Modelling, Data Analytics and AI in Engineering

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ABOUT MadeAI

In today's dynamic landscape of science and technology, modelling, data analytics, and artificial intelligence (AI) have become essential catalysts for redefining problem-solving and driving innovation across industries. These advanced tools are not only transforming traditional approaches but are also unlocking new possibilities for tackling complex challenges in sectors as diverse as aerospace, automotive, chemical, construction, energy, healthcare, materials, and transportation. By integrating these powerful technologies, industries can achieve unprecedented levels of efficiency, precision, and adaptability, setting new standards for progress and competitiveness in a rapidly changing world.

Modelling, data analytics, and AI share foundational mathematical and computational frameworks, yet these disciplines are frequently studied in isolation within engineering and science programs, limiting their transformative potential. This siloed approach restricts the interdisciplinary collaboration needed to harness their combined strengths fully. To unlock their full potential as pioneering solutions at the forefront of engineering, it is essential to integrate these disciplines through a holistic, systems-based approach. By breaking down these barriers, we can foster innovative solutions that address complex, real-world challenges more effectively and elevate the impact of engineering on society.

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Interpretable Data-Driven Models for Predicting Cylinder Flow Noise Using Explainable Artificial Intelligence (XAI)

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Accurately predicting aerodynamic noise generated by flow over cylindrical structures presents a significant challenge in fluid dynamics, especially in engineering applications within the automotive and aerospace industries. Traditional Computational Fluid Dynamics (CFD) methods, such as Direct Numerical Simulation (DNS), offer high-fidelity predictions but demand extensive computational resources and time. This research investigates the potential of Machine Learning (ML) techniques as an alternative to conventional CFD methods for predicting aerodynamic noise, focusing on pressure fluctuations in incompressible flow over a cylinder.

Flow-induced noise prediction is crucial for optimizing structural designs for noise reduction and enhancing aerodynamic performance. However, the high computational cost of DNS limits its practical application, creating a demand for efficient, data-driven predictive models. ML-based approaches provide the advantage of learning complex relationships from data, allowing for fast and reliable predictions. While ML has been utilized in various engineering fields, its application in aerodynamic noise prediction remains underexplored. This study intends to fill this gap by developing an ML model capable of accurately forecasting pressure fluctuations in-cylinder flow, thus offering a computationally efficient alternative to DNS.

A dataset was generated using DNS simulations of flow over a circular cylinder at varied Reynolds number and Mach number values. The dataset consists of 150 time series snapshots of pressure fluctuations, with 100 snapshots designated for model training and 50 for testing. The ML model employs linear regression to predict instantaneous fluctuating pressure values. The governing equations for compressible flow—mass conservation, momentum conservation, and energy conservation—were implemented using an in-house computational solver, HiPSTAR. A high-resolution numerical approach, incorporating a fourth-order compact finite- difference scheme and Runge-Kutta time integration, was utilized for DNS simulations. Model performance was assessed using Mean Squared Error (MSE) as the cost function, optimized through gradient descent.

The trained ML model significantly reduced cost function values over training epochs, demonstrating effective learning and optimization. Comparisons between predicted and actual fluctuating pressure values showed high accuracy, with minimal deviations observed in contour plots and directivity patterns. While the ML model captured radial pressure variations effectively, slight discrepancies appeared in the azimuthal direction, indicating the influence of acoustic disturbances. Root Mean Square (RMS) pressure analysis further validated the model's predictive capability, revealing close agreement between predicted and actual values.

To gain deeper insights into the influence of input features on pressure fluctuations, Explainable Artificial Intelligence (XAI) is employed. SHapley Additive exPlanations (SHAP), a game-theoretic framework, is utilized to interpret the ML model at both local and global levels, identifying the contribution of each input parameter to the predicted

pressure fluctuations. Additionally, Partial Dependence Plots (PDP), a model-agnostic XAI technique, provides a graphical representation of how variations in selected features impact the model's predictions. This visualization helps determine whether the relationship between features and pressure fluctuations is linear, monotonic, or more complex.

By integrating XAI techniques, this study improves the interpretability of ML predictions, connects data-driven models with fluid dynamic insights, and understands the impact of key aerodynamic parameters on flow-induced noise, which aids in creating more efficient and optimized structural designs. This strategy not only lessens the dependency on computationally intensive DNS simulations but also speeds up the design process by allowing for data-efficient predictive modeling.

This study's results contribute to the advancement of ML-based aerodynamic noise prediction. They demonstrate the potential of data-driven methods to capture pressure fluctuations accurately. Integrating ML and XAI in this context provides engineers with valuable tools for optimizing aerodynamic performance and strategies for noise reduction in applications such as automotive and aerospace design.

Keywords: Aerodynamic noise, Cylinder flow, Machine Learning, Compressible Flow, Reduced Order Model

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AI-based Motor Abnormal Signal Detection

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This study uses accelerometers to measure motor vibration signals, and after signal processing, uses them as AI recognition training data to identify the status of the motor. Abnormally status with five situations, which are 1. Normal 2. The rotor is unbalanced 3. Bearing loss is blocked 4. The base is not fixed. 5 Abnormal and violent shaking . Use the accelerometer sensing module to measure the motor vibration signal, conduct wavelet conversion on the measured time domain vibration signal to obtain its time-frequency diagram, and then convert the time-frequency diagram into a grayscale image for AI image recognition. The goal of eliminating the need for maintenance personnel is required to check and obtain the situation of motor failure. The results show that the actual measurement results of the time- frequency grayscale image converted from the vibration signal corresponding to the above five different situations are very discernible and the identification results are clear.

The overall hardware architecture is shown in Figure 1. First, we use a frequency converter to convert the bidirectional power supply into three phases to control the operation of the three- phase AC motor. Then, use a sensor to receive the vibration signal and transmit the sensed time domain vibration signal to the development board. The development board used Cypress Fx3 processor to process accelerometer sensing signal and the results are sent to the computer

through mutual communication and transmission. Finally, the computer stores the signal data and performs subsequent data processing procedures based on AI model.

Fig. 1 The proposed system architecture for motor signal detection

The setup of the hardware arrangement is shown in Figure 2. First, the

frequency inverter with 220V power supply, are supply the power for a three-phase AC motor. Then, the accelerometer sensor is placed to near the motor on the platform. Because the electromagnetic wave of the motor will interfere with the sensing module used, it may cause signal errors. After fixing the sensing module (CBM), the signal of sensing module is sent the development board for processing. Finally, the results of development board are transmitted to the computer via USB port.

Keywords: accelerometer, vibration signal, wavelet transformation, AI recognition.

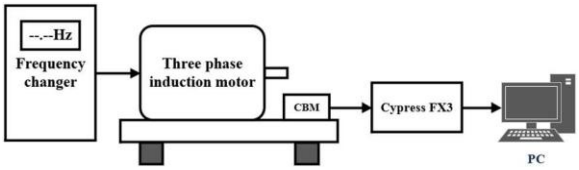
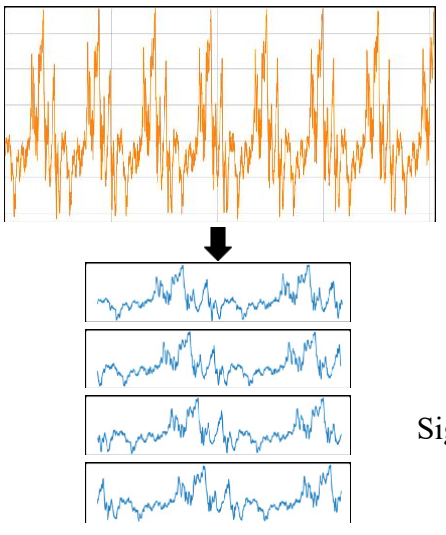


Fig. 2 The system setup for the proposed architecture.

The overall process is to extract the data of the vibration signal measured by the vibration sensing module, obtain the time-frequency diagram through wavelet transformation, then convert the time-frequency diagram to grayscale and adjust the size, and then store the required training set and test set respectively. The time-frequency data is trained with AI model, and finally verification and testing.The simulation of motor abnormality is split to : 1. Normal 2. Unbalanced rotor 3. Bearing loss and obstruction 4. The base is not fixed 5. Abnormal and violent shaking, the above conditions , mainly for load processing of motor rotors, and for abnormal simulation at rotating speeds with obvious shaking.

To create training data, use the corresponding measurement software provided by ADI, use
Cypress FX3 and connect to the CBM measurement module to measure and store time- frequency data. Among them, the CBM module samples 4096 points of time domain vibration at a time. For the signal, the sampling frequency is set to 6.875kHz. The data is converted into a waveform diagram and divided into 4 segments. 1024-point wavelet conversion is performed respectively. There are 4 images can be obtained in one acquisition of the signal. The time- frequency diagram after wavelet conversion is shown in Figure 3. Each time-frequency diagram is then converted into a grayscale diagram and resized to obtain the time-frequency diagram of the motor condition that is to be used as training data.



Time signal

Signal Segementation

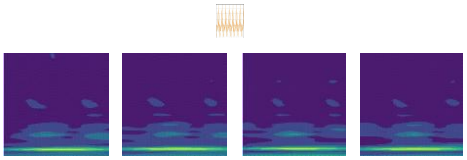


Fig. 3 Four time-frequency graphs with one sampling

Ecological Momentary Assessment of Bipolar Disorder Symptoms and Cohabiting Partner Affect over Time

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Background - The World Health Organization ranks bipolar disorder [BD] as the 7th leading cause of disability. The effects on those with BD is well described, less so the impact on cohabiting partners, and any interactions between the two. This requires *in vivo* data collection measured each day over several months.
Objectives - We set out to demonstrate the utility of ecological momentary assessment with BD couples measured using yoked smartphone apps. When randomly prompted over time, we assumed distinct patterns of association would emerge between BD symptoms [both depression and hypo/ mania] and partner mood [positive and negative affect].
Methods - For this pilot study, we recruited an international sample of young and older adults with BD and their cohabiting partners where available. Both participants and partners downloaded separate apps onto their respective smartphones. Within self-specified 'windows of general availability' participants with BD were randomly prompted to briefly report symptoms of depression and hypo/mania [i.e., BDS_x], positive and negative mood [i.e., POMS-15; partners] any important events of the day [both]. The partner app was yoked to participant app so that the former was prompted roughly 30 minutes after the participant with BD, or the next morning if outside the partner's specified availability.
Results - Four couples provided 312 matched BD symptom/partner mood responses over an average of 123 days [range 65 – 221 days]. Both were GPS- and time-stamped [M = 3hrs, 11min between questionnaires, SD = 4hr, 51min]. Total depression had a small but significant association with positive [r = -.14, P = .02] and negative partner affect [r = .15, P = .01]. Yet total hypo/mania appeared to have no association with positive partner affect [r = -.01, P = .87]; instead, negative partner affect was significantly correlated with total hypo/mania [r =.26, P = .01]. However, when we look specifically at BD factors, we see that negative partner affect is associated only with affrontive symptoms of hypo/mania [r =.38, P = .01]; elation/loss of insight appears unrelated to either positive [r =.10, P = .09] or negative partner affect [r =.02, P = .71]. Yet affrontive symptoms of hypo/mania were significantly correlated with negative affect but only when couples were together [r =.41, P = .01], not when apart [r = .22, P = .12]. That is, these angry interpersonal symptoms of hypo/mania appear to be experienced most negatively by spouses when couples share the same GPS coordinates.
Conclusions - These initial findings demonstrate the utility of *in vivo*, ambulatory data collection in longitudinal mental health research. Preliminary analyses suggest different BD symptoms are associated with negative and positive partner mood. These negative effects appear greater for hypo/mania than depressive symptoms, but proximity to the person with BD is an important factor.

KEY WORDS: bipolar disorder, couples, dyadic analyses, ecological momentary assessment

An Extended Ising Model

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The classical Ising model is expressed as a quadratic function. This quadratic function is commonly referred to as a Hamiltonian, for example,

$$E_W = -\sum_{i\neq j}\sum_{j} x_i x_j - \sum_i b_i x_i = -\frac{1}{2}\boldsymbol{x}W\boldsymbol{x}^T - \boldsymbol{x}B^T, \quad (1)$$

where $\boldsymbol{x}$ is a row vector, each element in $\boldsymbol{x}$, x_i, is a binary variable, taking values of either in
{-1, 1} or in {0, 1}. The diagonal elements of the symmetric matrix W are all zeros, and B is a row vector. This Hamiltonian is also known as the energy function or the objective function.

Obtaining W and B for a given problem is not an easy task. The Hebb's law of association gives a closed-form formula to obtain W [1]. There is no known general formula to find B, which in general is not unique for a problem.

The method we are presenting in this paper is inspired by the Ising model and it overcomes the three drawbacks of the Ising model. The three drawbacks are as follows.

1) When given a set of stable states of n binary variables, it may not be possible to construct an associated Ising model with n variables.

2) When a valid Ising model is found for a set of stable states, the energy function values corresponding to those stable states may be different. Some of them are local minima.

3) The Lagrange multiplier is treated as a hyper parameter. The optimization problem by treating a Lagrange multiplier as a hyper parameter does not work well.

When we are given a set of M stable states: $\boldsymbol{x}^{s1}, \boldsymbol{x}^{s2}, \ldots, \boldsymbol{x}^{sM}$, we define the energy function E as

$$E(\boldsymbol{x}) = \prod_{i=1}^{M} \|\boldsymbol{x} - \boldsymbol{x}^{si}\|^2 = \sum_{k=0}^{2^n-1} a_k \prod_{i=1}^{n} x_i^{k_i}, \quad (2)$$

which has a distinguishing property that $E(\boldsymbol{x})$ always satisfies $E(\boldsymbol{x}) \geq 0$, and $E(\boldsymbol{x}) = 0$ if and only if $\boldsymbol{x}$ is a stable state. In other words, all stable states reach the global minimum of the energy function $E(\boldsymbol{x})$. In (2), k has an M-bit binary representation $k_1 k_2 \ldots k_M$ with $k_i \in$
{0,1}. We will apply this new model (20) to the three examples in the previous section.

The variables can be updated one variable at a time. We assume that we want to

update the variable x_i. Let E^0 be $E(\boldsymbol{x})$ with $\boldsymbol{x}$ being the current state except that x_i is clamped to 0. Let E_i^1 be $E(\boldsymbol{x})$ with $\boldsymbol{x}$ being the current state except that x_i is clamped to 1. If $E^0 < E^1$, x_i is updated to 0. If $E^0 > E^1$, x_i is updated to 1. If $E^0 = E^1$, x_i is not updated (or updated to 1 or 0 randomly). In other words, the update formula is

$$x_i = step(E^0 - E^1), \tag{3}$$

where the step function is defined as

$$step(t) = \begin{cases} 1, & t > 0 \\ 0, & t < 0. \end{cases} \tag{4}$$

For the new energy function (2), the proposed neural network consists of n primary neurons: $x_1, x_2, \ldots, x_n$, and some necessary secondary neurons, such as $x_1x_2, x_1x_3, x_2x_3, \ldots,$ $x_1x_2x_3 \ldots x_n$. The secondary neurons are functions of the primary variables; we call them 'helping functions' in this paper. All these neurons are the terms appeared in the update formulas (3). In an n-bit problem, there are n primary neurons and there are at most $2^n - n$ secondary neurons. The n primary neurons are the inputs and the outputs as well. There are n update rules (i.e., formulas) for the primary neurons.

The proposed network has explicit closed-form update formulas. In other words, no training is required. The network is able to memorize a set of solutions (i.e., stable states). When a random n-bit input is assigned to the primary neurons, the network will update the neurons using the update rules. Each rule has a nonlinear activation function: step(t) as defined in (4). We assume that one neuron is updated at a time. We also assume that when $t = 0$, the function step(t) does not activate any updates for the variable bit in concern. When no action is performed for one particular neuron (i.e., a particular bit), a different neuron (i.e., a different bit) will be randomly selected for the potential update.

The traditional Ising model has update formulas in the form of a nonlinear activation function of a linear function of binary variables. The extension of the Ising model allows the update formulas in the form of a nonlinear activation function of a weighted sum of products of the binary variables. For a set of pre-specified n-bit solutions, an energy function can be readily formed using these solutions as the global minima in the extended Ising model. As soon as the energy function is formed, the explicit closed-form update formulas can be obtained. On the other hand, The Hebbian rule works only when all the input patterns (i.e., the solutions) are orthogonal or uncorrelated. The extended Ising model has many applications. One application is the decoder of an error correction code. The codewords of the error correction code are the stable states. This decoder can be used for any block code, which may not be linear and may not have a parity check matrix. An advantage of the proposed energy function is

that it does not have a hyper parameter l, which is problematic.

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Keywords: Ising model, machine learning, neural network, error correcting codes, logic circuits

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Context Modelling for Cyber-Physical Systems

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Abstract: The estimation, gathering, analysis and processing of information is a crucial part of modern computer systems in today's big data era. Context information plays a special role here. Often it is the context which determines if something holds true or not. Further the amount of information for context is multitudes higher than the amounts of data we usually find in system modelling, or even big data. Often, ontologies are enhanced with databases to both capture the meaning of data as well as gather, collect and analyse huge amounts of data together. SysML v2 is another modelling language used in systems engineering, that both formally and informally captures knowledge across abstraction levels. Here, also informal requirements are captured. The complete system model is created and entails mechanical, electrical, software and AI systems. These models are then often simulated together by coupling different simulators including simulations of physics. Context is hard to assess, as it is very "right-brain." It often depends on several other factors that are context related as well. And often the context is even for the observer hard to grasp, understand and process. This paper gives an overview of our works to address the challenges of current context modelling. We start out by motivating the need for a precise and comprehensive new architecture to address challenges of context. Past works [2] made an overview of the topic and tried to establish a common definition. For the sake of clarity and appropriateness we are using the Ontology Web Language (OWL) as the foundation to address the challenges. The modularity and flexibility in handling concepts is a major advantage to other modelling languages. Further in the IoT or Semantic Web pyramid the language is closest to the level of context which is above information and above data. So far we have been designing knowledge bases with a hand-crafted ontology [6] and we populate it with LLMs [5, 7]. These knowledge bases contain mostly entities of system engineering artifacts, their functions, properties, parts and software. Scaling this knowledge base is a challenge and context modelling is its successor and represents next steps. Currently there are few context models out there and they themselves are different and have different definitions [8, 3, 4] . In general entities are separated from their context. And elements like activities, locations, time, roles, profiles, environments and more are designated as context information. In Basic Formal Ontology (BFO) context can be viewed as the specifically dependent continuant, which is distinct from the independent continuant and the generally dependent continuant [1].

We give an outline of levels of context and define each level. Based on the definitions and framework, we go through a use case in detail: a distributed cyber-physical system for seismic activity recognition and earth quake estimation. Recently, new estimations prognosed a 75-82% probability or chance of an earthquake occuring in Japan. This earthquake is expected to have a strength of 8 on the Richter scale of magnitude and is supposed to occur within the next 30 years. These estimations are valid for the Nankai rift and could lead to hundreds of thousands of deaths. A cyber-physical system measures seismic data and various context information. From the system to its environment to its larger contexts the model is constructed. Building upon prior work the context model is created from the GENIAL! Basic Ontology (GBO) from systems engineering and electronics and the OWL Ontology of Consciousness (OOC), which provides firm foundations for context modelling. The use case exemplifies context on various levels and illustrates challenges of definition, measuring and modelling.

Finally we include and touch upon the modelling of non-linear dynamical systems. These systems need to be included when it comes to a discussion of modelling of contexutal systems and in AI. Here, a short deviation in initial conditions can lead to a completely different trajectory and even give surprising or astonishing output conditions.

We conclude that context modelling is one of the new upcoming frontiers of big data and AI. And further that much effort is needed to construct, refine and check the quality of those new contextual systems.

Keywords: context modelling, context, system, gbo

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Automatically Calibrated Hand-Eye System for Robotic Arms Based on Neural Network Integration

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It's well known that robotic arms can perform precise and repetitive tasks at high stability and efficiency for smart manufacturing and industrial automation. However, the spatial relationship calibration between the robotic arms and the cameras, called hand-eye calibration, is a crucial step for precise control of the arm's movements in practical applications. Traditional hand-eye calibration methods usually require manual operation, which is cumbersome, time- consuming, and prone to human error, leading to inaccurate calibration results. Therefore, this study developed an automated hand-eye calibration system using convolutional neural networks, calibration chessboard, and four corners of feature reference. A confusion matrix is an essential tool in machine learning and statistics for evaluating the performance of a classification model. In the Combined model, the prediction accuracy for RB, RT, and LB reaches 1.00, while the prediction accuracy for LT is 0.80. Regarding background false positives, RT and LT account for 0.56 and 0.44, respectively. Three training models were compared and Separated_Enhanced was selected as the recognition model for the automated hand-eye calibration, achieving an overall recognition accuracy of 98%. This study successfully established an automated hand-eye calibration system for robotic arms based on neural networks. This not only reduces the possibility of human error but also significantly improves the speed and accuracy of calibration. The system's automation greatly reduces the workload of operators, making the hand-eye calibration process simpler and more efficient.

Keywords: Automatically, Calibration, Hand-Eye, Convolutional Neural Networks, Feature Reference.

Prediction of Electric Vehicle Energy Consumption Using Multilayer Perceptron Models

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At present, the world is transitioning from the use of combustion engine vehicles to electric vehicles (EV) to mitigate pollution contributing to global warming. However, efficient energy utilization remains a critical consideration to maximize the driving range of EVs. This study investigates the energy consumption of EVs through experiments that collect various operational parameters, including vehicle speed, acceleration, road slope, carried load, battery temperature, electric current, voltage, and battery state of charge. The objectives of this study were to analyze these parameters, identify relationships, and predict EV energy consumption using machine learning specifically employing multilayer perceptron algorithms. Shapley technique was used to explain the relationships among variables. The results demonstrate that the machine learning model achieved a high accuracy with an R^2 value of 0.9968, a mean absolute error of 3.4398, and a root mean square error of 5.5998, based on test data validated through 10-fold cross-validation. Additionally, the findings indicate that electric current is the most influential factor in EV energy usage, followed by vehicle speed, which has the second- highest impact. This study provides insights that may assist researchers in understanding the interactions between various factors influencing EV energy consumption and contribute to the advancement of EV efficiency research.

Keywords: artificial neural networks, clean energy, machine learning, transport engineering

An Incremental Learning Approach for Efficient Detection of Emerging Type of SQL Injections

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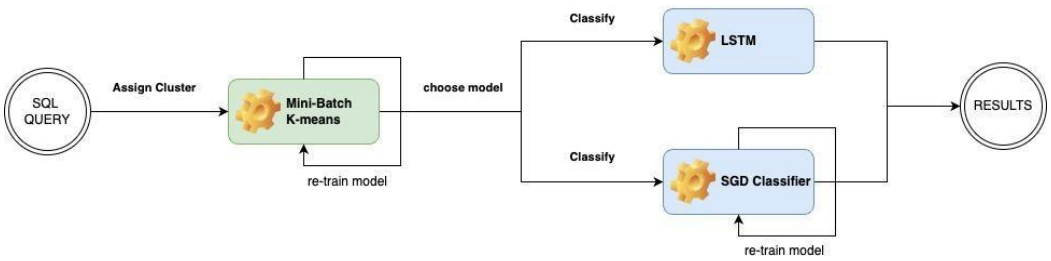
Current supervised learning models such as Support Vector Machine, Multilayer Perceptron (MLP) and Convolutional Neural Network (CNN) predict common structure language query injection (SQLi) at hyper accuracy. However, a study shows that such accuracy could decrease drastically if unseen SQLi is inputted without manual re-training (Issakhani et al., 2023). Our developed solution incorporates the use of Incremental Learning, along with Large Language Model (LLMs) and those previous models to sustainably manage emerging types of SQLi attack. We fine-tuned LLMs for SQLi feature extraction, trained our models with up-to-date SQLi payloads and simulated incremental learning in selected classification and clustering models to observe their behavior. Our models show promise in offering cost-effective mitigation to the problem.

To optimize our solution away from manual inspection and frequent offline retraining which are resource-heavy, we looked into possible use of Large Language Model (LLMs), Incremental Learning and Unsupervised Learning to complement the well-known supervised learning model. First, LLMs have shown excellent performance in tasks related to natural and computer language processing (see, for example, Brown et al. (2020) and Shah et al. (2023)). Second, incremental learning is a common technique to fit data drifting efficiently (Mugisha et al., 2024). Third, unsupervised learning models are capable of exploring hidden patterns in data, possibly in new types of unseen attacks (Hashana et al., 2023). While it is challenging to invent new types of SQLi attacks, we will be blindfolding our model from certain data to estimate its behavior upon encountering an emerging type of attack.

We advance a multi-model machine learning algorithm which comprises a main model and two supplementary models as shown in the figure below.



We utilized a highly accurate detection algorithm using a combination of Long Short-Term Memory (LSTM) and Bidirectional Encoder Memory from Transformers (BERT) as our main model. In addition, we deployed incremental / online learning on Stochastic Gradient Descent Classifier (SGD Classifier) to keep adapting itself to new types of

SQL injection attack. The Mini-Batch K-Means clustering was then used to identify possible emerging types of attack and decide which of the preceding classification models is most likely to be more accurate. All three models were pre-trained on the current up-to-date SQL injection query. However, SGD classifier and Mini-Batch K-means continued to incrementally learn on new query that was sent for classification and fed back for online re-training.
In our main model, LSTM and BERT complimented each other well giving an final accuracy of over 97.40% and a loss of 0.1044 highlighting the model's capacity to leverage BERT's contextual embedding and LSTM's sequential pattern recognition, ensuring precise and reliable classification of SQL injection inputs.

