could significantly enhance simulation accuracy while reducing computational costs. Unlike traditional ML models, which rely heavily on large datasets, PINNs incorporate physical laws directly into the loss function, enabling robust predictions even in data-scarce scenarios. This approach not only ensures consistency with underlying physics but also reduces the computational resources required for high-fidelity CFD simulations.

Furthermore, SciML's capacity for scalability and flexibility extends its applicability beyond CFD to a wide range of engineering problems, including turbulence modeling, inverse problem-solving, and boundary condition estimation. By enabling real-time predictions and iterative design optimization, SciML facilitates the development of innovative solutions in turbine technology, such as improving efficiency, minimizing emissions, and integrating renewable energy systems.

The findings from this internship validate the importance of adopting interdisciplinary approaches that leverage the strengths of both data-driven and physics-based methodologies. As SciML continues to evolve, its role in advancing sustainable energy solutions and addressing the pressing challenges of modern engineering will undoubtedly expand, reinforcing its significance in the future of technology and innovation.

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