In our supervised supplementary model, SGD Classifier could perform as accurately as the offline model that re-trained the entire dataset again while performing significantly less computation. In our simulation experiment, It predicts SQLi on average at 99% accuracy for unseen type while experiencing merely 1.8% accuracy decrease to 97.5% for seen type due to model forgetting. This provides a prospect to enhance computational efficiency and scalability by replacing manual retraining with online learning. Additionally, LLMs is proved useful in vectorising SQL query in our process of feature extraction. High accuracy achieved implies that the LLMs-extracted data is relevant to decision-making.

For our clustering model, the incremental clustering approach with the mini-batch K-Means algorithm we advance has over 85% correctly determined clusters compared to the original. This model could then be used to simulate online clustering of SQL query decently accurately without offline re-clustering at a regular juncture. This possibly enhances the speed of computation in the context of SQLi detection.

In short, Incremental learning is capable of mitigating accuracy drop when models encounter emerging types of attack at low and scalable computational cost. Application of incremental learning on unsupervised learning clustering unveils its potential to distinguish seen and unseen types of SQLi attack online.

Keywords: SQL Injection, Machine Learning, Supervised Learning, Unsupervised Learning, Large Language Model, Incremental Learning

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Identifying Change Points in Seasonal Hydrological Data using a Genetic Algorithm Approach

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Change point detection in climate time series is a complex task due to inherent seasonality, trends, and serial correlation within the data. We present an approach that integrates regression modeling with autoregressive error structures to effectively identify abrupt regime shifts in climate datasets. The proposed model decomposes the observed time series X_t into seasonal means, a linear trend component, and regime shift offsets, while capturing serial correlations through a periodic autoregressive (PAR) process that varies by season. Parameter estimation is achieved using the iterative Cochrane–Orcutt procedure, which simultaneously estimates regression coefficients and autoregressive parameters via the Yule–Walker method. To balance model fit and complexity, the Minimum Description Length (MDL) principle is used as the objective function, incorporating penalties for the number of change points, their positions, and the autoregressive order. Given the combinatorial nature of selecting change points and AR orders, a multi-island genetic algorithm (GA) is utilized to explore the model space. The GA employs chromosome representations that encode both change point locations and AR orders, and utilizes genetic operators such as crossover, mutation, and migration to optimize the MDL score.

The methodology is validated through synthetic data generation that mirrors real climate series characteristics, including induced change points and controlled shift magnitudes. Performance assessments indicate the GA-based model selection effectively identifies true change points under varying conditions of shift magnitude and autocorrelation.

Keywords: Change point detection, Climate time series, MDL, GA

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Predicting Soybean Prices in International Futures Markets Using AI Techniques

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The vegetable oil industry, particularly reliant on soybean oil, plays a crucial role in Thailand's economy and food security. However, the sector faces significant challenges due to global market volatility and Thailand's heavy dependence on imported soybeans, which account for 85–90% of the country's usage. Accurate price forecasting is critical to mitigating risks, optimizing procurement strategies, and supporting sustainable planning. This study investigates the application of three machine learning models—ARIMA, Artificial Neural Networks (ANN), and Support Vector Regression (SVR)—for forecasting soybean futures prices. Data was collected from key sources, including the Soybean Future Price dataset, USDA Demand & Supply reports, WASDE projections, and external factors such as crude oil prices, exchange rates, and weather patterns. These models were rigorously evaluated using the Mean Absolute Percentage Error (MAPE) metric to compare their performance. The results reveal that ARIMA achieved the highest predictive accuracy, with a test MAPE of 4.410258, outperforming ANN (12.307427) and SVR (14.844223). This highlights ARIMA's robust capability in time-series forecasting, effectively capturing trends and temporal dependencies. While ANN and SVR showed promise in modeling non-linear relationships, their performance lagged behind ARIMA under volatile market conditions. The findings emphasize the importance of integrating diverse data sources and selecting appropriate models to improve forecast reliability. This study underscores the potential of machine learning in supporting strategic decision-making for stakeholders in the soybean market, paving the way for more resilient and adaptive agricultural systems in Thailand and beyond.

Keywords: Soybean Price Forecasting, Machine Learning Models, International Futures Markets

Deep Learning for Industrial-Scale Modeling of the Basic Oxygen Furnace Process

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Abstract: The basic oxygen furnace (BOF) steelmaking process is a cornerstone of modern steel produc- tion, where accurate modeling is critical for optimizing operations, improving process control, and enhancing energy efficiency. This study investigates the application of advanced deep learning models, including deep transformers, to model the BOF process. Representing the first extensive deployment of such architectures on BOF operational data, we evaluated multiple state-of-the-art models using a comprehensive dataset com- prising over 10,000 samples from a large-scale industrial setting. Our research introduces novel approaches tailored to the complexities of BOF data, leveraging insights from exploratory data analysis to enhance pre- dictive performance. The proposed models demonstrated improvements in accuracy compared to traditional methods, highlighting the transformative potential of deep learning in optimizing industrial processes.

Keywords: BOF Steelmaking, Deep Learning, Industrial Digitalization, Transformers

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Optimisation for recycled concrete performance

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Abstract

Concrete is a very effective material for the construction of buildings and infrastructure around the world. Unfortunately, typical concrete is a large contributor to CO_2 emissions and consumption of natural reserves. CO_2 Concrete allows the mitigation of these downfalls by carbonating recycled aggregate, reducing CO_2 emissions, reusing crushed masonry materials and conserving virgin aggregate. CO_2 Concrete can also be considered reliable as its compressive strength can be accurately predicted by both regression analysis and artificial neural networks. The artificial neural network created for this paper allow accurate prediction of the compressive strength for CO_2 Concrete. The artificial neural network exhibited a strong relationship with the experimental specimens, revealing a multiple R of 0.98 and an R square of 0.95. The artificial neural network was also validated by 22 laboratory validation concrete mixes. The artificial neural network displayed an average error of 1.24 MPa or 3.43% in the validation mixes with 59% of concrete samples within 3% error and 77% being within 5% error. The successful prediction of compressive strength of CO_2 Concrete can help a greater mainstream use of the green material.

Keywords

CO_2 Concrete; Recycled Aggregate Concrete; Green Product; Waste Recycling; Energy Conservation; Regression Analysis; Artificial Neural Network

Application of AI methods to recognition of the liquid–gas flow regime using gamma absorption technique

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Two-phase liquid-gas flows in pipelines occur frequently in the mining, nuclear, and oil industry. One of the non-contact techniques useful for studying such flows is the gamma ray absorption method. An analysis of the signals from scintillation detectors allows us to determine the number of flow parameters and to identify the flow regime.

In this work, four types of liquid-gas flow regimes as a slug, plug, bubble, and transitional plug – bubble were evaluated using AI methods. The experiments were carried out for water-air flow through a horizontal pipeline. Two sealed Am-241 gamma ray sources and a NaI(Tl) scintillation detectors were used in the research. Based on the measuring signal analysis in the time snd frequency domains, seventeen features were extracted (e.g. mean value, standard deviation, skewness, kurtosis, 3rd and 4th order moments, selected value of normalized autocorrelation function, and parameters extracted from the signal spectrum for one detector and the cross-spectral density: maximum amplitude of the spectral densities, weighted average frequencies and variance of spectral densities) which were used at the input of the classifier. Six computational intelligence methods: K-means clustering algorithm, single decision tree, probabilistic neural network, multilayer perceptron, radial basic function neural network and support vector machine were used for a two-phase flow regime identification. It was found that all the methods give good recognition results for the types of flow examined. These results confirm the usefulness of gamma ray absorption in combination with artificial intelligence methods for liquid-gas flow regime classification.

Keywords: two-phase flow, gamma-ray absorption, pattern recognition, artificial intelligence, artificial neural networks.

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A Particle Swarm Optimization Approach to Sensor Placement for Structural Health Monitoring

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Structural Health Monitoring (SHM) is crucial for assessing the conditions of existing structures and civil infrastructures and identifying possible damage at early stages. The placement of advanced sensors has made Structural Health Monitoring methods more innovative. However, the deployment of these developed monitoring devices in large-scale structures in an arbitrary way often results in an excessive amount of online SHM data, increasing computational cost without significantly improving damage detection accuracy. Optimizing the locations of available sensors is essential for collecting high-quality measured data and reducing the computational cost and data redundancy.

Various approaches have emerged to determine the most effective optimal sensor configurations for damage detection and structural health monitoring purposes. This study presents a novel optimal sensor placement framework that integrates the famous Particle Swarm Optimization (PSO) and Ensemble Kalman Filter (EnKF) approaches for system identification and improved SHM. The suggested Particle Swarm Optimization and Ensemble Kalman Filter (PSO-EnKF) approach is based on the swarm intelligence theories of the PSO algorithm to iteratively adjust and optimize the locations of candidate solutions or particles (sensors) based on their fitness value. This fitness function is defined by the difference between the actual sensor measured data and the EnKF predicted values. The ability of the PSO technique to balance exploration enables effective convergence toward an optimal sensor layout, while the power of the EnKF data assimilation method to update the structural system state using measured data provides a robust framework for real-time system identification.

The robustness of the proposed PSO-EnKF methodology is validated using a ten-story reinforced concrete building subjected to seismic excitation. The performance of the suggested PSO-EnKF approach, in terms of accuracy in detecting structural changes, convergence ability to optimal sensor placements and computational efficiency, is tested by comparing its results to the brute-force search methodology outcomes.

This work highlights the ability of the PSO approach in optimizing available sensor locations and enhancing SHM efficiency. The proposed PSO-EnKF methodology offers a flexible solution for real-world structure and infrastructure monitoring.

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Keywords: Structural Health Monitoring, Optimal Sensor Placement, Particle Swarm Optimization, Ensemble Kalman Filter, Seismic Monitoring, System Identification, Damage Detection

Optimized Attention U-Net for Retinal Vessel Segmentation Across Multiple Data Representations

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The length, width, tortuosity, branching patterns, and angles of retinal blood vessels can be utilized for diagnosing, screening, treating, and monitoring a range of cardiovascular and ophthalmologic conditions, such as diabetes, hypertension, arteriosclerosis, and choroidal neovascularization [1].

Automated vasculature detection and analysis play a key role in enabling diabetic retinopathy screening programs [2]. They also aid research into the relationship between vessel tortuosity and hypertensive retinopathy, the assessment of vessel diameters for diagnosing hypertension, and the advancement of computer-assisted laser surgery. Moreover, automated generation of retinal maps and identification of branch points have been used in temporal or multimodal image registration and the synthesis of retinal image mosaics. Finally, the retinal vascular tree is uniquely distinctive to each individual, making it a promising tool for biometric identification.

In the study presented, the Attention U-Net was implemented. After initial testing it turned out to produce better results than standard U-Net architecture. Attention U-Net is a variation that integrates attention mechanisms to focus on relevant regions within an image. It is often used in segmentation of medical images. In terms of the presented study, applying this architecture allows for achieving higher value of Intersection over Union. The neural network consists of 5 encoder blocks (with an increasing number of filters: 32, 64, 128, 256 and 512) and 5 decoder blocks. With convolution block containing 6 layers (2 convolution, 2 batch normalization and 2 activation layers), and *relu* as activation function. There were 5 different input conditions considered: original RGB images, grayscale images and images based on R, G and B channels of RGB color space model.

The results showed that there is a difference between the segmentation results for particular channels of RGB color space model. The mean DICE value for test set in case of R channel was 0.848, which is comparable to the results of grayscale image (0.856). In the case of G channel, the results were the worst, with DICE value equal to 0.712 and for B channel 0.814. The best results were achieved for RGB image with the mean DICE value equal to 0.909. What is interesting to see is that most information is stored in channels R and B of RGB image. Moreover, the results of R channel are comparable to results of grayscale images. The study also showed how the size of an input image influences the accuracy of the result. The conclusion drawn is that there is an adequate resolution of an image, which is more suitable for segmentation and

returns more accurate results.

The presented results were compared with adaptive local thresholding methods. In all cases, the achieved segmentations were better in the case of Attention U-Net implemented and proposed, which can be explained for example by differences in illumination between particular images.

This study shows that there is not one proper way of segmentation in case of retinal vessel extraction. There are a lot of methods existing and all of them possess their strengths and limitations [3]. The presented method allows for really good segmentation results, which can help in a lot of fields. The question raised during this project concerns the validity of accuracy metrics for segmentation. In the case of small object segmentation, we deal with a lot of bias which cannot always be resolved by assigning weights or applying other known methods. Further research should focus on implementing other methods which would allow for better verification of accuracy for segmentation results.

Keywords: image segmentation, attention U-net, color space models, retinal vessel segmentation

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Evaluation of Machine Learning and Physical Models for PV Power Forecasting: A Multi-Site Validation Approach

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Photovoltaic (PV) power generation, along with wind power, is a critical renewable energy source for achieving carbon neutrality. As of 2023, the combined PV and wind power generation in the Korean electricity market reached 56.562 GWh, accounting for 9.6% of the nation's total electricity production. This share has been steadily increasing each year. However, the intermittent nature of solar and wind power presents significant challenges for grid stability, as fluctuations in output make accurate power generation forecasting difficult. To mitigate the growing variability of renewable energy generation, the Korean electricity market introduced a power generation forecasting system in October 2021, which provides financial incentives based on forecast accuracy. This study systematically compares various PV power forecasting models, with a particular emphasis on their applicability in real-world electricity market operations. Unlike previous studies that primarily focused on forecasting accuracy, this research evaluates the economic impact of forecasting accuracy by estimating potential financial incentives. Additionally, by validating the models with data from multiple locations, this study enhances the generalizability of forecasting methodologies. The findings offer practical insights into the integration of PV power forecasting for grid stability management and real-time operational strategies.

Various approaches exist for PV power forecasting, including physical models, statistical models, and machine learning models, each with distinct characteristics. The models employed in this study are as follows:

- **Physical Model:** The HDKR model, based on photovoltaic theory, utilizes a diode model to compute power generation using solar irradiance and surface temperature as input variables.
- **Statistical Model:** Linear regression and ARIMA models estimate power generation by

deriving coefficients from time-series power generation data and meteorological data collected from power plants.

- **Machine Learning Model:** Support Vector Regression (SVR) and Deep Neural Networks (DNN) predict power generation by learning from time-series data, leveraging advanced AI techniques to achieve high accuracy.

Key variables influencing PV power generation and time-series forecasting models include:

- **Meteorological Data:** Solar irradiance, temperature
- **Installation Conditions:** Site location (latitude, longitude, and elevation above sea level), tilt angle, azimuth angle, PV cell characteristics, inverter efficiency

[a] Presenting Author

- **Measurement Data:** Power generation, global horizontal irradiance, tilted plane irradiance, PV cell surface temperature
- **Measurement Conditions:** Time intervals, measurement periods (number of data points)

The physical model calculates PV power generation by determining the solar irradiance incident on the PV module surface using location and weather data. This computed irradiance, along with cell surface temperature, is then used to estimate PV power output through photovoltaic theory equations and efficiency models. The HDKR model [1], employed in this study, determines tilted plane irradiance by incorporating tilt and azimuth angles. It refines the Hay & Davies model by integrating the anisotropy index and horizon brightening factor, making it one of the most robust models for tilted irradiance analysis. For the statistical and machine learning models, the same input data as the physical model were used. The dataset consists of 8,760 hourly measurements collected over one year, divided into training and validation sets. The independent variables selected during model training were solar irradiance and temperature, while the target variable was PV power output. The trained forecasting models were evaluated by comparing their predicted outputs with actual power generation data from different locations, ensuring a rigorous validation process.

All forecasting models were implemented using open-source software provided by Scikit-learn [2], and the development environment was based on Python scripts executed in Colab [3]. The performance of each model was assessed using key statistical metrics, including the coefficient of determination (R^2), the normalized root mean square error (nRMSE), and the normalized mean bias error (nMBE). Additionally, forecast accuracy was evaluated using the error rate (%) formula defined in Korean regulations, and the potential financial incentives were estimated based on accuracy levels.

Keywords: Photovoltaic (PV) power generation, Solar energy forecasting, Machine learning models, forecasting accuracy, Power grid stability

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Novel REST block for Gradient Optimization in Deep Learning Models

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Deep learning surpasses traditional machine learning methods in image segmentation tasks by autonomously discerning pertinent features from the input, yielding remarkable outcomes. Optimizing algorithms are an important feature of training deep learning models which aid to minimize loss and modify the model's parameters. In training deep learning models, unstable gradient poses a challenge. The optimizing algorithm mostly use gradient descent to learn and tune up model parameters. The problem of unstable optimizing algorithm in deep learning can lead to the issue of gradients becoming either too small (vanishing gradients) or too large (exploding gradients) during the training of deep neural networks. If the gradient of the loss is too low or too high it effects the ability of the optimizer algorithm to learn properly. Models based on fewer/shallow layers, such as Convolution Neural Network (CNN) as well as deeper/dense layered variants like U-Net have shown prominent segmentation results. However, they often suffer from unstable optimizing algorithm and overfitting during the training process particularly in the initial layers of the model.

In order to stabilize the optimizing algorithm, we propose a novel block which comprises of four sub-blocks collectively called the REST block; Residual Block, Efficient Channel Attention, 2D convolution layers, Stochastic Depth and a three-layered Dense Block with three feature maps to reduce computational cost. The REST is embedded in the decoder layer of the U-Net model after the last up-sampling convolution. In the CNN model, REST is integrated after each maxpooling layer to recalibrate the feature maps before they are fed into the next stages of the network. Some features of REST are used after the first and fifth Conv2D layer, where overfitting is more likely to happen. The aforementioned models were successfully able to suppress the unstable gradient in order to improve optimizing algorithm and overcome overfitting of the model. The model was tested on three imbalanced medical datasets including DRIVE, BUS2017 and CVC-Clinic.

The experimental results show that neural network models having deep as well as shallow layers, embedded with REST block helps to mitigate the unstable

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gradient issue. While being trained, the suggested model significantly reduced the convergence time by sharply minimizing the loss up to 0.004% and increasing accuracy to 99.7% in comparison with other models. Comparison of models integrated with state-of-the-art REST block show promising results by reaching 0.982± 0.002 in terms of testing accuracy while using 95% confidence interval on five-fold cross validation.

Keywords: Vanishing Gradient, Exploding Gradient, Optimization, Deep learning, Stabilizer, Overfitting, Segmentation.

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Causal CNN-based Virtual Sensor in Industrial Aircraft Vapor Cycle System

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Abstract:

In aircraft, the Vapor Cycle System is used to manage the cooling needs of the cabin and can also be used to cool the engines. In such systems, the mass flow sensor plays a key role in a variety of monitoring and control tasks. However, physical sensors may be inaccurate, heavy, cumbersome, expensive, or highly sensitive to vibrations—limitations that are particularly critical when embedded on an aircraft. Designing a virtual sensor, using inputs from standard on-board sensors, is therefore an attractive alternative.

This paper has two main objectives. First, we propose a data-driven model based on a Causal Convolutional Neural Network to estimate the mass flow through the compressor. Our results show that it significantly outperforms the standard Polynomial Regression approach (thermodynamic maps), both in terms of Mean Square Error and the Engineer Performance metrics. Second, we introduce a semi-automatic segmentation method to compute these Engineer Performance metrics on real datasets, as the conventional Mean Square Error metric alone may pose risks when analyzing the dynamic behavior of Vapor Cycle Systems.

Keywords: Deep Learning, Convolutional Neural Network (CNN), Vapor Cycle System (VCS), Virtual Sensor

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Nomenclature

$\dot{m}$	Compressor Mass Flow	kg s^{-1}
ω	Compressor Motor Speed	rad s^{-1}
C	Compressor Motor Torque	N m
P_{in}	Compressor Inlet Pressure	Pa
P_{out}	Compressor Outlet Pressure	Pa
T_{in}	Compressor Inlet Temperature	K
T_{out}	Compressor Outlet Temperature	K

1 Introduction

In physical systems, it is crucial to measure certain quantities. Traditionally, physical sen- sors have been used for this purpose, but they can be expensive, cumbersome, and require maintenance. Sometimes there are no physical sensors for the quantity of interest. As an alternative, virtual sensors have emerged as a cost-effective and reliable method for mea- suring physical data based on other physical sensors [1]. In complex physical systems, it is sometimes hard to derive physically meaningful equations to construct a virtual sensor. Therefore, using machine learning models to design a virtual sensor has become a popular re- search direction in recent years [1–7]. In this paper, we propose and evaluate a virtual sensor based on Machine Learning (ML) for estimating an important physical quantity (Compres- sor Mass Flow) in the Vapor Cycle System (VCS) of LIEBHERR in airplanes.

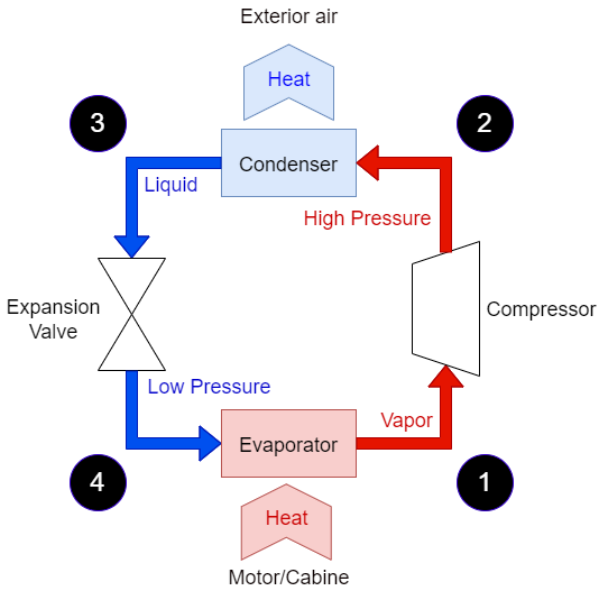

Figure 1: Vapor Cycle System (VCS)

Background of the VCS: The function of this system is to reduce and control the temperature of a medium by transferring its heat to the refrigerant (Evaporator) and then to transfer the heat from the refrigerant to an external medium (Condenser). The Compressor and the Expansion Valve bring the refrigerant fluid in the appropriate conditions of pressure and temperature for heat transfer. A typical refrigeration cycle comprises four stages through which the refrigerant undergoes: compression (from point 1 to point 2), condensation (from point 2 to point 3), expansion (from point 3 to point 4), and evaporation (from point 4 back to point 1) [8, 9]. This system is represented in Figure 1. The cycle is defined by these transitions that are represented in Figure 2. VCSs are used in aircraft for cooling the cabin and the motors down. For control purposes, it is necessary to accurately measure the mass flow through the compressor with a small response time, lest it could lead to control instability [10] and surge phenomenon [11]. This mass flow can be expressed as the ratio of the power supplied to the fluid by the enthalpy difference between the outlet and the inlet of

the compressor [2] :

$$\dot{m} = \frac{C\omega(1-\alpha_{loss})}{h_2 - h_1} \overset{(\star)}{=} \frac{C\omega(1-\alpha_{loss})}{h(T_{out}, P_{out}) - h(T_{in}, P_{in})}$$

where h(P, T) is the enthalpy of the refrigerant fluid in vapor phase at temperature T and pressure P. α_{loss} is the proportion of dissipated energy and cannot be measured.

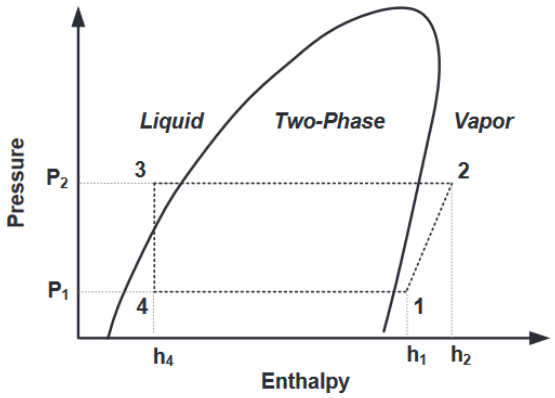

Figure 2: Vapor Cycle on Pressure-Enthalpy diagram [9]

On the ML-based virtual sensor: There are two standard physical mass flow sensors, the Coriolis [12] and Venturi [13] flowmeter. The first one is highly accurate but not robust to vibrations and hence not adapted to aircraft systems. The second one requires adding a bottleneck that induces a loss of charge and deteriorates the efficiency of the system. This leads to the need for a virtual sensor based on other embeddable sensors. Unfortunately, there are no obvious physical equations that give the flow in function of these measured quantities with sufficient accuracy.

In the laboratory of LIEBHERR Aerospace in Toulouse, experiments were done on an indus- trial VCS. Several physicals quantities were recorded at a high frequency during 30 hours, including the mass flow measured with a Coriolis flowmeter. Indeed, even though the Coriolis flowmeter is not embeddable in aircraft, it is an excellent sensor for measuring the mass flow during the experiment in the laboratory. Those measures pave the way to adopt a supervised machine learning framework to predict the mass flow from other physical quantities (defined in the Nomenclature and exposed in Figure 3). Similar experiments were done in [2] without the torque measure C and in [3] with additional data on the Condenser and the Expansion Valve.

State-of-the-art and main contributions: In [2] an evaluation of statistical models based on Poly- nomial Regression (PR) is conducted. A CNN based on 2d convolutional networks (usually used to analyze images) is tested in [3] and it is shown to outperform the PR models. The issue with the existing CNN approach is that no guarantee of physical properties are ana- lyzed. In this article, we propose a different CNN architecture to guarantee time-translational invariance, insensitive to the order of input features, and causal properties for real-time es- timation. The architecture is adapted from [6] for unsupervised learning of time series, with applications to classification and regression problems.

By expanding the scope of applications, one finds in the literature several models for de- signing

virtual sensors [4–7, 14]. In [5], a CNN with recurrent skip connections is trained on simulated data, fine-tuned on real data to estimate physical quantities in electrical induction motors, and evaluated with electrical engineering metrics.

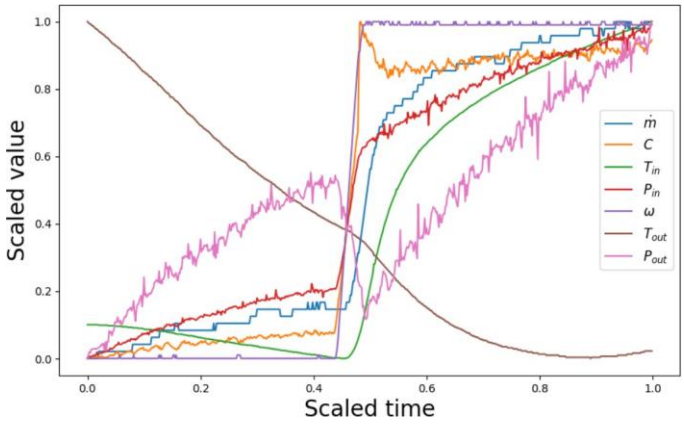

Figure 3: Scaled measures

The main contribution of this article is to show that the proposed CNN significantly outper- forms the PR model on the novel LIEBHERR dataset. To compare the difference between these models, we further propose a semi-automatic evaluation method to compute similar engineering metrics as in [5]. The novelty is that we work on a real dataset so it is needed to introduce a segmentation step of time series based on peak detection.

The rest of the article is organized as follows. In Section II, PR and the proposed CNN models are detailed. In Section III, a two-fold evaluation method is explained, integrating machine learning metrics and engineering ones. The engineer's metrics are computed after a segmentation step, that enables to compute a multitude of metrics and to perform statistics analysis. Finally, the results are presented and discussed in Section IV.

2 ML Models

We aim to develop a model 8capable of predicting real-time mass flow $\dot{m}$ based on specific measurements. Although equation ($\star$) relates these variables, the quantity α_{loss} is absent from our measurements. To circumvent this lack of physical relationship, we will rely on experimental data to construct two statistical models: Polynomial Regression (PR) and Convolutional Neural Networks (CNN). Each recording consists of a variable-length, multi- variate time series containing seven measures, as represented in Figure 3.

Polynomial Regression: Statistical models are used in thermodynamics to determine the state function of a system at equilibrium from experiments. These models are called maps, and a standard way to create them is Polynomial Regression (PR) [15]. Our baseline approach is PR as in [2,3,15] and hence the model is static. It involves fitting a second-order polynomial function without cross-terms to the data points obtained from experimental recordings. This function was then used to predict the mass flow on the test recordings for evaluation. It is important to note that the prediction at time t depends only on the measures at time t.

$$\hat{\dot{m}}_t = \alpha +$$

$$\sum_{i=1}^{6} \beta_i x^{(i)} + \gamma_i t^{(i)} x \quad ,$$

where $\hat{m}_t$ is the estimated mass flow at time t,$x_t = (C_t, \omega_t, P_{in,t}, T_{in,t}, P_{out,t}, T_{out,t})$ is the vector of input measures at time t, $\alpha \in R$ and $\beta, \gamma \in R^6$
are the model parameters.
In [2], the authors propose to use the equation $(\star)$ by estimating the missing value α_{loss} with a polynomial of other measures and found more precise and consistent results. Combining physical and statistical approach could be interesting, but this is not in the scope of this paper.

Convolutional Neural Network [16, 17]: A Convolutional Neural Network (CNN) is a series of convolution layers with adjustable coefficients, designed to minimize a loss function during the training process. We shall first specify the convolutional layer that we use in this paper and then analyze its physical properties. We then specify the proposed CNN architecture and discuss its advantage with respect to the standard Polynomial Regression model.

Let $x \in R^{I \times T}$ with x_t^i the i-th feature at time $t \in \{1, ..., T\}$. The causal one-dimensional convolution **(Conv1D)** is defined as

$$y_t^j = Conv1D(x) = \sum_{s=t-k+1}^{t} x_s^i w^{j,i},$$

$$1 \le i \le I \quad s = 0$$

where y^j_t is the j−th output channel at time t, $I \in \mathbb{N}$ is the number of input channels, $k \in \mathbb{N}$ is the kernel size, $w^j \in \mathbb{R}^{I \times k}$ the kernels of the j−th output channel. This convolution is performed with zero padding, meaning that $x_t = 0$ for $t < 0$. To compute the output at time t the model uses the measurements $(x_{t-k+1}, x_{t-k+2}, \ldots, x_t)$ which are all anterior to t, this is a way to model causality [18].
In [3], the CNN is based on two-dimensional convolution **(Conv2D)** defined as

$$y^{j,l}_t = Conv2D(x) = \sum_{i=0}^{d-1} \sum_{s=0}^{k-1} x^{l-\lfloor d/2 \rfloor + i}_{t-\lfloor k/2 \rfloor + s} w^{j,i}_s,$$

where $w^j \in \mathbb{R}^{k \times d}$ are the kernels of j−th output channel of size $k \times d$. There is one more exponent 'l' on y because the convolution is also performed on the dimension of features.

In this paper, we propose a one-dimensional causal CNN with skip connections [19]. The complete architecture is detailed in Figure 4 and is similar to the one used in [6]. A skip connection creates a shortcut from an early layer to a later one, linking the input of a convolutional block straight to its output [19]. Since various layers of a neural network capture distinct feature "levels," skip connections assist in preventing a drop in performance as more layers are added [19]. The CNN is trained with the MSE Loss. To accelerate the training, we also apply the weight normalization [20] to re-parameterize the weights of each convolutional layer.

Physical properties in CNN

- Causality: Aiming to perform real-time estimation, the CNN has to be causal [18]. Thus, the model will only use present and past measures.
- Equivariance to time-translation: As demonstrated in [21], CNNs are equivariant to translation in the dimension of convolution. Time-translation equivariance is an im- portant property of physical systems, since the physical law does not evolve through time.
- Insensitivity to input-feature order: The order of features in x is arbitrary and has no physical meaning.

  In causal Conv1D, the j−th output channel at time t is

$$y^j_t = \sum_{i=1}^{I} \sum_{s=0}^{k-1} x^i_{t-s} w^{j,i}_s$$

  where I is the number of input channels. If the input channel of x is permuted (by π) to $\tilde{x}^i_t = x^{\pi(i)}_t$, then one can find an equivalent CNN with kernel $\tilde{w}^{j,i}_s = w^{j,\pi(i)}_s$ to have the same output y^j_t. This property does not hold in general if one uses the Conv2D layer.

Advantage of CNN over PR:

- Capturing Local Patterns [22]: CNNs are designed to capture local patterns and fea- tures within the data. In the context of time series, local patterns can represent short- term temporal dependencies, which are crucial for understanding the dynamics of the time series. PR, on the other hand, cannot effectively capture these local patterns as it does not use past measures for predictions.
- Automatic Feature Extraction [22]: During the training step, CNNs automatically learn the relevant features from time series. PR uses directly the measures from sensors, which might not capture all the relevant information in the time series.
- Handling Non-Linear Relationships [22]: Time series data often contains complex non- linear relationships between the input and output variables. CNNs with their multiple layers and non-linear activation functions can better model these non-linear relation- ships compared to the PR, which is inherently limited to polynomial relationships. The activation functions of our model are LeakyReLU [23] :

$$\forall x \in \mathrm{R}, \mathit{LeakyReLU}(x) = \begin{cases} x & \text{if } x \geq 0 \\ 0.1x & \text{elsewhere} \end{cases}$$

PR has the advantage of being simple to train and easy to understand, as it only involves 13 parameters. On the other hand, CNN are considerably more complex, requiring the tuning of 2, 700 parameters and involving more sophisticated computational processes.

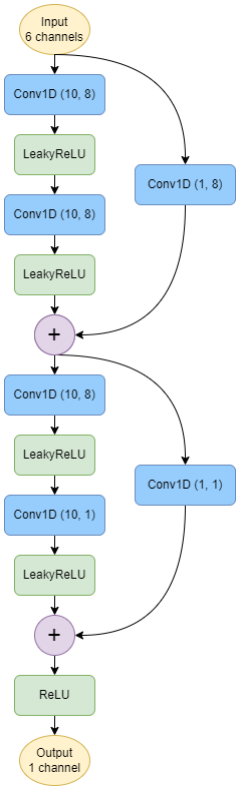

Figure 4: Feedforward CNN
Conv1D (kernel size, number of output channels)

3 Evaluation

EP Metrics: To evaluate the performance of the ML methods, a dataset of systems mea- sures and their corresponding mass flow was split into training (64%), validation (18%), and testing (18%) sets. The training set was used to train the ML models, the model which had the smallest validation loss was selected, and the testing set was used to evaluate their performance. The performance of the ML models was evaluated using the MSE and engi- neering performance (EP) metrics that are standard in engineering fields and well-suited for analyzing dynamical behavior [5]. The EP metrics are defined as follows:

- $\Delta t_{80\%}$, $\Delta t_{10\%}$ [5]: 80% (resp.10%) response time ($t_{80\%}$, $t_{10\%}$) is the time value at which the response signal has covered 80% (resp.10%) of the ramp amplitude. $\Delta t_{80\%}$ (resp. $\Delta t_{10\%}$) is the absolute difference between the true and predicted $t_{80\%}$ (resp. $t_{10\%}$)
- Δt_{peak} [5]: Peak delay is the absolute delay between the predicted signal and the target one.
- Δt_{conv}: for a signal containing a ramp followed by a static state, t_{conv} is the time when the signal has converged to the final valued with 3% of tolerance. Δt_{conv} is the delay between the predicted and true t_{conv}.
- E_{abs} (resp. E_{rel}): Absolute (resp. relative) error on static states.

In order to compute a lot of characteristic times and static errors (EP metrics), a first step of segmentation was developed to identify the ramps ($\Delta t_{80\%}$, $\Delta t_{10\%}$, and Δt_{conv}), the overshoots and undershoots (Δt_{peak}) and the static states (E_{rel} and E_{abs}). Eventually, we have, for each of those metrics, several instances. To represent their distributions, we consider their 90% quantile.

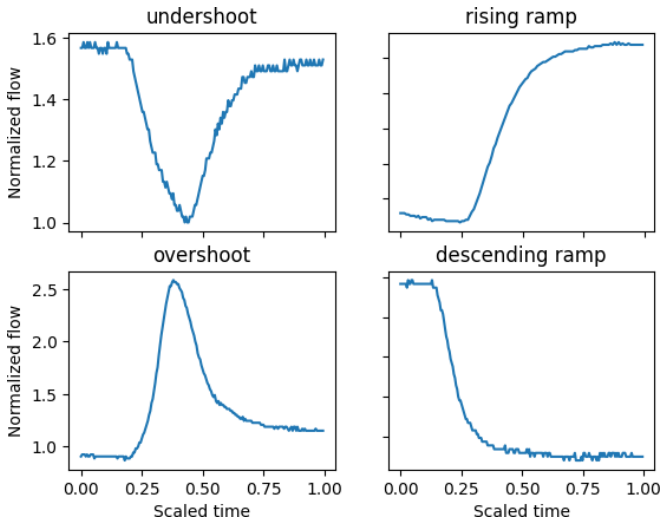

Figure 5: Templates of patterns

The segmentation process: It consists of four steps. The patterns of interest are presented in Figure 5. The first step consists in selecting windows in the dataset that will constitute a set of candidates for being one of the patterns. For this purpose, a Butterworth [24] pass band filter of order 6 is applied to the flow with system-specific cutting frequencies. The frequency peaks are detected via the scipy function *'find peaks'* as shown in Figure 6. The candidates are symmetric windows around the detected peaks. Then, a Dynamic Time Warping (DTW) k-means clustering [25] with 6 clusters is performed on the normalized signals (Figure 7 in Appendix). DTW, while not a true distance measure, serves as an effective metric for clustering patterns. Specifically, two signals exhibiting identical patterns, albeit with a mere time delay, will manifest a small DTW value. This is evident in Cluster 2 of Figure 7, where even if overshoots happen at varying times, they remain closely aligned in terms of DTW. The identification of patterns is as follows:

- Cluster 1: Undershoots
- Cluster 2: Overshoots
- Cluster 3: Descending ramps
- Cluster 4: Rising ramps

Cluster 5 and 6 correspond to other phenomenons like sinusoids. At this step, there are in clusters 1-4 some bad candidates. Aiming to remove those, we take the intersection with a DTW ball centered on the centers. A last manual selection is applied. Finally, we obtain satisfying numbers of each pattern (table II).

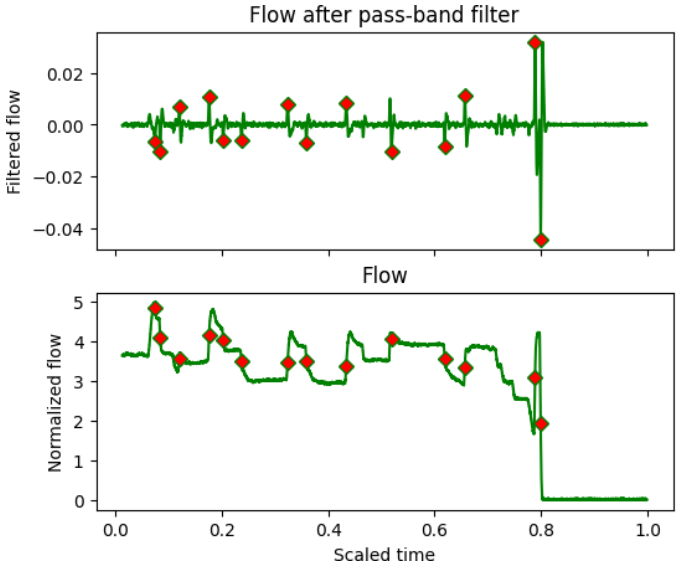

Figure 6: First selection of candidates

	train	test
Rising ramps	30	8
Descending ramps	35	5
Overshoots	79	12
Undershoots	22	8

Table 1: Number of patterns detected in each set

4 Results

Our study at LIEBHERR presents its results in a normalized manner due to the sensitivity and protection of the VCS data. Even so, the obtained results can provide a clear comparison between the performance of PR and CNN models.

As tabulated in Table III, the Convolutional Neural Network (CNN) model demonstrates superiority over the PR model both in terms of Machine Learning (ML) metric (MSE) and Engineering Performance (EP) metrics. The CNN model particularly excels in predicting static errors and Δt_{conv} (convergence time).

As per the results, the CNN model outperforms the PR model by reducing the MSE from 0.18 to 0.06, the absolute error (E_{abs}) from 0.73 to 0.28, and the relative error (E_{rel}) from 28% to 14%. Furthermore, it provides a more accurate prediction of Δt_{conv} and $\Delta t_{80\%}$. PR has better results on $\Delta t_{10\%}$ and less good results on Δt_{peak}, however the differences are not significant. Thus, a better dynamic behavior is captured by the CNN model. Examples of predictions on patterns of interest can be found in Figure 8 in Appendix.

	PR		CNN	
	train	test	train	test
MSE	0.2	0.18	**0.063**	**0.06**
E_{abs}	0.53	0.73	**0.19**	**0.28**
E_{rel}	21%	28%	**11%**	**14%**
$\Delta t80\%$	65	20	**33**	**17**
$\Delta t10\%$	92	**3**	**17**	3.6
Δt_{conv}	97	44	**74**	**14**
Δt_{peak}	**9**	7.1	11	**7**

Table 2: Comparaison on MSE and 90% quantile

5 Conclusion

The study demonstrates that ML algorithms, specifically CNNs, can effectively function as virtual sensors in estimating physical quantities such as mass flow in aircraft compressor systems. Compared to PR, the causal one-dimensional CNN model, with the ability to capture dynamic behavior and non-linear relationships, outperforms in terms of MSE and EP metrics. The computation of multiple EP metrics on a large real dataset was performed via a semi-automatic segmentation method proposed in this article. The contribution is, on one hand, the design of a CNN-based model for estimating the flow in an industrial dataset from LIEBHERR Aerospace. On the other hand, the engineering evaluation is performed on several instances of ramps, overshoots, and undershoots.

Future work will focus on improving these models by using physical knowledge. For the virtual sensor of mass flow, the author of [2] proposed to use an incomplete equation ($\star$). There exists multiple other methods to integrate physical knowledge into ML Models [26].

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Appendix

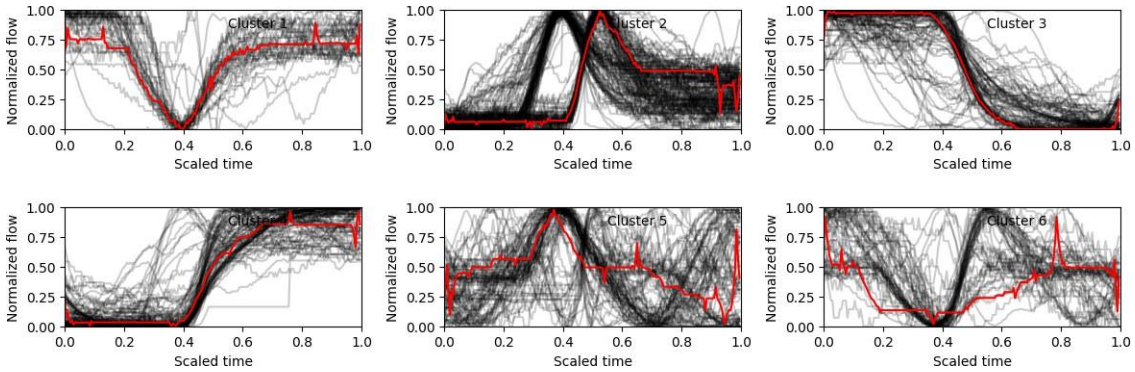
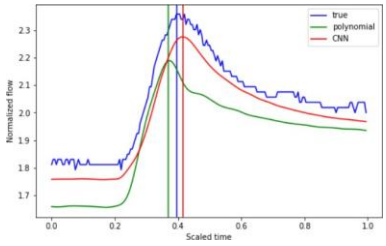
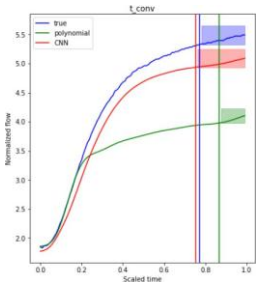


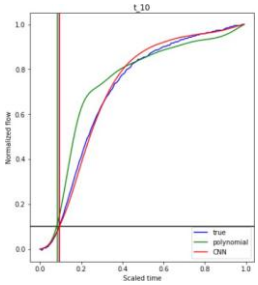
Figure 7: Clusters with the DTW K-means algorithm. The centers are represented in red.



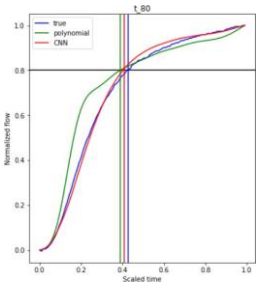
(a) Δt_{peaks}



(b) Δt_{conv}



(c) $\Delta t_{10\%}$



(d) $\Delta t_{80\%}$

Figure 8: On (a) Δt_{peaks} is computed from an overshoot. In (b) Δt_{conv} is computed from a rising ramp with the two predictions. On (c) and (d) there is the same ramp as (b) but the three signals are scaled in order to have the same initial and final value. In this manner it is easier to compute $\Delta t_{10\%}$ and $\Delta t_{80\%}$.

Spatial Patterns of Loss of Access to Urban Critical Infrastructure During Disasters

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Abstract: This study presents a novel framework integrating geographic information systems (GIS) with network analysis to assess the resilience of urban critical infrastructure during extreme events. By leveraging remote sensing data and socio-demographic information across diverse regions including North America, Asia, and Oceania, the research identifies distinct vulnerability patterns for disasters such as floods, hurricanes, earthquakes, and explosions. Using network metrics and simulations, it evaluates both robustness and resilience, revealing differential impacts on populations based on factors like sex, age, and poverty. The findings underscore the need for tailored strategies to enhance infrastructure resilience, emphasizing region- specific approaches for effective disaster preparedness and urban planning.

Keywords: urban resilience, natural disasters, explosions, spatial patterns, sociotechnical analysis, complex networks, access to critical services

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* Presenting author

This study introduces an original framework developed and applied to assess the resilience of urban critical infrastructure during extreme events [1, 2, 3]. The approach integrates advanced geographic information systems (GIS) with network analysis tools, utilizing open- source remote sensing data from post-disaster scenarios, vector datasets of infrastructure networks, and socio-demographic data to evaluate the impacts on both critical infrastruc- ture and affected populations. Through this comprehensive approach, distinct geospatial patterns of infrastructure vulnerability were identified in urban areas affected by major disasters such as floods, mudslides, hurricanes, earthquakes, and industrial or nuclear ex- plosions. The research spans diverse geographical regions, including North America (e.g., U.S. Florida and Washington D.C.), Asia (Turkey, Lebanon, Kyrgyzstan), and Oceania (In- donesia). This multi-regional analysis enables a comparative assessment of infrastructure resilience across different climatic and socio-economic contexts, providing valuable insights for disaster preparedness and urban planning strategies globally.

The methodology of this work enables the investigation of underlying determinants of nat- ural disasters by integrating findings from urban studies, network analysis, and disaster risk reduction research while employing GIS-based methods. Satellite and aerial remote sensing technologies can provide valuable data for identifying affected regions, evaluating post-disaster damage, and supporting predictive models that forecast urban susceptibility to catastrophic events. These datasets are publicly available through space agencies, govern- ment bodies, and private companies. The OpenStreetMap platform offers high-quality data regarding the location of essential services and

transportation network layouts. Utilizing these and other public sources, the study quantifies damages sustained by cities affected by catastrophes. Furthermore, we assess whether there are observable signs of overall system robustness and resilience in post-recovery states. The methodological framework continues an evolving research thread [1, 2, 3] and is grounded in Alexander's conceptualization of fit as the absence of misfit [4]. Given that future disaster events are inherently unpredictable, it is advisable to prioritize preparedness over reliance on forecasts alone [5]. Overall, this research identifies vulnerabilities in people's access to critical infrastructure during catas- trophic events events rather than focusing narrowly on specific procedures.

Robustness and resilience of cities are assessed through measures such as shortest path lengths, network efficiency, clustering, effective resistance, and edge betweenness centrality. These metrics help evaluate how well a city's infrastructure holds up during disasters (ro- bustness) and its ability to recover afterward (resilience). To determine the loss of access to essential services, preserved connectivity is calculated by tracking all edges in the network subgraphs where at least one service has been disrupted after each catastrophic event. This approach ensures that we understand which populations lose access to critical infrastructure. Additional probabilistic analysis is conducted using a Markov chain stochastic process, sim- ulating various scenarios to predict potential outcomes and impacts of disasters on different parts of the city.

Findings reveal unique patterns for each disaster type. Floods create isolated islands in the network, leading to loss of access for populations concentrated in these areas. Hurricanes and earthquakes have randomly distributed effects, with hurricanes particularly affecting residential areas and network corners. Explosions create large homogeneous affected regions within specific parts of the city. All disasters significantly impact societal groups differently based on factors like sex, age, and poverty levels. Therefore, strategies to enhance resilience should be tailored to each case, such as in flood-prone areas, decentralizing critical services in low-lying or coastal zones is recommended. For explosion-risk regions, increasing redundancy of services outside risky urban parts is suggested. This approach ensures that cities can better withstand and recover from disasters by addressing specific vulnerabilities based on disaster type and societal demographics.

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Conceptual modeling and analysis of blockchain integration in data spaces: Challenges and solutions for security and data protection

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The ongoing digitalization of the economy and the rapid increase in data flows mean that companies are increasingly reliant on sharing data and using new data sources to remain competitive and drive new innovations. Joint collaborations in conjunction with data exchange are leading to the development of data spaces. To ensure the security and data protection- compliant handling of data spaces, this thesis examines the challenges and possible solutions through the integration of blockchain technology. In this regard, a conceptual model is developed that addresses the identified challenges using the IDS reference model. With the help of morphological analysis, blockchain types, encryption algorithms, consensus mechanisms and data management, among other things, can be identified and used in the model. Security mechanisms offered by the blockchain in this context are asymmetric encryption and smart contracts, which can be used to ensure data security and compliance with governance guidelines. Through the theoretical case study and the concluding discussion, the decisive advantages of blockchain integration in data spaces could be demonstrated based on the model evaluation, regarding an improvement in data integrity and traceability and unalterable storage of all data flows and interactions by creating transparency. Strengthening data sovereignty leads to increased trust in data and data spaces with the help of access and usage control through smart contracts. Smart contracts ensure the enforcement of defined regulatory provisions such as the general data protection regulation. The scalability and interoperability between data spaces and blockchains is ensured by standardization such as APIs and decentralized applications as interfaces as well as standardized components of the International Data Spaces. Although not every identified mechanism has been implemented in the model and challenges remain, the conceptual model provides a solid foundation for future optimization and research.

Keywords: Data Spaces, blockchain technology, IDS reference model, data security, data protection, smart contracts

The Pareto front of PINNs for temperature reconstruction from 3D velocity fields in mixed convection

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Abstract: We demonstrate the temperature reconstruction potential of PINNs for a mixed convective flow in a cuboid cavity based on tomographic particle image velocimetry data provided for a sub-volume of the cavity. To optimise the loss weighting strategy for this application and to gain insight into the training processes, the associated Pareto front will be analysed.

Keywords: PINN, mixed convection flow

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Physics-informed neural networks (PINNs) provide a versatile data assimilation framework to solve problems in fluid mechanics [1]. A particular application of PINNs is the recon- struction of temperature fields from 3D velocity fields, which allows the determination of convective heat fluxes, which are essential for many engineering problems such as the de- sign of ventilation systems for passenger compartments of trains or aircraft (see e.g. [2]). Our previous work showed that this kind of temperature reconstruction is possible for the canonical case of Rayleigh-Bénard convection, which is driven by buoyancy forces only [3].

However, in engineering applications, thermal convective flows often include a forced con- vection component. To bridge the gap to engineering applications, we investigate the tem- perature reconstruction capabilities of PINNs for mixed convection flow in a generic cuboid geometry at a Rayleigh number $Ra = 1.5 \times 10^8$, Prandtl number $Pr = 0.71$ and Reynolds number $Re = 7100$ [4]. Figure 1 shows an intermediate result of the fitted velocity field of an existing measurement [4] as vectors, which are colour-coded by the reconstructed temperature field.

One complication introduced by these data is that the buoyancy forces are now superimposed by additional inertial forces, making it more difficult to reconstruct the correct temperature field. Furthermore, the measured velocity vector fields contain partly systematic measure- ment errors that need to be corrected by the PINN. Both aspects require an update of the established [3] strategy for weighting the different loss components. Therefore, we plan to investigate the Pareto front (see [5]) of the present temperature reconstruction task in or- der to find an optimal setting and to gain a deeper understanding of the training process. An example of this is shown in Figure 2, where the losses for both the partial differential equations (PDEs), Navier-Stokes and energy equations, and for the measurement data are plotted for a 10^4 epoch training process, for which the data loss weight

λ_{data} was varied by a factor of ten: $\lambda^{\#1}_{data} = 10\lambda^{\#2}_{data}$. The result of the weight variation is that a lower PDE loss is obtained for case #2, while the data losses of this case remain higher. Since the data

is subject to errors, the determination of an optimal configuration is not trivial. For this reason, we will also consider an existing direct numerical simulation data-set, representing a digital twin of the measured data, to verify the PINN results.

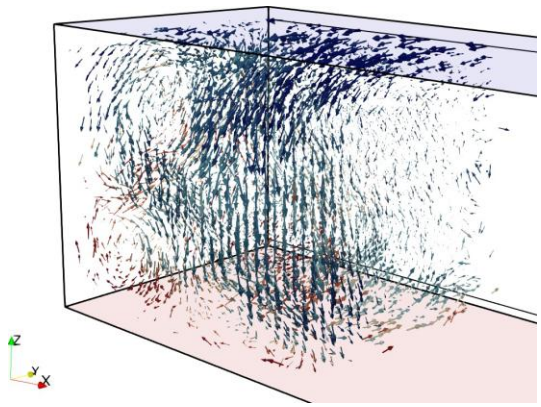

Figure 1: Exemplary instantaneous fields of the adapted velocity vectors and the reconstructed tem- peratures provided (color-coded from blue to red, i.e. cold to warm) by the PINN for a flow domain bound

by a heated plate at the bottom (red) and a cooled plate at the top (blue). In- and outlet openings exist along the rear top and bottom edges, respectively.

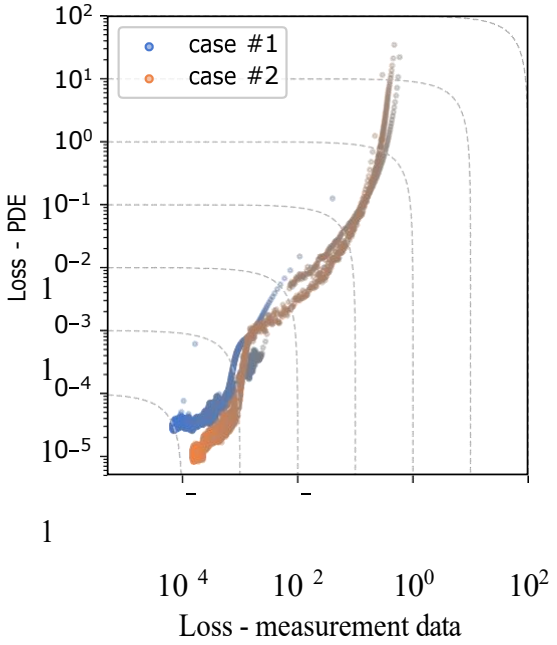

Figure 2: Loss of the PDEs (Navier-Stokes and en- ergy equations) over the loss of the measurement data over a training process of 10^4 epochs for two cases with a varying data loss rate: $\lambda_{data}^{\#1} = 10\lambda_{data}^{\#2}$.

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Federated Learning Under Attack: Threats, Challenges, and Defense Strategies

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Abstract: Federated Learning (FL) has gained significant traction as a decentralized machine learning paradigm that enables collaborative model training across distributed nodes while preserving data privacy. By allowing devices to train local models and aggregate their updates via a central or decentralized coordina- tor, FL mitigates data-sharing risks and is particularly suitable for privacy-sensitive applications, including Internet of Things (IoT) networks, industrial control systems, and critical infrastructure protection [1]. How- ever, its distributed nature also introduces critical security risks, such as adversarial model manipulation, Byzantine attacks, and malicious node infiltration [2]. These vulnerabilities not only degrade model perfor- mance but also raise concerns about the trustworthiness and reliability of FL in real-world deployments. A key challenge in securing FL lies in managing adversarial behaviours and trust issues among participating nodes. While decentralization helps preserve privacy, it also raises concerns about data integrity, model reli- ability, and secure communication [3]. The presence of untrusted or compromised participants can degrade model performance, hinder convergence, and lead to unintended biases in learning outcomes. Additionally, the heterogeneity of data distributions, common in FL environments, complicates security challenges by making it more difficult to detect anomalous behaviours and ensure robust model updates. To address these threats, various defence strategies have been explored, including anomaly detection mechanisms, resilient aggregation techniques, and cryptographic protocols designed to enhance trust and mitigate the impact of malicious actors [4].

One promising avenue for enhancing the security and resilience of FL is the adoption of distributed and trust-enhancing architectures. Decentralized frameworks provide a tamper-resistant approach to managing model updates, enforcing trust among participating nodes, and reducing reliance on a central authority. By leveraging mechanisms such as distributed authentication, consensus protocols, and transparency-enhancing technologies, FL can improve its resistance to unreliable or malicious contributions while maintaining system integrity [5]. Additionally, automated verification processes can help validate model updates dynamically, ensuring robustness without introducing significant overhead. However, these distributed approaches also bring challenges related to computational efficiency, communication overhead, and scalability, particularly in resource-constrained environments such as IoT networks. The need for ongoing advancements in lightweight coordination mechanisms, efficient resource allocation, and optimised storage strategies is essential to ensure seamless and secure FL deployments in diverse environments. [6].

Beyond centralized security measures, distributed defence mechanisms have gained traction as effective strategies for ensuring the integrity and reliability of federated learning environments. Traditional security strategies often rely on centralized monitoring, which can introduce single points of failure, latency issues, and privacy concerns due to the need for data aggregation. In contrast, decentralized security approaches leverage the distributed nature of FL itself, enabling real-time detection and mitigation of potential threats without compromising data confidentiality. These methods often incorporate techniques such as anomaly detection, secure multi-party

computation, and privacy-preserving analytics to identify deviations in model updates and detect malicious behaviours [9].

One notable advancement in this direction is the implementation of distributed intrusion detection mech- anisms that operate collaboratively across participating nodes [7]. These systems analyse patterns in lo- cal model updates to identify inconsistencies, outliers, or adversarial influences that may indicate security breaches. By employing privacy-preserving techniques such as differential privacy and secure aggregation, these frameworks can enhance resilience against poisoning attempts while maintaining compliance with data protection principles. Additionally, novel aggregation techniques and consensus-driven verification mecha- nisms further strengthen the robustness of FL against adversarial perturbations. The effectiveness of these distributed security strategies depends on their adaptability to heterogeneous network environments, the scalability of their detection algorithms, and their ability to operate efficiently in resource-constrained set- tings. Recent approaches in this area focus on optimizing computational overhead, improving detection accuracy in non-IID data distributions, and integrating adaptive threat response mechanisms to enhance the overall security posture of FL deployments [8]. As FL continues to be adopted in critical applications, ensur- ing its resilience against emerging threats through distributed, intelligent, and scalable security architectures remains a key challenge.

This work advocates for a security-first approach to FL by leveraging distributed solutions to protect against external threats and malicious interference. By enhancing FL with decentralized trust mechanisms and anomaly detection techniques, we aim to ensure its robustness in adversarial environments while maintain- ing privacy and efficiency. Furthermore, we explore how FL itself can serve as a tool for network security, enabling collaborative threat detection and mitigation without compromising sensitive data. Our approach underscores the importance of distributed intelligence in securing both the learning process and the underly- ing network infrastructure. By considering a range of real-world scenarios, including IoT, smart homes and industrial settings, this perspective can be adapted to meet diverse requirements. This approach ultimately opens up possibilities for the emergence of more resilient and adaptive security frameworks in large-scale, decentralised environments.

Keywords: Cybersecurity, Federated Learning, Distributed Systems, Threats and Defenses

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Automated IoT vulnerability classification using Deep Learning

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Abstract: Technological advancements in the development of low-power chips have enabled everyday objects to connect to the Internet, giving rise to the concept known as the Internet of Things (IoT). It is currently estimated that there are approximately 16 billion IoT connections worldwide, a figure expected to double by 2030 [1]. However, this rapid growth of the IoT ecosystem has introduced new vulnerabilities that could be exploited by malicious actors. Since many IoT devices handle personal and sensitive information, threats to these devices can have severe consequences [2]. Moreover, a series of cybersecurity incidents could undermine public trust in IoT technology, potentially delaying its widespread adoption across various sectors [3].

Common Vulnerabilities and Exposures records (also known by their acronym as CVEs) [4] is a public cata- loging system designed to identify and list known security vulnerabilities in software and hardware products. This system is developed and maintained by MITRE with the support of the cybersecurity community and sponsored by the U.S. Department of Homeland Security (DHS) through the Cybersecurity and In- frastructure Security Agency (CISA). CVE provides a reference database that enables security researchers, manufacturers, and organizational security managers to more effectively identify and address security issues.

In our study, we have focused on CVEs exclusively oriented towards IoT systems, with the aim of analyzing the main vulnerabilities detected from 2010 to nowadays as a basis for detecting the main attack vectors in IoT systems. As part of this effort we have created the following dataset [5].

CVEs records include various metrics such as:

- Common Weakness Enumeration (CWE) [6], mainly focused on technical classification of vulnerabilities.
- Common Vulnerability Scoring System (CVSS) [7], which reports about different metrics such as the attack vector, the severity of the vulnerability or the impact level of the exploitation of the vulnerability. This is one of the most informative metric.
- Stakeholder-Specific Vulnerability Categorization (SSVC) [8], oriented towards help cybersecurity team to handle properly the vulnerability.

These metrics allow security teams on the one hand to prioritize, such vulnerabilities within their security program, evaluating efforts to mitigate them. But according to our analysis of our dataset, around the 14% of CVEs records do not contain any metric. Around the 83% of CVEs registries contain CWE metric (an ID or its textual description). This metric, as it is explained before, only reports about the type of vulnerability from a technic point of view. Only the 10% of CVEs registries contain SSVC metrics. And CVSS, in its different versions, appears only in the 40% of the studied CVEs registries.

Additionally, most of studied records includes metrics a retrospectively, several weeks or months later the vulnerability is disclosed. Thus, cybersecurity teams must trust their previous knowledge in order to distinguish which vulnerabilities are relevant and which not.

To tackled this situation, our proposal is focused in the application of Deep Learning techniques

in order to classify the severity of CVE records from its textual description. Textual description is a mandatory field that is present in all CVEs records. To achieve this objective, we trained the BiLSTM [9] algorithm using the CVE records with CVSS metrics and its description field; and performed a comparative study of different hyperparameter configurations to find the optimal configuration. The metrics for model evaluation that have been studied are accuracy, loss and F1-score,

Keywords: vulnerabilities, natural language processing, cybersecurity, Internet of Things

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Inferring Temperature Fields in the PIV Measurement Plane from Two-Component Velocity Data using PINNs: Case Rayleigh-B´enard Convection

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Abstract: Recent studies revealed the capabilities of physics-informed neural networks (PINNs) to predict instantaneous temperature fields in turbulent convective flows using three-dimensional (3D) velocity fields [6, 4]. Inferring the temperature in thermally-driven flows is highly relevant in various technical applications that require precise analysis and control of heat transfer, such as the design of interior ventilation systems in aircraft or train cabins, to optimize air circulation and ensure thermal comfort [1]. As 3D velocity mea- surements are still demanding in terms of equipment, we investigate whether relying onto two-dimensional (2D) measurements only is feasible. A classical experimental technique is particle image velocimetry (PIV), which, in its simplest form, provides planar fields of the two in-plane velocity components. While PINNs have already shown great potential for improving the quality of PIV measurements [2], in this study, we challenge the PINN approach to reconstruct temperature fields using only planar two-component velocity data within a cubic Rayleigh-B´enard Convection (RBC) cell.

Leveraging available direct numerical simulation data at Ra = 10^7 and Pr = 0.7 enables the direct validation of the PINN-predicted fields. The PINN loss formulation typically has the following main contributions: a data loss term and loss terms incorporating the residuals of the governing partial differential equations and the boundary conditions [5]. To address the lack of information perpendicular to the PIV plane, we minimise the residuals in an enclosing 3D domain D, as motivated in [3], together with weighted dynamic sampling strategies. The thickness δ_x of D has to be chosen carefully within $0 < \delta_x \leq H$ depending on the characteristic flow length scales. Since only the two in-plane velocity components are available, the PINN has considerable freedom when reconstructing the orientation of the out-of-plane velocity component. Consequently, it is necessary to include additional constraints to account for the global in-plane mass conservation.

Current results of the temperature predictions show encouraging results with a Pearson Correlation Coeffi- cient $\rho_T = 0.92$ (fig. 1 right). As we have only partial knowledge of the 3D velocity field, guiding the PINN towards the global minimum is more difficult. Therefore, a challenge in this work is developing an effective strategy for handling the additional physical constraints.

Our method serves as a foundation for future research focused on inferring temperature fields through in-field measurements in industrial applications. To demonstrate its applicability, we will apply it to real PIV data and compare the results with temperature fields measured via Particle Image

Thermometry (PIT).

Keywords: Physics-informed Neural Networks, Rayleigh-B´enard Convection, PIV

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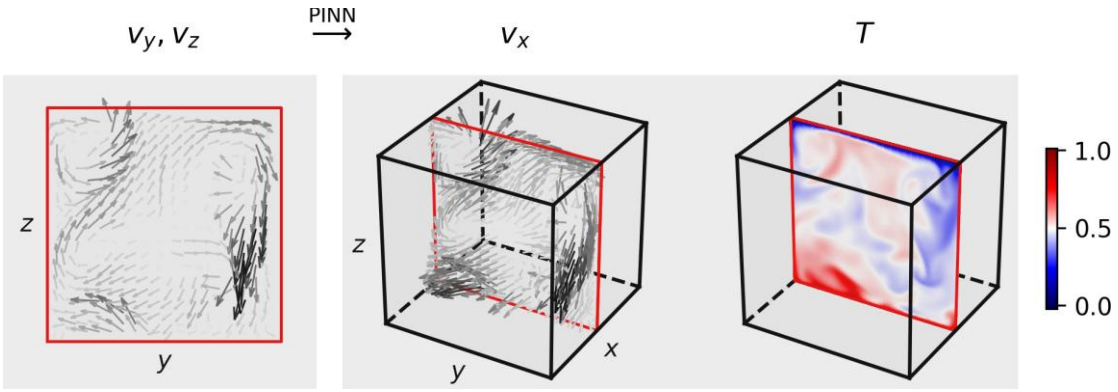

Figure 1: Schematic of a cubic RBC cell with height H for the test case Ra = 10^7 and Pr = 0.7. We train a PINN with the two in-field velocity components on the vertical plane $A : x = 0.5\ H$ (left) and by minimising the residuals of the PDEs within a 3D collocation layer around A to obtain the out-of-plane velocity component (middle) and the temperature field (exemplary result on the right).

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Modelling engineering structures from LiDAR data using Msplit estimation

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Light Detection and Ranging (LiDAR) systems can provide a massive number of measurements of an object of study in a relatively short time. This is why the method has numerous practical applications in civil and environmental engineering, architecture, and surveying. The last decades have brought significant progress in equipment accuracy, mobility, and acquisition speed. One can distinguish three major scanner types: airborne (ALS), terrestrial (TLS) and mobile (MLS). There is no doubt that TLS is the most accurate, and therefore, that technique is often used in civil engineering and surveying. On the other hand, ALS can bring vast information about large areas of study and is quicker to apply than TLS. However, its accuracy is much lower (the same remarks concern also MLS). Regardless of the technique applied, laser scanner observations usually create point clouds, which always require post-processing. Data processing is aimed at modelling the object of study, and it is necessary to obtain more accurate final products.

There is no doubt that the least-squares estimation is the most popular because of the simplicity of computation. The method in question is sufficient for simple objects like engineering structures (retaining walls, buildings, dams, etc.). For more complex constructions (e.g., bridges), the point cloud can be divided into several parts related to the simple surfaces. However, in the case of objects with no regular shapes like terrain, forest, vegetation cover, etc., even such an approach is not sufficient. In the case of such objects, one usually applies more complex methods based on segmentation, filtering or generalization.

Msplit estimation is one of the modern methods that has successfully processed LiDAR data. It is especially useful in processing data from engineering structures; however, it was also applied to determine terrain profiles. Generally speaking, the method is a generalization of M-estimation, which assumes splitting the functional model into at least two competitive ones. During the iterative process, the observations are assigned to either of such models in an automatic and autonomic manner. Such a unique feature makes the method applicable in modelling engineering structures, which is also why Msplit estimation might overperform conventional modelling methods. Another advantage of Msplit estimation is its robustness against outliers. The method in question can withstand a high share of outliers, more than conventional robust methods, for example, belonging to the class of M-estimation.

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The research presents the applications of two basic variants of M_{split} estimation in modelling engineering structures. The building roofs are modelled from ALS data, whereas the building walls and beam deformation are from TLS data. The obtained results prove that M_{split} estimation is an interesting alternative to conventional data processing methods. The test shows that M_{split} estimation can deal with a higher share of outlying observations than robust M-estimation methods.

Keywords: M_{split} estimation, LiDAR data, ALS, TLS, engineering structures

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Adversarial Attacks on Convolutional Neural Networks with General Purpose Optimization Software

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Abstract: It has been known for several years that sophisticated state-of-the-art image classification tools are vulnerable to adversarial attacks. A surprisingly small, carefully chosen, perturbation to an image can cause a change in classification [4, 12]. There is a growing literature on the development of algorithms that create attacks, and those that identify and mitigate against them [2]. The recent International AI Safety Report[1] makes the point that *"Improved understanding of model internals has advanced both adversarial attacks and defences without a clear winner."* There is also recent theoretical evidence that, under reasonable assumptions, it is inevitable that classification tools will be susceptible to attack [10, 11]. Such vulnerabilities have important implications for safety, security, privacy and ethics, and hence for regulation. Indeed, the European Union AI Act requires that *"High-risk AI systems shall be resilient as regards to attempts by unauthorised third parties to alter their use, behaviour, outputs or performance by exploiting the system vulnerabilities."*

Designing an attack algorithm involves a number of choices, including: whether to attack the loss function or the output from the network, how to measure the perturbation size, and what constraints to place on the perturbation. Many customised optimization approaches have been developed; including, for example, the fast gradient sign method [4], DeepFool [8], and projected gradient descent [6].

In this talk, we will discuss the alternative approach of using high-quality, general purpose nonlinear opt- mization software to compute an adversarial perturbation. To do this, we focus on routines from the NAG Numerical Library [9]. The main advantages of this set-up are: (i) the optimal perturbation in any p-norm can be sought, (ii) constraints, such as bounds on pixel sizes, can be specified naturally, (iii) in principle, the full nonlinear constrained optimization problem is tackled (with any required linearisations taking place un- der the hood by the optmization routines). The talk will summarize a range of computational experiments; in summary, we found this approach to be convenient and flexible, and to provide results that were at least comparable with customized attack algorithms.

It is interesting to note that traditional optimization algorithms are not considered feasible for the type of large-scale problems that arise when *training* modern neural networks [3]. However, in the context of *attacking* a trained network, we have found that they can be effective. We also note that for very high resolution images, where the problem dimension is large, it is possible to design effective attacks by focusing on relevant portions of an image [1], thereby reducing dimension.

As an illustration, on the left in Figure 1 we show an image of a digit 4 from the MNIST data set [5] that was correctly classified by a simple convolutional neural network. Regarding the pixels as forming a vector $x \in \mathrm{R}^N$,with $N = 784$ we use Δx to denote a corresponding perturbation. The other two images show the effect of small Euclidean norm perturbations that cause misclassification as a digit 9. The perturbation
found by the NAG routine (centre) has a smaller Euclidean norm than the DeepFool perturbation (right). It is also notable, however, that the NAG perturbation has produced a more "obvious" 4 $\rightarrow$ 9 alteration, even though it has smaller Euclidean norm.

In Figure 2 we show the result of attacks on a Resnet-50 architecture[2] with examples from Imagenet [7] in dimension $N = 512 \times 512 \times 3 = 786432$.

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Keywords: Convolutional Neural Network, Stability, Image Classification

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[1]https://www.gov.uk/government/publications/international-ai-safety-report-2025 [2]https://huggingface.co/microsoft/resnet-50

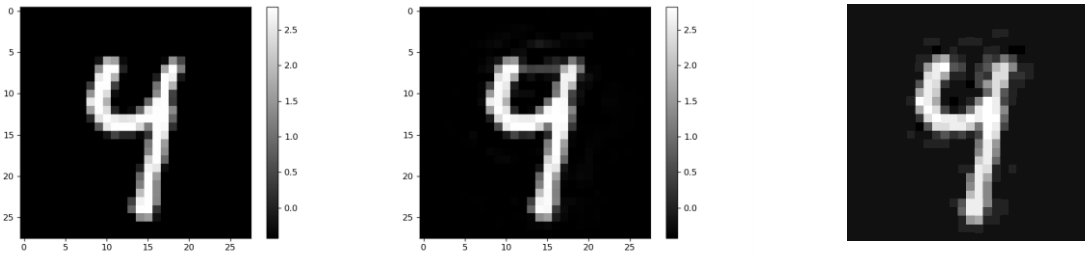

Figure 1: Left: Original image. Middle: 4 → 9 NAG, $/l\Delta x/l^2 = 5.9$. Right: 4 → 9 DeepFool, $/l\Delta x/l^2 = 10.6$.

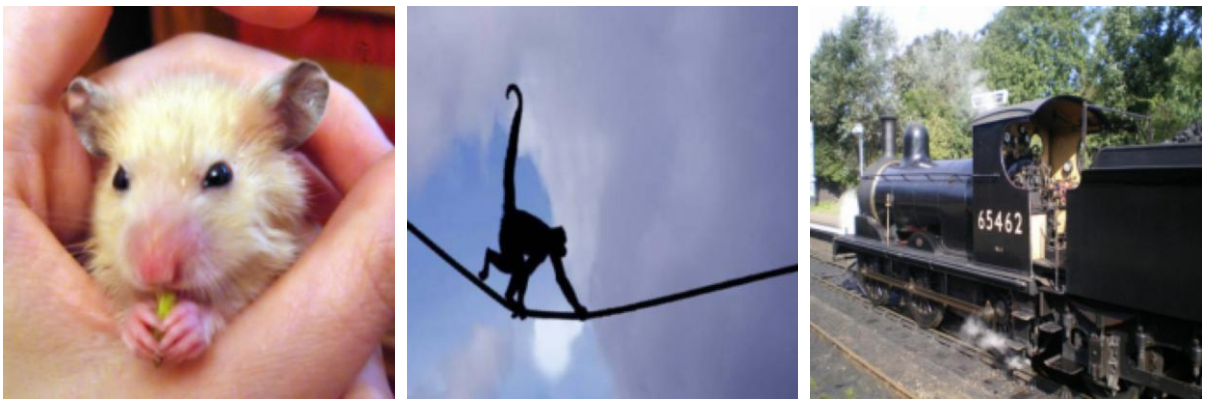

Figure 2: Adversarially perturbed images: hamster → gas pump, spider monkey → water jug, steam locomotive → tobacco shop.

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Inferring Optimal Measurement Sequences

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Abstract:

In many circumstances, data collection incurs a cost. This cost may be in terms of acquisition time, invasion of or damage to the environment and storage. Identifying which, out of a range of data measurements, to collect next is potentially a valuable cost saving activity. Importantly, it also facilitates fast decision making [1]. Data minimisation is also an important consideration for compliance with data protection laws worldwide [1]. In defense situations, the requirement for covert human intelligence means that the act of taking measurements can also pose a security risk [2].

In this work, our overall aim is to identify an optimal measurement sequence from a range of possible measurement sequences. We develop an active sequential inference algorithm that uses a low dimensional data representation to infer its high dimensional state conditional on measurements of that state. Reducing dimension allows for more efficient exploration of the space of state possibilities. The state and types of tasks we are primarily interested in are image/scene reconstruction and related classification tasks using photon based imaging and sensing technology such as a single pixel camera [2, 3]. However, the method is applicable to a broader range of activities.

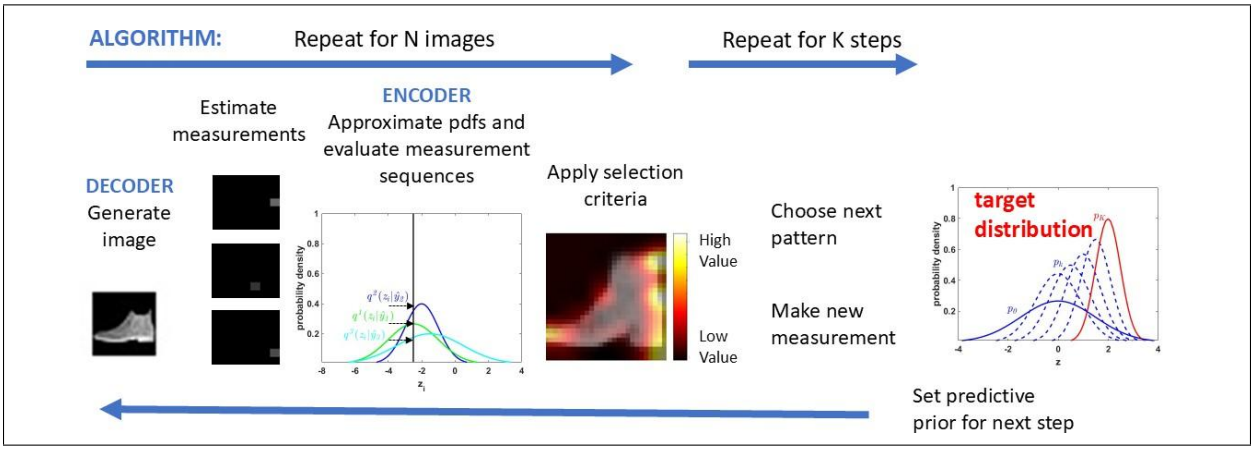

Figure 1: Illustration of the proposed algorithm to select an optimal measurement sequence.

We customise a generative probabilistic model to provide the agent with different reconstruction scenarios conditional on measurement sequences. A variational autoencoder (VAE)[4] is an AI tool which can model the representative space of a high dimensional 2D or 3D scene as a low dimensional latent space. VAEs comprise an encoder (a map from data space to a low dimensional latent representative space) and a decoder (a map from the low dimensional space back to data space). A VAE accomplishes this by employing an encoder network to approximate the genuine posterior distribution with a learned approximation. Samples from the prior on the latent space can be pushed

[3]through the decoder in order to obtain new generated data. Similarly, samples from the posterior can be pushed through the decoder in order to obtain data conditional on the input data. Here we adapt the encoder to map measured data to the latent space. This necessitates creating a training set of measurement sequences. Once trained, the custom encoder and the original decoder are used by the algorithm to sequentially reason about the full state and choose the next measurement. The model we are inferring over is capturing both the (approximate) data-generating process and the noisy measurement model.

Ours is a hybrid approach, in a similar spirit to [5] but novel in our context, as we combine the strengths of VAE and stochastic variational inference SVI [6]. We use the custom encoder to choose between patterns and SVI when a pattern has been selected for inferring the posterior distribution parameters based on actual measurements. The algorithm is developed to actively select the next best measurement. It starts by pushing samples from the prior distribution on the latent space through the decoder to obtain candidate images. Possible measurements on these candidate images are estimated, forming an indexed set. The problem can be thought of as choosing the next measurement index from a set of possible measurement indexes. See Figure 1 for an illustration of the algorithm in action. The custom encoder or SVI is used to characterise the posterior distribution and hence provide a score under that distribution for each possible measurement index for each candidate image. There are different ways to define this score. We consider two approaches. First, we choose the index with the highest average (over the candidate images) likelihood score. Second, we choose the index with the least uncertainty score. The aim is to develop a method that is flexible to the task context and measurement basis.

Starting from no measurements and a normal prior on the latent space, we consider alternative strategies for choosing the next measurement and updating the predictive posterior prior for the next step. The algorithm is illustrated using the Fashion MNIST dataset and a novel convolutional Hadamard pattern measurement basis. We see that useful patterns are chosen within 10 steps, leading to the convergence of the guiding generative images. Compared with using stochastic variational inference to infer the parameters of the posterior distribution for each generated data point individually, the partial VAE framework can efficiently process batches of generated data and obtains superior results with minimal measurements.

Keywords: Bayesian Inference, Active Measurement

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* Presenting author

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β-VAE Extraction of Fault Features from Vibration Signals for Condition Monitoring

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Abstract: Condition monitoring (CM) of rotating machines is crucial, as maintenance practices significantly affect a machine's lifetime, uptime, and downtime. Additionally thanks to the increasing volume of data obtained from monitoring such machines, recent trends in CM have shifted towards automation. Commonly utilized approaches include rule-based methods and more recently methods based on artificial intelligence (AI) [1]. The AI-based methods can be feature based, where the user identifies which features are necessary, which might contain information derived from the sensors, such as the amplitude of certain frequencies. However, this relies on having a good understanding of the underlying system to be able to select sufficient features. On the other hand, data-driven approaches integrate the feature extraction process to the network architecture. Examples of this include deep-learning (DL) models, where you can give raw time-series signals as input, such as convolutional networks or recurrent network architectures.

However, AI-based approaches come with their own challenges. First, operating conditions can differ significantly. For example, ship thrusters experience significant variation in the operating conditions due to ever-changing sea conditions. Changing operating conditions can be mistaken for faulty behavior if the AI model is not specifically trained to differentiate such changes or unless deliberate preprocessing for different conditions, such as RPM, is applied [2]. Secondly, there exists inherent variation between different instances of similar machines, which poses challenges for fleet-level generalization. While some studies demonstrate that DL models can generalize to machines outside the training set, these tests often occur in controlled environments with limited fault types and predefined operating conditions [3]. The results may not fully reflect the complexity of real-world industrial applications, where faults develop gradually under diverse conditions, such as fluctuating loads, environmental factors, and sensor noise.

Furthermore, DL models require significant amounts of labeled fault data to perform well, but industrial data is often imbalanced, with rare but critical faults being underrepresented. This limitation makes it essential to explore methods that improve generalization, such as using transfer learning or combining fault diagnosis with anomaly detection to capture previously unseen conditions.

However, even with hours of vibration data from a specific breakdown instance, it is still usually from the same installation and from a specific component, and after the component is changed, the signal might change, rendering a model trained on the previous data unusable. Thus, identifying a machine breakdown requires monitored breakdown events from all machines in a fleet, which is unrealistic in an industrial setting. This creates a need to isolate fault specific information from a signal with patterns related to noise and operating conditions. A method of normalization applied to the vibration samples in a way, where most of the unnecessary information is left out, has potential to vastly improve the accuracy of intelligent fault diagnosis (IFD) models.

To overcome these challenges, a β-VAE (variational autoencoder) model transformed to work with vibration signals instead of images is employed. This type of approach has been demonstrated to isolate features from images into different sections of the latent space vector [4]. The model architecture is used to isolate the operating speed, operating conditions, installation specific differences and underlying faults to the latent dimensions.

A dataset that includes to-be isolated quantities is utilized, for example the Aalto Gear Fault dataset [5]. The goal is to simplify the CM process by condensing specific information into specific parts of the latent space, which allows the removal of unwanted changes in the input sample. Thus, only fault specific information can be utilized for fault diagnosis. Additionally, the β-VAE is able to produce the same faults over different conditions or machines by informally modifying the latent

representation. With this work, we provided a proof-of-concept model showing the ability of the β-VAE to isolate critical features for CM, and with further work improving on this concept might lead us to a more general CM model capable of fleet-level diagnosis.

The method we propose extracts important fault features that can be used for condition monitoring and discards unnecessary features such as RPM and load (i.e., operating conditions) - in cases where it is desired. In general, this signifies that we propose an intelligent *filter* to the vibration signal, which detects the important information, extracts it and relays it further for the actual inference phase as shown in Figure
1. We see that this preprocessing step improves the accuracy and generalization of deep-learning based IFD algorithms, which has been identified as a critical issue in DL-based CM methods [6].

Keywords: β-VAE, condition monitoring, intelligent fault diagnosis (IDF), deep learning (DL)

* Presenting author

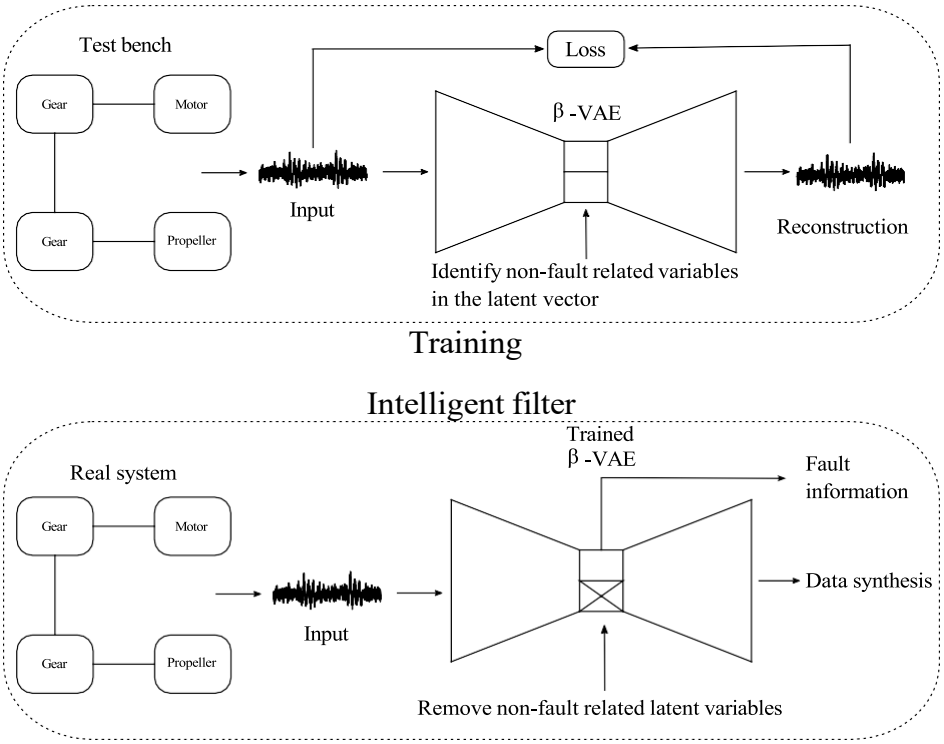

Figure 1: Proposed method: We train a β-VAE model with a test bench with varying installations, operating speeds, loads and faults. Then we identify from the latent space vector, which components are related to which features, and then we test the model with another system, where we set the unnecessary information to a known state, to ease inference on the state of the machine.

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Enhancing Renewable Energy Site Planning through Artificial Intelligence: an Italian Case Study

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Abstract: The global transition toward renewable energy has gained unprecedented momentum in recent years, driven by mounting environmental concerns and an urgent need for sustainable solutions. Leading this transformation, the European Union (EU) revised its Renewable Energy Directive in 2023, raising the EU's binding renewable target for 2030 to a minimum of 42.5%, up from the previous 32% target, with aspirations to reach 45% [1]. This means almost doubling the existing share of renewable energy in Europe. Germany stands as an exemplar among EU member states in this transition. The nation has already achieved its ambitious target of 55% renewable energy usage by 2030 ahead of schedule, as documented in its latest energy report [2]. However, the shift toward renewable energy sources presents considerable challenges regarding reliable power generation estimation and efficient site planning. The inherent variability and intermittency of renewable sources, particularly wind and solar power, introduce significant uncertainties in energy production forecasting, directly impacting grid integration, energy storage planning, and project feasibility assessments.

Addressing these challenges requires precise estimations of key environmental parameters that significantly influence renewable energy production, including wind patterns, solar radiation, temperature, and atmo- spheric pressure. Real historical and current data represent the most reliable foundation for these esti- mations, helping investors and developers avoid significant over- or underestimation of energy production potential that could lead to suboptimal system designs, inaccurate financial projections, and compromised plant performance. For instance, even small variations in measured wind speeds can substantially affect pre- dicted wind turbine output, while imprecise solar irradiance data can significantly impact solar Photovoltaic (PV) production estimates. Moreover, accurate weather data facilitates understanding of seasonal variations and extreme weather events that could impact facility operations, enabling better risk assessment and more reliable long-term planning for renewable energy projects.

However, obtaining site-specific weather parameters poses significant challenges, particularly in remote or developing regions with limited weather monitoring infrastructure. This data scarcity, combined with the high costs of installing and maintaining comprehensive weather stations, often necessitates reliance on Re- gional Climate Models (RCMs). While these models provide reasonable approximations of local weather patterns by downscaling data from larger meteorological datasets and incorporating topographical features and land use characteristics, they introduce additional uncertainty into renewable energy assessments. De- spite offering comprehensive large-scale forecasts, RCMs often struggle with local predictions due to complex terrain features, microclimate effects, and site-specific atmospheric conditions [6].

To overcome these limitations while leveraging the effectiveness of regional climate models, advanced fore- casting systems have emerged as crucial tools in recent decades. Deep Learning (DL), a key branch of Machine Learning (ML), has shown particular promise in renewable energy predictions [3, 4, 5]. Thus, DL techniques have become fundamental in developing sophisticated forecasting models, offering enhanced pre- cision and adaptability for managing complex renewable energy networks. These approaches prove valuable for both future weather parameter predictions and improving historical and current data accuracy, thereby supporting more informed renewable

energy site planning decisions.

In this context, the present work proposes an innovative integration of Artificial Intelligence (AI) to en- hance the accuracy of weather data generated by traditional meteorological models for renewable energy site planning. In detail, the research employs the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5) as a RCM, enhanced by a Recurrent Neural Network (RNN) implementing a hybrid approach. This RNN, previously validated by the authors [7], combines actual weather measurements with MM5 data to achieve more accurate weather parameter estimations. These enhanced weather predictions serve as cru- cial inputs for optimising renewable energy systems, particularly photovoltaic and wind power installations. The study utilises a comprehensive Python-based analytical framework that processes climatic parameters including solar radiation, ambient temperature, wind speed, and direction for precise resource assessment. This framework applies rigorous mathematical equations to estimate renewable power generation potential for a specific location in southern Italy. The methodology provides more reliable estimations to support energy site planning in regions like Italy, which possess substantial renewable energy potential but require accurate assessment tools for optimal development.

Keywords: Renewable Energy, Recurrent Neural Networks, Regional Climate Models, Weather Forecasting, Resource Assessment, Energy Production Estimation

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PINNs for operator equations with stochastic data

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Abstract: Uncertainty quantification (UQ) is paramount in domains ranging from aerospace exploration to electronic design automation. Uncertain data or source term delivers an abstract operator equation with stochastic data of the form:

$$A u(\omega) = f(\omega) \quad \text{P-a.e. } \omega \in \Omega. \tag{1}$$

We aim at computing the statistical moments for $u(\omega)$, as being for any integer $k \geq 1$:

$$M^k[u] := \int_\Omega u(\mathbf{x}_1, \omega) \cdots u(\mathbf{x}_k, \omega) d\mathbb{P},$$

the latter amounting to solving the following tensor operator equation:

$$(A \otimes \cdots \otimes A) M^k[u] = M^k[f]. \tag{2}$$

Tensor operator equations are prone to the infamous curse of dimensionality [1]. To circumvent this limi- tation, it is common in the literature to couple: (i) numerical schemes such as finite or boundary element methods with (ii) sparse tensor approximation [1, 2].

In this work, we apply Physics-Informed Neural Networks (PINNs) [3] to tensor operator equations, referring to them as Tensor PINNs (TPINNs). These novel PINNs inherit the following interesting properties:

- ✓ They scale well with increasing k;
- ✓ They require minimal modifications—specifically, adapting data generation—to existing PINNs code;
- ✓ They allow for the consideration of time-dependent and non-linear problems;
- ✓ They can be extended to ill-posed inverse problems.

Inspired by the framework in [4], we establish a bound for the generalization error of vanilla (V)-TPINNs. This result enhances our understanding of TPINNs and provides a strong theoretical background for their formulation. An example of a V-TPINN is illustrated in Fig. 1, where Σ_θ^k approximates the unknown $M^k[u]$ in (2). We propose two types of architectures, *vanilla* and *multi-output* TPINNs, and analyze their respective advantages and limitations. Extensive numerical experiments are conducted with DeepXDE open-source library [5], including comparison with traditional methods—specifically, finite element methods; demonstrating applicability and performance while opening up promising new research directions. For example, we represent $\mathrm{diag}(\Sigma_\theta^k)$, $k = 2$ for V-TPINNs in Fig. 2, showcasing their robustness and practical relevance.

Keywords: Physics-Informed Neural Networks, Uncertainty Quantification, Tensor Operator Equations.

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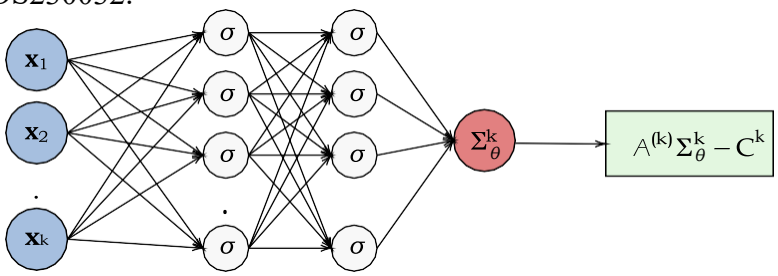

Figure 1: Schematic representation of a V-TPINN. The neural network has 2 hidden layers. The residual corresponds to (2), with $C^k := M^k_\theta[f]$ and Σ^k the approximate.

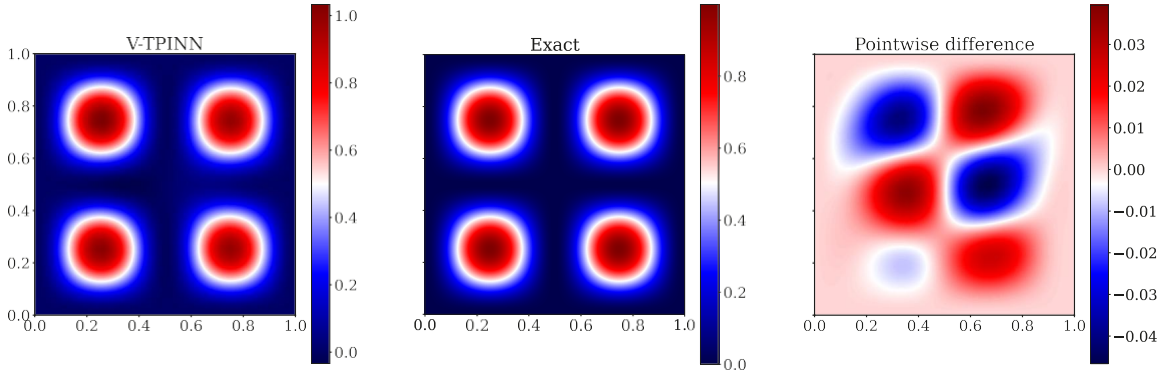

Figure 2: Helmholtz 2D: Solution and pointwise error of V-TPINN for diag(Σ^k_θ) and a separable right-hand side.

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Improving ML Based Lidar Processing Algorithms with High-fidelity Synthetic Data

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Abstract: This study investigates the application of Machine Learning (ML) techniques for automatic, rapid, and accurate processing of wake vortices in lidar (light detecting and ranging) measurements. The research focuses on assessing the effectiveness of using high-fidelity synthetic data to train vortex detection pipelines, addressing the challenges posed by error-prone labeled measurement datasets. The study com- pares the performance of synthetic datasets to real measurements in training ML models for wake vortex characterization. Results indicate that synthetic data can significantly enhance the quality and accuracy of neural networks in this domain. Synthetic datasets prove particularly valuable in augmenting limited or noisy measurement data, leading to more robust and generalizable models. Furthermore, the research demonstrates that synthetic data can be used to fine-tune neural networks for specific scenarios or con- ditions. This capability allows for the customization of ML models to particular atmospheric conditions, aircraft types, or measurement setups, enhancing their performance in targeted applications. In conclusion, the integration of synthetic data with measurement data in training neural networks for wake vortex detec- tion and characterization shows promising results. This approach not only improves the overall quality of the models but also enables their adaptation to various operational contexts, potentially advancing the field of aircraft wake vortex monitoring and safety.

Keywords: Aviation safety, Lidar, wake vortex detection

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* Presenting author

1 Introduction

Wake vortex encounter occur when a follower aircraft flies into a wake vortex produced by a generator aircraft flying ahead. They are most common and dangerous during the final approach and landing phase of an aircraft, as aircraft share similar glide paths and their low altitude does not allow for major piloting maneuvers. Also emerging air vehicles such as air taxis, may experience wake vortex encounters when a vertiport is installed in the vicinity of a runway. Lidar devices are a well suited instrument to detect wake vortices at airports [1], see Fig. 1. Previous studies have shown, that ML offers powerful tool to detect and characterize wake vortices on lidar scans [2, 3], see Fig. 2. The dataset presented in [2] has been generated employing high fidelity hybrid

RANS/LES Simulations.

2 Results

A data processing pipeline, like in [4] employing the Computer Vision tool Yolov4 and a fine tune convolutional neural network (CNN) has been trained with measurements as well

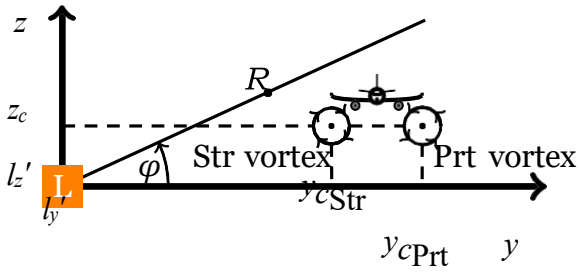

Figure 1: Schematic of the lidar set-up with the starboard (Str) and port (Prt) vortices, where L represents the lidar placed in the LES domain [3].

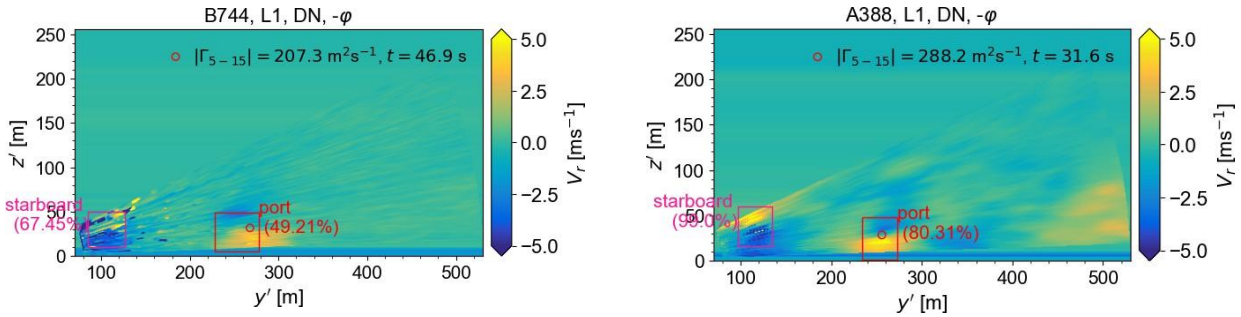

Figure 2: Noisy lidar scans with wake vortex structures. Symbols depict labels, boxes depict results from the ML detection pipeline, trained with synthetic data.

as synthetic data. Figure 2 shows the effectiveness of the NN. While the original labeling algorithm applied to the measurements fails to detect the starboard vortices in the fairly noisy part of the scan, the synthetically trained NN correctly finds the starboard vortex being at the edge of te scan.

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AI-Driven Analysis of FTTH Network Print Overlaps Using Deep Neural Networks and Heuristic Rules

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Abstract:

The deployment and management of Fiber To The Home (FTTH) networks present significant challenges for operators, particularly in resolving fiber address ambiguities and calculating overlaps between FTTH access lines from different providers. This study integrates Deep Neural Network (DNN) techniques with Expert Systems Heuristic Rules to analyze FTTH network print graph databases, enhancing data quality to comply with CNMC (National Commission on Markets and Competition) regulations and optimize fiber deployment and service offerings. Our approach explores Neo4j graph databases as the FTTH network print data source. The goal is to accurately determine diverse FTTH network prints within a given area and identify street addresses where multiple operators provide fiber services with a high degree of confidence.The proposed AI- driven engine comprises two primary components. The first block extracts and categorizes data from Neo4j, employing heuristic functions to compare data from different operators. The similarity between datasets is normalized with a heuristic filter identifying potential address matches. The second block applies a Deep Neural Network (DNN) to analyze these potential matches, determining the probability that data points correspond to the same street address. This innovative AI-driven methodology shifts away from traditional manual query-based analysis, enabling independent data evaluation and resolving inconsistencies in non- homogenized databases. The effectiveness of the DNN model is validated using key performance metrics, including Mean Squared Error (MSE) and Mean Absolute Error (MAE). The results demonstrate that the proposed system accurately delineates FTTH network prints and identifies overlapping access lines at the street level. By streamlining fiber service deployment and enhancing regulatory compliance, this approach offers a significant advancement in FTTH network management.

Keywords: Artificial Intelligence, Fiber To The Home (FTTH), Deep Neural Networks (DNN), Graph Databases, Neo4j, Heuristic Rules, National Commission on Markets and Competition (CNMC).

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Transfer Learning on Frequency-Domain Data of Vehicle Finite-Element-Simulations in Vibroacoustics

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In the early stages of vehicle development, surrogate models and machine learning play an increasingly important role – especially in order to optimize the comfort and noise generation in the interior more efficiently through finite element simulations of the body. A well-known disadvantage of surrogate models based on neural networks is the high demand for time- consuming simulations to provide a sufficient data basis for training, validation, and testing.

In this work, the methodology of transfer learning is investigated based on real vehicle simulations in order to overcome this disadvantage. The transfer learning methodology uses a pre-trained neural network of vehicle A to train a surrogate model for a vehicle B with significantly less data. The data basis consists of frequency-dependent mechanical transfer admittances from vibroacoustic simulations, which characterize the vibration propensity of a structure and describes a typical evaluation parameter in vibroacoustics.

We evaluate this methodology for different vehicles based on the performance of the neural networks. With good performance of the transfer learning step, time-consuming finite element simulations can be saved to train surrogate models for vehicle design. To the best of our knowledge, the investigation of transfer learning on time-consuming, real finite element simulations of different vehicles has not been available in the literature yet. Furthermore, this work is characterized by frequency-domain data.

Keywords: transfer learning, neural network, frequency-domain data, vibroacoustics, vehicle, surrogate model of finite-element simulation, car

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PINN + electric circuit analogy to heat flow: an intuitive off-the-shelf framework for buildings temperature modeling and control

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Abstract: Full-scale and accurate modeling of indoor microclimate can help managing different optimization targets such as reducing the overall energy use and operation cost of a building, while keeping or increasing thermal comfort [1]. However, proper modeling using physical laws and properties requires expert work, and using "off-the-shelf" AI requires months or years of carefully collected and curated data [2]. Moreover, both approaches require expensive computing equipment [2]. Here, we propose a truly off-the-shelf approach, which combines the principles of electric circuit analogy to heat flow [3] and physics-informed neural networks (PINNs) [4].

The electric circuit analogy to heat flow allows for an understandable visual representation of the heat equation — including all the different energy transfer modes — while simplifying the formulation of the differential equations that govern the building to be modeled [3]. Further, PINNs offer the possibility to integrate the governing differential equations of the building into the loss function and test the correctness of the approximated solution using a predefined set of points and the boundary conditions. This allows for fast convergence, especially when approximating non-linear functions [4]. PINNs can also solve the inverse problem (finding the coefficients of a differential equation) and approximate the modeled temperatures simultaneously [4].

In this work, we develop a family of models capable of learning the physical parameters of a building, such as insulation R-values, AC power output, and window area, with high data efficiency. We extend the use of electrical engineering tools by using Bode plots [3] for accurate indoor temperature drop/increase prediction as a function of the weather forecast and current indoor temperature.

Our approach is intuitive and dynamic, offering different possible resolutions, building architectures, and complexities. Another advantage of this method is the possibility of validating model results using circuit simulators such as PySpice [5] or KiCad [6]. Furthermore, a single model can be easily tuned by non-experts by turning on or off the parameters associated with specific physical elements, such as the number of windows and the availability of heat sources or heat sinks, while using comparably small datasets or online training. Using relatively small neural networks, one can enhance a building's capabilities. As an example, we explore the use of a small model to

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predict the time of demand response events, using an easy-to-understand and computationally inexpensive lumped thermal model, allowing for planning and maximizing the economic benefits of demand response participation. Thanks to the data efficiency of PINNs, learning the unique physical properties of the building can be done locally using inexpensive equipment, allowing for fast partial or total deployment.

Keywords: PINN, microclimate control, microclimate modelling, physics-informed neural network, demand response

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A Dynamic Distance Social LSTM for Predicting Pedestrian Trajectories in Crowded Environments

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Abstract: This work introduces dynamic distance Social Long Short-Term Memory, a deep learning approach for pedestrian trajectory prediction in crowded environments. The approach integrates a new dynamic distance-based loss function into Social Long Short-Term Memory, enhancing collision avoidance without compromising displacement accuracy. The method is trained and evaluated on a heterogeneous density dataset and four homogeneous density datasets, covering various crowd-density levels. Experimental results show that the proposed approach outperforms baseline methods in reducing collision rates without decreasing displacement accuracy and, in most cases, even improving it.

Keywords: Deep Learning, Social LSTM, Pedestrian Trajectory Prediction, Collision Avoidance

1 Introduction

Predicting pedestrian trajectories in crowded environments is crucial for engineering ap- plications such as intelligent transportation, robot navigation, urban planning, and event management. While deep learning has advanced trajectory forecasting, many models still struggle to prevent overlaps and collisions in high-density scenarios. A recent deep learning- based method attempted to address this issue [1], but it remains ineffective in high-density crowds, where it forecasts overlapping trajectories. This highlights the need for a model that can prevent collisions without increasing displacement error across varying crowd densities.

2 Proposed Approach

To address the above gap, this study proposes an approach that integrates Social Long Short-Term Memory with a novel dynamic distance-based loss function. The new loss func- tion plays a critical role in enhancing Social Long Short-Term Memory's ability to learn collision avoidance without compromising distance-based performance in real-world crowded scenarios. This loss function (loss = ADE + λ × DDC) combines the Average Displacement Error (ADE) with a Dynamic Distance-based Collision penalty (DDC). The Average Dis- placement Error helps maintain or improve the performance of distance-based metrics, while the Dynamic Distance-based Collision penalty prevents close proximity between individuals to reduce collision occurrences. Here, λ is a predefined weight that controls the influence of the collision penalty on the overall loss function. The Dynamic Distance-based Colli- sion penalty quantifies the total overlap distances between individuals at each time step. It dynamically adjusts a circular personal space around each pedestrian based on their ground-truth future trajectories. The radius of this space is adaptively modified according to the actual crowd density, ensuring that the model penalizes potential collisions while preserving natural movement behavior.

* Presenting author.

3 Preliminary Evaluation and Results

The proposed approach was evaluated against two Social Long Short-Term Memory-based methods: one optimizing distance-based accuracy [2], serving as the baseline, and another integrating Time to Collision alongside distance-based performance [1]. All models were implemented using the TrajNet++ framework [3] with hyperparameters from Ref [1]. The training and evaluation were conducted on five pedestrian trajectory datasets collected from the Festival of Lights in Lyon [1], including a heterogeneous density dataset and four ho- mogeneous density datasets categorized by density based on the classification in Ref [1]. Performance was assessed using Average Displacement Error and Final Displacement Error (FDE) for accuracy, while the prediction Collision Rate metric (CR) [3] measured collision occurrences. As shown in Table 1, the proposed approach reduced collisions in heteroge- neous, high, and very high density datasets while improving distance-based performance. In contrast, Time to Collision-based Social Long Short-Term Memory failed to reduce colli- sions without increasing displacement error. Both models successfully reduced collisions in low density and medium density datasets; however, our approach outperformed the Time to Collision-based model, achieving a 14.6% greater reduction in low density and 8.3% in medium density datasets.

Table 1: erformance comparison across a heterogeneous dataset and four homogeneous datasets (Low Density, Medium Density, High Density, and Very High Density). 'Diff.' represents the difference relative to the baseline model. 'Heterog.' refers to the heterogeneous dataset.

Model	Heterogen. Value	Diff.	Low Density Value	Diff.	Medium Density Value	Diff.	High Density Value	Diff.	Very High Density Value	Diff.
The baseline [2]										
ADE (m)	0.257	–	0.499	–	0.345	–	0.241	–	0.259	–
FDE (m)	0.473	–	0.949	–	0.671	–	0.418	–	0.456	–
CR (%)	39.3	–	40.62	–	29.21	–	33.8	–	51.29	–
Time to Collision [1]										
Optimal λ	0.001	–	0.001	–	0.002	–	0.001	–	0.002	–
ADE (m)	0.288	0.031 ↑	0.469	−0.03 ↓	0.307	−0.038 ↓	0.251	0.01 ↑	0.319	0.06 ↑
FDE (m)	0.532	0.06 ↑	0.904	−0.045 ↓	0.549	−0.122 ↓	0.435	0.017 ↑	0.577	0.121 ↑
CR (%)	26.1	−13.2 ↓	37.5	−3.12 ↓	20.6	−8.61 ↓	19.3	−14.5 ↓	38.7	−12.59 ↓

The proposed approach								
Optimal λ	0.003	–	0.01	–	0.01	–	0.001	–	0.002	–
ADE (m)	0.248	−0.01 ↓0.463		−0.036 ↓ 0.323		−0.022 ↓	0.239	−0.002 ↓	0.238	−0.021 ↓
FDE (m)	0.445	−0.028 ↓0.876		−0.073 ↓ 0.621		−0.05 ↓	0.413	−0.005 ↓	0.42	−0.036 ↓
CR (%)	29.9	−9.4 ↓ 22.9		−17.72 ↓ 12.3		−16.91 ↓	25.5	−8.3 ↓	47.4	−3.89 ↓

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Vulnerability Analysis of Transformer-based Optical Character Recognition to Adversarial Attacks

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Abstract: Recent advances in Optical Character Recognition (OCR) have been propelled by transformer- based architectures that integrate computer vision and natural language processing. In particular, Transformer- based OCR systems (TrOCR) have achieved state-of-the-art accuracy on both printed and handwritten texts by utilizing global attention mechanisms to capture long-range dependencies [5].

It is well known that deep learning techniques are vulnerable to adversarial attacks [8]. In this work, we extend existing adversarial attack methodologies to evaluate the security of TrOCR systems. We focus on two types of attacks: untargeted attacks, which aim to broadly degrade recognition performance as quantified by an increased Character Error Rate (CER), and targeted attacks, in which minimal perturbations force the model to produce a specific token or sentence. We mainly consider handwritten text from the IAM dataset [6].

We adapt classical methods including the Fast Gradient Sign Method (FGSM) [4], DeepFool [7], and the Carlini & Wagner (C&W) attack [2] to address the challenges of token-level adversarial attacks. In the TrOCR pipeline, input images are preprocessed and encoded as sequences of patch representations using a Vision Transformer [3] before a language model decoder generates the final text output [9]. By computing gradients relative to a token-based cross-entropy loss, our approach identifies perturbation directions that significantly impair the recognition process.

Figure 1 presents two adversarial attack scenarios side by side. Subfigure 1a displays a targeted adversarial attack using the C&W algorithm with increasing perturbation levels, while Subfigure 1b shows how a tar- geted attack forces the system to output a specific sentence. These examples emphasize that even minute perturbations—imperceptible to human observers—can significantly alter the OCR output.

Our experimental studies reveal that while TrOCR is highly vulnerable to untargeted attacks—with a CER exceeding 1 under minimal noise—it is slightly less vulnerable to targeted attacks, allowing success ratios around 25%. These findings highlight the critical need for robust defense mechanisms, especially as OCR systems are deployed in security- and compliance-sensitive environments.

Acknowledgements

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Keywords: adversarial attacks, optical character recognition, transformer, robustness

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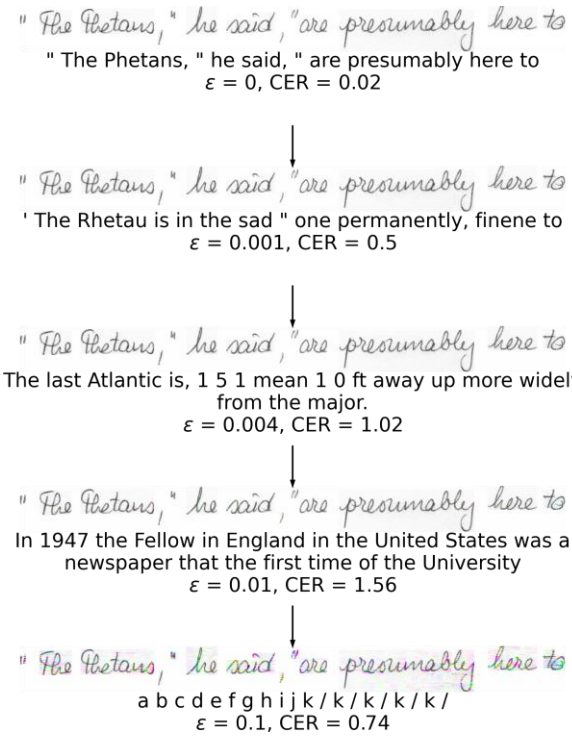
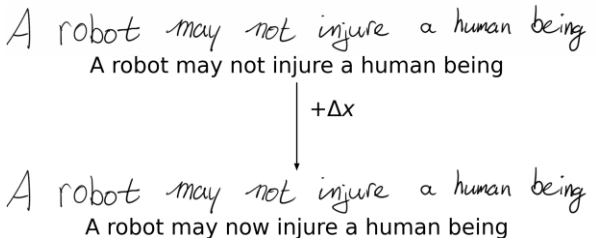


(a) Images perturbed using the C&W algorithm with increasing ϵ values, where ϵ denotes the noise amplitude added to the image. Lower ϵ results in subtle perturbations and low Character Error Rates (CER), indicating high recognition accuracy, while higher ϵ produces noticeable noise and high CER, signifying degraded OCR performance. The target text is: "The Thetans," he said, "are presumably here to.



(b) Targeted adversarial attack on the TrOCR system using an extended Carlini & Wagner method. The top image shows the original handwritten sentence, correctly recognized as "A robot may not injure a human being." After adding an imperceptible perturbation Δx, the system outputs the attacker-specified target "A robot may now injure a human being." This example, inspired by Asimov's first law of robotics [1], demonstrates how minimal noise can force a substantial change in the OCR output.

Figure 1: Adversarial attacks applied to the TrOCR system.

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AI-Driven Data Analytics for solar energy forecasting and CO2 reduction in the Amazon Basin

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Abstract:
The application of Data Science and Artificial Intelligence (AI) has become essential in optimizing solar energy generation, particularly in challenging regions like the Amazon basin[1,2]. This work presents a case leveraging machine learning techniques to enhance solar energy predictions using existing solar power stations in Brazil, satellite and weather data. Building upon Marques et al. (2023), the approach integrates Data Analytics tools and Machine Learning algorithms, such as Random Forest (RF) and Light Gradient Boosting (LGB), for the forecasting of solar electric energy generation, based on time series analysis. First, data from four existing solar power units, in central Brazil, were handled to stablish a technical relation, or 'SE function', between solar incidence and electric power generation. After a technical evaluation, the 'SE function' is used in the region of Manaus/Brazil, to forecast the amount of eletricity that could be generated from solar energy incidence. This application aims to reduce the amont of CO_2 generated by the thermal power units, which burn natural gas, around Manaus. Equally important, the use of solar energy in the Amazon Basin dims the logistic burdens to transport oil fuel to that region. Results show a potential reduction of up to 6% in the energy from the thermal units. This research highlights the potential of AI-driven data analytics to address the variability of solar resources in the Amazon basin and supports sustainable energy development through proven engineering solutions.

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[2] Neural Networks Forecast Models Comparison for the Solar Energy Generation in Amazon Basin https://doi.org/10.1109/access.2024.3358339 .

Keywords: Solar Energy, Data Science, Artificial Intelligence, Renewable Energy, Machine Learning, Time Series Forecasting

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A Physics Informed Diffusion Model with Data from a CFD Model

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Training and testing physics informed diffusion models (PIDM) require as the baseline generated data by computational fluid dynamics (CFD) models. Fundamentally, data from CFD will serve to prove capabilities of PIDM related to learning the complexity of fluid dynamics derived from nonlinear partial differential equations (i.e. Navier-Stokes). Also, to provide pre- trained PIDM according to expected needs from the field. Here we present a study showing the path from a set of numerical results of a CFD model, which was used as input data to a PIDM. This set of numerical results was achieved under turbulence conditions following unsteady state Reynolds-averaged Navier-Stokes (RANS) equations for a domain including walls. The pipeline covered the following steps: 1. Conversion of each numerical result to an image, 2. Development of a PIDM and its training, and 3. Testing the PIDM for prediction.

Conversion of each numerical result from CFD models of the velocity field was accomplished by spatially restructuring its resolution into spatially uniform data by means of images. Afterwards, those images were used to train a diffusion model (DM). In addition, a physics informed condition was proposed in function of the velocity changes over time together with distance to walls within the domain, which served to process additional information meanwhile residuals generated a set of images which were processed by a PIDM. Test of DM and PIDM were conducted by comparing its results against CFD data as ground truth. Also, it was explored how much a PIDM can be useful for predictions as well as the zones within the domain where error prevailed.

For this study, training stage of DM and PIDM implied the use of 1008 images whereas testing was covered with 144 images. In specific, 69 images out of 144 were chosen for assessing performance of DM and PIDM at reproducing the velocity field. It was found that that physics informed condition incorporated in our PIDM aided to have better performance than DM at generation of images. Furthermore, generated images analysis allowed us to identify zones close to walls that had significant error with respect to the rest of the domain for DM and PIDM, however, PIDM was able to mitigate it. With these findings, we claim that PIDM under limited training can become a viable choice to represent fluid dynamics. Additionally, our methodology can be used to pre-train PIDM from CFD data which can later be deployed to continue its calibration with experimental data and its potential use for monitoring, prediction and control.

Keywords: artificial intelligence, CFD, diffusion, generative data, RANS models, turbulence

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Predicting Cancer Immunotherapy Outcomes Using Machine Learning: A Combined Analysis of Mechanistic and Clinical Metrics

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Immune checkpoint inhibitors (ICIs) have transformed cancer treatment, offering significant benefits to some patients while showing limited efficacy in others. Even within the same individual, different tumor lesions may react differently. It is essential to identify which lesions are responding or not early on to optimize treatment decisions. A reliable predictive model could help clinicians decide whether to continue ICI therapy, make modifications, or introduce other treatments for lesions that are not responding.

In this paper, we present a novel approach that combines a mechanistic tumor modeling framework with machine learning (ML) techniques to evaluate and predict lesion-specific responses to ICIs. A previously developed and validated mechanistic model has demonstrated its ability to predict cancer immunotherapy outcomes by tracking tumor volume changes over time following ICI initiation [1-3]. Through model analysis, we identified several key mechanistic parameters that distinguish between responders and non-responders, including μ (the T-cell-mediated tumor kill rate), Λ (the anti-tumor immune state), and $\alpha 1$ (the tumor growth rate after initial restaging).

We first applied this mechanistic model retrospectively to CT imaging data of 165 tumors from 93 patients undergoing ICI therapy. Next, we trained an XGBoost ML model using these mechanistic parameters along with clinical features such as neutrophil count, neutrophil- to-lymphocyte ratio, age, and race. The dataset was divided into training (n = 99), testing (n = 33), and validation (n = 33) groups, and then standardized for ML analysis. To assess predictive accuracy, we evaluated the ML model under three different conditions: (1) full time-course data, (2) data limited to the first two follow-ups, and (3) data only available at the first restaging, excluding the immune-mediated tumor killing parameters μ and Λ. To further interpret model predictions, SHAP (SHapley Additive exPlanations) analysis and permutation-based ranking were used to identify the most significant features for predicting treatment responses.

Our findings revealed significant differences in model parameters

between lesions classified as responders (with smaller final tumor volumes) and non-responders (with larger volumes) (Figure 1; $p < 0.01$). Notably, the ML model achieved 82% accuracy with full time- course data, 82% accuracy with two follow-ups (but with slightly reduced sensitivity), and 76% accuracy with first restaging data. Although accuracy decreased with earlier predictions, these results demonstrate the feasibility of using this model in clinical settings during the critical window shortly after treatment starts. SHAP analysis identified Λ (anti-tumor immune state) and $\alpha 1$ (growth rate at first restaging) as key predictive features. Notably, the model displayed consistently higher specificity compared to sensitivity, showcasing its strength in detecting non-responding lesions. This capability may allow oncologists to adapt ineffective ICI treatments sooner (e.g., by introducing targeted therapy for non-responsive lesions), enabling a shift to alternative therapeutic strategies. Ultimately, this could enhance patient outcomes while minimizing their exposure to unhelpful treatments.

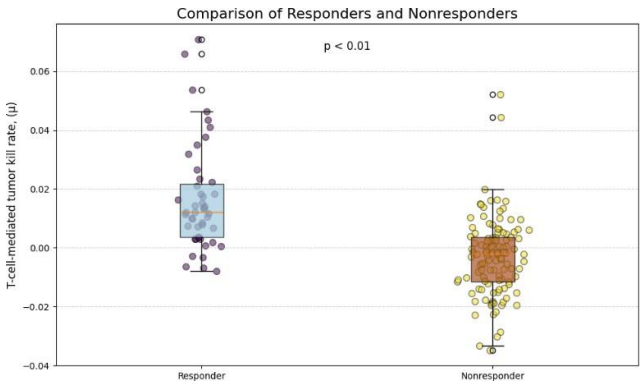

Figure 1: Comparing distribution of mechanistic model results for μ of responders ($n = 47$) and non- responders ($n = 118$) using Mann-Whitney U test.

In conclusion, our study underscores the potential of hybrid mechanistic-ML modeling in predicting lesion-specific responses to ICIs. Importantly, this model relies solely on standard imaging and blood markers, making it straightforward to implement in clinical practice. By facilitating early identification of non-responders, our approach aims to support timely treatment adjustments and enhance personalized cancer care.

Keywords: Cancer immunotherapy, engineering medicine, mathematical modeling, translational medicine, tumor-immune interaction

Acknowledgements

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Extending Graph Deviation Network for More Effective Anomaly Detection

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Graph Deviation Network (GDN) is a representative GNN-based model for anomaly detection that learns graph structures from sensor data, allowing it to more effectively capture complex dependencies between sensors compared to traditional deep learning models. However, GDN relies on limited statistical measures such as the median and interquartile range (IQR), primarily focusing on detecting point anomalies at individual time steps. As a result, it struggles to effectively identify contextual anomalies and collective anomalies.

To overcome these limitations, this study proposes an advanced anomaly detection method that leverages various statistical characteristics of residuals, including the mean, standard deviation, skewness, kurtosis, and quantiles. The proposed approach maintains GDN's graph structure learning framework while incorporating additional distribution-based features to enhance anomaly detection performance.

This study introduces an anomaly detection methodology that extends beyond simple magnitude-based detection in graph-based models, incorporating both distributional context and multivariate context to improve anomaly identification.

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Keywords: Anomaly Detection, Graph Deviation Network, Distribution-based Features

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Size-Aware SIoU: Enhancing Bounding Box Regression for Small Object Detection

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The performance of object detection models heavily depends on the design of bounding box regression loss functions. While existing IoU loss variants, such as CIoU and DIoU, improved bounding box prediction by incorporating center distance and aspect ratio differences, they showed limitations in small object detection due to not considering the relative importance of object size.

Recent SIoU enhanced localization performance by introducing angle cost, but still faces performance degradation in small object detection. This is because existing loss functions calculate the same loss values regardless of object size and shape, failing to properly reflect the relative importance of small objects.

To address this issue, we propose Enhanced SIoU for Small Object Detection, a new IoU loss function that combines relative distance cost and size weighting with the SIoU loss function. Experiments on YOLOv8 demonstrate that our proposed loss function improves both mAP@0.5 and F1 scores compared to existing methods. This study presents a practical solution for enhancing small object detection performance by presenting an effective loss function that considers object size and relative distance.

Acknowledgments: This work was supported by Institute of Information & communications Technology Planning & Evaluation (IITP) grant funded by the Korea government(MSIT) No.RS-2021-II212068, Artificial Intelligence Innovation Hub) and funded by the Korea government(MSIT) (2022-0-00215).

Keywords: Computer Vision, Object Detection, YOLO, Intersection over Union, Loss Function

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Leveraging Neural ODEs and Graph Network Simulators for Improved Particle-Based Simulations

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Abstract:

Simulation of fluids is a widespread task in many application domains. For example, it is used in wave modeling, vehicle wading through water, spray painting or air flow around plane foils, just to name a few. There are two primary methods to simulate fluids: the Eulerian approach and the Lagrangian approach. The Eulerian approach discretizes the domain into a finite number of cells and computes the fluid properties for these cells. Computational Fluid Dynamic (CFD) simulators utilize this method to simulate fluids and achieve high precision; however, the computation time increases with the number of mesh cells. To simulate microscopic effects such as spray or droplets, the discretization of the mesh must be fine enough to capture these phenomena, which leads to extensive computational cost. An alternative that excels in these scenarios are Lagrangian-based simulators. In this case, the fluid is represented as particles that move freely through the simulation domain. The most prominent particle-based method is called Smooth Particle Hydrodynamics (SPH) [1]. Unlike traditional mesh-based fluid simulations, the Lagrangian nature of this approach reduces the discretization cost as only the fluid not the underlying grid must be sufficiently fine resolved. This allows SPH to represent small fluid structures, such as splashes or fluid surfaces, more efficiently. Particles within a certain distance influence each other through the governing Navier-Stokes equations, with the influence being weighted by the distance between particles. To capture all relevant effects, a sufficiently fine discretization is necessary, making the method computationally expensive and infeasible to compute in real time, especially large systems where numerous individual droplets are present, like in spray painting processes. In order to reduce simulation time and computational cost while maintaining the precision of scientific simulation methods such as SPH, artificial neural networks (ANNs) are incorporated into first- principle and scientific computing models. This approach is part of the field of Scientific Machine Learning (SciML), where scientific data sets and knowledge of the underlying physical principles are combined with data-driven Machine Learning (ML).

We propose to leverage the experience of decades on solving Ordinary Differential Equations (ODEs) for applications in more complex simulation scenarios. The idea is to formulate the Graph Network Simulators (GNS) approach [3] as a Neural Ordinary Differential Equations (NeuralODE) [4]. Although GNS are structurally NeuralODEs, they have not been considered as such in related work, and developments in this direction have, therefore, been ignored thus far. The use of more sophisticated numerical solvers allows us to use adaptive time stepping or stiff solvers. Additionally, we can swap out the solver based on the requirements of the system results. While a simple solver produces an output more quickly, a more complex solver can improve the accuracy of the solution of the same system without starting over the training process. Sanchez- Gonzales et al. [3] propose GNS, a method for particle-based fluid simulation that calculates the behavior of fluids based on moving particles. As our work is based on this method, it is described in more detail. In this approach, a graph is constructed with the particles as its nodes. Edges are then inserted between directly neighboring particles within a predefined radius that influence each other (similar to standard SPH approaches). Particles represent either fluid or solid, allowing fluid-solid interaction to be inherently learned. The architecture of GNS consists of three multi-layer perceptron networks: ENCODE, PROCESS, and DECODE. First, the states of the particles and

information of the edges, which contain i.e. the distance between the particles, are encoded into a high dimensional representation through the ENCODE network. Second, the particles exchange information with their neighbors a predefined number of times through the PROCESS network. Finally, the DECODE network recovers the state derivative from the high dimensional representation. A differential equation solver calculates the new system state from the state derivative. This procedure is repeated iteratively over time. One of the key features of GNS is that the model is trained locally on the interaction between particles instead of a global representation. This makes it possible to use a simpler scenario for the training and extrapolate the learned physics to more complex simulations as shown in [3]. The model does not require training on data from these complex scenarios. In the original method and implementation [3] the usage of the model is limited, as it is (a) trained with a fixed time difference between data points in the training data leading to sub-optimal generalization capabilities (see [5]), (b) limited to a simple forward Euler ODE solver, which possesses only first-order accuracy and therefore limits the applicability to highly dynamic simulation scenarios and (c) a mixture of model equations and solving process hindering the use of the full power of ODE solver theory and software. We eliminate these limitations with our method.

To evaluate our method, we use, among others, a 3D dataset provided by [2]. Each trajectory in this dataset consists of up to three randomly placed fluid bodies within one of ten different containers. The shape of the fluid body is selected from the following list: cube, cone, ball, cylinder and torus. The size and orientation as well as the initial velocity of the fluid bodies are varied. The only external force is gravity and the simulation time of one trajectory is 16 s with a sampling rate of 0,02 s. There are 200 train and 20 test trajectories within the dataset. A comparable dataset is used in [3], so our results will be compared against GNS [3] and Deep Momentum Conserving Fluids [2]. The data was generated with the divergence-free SPH (DFSPH) method inside the tool SPliHSPlasH. Despite no hyperparameter tuning and code optimization, our preliminary results indicate that we reach at least same interference times as [3] (see Figure 1).

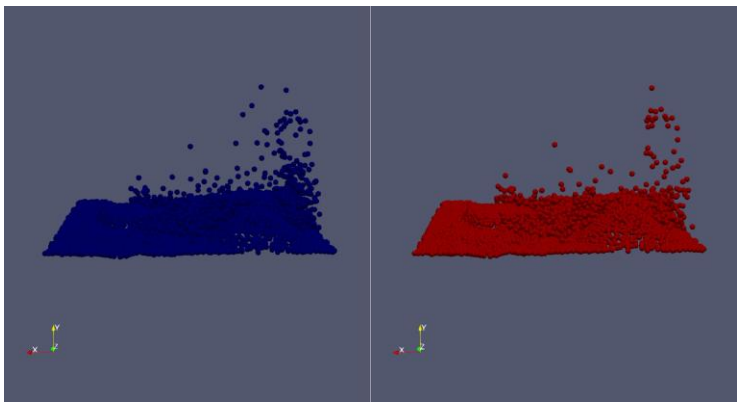

Figure 1: Preliminary results - left: ground truth - right: our result.

Keywords: NeuralODE, Scientific Machine Learning, Graph Network Simulators

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Comparing Methods for Automated Generation of System Models in SysML v2

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In recent decades, the development of automobiles has become increasingly complex, due to the integration of software and electronics in modern products and growing customer demands for functionality. Simultaneously, stricter regulations for demonstrating functional safety further complicate product development. As a result, engineers face challenges in managing the rising number of interdependencies between systems and ensuring compliance with evolving safety regulations.

To address the increasing complexity, establishing digital models of the system following the idea of model-based systems engineering (MBSE) during product development has emerged as a key strategy. These models help in representing the interdependencies between the systems, identify errors earlier in the development process, and serve as documentation for functional safety compliance. However, the creation of such models demands expertise and significant time investment, even for experienced professionals. Parts of the information needed for building such models can be found in product specification documents. This information is typically embedded in documents in textual, natural language representations and therefore unstructured and difficult to process efficiently.

Traditional, manual methods for extracting and structuring this information for modeling are time-consuming and prone to inconsistencies, increasing the risk of errors and inefficiencies. Recent advancements in artificial intelligence, particularly large language models, and the introduction of the code-based systems modeling language SysML v2 offer new opportunities for automating the modeling process. Improved access to data within natural language requirement specifications enables more systematic extraction and structuring of information. Building on this, the automation of system model generation may become possible, which represents a major step forward. This shift has the potential to significantly reduce manual modeling efforts, thereby lowering the barrier to adopt system models in product development processes. For model generation from text, different approaches have been proposed in literature, yet a direct comparison between approaches, specifically for SysML v2 model generation has not been carried out.

In this paper, two approaches for model generation are implemented and compared to address the challenge of bridging the gap between textual requirement specifications and SysML v2 code. These approaches aim to facilitate an automatable and seamless transformation of natural language descriptions into structured, code-based SysML v2

models, thereby enhancing the efficiency and accuracy of the modeling process. The comparison includes key aspects to differentiate the approaches, such as data security, flexibility, accuracy, and required computing power. By systematically analyzing these factors, this paper evaluates both conceptual frameworks and practical implementations, providing a comprehensive overview of possible solutions and their trade-offs. The evaluation will be carried out using the example of an electric window opener system with anonymized data from an automotive manufacturer.

Keywords: Model-based Systems Engineering, SysML v2, Code Generation, Requirements, LLM, Engineering, Mechanical Engineering

Machine Learning for Fatigue Life Prediction of Additively Manufactured 316L Stainless Steel

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Additive manufacturing (AM), commonly known as 3D printing, has transformed the landscape of industrial production, enabling the creation of intricate geometries that are unattainable via conventional manufacturing methods. Among the materials used in AM, 316L stainless steel (316L SS) has emerged as a cornerstone, celebrated for its exceptional corrosion resistance, high-temperature strength, and mechanical versatility. This material finds application in critical sectors such as aerospace, automotive, and biomedical industries, where components are often subjected to cyclic loading conditions, making fatigue life a critical consideration. Despite its advantages, assessing the fatigue behavior of 316L SS is complex and resource-intensive, particularly when fabricated through different AM techniques that introduce unique microstructural characteristics. Addressing these challenges, this study explores the integration of machine learning (ML) into fatigue life prediction, presenting a data- driven alternative to traditional experimental approaches.

The study begins with a comprehensive bibliometric analysis to uncover research trends, collaborations, and key contributions in the domain of ML applications to fatigue analysis in AM materials. This analysis reveals a burgeoning interest in leveraging ML for predictive modeling in material science, driven by the need to optimize AM processes and reduce dependence on extensive physical testing. The subsequent literature review delves into the nuances of AM techniques for 316L SS, highlighting the impact of manufacturing parameters, such as build orientation, surface finishing, and heat treatments, on mechanical properties and fatigue behavior. Building on this foundation, a dataset of 274 data points was compiled from diverse literature sources, encompassing 29 distinct conditions with varying mechanical properties and fatigue parameters.

Four state-of-the-art ML models, including Random Forest (RF), Extreme Gradient Boosting (XGB), Support Vector Regression (SVR), and Multilayer Perceptron (MLP), were developed and rigorously evaluated. The models were trained using features categorized into mechanical properties (e.g., Young's modulus, yield strength, ultimate tensile strength, elongation) and fatigue conditions (e.g., frequency,

minimum stress, maximum stress). Comprehensive preprocessing techniques, including normalization and logarithmic transformation, were employed to enhance predictive accuracy. Among the models, the MLP demonstrated superior performance with the highest R-squared value (0.877) and the lowest root mean squared error (0.4944), affirming its robustness in capturing the complex relationships between input features and fatigue life.

To provide interpretability, the Shapley Additive exPlanations (SHAP) framework was utilized to identify key factors influencing fatigue life predictions. Maximum stress (σ_{max}) emerged as the most impactful feature, exhibiting a linear inverse relationship with fatigue life.

Other significant contributors included elongation and minimum stress (σ_{min}), which showed nonlinear influences. Partial dependence plots (PDPs) were employed to visually interpret these relationships, offering insights into feature interactions and their effects on predictions. These

findings underscore the potential of ML in unraveling the intricate dependencies governing fatigue behavior, enabling more informed decision-making in material and process design.

The integration of ML into fatigue life prediction of AM-fabricated 316L SS components offers transformative implications for industrial applications. By reducing reliance on exhaustive experimental campaigns, this approach accelerates the development of robust, optimized designs, paving the way for enhanced durability and reliability in critical applications. This study not only demonstrates the feasibility of data-driven fatigue life prediction but also highlights the broader applicability of ML techniques to other alloys and manufacturing contexts. Future research directions include expanding the dataset to incorporate real-time monitoring data and exploring the generalization of ML models across diverse materials and AM processes. In doing so, this work bridges the gap between advanced manufacturing technologies and artificial intelligence, fostering a synergistic relationship that drives innovation in material science.

Keywords: Fatigue, Additive manufacturing, 316L stainless steel, Machine learning,

Decoding Biofilm Complexity: Evaluating General vs. Specialized Deep Learning Models for 3D Cell Segmentation

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Biofilms are complex microbial communities with critical implications in healthcare, environmental science, and biotechnology. Quantitative analysis at the cellular level of biofilms is essential for understanding their structure and behavior, but segmentation remains a challenge due to imaging variability and biofilm heterogeneity. Deep learning has shown promise in addressing these challenges, yet it is unclear whether general-purpose models or task-specific architectures perform better in biofilm segmentation.

This study evaluates two categories of deep learning models for 3D biofilm cell segmentation: (i) foundational models, like segment-anything models, designed for broad applicability, and (ii) specialized biofilm segmentation models trained for bacterial cell detection. The analysis uses early-stage Pseudomonas aeruginosa biofilms and evaluates segmentation accuracy through various metrics against reference datasets.

Our findings reveal distinct trade-offs between generalizability and task-specific accuracy. While all methods leverage deep learning, architectural differences significantly influence segmentation performance. The results indicate that while the models show promise, they still struggle with robust segmentation across diverse biofilm conditions. We suggest that hybrid methodologies, integrating foundational models' strengths with task-specific refinements, may improve segmentation reliability and versatility.

By comparing these model categories, we provide valuable insights into the optimal strategies for biofilm cell segmentation, contributing to the development of more reliable tools for biofilm research with applications in infection control, environmental monitoring, and biotechnology.

Keywords: Biofilms, Cell Segmentation, Deep Learning, 3D Confocal Images, Quantitative Analysis

The development of a model of artificial neural network to predict the stability of homogeneous and dry slopes: a comparation with the limite equilibrium, stability charts and stability equations

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Climate changes and the lack of control over human occupation in risk-prone areas increases the occurrence of natural disasters, endangering lives, property and urban infrastructure. In this context, the movement of masses exhibit many uncertainties due to their complex behavior and high heterogeneity. Many techniques have been developed to help determine the stability of slopes, however more precise and efficient alternatives are still needed. Artificial intelligence has advanced significantly in various applications, making it essential to explore the technique in the field of slope stability analysis. This study aims to develop an artificial neural network model to predict the safety factor of homogeneous, dry slopes. The neural network was trained using 455 samples generated in the Slope/W software, using the Morgenstern-Price method. Different arrangements of the architecture were tested in order to find the model with the best results. The final architecture consisted of a structure with four hidden layers, a total of 95 hidden neurons and ReLU activation functions, adopting the Adam optimizer. Excellent results were obtained, with a correlation coefficient (r) of 0.999, a mean absolute error (MAE) of 0.0258 and a mean squared error (MSE) of 0.0014. In the comparison with the consolidated limit equilibrium methods and stability equations, the model presented satisfactory results. However, discrepancies arose in comparisons with stability charts, suggesting that the model was not able to generalize adequately to data outside the training range. Despite this limitation, the artificial neural networks showed significant learning capacity, achieving predictions very close to those obtained by consolidated methods. This study highlights the potential for improving the model by incorporating more advanced artificial neural network techniques, along with the inclusion of more complex slopes condition and an extended training data range.

Keywords: artificial neural networks; artificial intelligence; slope stability; safety factor.

Interpretable Data-Driven Models for Predicting Cylinder Flow Noise Using Explainable Artificial Intelligence (XAI)

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Accurately predicting aerodynamic noise generated by flow over cylindrical structures presents a significant challenge in fluid dynamics, especially in engineering applications within the automotive and aerospace industries. Traditional Computational Fluid Dynamics (CFD) methods, such as Direct Numerical Simulation (DNS), offer high-fidelity predictions but demand extensive computational resources and time. This research investigates the potential of Machine Learning (ML) techniques as an alternative to conventional CFD methods for predicting aerodynamic noise, focusing on pressure fluctuations in incompressible flow over a cylinder.

Flow-induced noise prediction is crucial for optimizing structural designs for noise reduction and enhancing aerodynamic performance. However, the high computational cost of DNS limits its practical application, creating a demand for efficient, data-driven predictive models. ML-based approaches provide the advantage of learning complex relationships from data, allowing for fast and reliable predictions. While ML has been utilized in various engineering fields, its application in aerodynamic noise prediction remains underexplored. This study intends to fill this gap by developing an ML model capable of accurately forecasting pressure fluctuations in-cylinder flow, thus offering a computationally efficient alternative to DNS.

A dataset was generated using DNS simulations of flow over a circular cylinder at varied Reynolds number and Mach number values. The dataset consists of 150 time series snapshots of pressure fluctuations, with 100 snapshots designated for model training and 50 for testing. The ML model employs linear regression to predict instantaneous fluctuating pressure values. The governing equations for compressible flow—mass conservation, momentum conservation, and energy conservation—were implemented using an in-house computational solver, HiPSTAR. A high-resolution numerical approach, incorporating a fourth-order compact finite- difference scheme and Runge-Kutta time integration, was utilized for DNS simulations. Model performance was assessed using Mean Squared Error (MSE) as the cost function, optimized through gradient descent.

The trained ML model significantly reduced cost function values over training epochs, demonstrating effective learning and optimization. Comparisons between predicted and actual fluctuating pressure values showed high accuracy, with minimal

deviations observed in contour plots and directivity patterns. While the ML model captured radial pressure variations effectively, slight discrepancies appeared in the azimuthal direction, indicating the influence of acoustic disturbances. Root Mean Square (RMS) pressure analysis further validated the model's predictive capability, revealing close agreement between predicted and actual values.

To gain deeper insights into the influence of input features on pressure fluctuations, Explainable Artificial Intelligence (XAI) is employed. SHapley Additive exPlanations (SHAP), a game-theoretic framework, is utilized to interpret the ML model at both local and global levels, identifying the contribution of each input parameter to the predicted pressure fluctuations. Additionally, Partial Dependence Plots (PDP), a model-agnostic XAI technique, provides a graphical representation of how variations in selected features impact the model's predictions. This visualization helps determine whether the relationship between features and pressure fluctuations is linear, monotonic, or more complex.

By integrating XAI techniques, this study improves the interpretability of ML predictions, connects data-driven models with fluid dynamic insights, and understands the impact of key aerodynamic parameters on flow-induced noise, which aids in creating more efficient and optimized structural designs. This strategy not only lessens the dependency on computationally intensive DNS simulations but also speeds up the design process by allowing for data-efficient predictive modeling.

This study's results contribute to the advancement of ML-based aerodynamic noise prediction. They demonstrate the potential of data-driven methods to capture pressure fluctuations accurately. Integrating ML and XAI in this context provides engineers with valuable tools for optimizing aerodynamic performance and strategies for noise reduction in applications such as automotive and aerospace design.

Keywords: Aerodynamic noise, Cylinder flow, Machine Learning, Compressible Flow, Reduced Order Model

Watchapon Rojanaratanangkule
Presenting Author

Decentralizing Predictive Healthcare: Evaluating Federated Learning for Cost Estimation in Acute Myocardial Infarction

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Background:
Multicentric studies are essential for developing robust predictive models in healthcare, yet privacy concerns, data heterogeneity, and heteroskedasticity often constrain them. Federated Learning (FL) provides a decentralized framework for collaborative model training, ensuring data privacy while handling institutional variability. Containerization technologies like Docker have emerged as state-of-the-art solutions for scalable and reproducible FL implementations, optimizing communication efficiency and deployment across distributed environments.

Aim:
This study evaluates FL's ability to preserve privacy, manage variability, and achieve stable convergence while predicting the cost of care for acute myocardial infarction (AMI) patients, comparing its performance to traditional centralized approaches.

Methods and Results:
The COSTAMI dataset on AMI care was partitioned into 9 clients by centre to simulate decentralized institutional data in a federated learning environment. In the initial phase a Generalized Linear Model (GLM) was first trained in a traditional centralized manner to establish a baseline for comparison. In the FL approach, each centre functioned as an independent client, training locally while a central server aggregated model updates using the Federated Averaging (FedAvg) algorithm. The Flower framework was employed for model transposition within a client-server architecture using Python. To optimize performance, multiple configurations of communication rounds, local epochs, and batch sizes were tested. Model convergence was assessed using loss functions and learning curves, with Mean Squared Error (MSE) and Mean Absolute Error (MAE) as evaluation metrics. The centralized GLM model yielded an MAE of €5560, whereas the FL approach exhibited a gradual decline in error and converged to a minimum MAE of €5497 after 50 rounds, with a fixed batch size of 32 and four communication epochs. Despite initial fluctuations, on different parameter combinations the FL model gradually converged, indicating its feasibility for predictive cost modelling under decentralized conditions.

Conclusions:
A significant difference in hospital days and total costs was observed across nine centres, reinforcing the variability in cost-effectiveness among different strategies. The federated model exhibited promising predictive accuracy, albeit requiring more communication rounds for stable convergence compared to the centralized GLM. The analysis of loss functions and learning curves confirmed that while FL incurs additional computational overhead due to communication constraints, it progressively stabilizes with appropriate hyperparameter tuning. Finally, FL demonstrates strong potential for privacy-preserving predictive modelling, offering an effective alternative to traditional centralized statistical analyses in healthcare cost estimation.

Keywords:
Federated Learning, Multi-centric study, Data Privacy, Containerization, Flower framework, Generalized Linear Model, Federated Averaging

Performance Comparison of CNN and AST Models for Environmental Sound Classification

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Abstract: Environmental sound classification (ESC) has gained significant attention in recent years, given its applications in surveillance, smart cities, fault detection in automobiles and acoustic-based quality con- trol in manufacturing . Deep learning models such as Convolutional Neural Networks (CNNs) and Audio Spectrogram Transformers (ASTs) have emerged as dominant techniques for feature extraction and clas- sification of environmental sounds. This study presents a comparative analysis of CNN and AST models in terms of their classification performance on the widely used ESC-50 dataset. The CNN model utilized in this research consists of multiple convolutional layers with max-pooling operations, followed by dense layers for final classification. The AST model, on the other hand, employs a transformer-based architecture designed to process Mel-Spectrograms only. Different stacked feature combinations were explored as input to CNN, including Log-Mel Spectrogram (LM), Spectral Contrast (SPC), Chroma (CH), Tonnetz (TZ), and Mel-Frequency Cepstral Coefficients (MFCCs). The following feature combinations were evaluated for the CNN: LM+SPC+CH, LM+TZ, MFCC+LM, LM, and MFCC+TZ.

Keywords: Environmental sound classification (ESC), Feature extraction, Stacked Features

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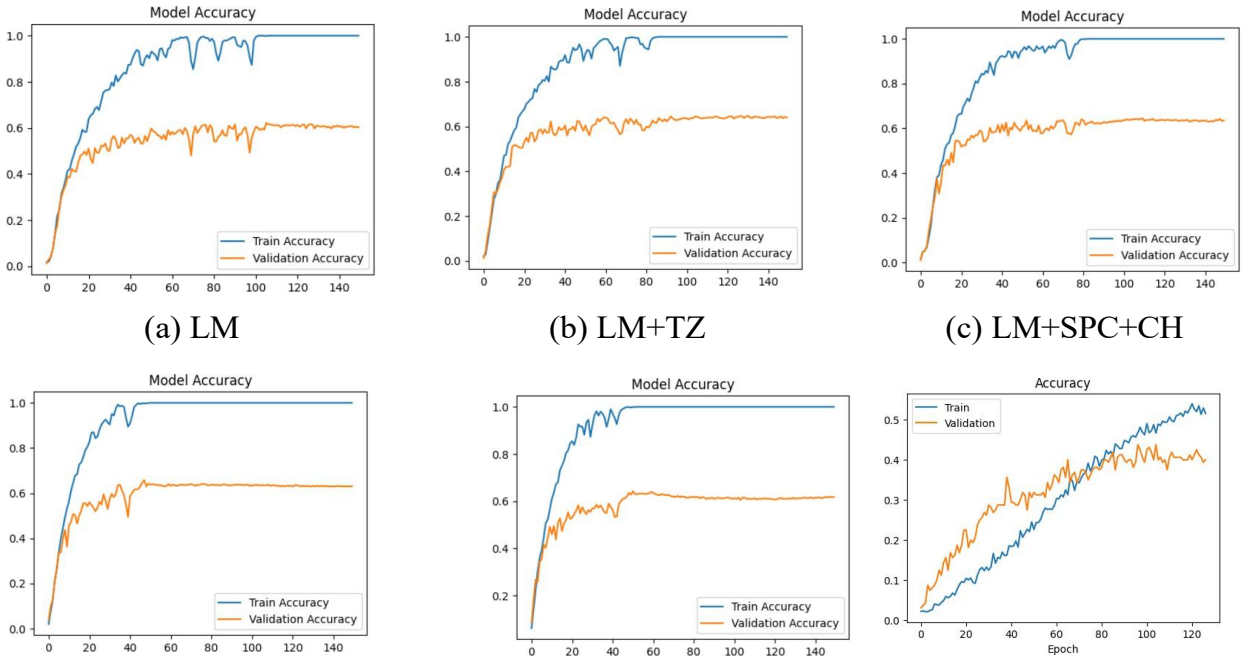
* Presenting author

Performance Comparison of Feature Combinations in CNN: We explored various stacked feature inputs. This approach was motivated by the fact that CNNs are compu- tationally lighter compared to transformer-based models like AST [1], making them more suitable for extensive feature combination experiments. Following the demonstrated effec- tiveness of stacked features in enhancing CNN performance for environmental sound classi- fication [2], we evaluated combinations such as LM, LM+TZ, LM+SPC+CH, MFCC+LM, and MFCC+TZ.

Comparison with AST Model: Compared with the AST model, the CNN and all stacked feature variants achieved superior performance, likely due to the AST's reliance on large datasets or careful pre-training to reach its full potential [1]. Since our study uti- lized the ESC-50 dataset without pre-trained models, CNN's ability to capture local patterns proved highly effective.

Model	LM	LM+TZ	LM+SPC+CH	MFCC+LM	MFCC+TZ	AST
Accuracy (%)	61.75	66.25	65.25	66.25	59.75	44.75

Table 1: Test accuracy for CNN and AST models.



(a) LM (b) LM+TZ (c) LM+SPC+CH

(d) MFCC+LM (e) MFCC+TZ (f) AST

Figure 1: Accuracy performance of different methods as a function of epochs: (a), (b), (c), (d), and (e) are CNNs with stacked features, while (f) is the AST model. The blue line represents the training accuracy, and the orange line represents the validation accuracy.

Conclusion: The results demonstrated that CNNs with stacked feature combinations, particularly LM+TZ and MFCC+LM, achieved superior performance, with test accuracies of 66.25%, outperforming the AST model, which achieved 44.75%. While CNNs excelled at capturing local patterns, especially with well-chosen feature combinations like LM+TZ, the AST's lower performance may be attributed to its need for larger datasets or pre-training [3]. These findings highlight the effectiveness of CNNs for small-scale datasets like ESC-50 and underscore the importance of feature selection in optimizing model performance [4]. Future research may explore transfer learning approaches with pretrained models leveraging the advantages of both architectures, potentially improving AST performance across diverse real-world applications.

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Surrogate modeling of the human cardiovascular system using MeshGraphNets

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Abstract:

The simulation of the human cardiovascular system is a crucial tool in medical research, clinical diagnostics, and biomedical engineering. By creating computational models of the heart, blood vessels, and hemodynamic processes, researchers can gain a deeper understanding of cardiovascular physiology and pathology. These simulations enable the study of diseases such as hypertension, atherosclerosis, and heart failure without invasive procedures. Additionally, they facilitate the development and optimization of medical devices, such as artificial hearts, by predicting their interactions with blood flow [1][2]. Simulations also play a key role in personalized medicine by tailoring treatments to individual patients based on their unique cardiovascular dynamics. To further drive the research and development in that field fast and accurate models are required, which can be achieved by combining machine learning and current physical modeling techniques.

As a foundation for our data driven approach the Pulse Wave Database [3] serves as a resource for the creation of cardiovascular meshes. This database contains extensive pulse wave measurements simulated with parameters that define various patients, capturing critical hemodynamic parameters such as arterial pulse waveforms, pressure distributions, and flow dynamics. The overall structure of the underlying model and an exemplary simulation is shown in figure 1. These measurements are essential for training our model to learn the physiological behavior of the cardiovascular system.

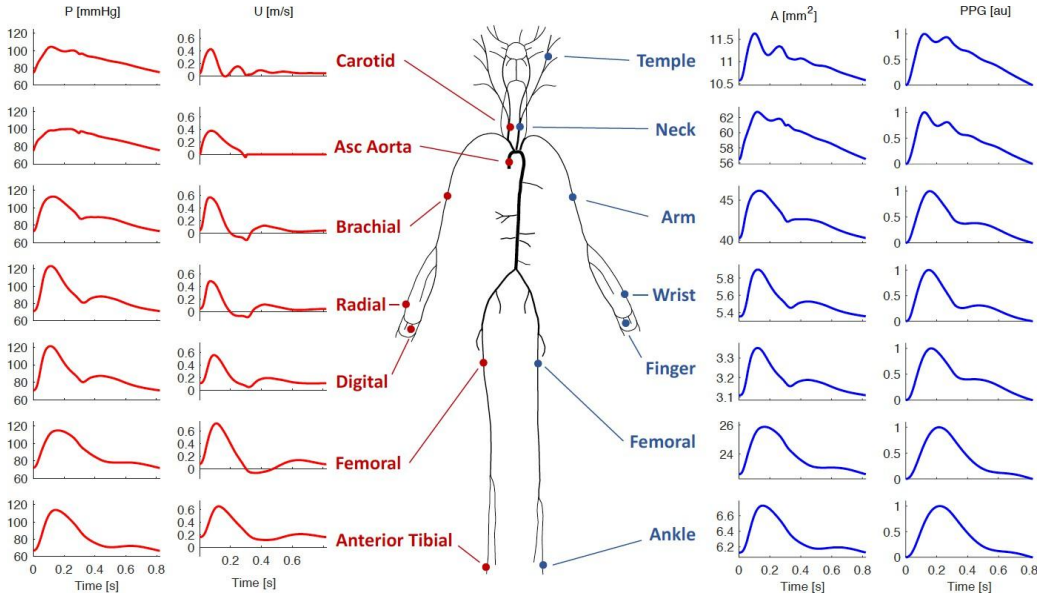

Figure 1: Simulation model of a 25-yr-old subject with the resulting pressure (P), flow velocity (U), luminal area (A) and photoplethysmogram (PPG)[3]

By leveraging data from the Pulse Wave Database, we extracted a mesh structure represented by the measurement sites and the connections between them. This allowed us to use the data for creating a surrogate model with MeshGraphNets [4]. MeshGraphNets leverage graph neural networks (GNNs) to learn underly- ing physical dynamics, enabling efficient and accurate simulations across different patient-specific vascular geometries.

One of the key advantages of MeshGraphNets is their ability to generalize beyond the specific meshes used during training. This makes them particularly well-suited for cardiovascular modeling, where anatomical variations between individuals—such as differences in artery size, bifurcations, and vessel elasticity—are significant. By learning spatial and temporal relationships in blood flow dynamics, our model can predict pressure, velocity, and other hemodynamic properties across a wide range of geometries with high fidelity.

Additionally, our implementation of MeshGraphNets as a NeuralODE [5] provides the flexibility of choosing either computationally efficient solvers to reduce simulation time while maintaining accuracy or accuracy- focused solvers for better results. On one hand, this efficiency is critical for real-time applications, such as online patient-specific diagnostics on wearable medical devices. On the other hand, a more accurate simulation provides an opportunity for a precise prediction of patient health based on current readings. With regard to performance the original model that was used for the Pulse Wave Database took, on average,
75.6s per pulse wave to simulate [6]. In contrast, the simulation time of our model ranges from 1.1s (explicit Euler) to 7.5s (Runge-Kutta of order 5(4)), depending on the choice of a more performant or more accurate solver, resulting in a speedup factor of around 10 to 70 times.

Keywords: MeshGraphNets, NeuralODE, Scientific machine learning (SciML), medical engineering

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Three-dimensional failure criterion for fiber reinforced polymers based on micromechanics informed neural network

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Abstract: The usage of fiber reinforced polymers (FRP) continues to increase due to their excellent specific properties and inherent lightweight potential. More recent developments focus on the application of FRP to laminates of increased thickness, further leveraging their benefits and opening up new areas of appliaction [1]. This inevetibly leads to more complex stress states in the laminates as opposed to the typically assumed plane stress conditions in thin laminates. Such generalized stress states pose a significant challenge to predicting the material's behavior, especially when it comes to failure.

The fundamental problem of complex stress states posing a major challenge to established failure theories was thoroughly investigated in the second world wide failure excercise (WWFE-II) [2]. The results sparked the development of further, more advanced models trying to close the identified gap. Daniel Camanho et al. continued with the concept of an invariant based theory and validated it experimentally for superimposed hydrostatic pressure [3]. Daniel incorporated micromechanical concepts into a macroscopic theory, allowing for pre-failure yielding of the laminate [4]. With increasing computational ressources, explicit modeling of the microscale became more prominent. Sun et al. made extensive use of simulations based on representative volume elements (RVE) to generate data which they used to refine the NU-Daniel criterion [5]. Chen et al. take this one step further and rely solely on data obtained from RVE simulations to train a machine learning (ML) model to assess stress states of up to three superimposed stress components simultaneously [6]. Wan et al. follow a similar approach of training an ML model based on the results of RVE simulations [7]. They, however, deviate from the absoulute prediction of a single failure point, but rather leverage experimental data to assess failure probability of 2D failure envelopes.

Despite the significant research effort and notable results, none of the works address the fundamental challenge of simultaneous superposition of all six stress components. In recent work of ours, we showed that the assessment of such 6D stress states is in principal possible, leveraging simulations of a validated RVE to train a neural network (NN) as classifier [8]. In the proposed work, we extend the results to obtain material effort under arbitrary stress states via a deep NN. This significantly enhances the usability of the resulting failure assessment network (failNet), by imporving both accuracy as well as interpretebility of the results.

The improvements is traced back to the fact that, as opposed to typical classification tasks, an exact representation of the boarder between the different classes is of the utmost importance. The advancement from a previously binary decision where minimal increases in the stress state had to lead to a sudden change in predicted class, to a continuous rating of the stress state leads to a much more robust training. In addition to that, the proposed failNet's prediction may be used to determine unexploited material capabilities and therefore potential to further reduce the material footprint of the structure at hand.

Approaches to ensure a representative generation of training for the failNet in the face of different failure modes will be elucidated. The capabilities of the proposed failNet will be compared to established failure theories both for classical 2D stress states as well as more complex superpositions.

Keywords: Fiber reinforced polymers, Failure modelling, Micromechanics, Machine Learning, Neural net- works

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When PINNs Meet MBDoE: Tackling Parameter Uncertainties in PDE-Based Process Models

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Abstract: The transition toward Industry 4.0 and digital twins necessitates hybrid modeling frameworks that bridge the gap between physics-based models and data-driven machine learning. Among these, physics- informed neural networks (PINNs) [1] have emerged as a compelling solution, embedding governing equations directly into neural network architectures to enforce physical consistency while leveraging process data. This dual capability positions PINNs as particularly promising for parameter identification in distributed parameter systems, where traditional methods for partial differential equation (PDE)-based models often struggle with computational complexity or sparse data [2]. Focusing on adsorption processes—a widely adopted unit operation in (bio)chemical manufacturing for high-purity separations—we investigate how PINNs can be synergized with model-based design of experiments (MBDoE) [3] to address critical challenges in uncertainty-aware process modeling and system identification.

Through systematic comparisons with classical parameter identification (CPI), which relies on numerical PDE solvers, we uncover a fundamental trade-off: while PINNs avoid costly numerical simulations, their parameter estimates may exhibit significantly higher uncertainties than CPI. By contextualizing PINN-based identification within functional data analysis (FDA) and principal differential analysis (PDA)—methods [4] that treat dynamical systems as functional observations—we reveal how PINNs inherently encode system- theoretic properties like differential flatness [5]. This concept, which enables algebraic parametrization of dynamical trajectories, exposes PINNs' over-reliance on input-dependent regularization, amplifying sensitivity to experimental imperfections. Consequently, minor deviations in boundary conditions or sensor noise propagate disproportionately into parameter uncertainties [6], a phenomenon poorly captured by standard MBDoE concepts. To resolve this, we propose a dual uncertainty quantification (UQ) strategy combining Monte Carlo sampling with a novel deterministic sensitivity analysis method. The latter significantly re- duces computational costs compared to conventional Monte Carlo approaches, enabling efficient MBDoE adaptations.

The proposed PINN-MBDoE framework (Fig. 1) demonstrates three pivotal insights:

- Trade-offs in industrial applicability: Despite improved precision in idealized settings, PINNs' uncer- tainty propagation limits their standalone use for high-stakes PDE parameter identification.
- Niche potential for ill-posed problems: PINNs' ability to regularize inverse problems through neural network architectures makes them uniquely suited for scenarios where CPI fails, such as sparse or noisy data regimes.
- Paradigm shift in experimental design: MBDoE must evolve to prioritize input profiles that simul- taneously satisfy PINNs' stability requirements and maximize parameter identifiability—a balance unaddressed by traditional criteria.

These findings advocate for a hybrid future where PINNs and CPI coexist, complemented by tailored MBDoE strategies that harness their respective strengths while mitigating weaknesses. The proposed computational advances not only enhance the reliability of PINNs in industrial contexts

but also provide a roadmap for integrating machine learning into physics-based workflows without sacrificing rigor.

Keywords: model-based design of experiments, physics-informed neural networks, distributed parameter systems, uncertainty quantification, parameter sensitivity analysis, adsorption processes

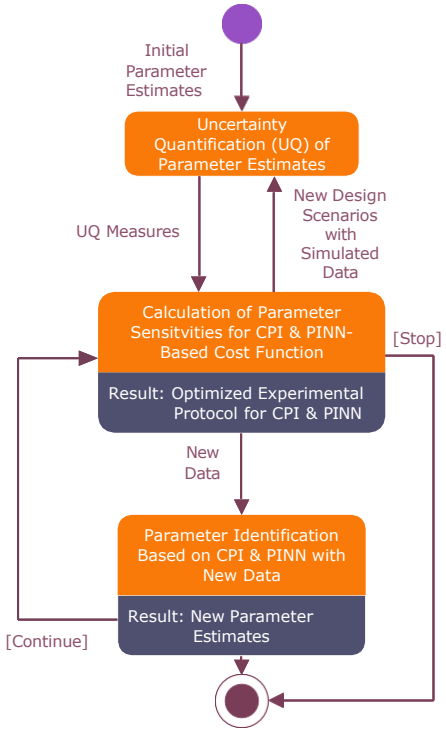

Figure 1: MBDoE workflow for CPI/PINN: Iterations of lab data and parameter identification.

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Data-driven Reconstruction of Cylinder Wakes Using POD and Convolutional Autoencoder

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The reconstruction of cylinder wakes is a critical area of research in fluid dynamics, with a wide range of applications in engineering design. Recent advancements in data-driven methods have introduced new techniques for analyzing and reconstructing complex flow fields. This study focuses on the use of autoencoders and proper orthogonal decomposition (POD) for the reconstruction of cylinder wakes. POD is a widely used method for reducing the complexity of high-dimensional data by identifying coherent structures in flow fields. This method involves decomposing a flow field into a set of orthogonal modes, which can be used to reconstruct the original flow field with reduced computational cost. Lumley (1967) first introduced POD in the context of turbulence analysis, and numerous subsequent studies (e.g., Meyer *et al.*, 2007; Shinneeb *et al.*, 2008; Thakurta & Balachandar, 2025) have demonstrated its effectiveness in capturing large-scale structures in wake flows. In machine learning, various variants of autoencoders have been used in reconstruction of data (Gu *et al.*, 2024; Laima *et al.*, 2023). Autoencoders are neural networks designed to learn efficient representations of data by encoding it into a lower-dimensional space and then decoding the data back to the original space. Comparative studies between autoencoders and POD have shown that both methods have their strengths and weaknesses. While POD is effective in identifying dominant modes and large-scale structures, it may struggle with capturing non-linear dynamics in the wake flow. Autoencoders on the other hand, particularly when trained with appropriate loss functions, can provide more flexible and accurate reconstructions of complex flow fields.

In this research, two different wakes obtained from non-intrusive particle image velocimetry (PIV) experiments are used for a comparative analysis of POD and autoencoders. Singular value decomposition (SVD) is applied in POD to extract the most energetic modes. The study focuses on two cases: a plain cylinder and a cylinder with a slot oriented parallel to the approach flow. The impact of the choice between the L1 norm (mean absolute error) and the L2 norm (mean squared error) in the autoencoders on reconstruction quality is explored, with the L2 norm known to be more sensitive to outliers and larger errors. Different latent space dimensions are investigated to assess their effect on reconstruction accuracy of the autoencoder.

A particle image velocimetry (PIV) system was used to measure the velocity field in the mid-depth horizontal plane, using a Powerview Plus 8 MP CCD camera with a 3312 × 2488-

Keywords: Autoencoder, PIV, POD, cylinder wake flow pixel resolution and Nikon AF NIKKOR 50 mm lens. The PIV images were analyzed, yielding a final interrogation

area size of 16 × 16 pixels. The velocity field resolution was 0.70 mm. Some selected wakes of the cylinders, which will be analyzed using POD and autoencoders, are shown in Figure 1. The streamwise instantaneous velocity component (u) is normalized by the mean bulk velocity (Um) of the approach flow. The horizontal and vertical axes are normalized by the cylinder diameter (d).

In the convolutional autoencoder (CAE) used in this study, the fully connected layers of a conventional autoencoder are replaced with convolutional layers. Figure 2 presents a schematic diagram of the CAE process. In the encoder, PIV images are compressed into a sparse, low-dimensional representation (latent space) through multiple convolutional layers. The decoder then utilizes this compressed information to reconstruct the velocity fields.

Detailed analysis and discussion of results will be provided in the presentation.

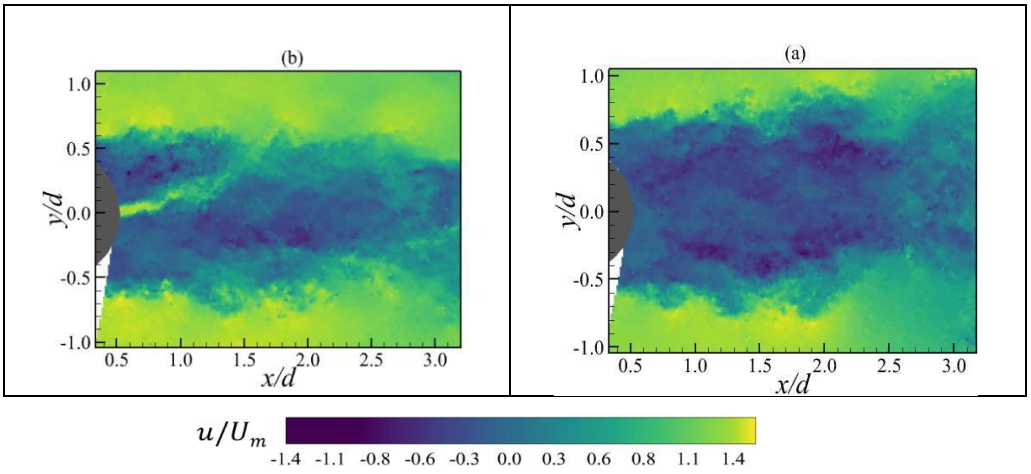

Figure 1: Streamwise PIV instantaneous velocity fields: (a) plain cylinder, and (b) cylinder with slot

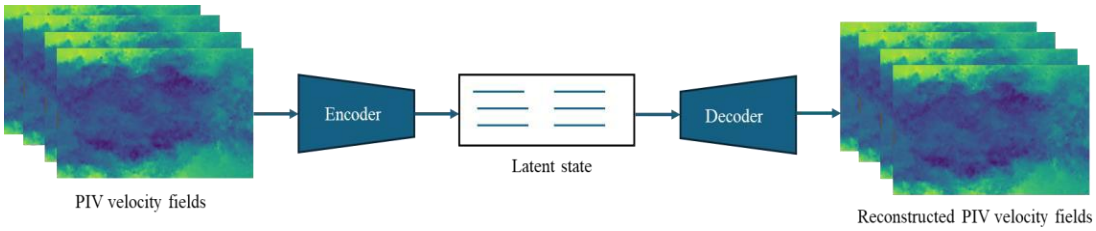

Figure 2: Schematic diagram of a convolutional autoencoder

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A stationarity-based method for wind turbine condition monitoring

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Wind power is a rapidly growing renewable energy source, with a record 117 GW of new capacity installed in 2023, bringing the global total to 1,023 GW [1]. However, operating wind turbines in harsh environments presents challenges, as failures in critical components like generators and gearboxes lead to costly downtimes and increased O&M expenses. To enhance reliability and reduce costs, developing efficient condition monitoring and fault detection methods is essential. SCADA-based solutions have gained popularity due to their low cost and accessibility. However, managing vast amounts of supervisory control and data acquisition (SCADA) data remains a challenge, leading to the growth of machine learning (ML) models and statistical approaches [2-4] for fault diagnosis.

Wind turbine monitoring faces challenges with statistical and ML-based methods relying on normal behavior models (NBMs) for specific components. NBMs use historical SCADA data to model normal operation state, detecting faults by analyzing deviations from expected values. While effective, this approach requires maintaining multiple NBMs for each wind turbine, which can be complex due to factors like turbine aging, component replacements, and sensor recalibrations. Moreover, updating NBMs demands expertise in statistics and ML, making implementation difficult and less practical for wind farm operators.

This study explores a novel data-driven approach for wind turbine condition monitoring without relying on NBMs. Based on time series stationarity, it introduces the use of the Augmented Dickey-Fuller (ADF) test, a well-known unit root test in econometrics, for anomaly detection in wind turbines. The method relies on a sliding window principle for time series data. Initially, the window is formed with a reference data set collected from a wind turbine under healthy condition. During the monitoring process, the data window is regularly updated with the latest samples recorded by the SCADA system. The ADF test evaluates the stationarity of the data within the window at each updating step, with abrupt changes in ADF t-statistics indicating potential faults. The method does not require NBMs and can simultaneously monitor multiple parameters. Its fault detection mechanism relies on tracking variations in stationarity of SCADA signals in the data window over time. Validation using two real SCADA datasets shows the method's effectiveness in detecting the abnormal temperature and gearbox fault. Key advantages of the method include eliminating the need for NBMs, enabling simultaneous monitoring of multiple parameters, making it a simple solution for practical applications.

Keywords: wind turbine; condition monitoring; fault detection; stationarity analysis; ADF test Acknowledgements: This work was performed within the scope of the

research grant No. UMO-2023/51/B/ST8/01253 financed by the National Science Centre, Poland.

Shifting steps	Samples removed from window					Existing samples in the window at each shifting step							
0						S_1	S_2	S_3	…	S_{N-2}	S_{N-1}	S_N	=> ADF test
1					S_1	S_2	S_3	S_4	…	S_{N-1}	S_N	S_{N+1}	=> ADF test
2				S_1	S_2	S_3	S_4	S_5	…	S_N	S_{N+1}	S_{N+2}	=> ADF test
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	=> ADF test
m-1		S_1	…	S_{m-2}	S_{m-1}	S_m	S_{m+1}	S_{m+2}	…	S_{N+m-3}	S_{N+m-2}	S_{N+m-1}	=> ADF test
m	S_1	S_2	…	S_{m-1}	S_m	S_{m+1}	S_{m+2}	S_{m+3}	…	S_{N+m-2}	S_{N+m-1}	S_{N+m}	=> ADF test
m+1	S_2	S_3	…	S_m	S_{m+1}	S_{m+2}	S_{m+3}	S_{m+4}	…	S_{N+m-1}	S_{N+m}	S_{N+m+1}	=> ADF test
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	=> ADF test

Sliding data window

Figure 1. On-line monitoring process is based on the consecutive accumulation of changes in stationarity of SCADA signals in the sliding data window [5].

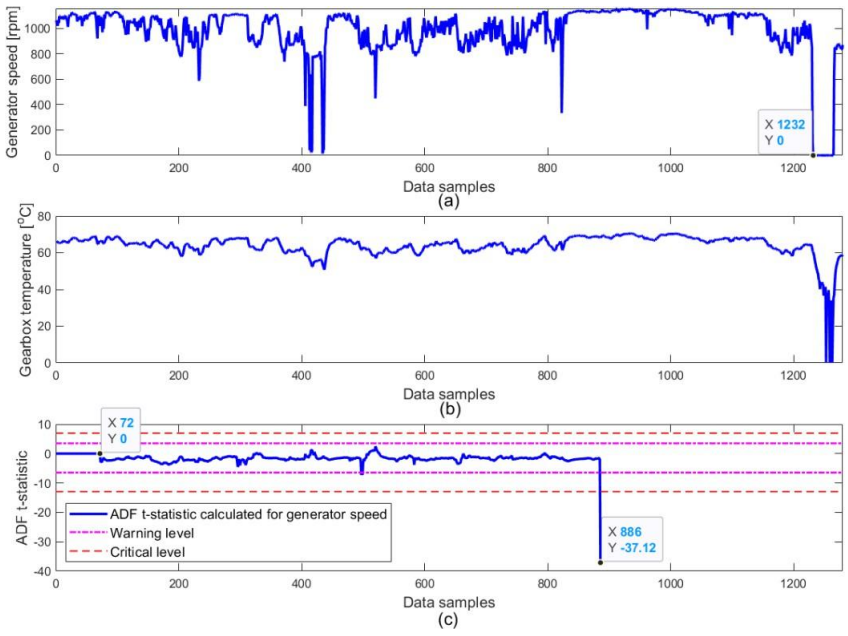

Figure 2. Detection of a gearbox fault [5].

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Automatic Discovery for Categorical Causality between Sets of Variables

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The discovery of categorical causality among sets of variables is an important issue in various subjects and applications. The traditional approaches are aiming at finding the latent variables or simulating the data by diagrams or differential equations. The methods normally rely on the assumptions about the mean, covariance, and errors, and sufficient samples for the reasoning is a normal requirement. In this work, we devise a measure, or a statistic, that could measure the strength of categorical causality and automatically detect the category causalities between a given set of variables. The method utilizes the concepts of non-parametric statistical testing, in particular the ranking methods, and a measure for category causality. By properly converting the raw data into ranks and processing the ranks via a list of procedures, we could then find the optimal pair of cause category and effect category and test their statistical significance. We implement this approach on a given set of five price indexes as our target for implementing the whole mechanism. This method is suitable for automatic detection of categorical causality.

Keywords: categorical causality; grouped variables; ranks; interval operations; commodity variables

Data-driven dislocation mediated plasticity

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In this paper, a data-driven approach to dislocation-mediated plasticity is presented. Within a dislocation density-based plasticity model incorporating effective disorder temperature, we analyze mechanical test data for various metals under diverse loading conditions and use large scale least squares method to determine the parameters of the theory. This approach enables accurate predictions of stress-strain behavior and temperature evolution for crystals under simple shear, tension/compression, and torsion over a broad range of strain rates and temperatures, where traditional crystal plasticity models fail. Furthermore, it captures size and Bauschinger effects, work hardening, and thermal softening. Next, we model notch-like defects to explore shear band instabilities, with predictions accurately matching Marchand and Duffy's experiments over a broad range of strain rates and temperatures. Finally, we apply this approach to the brittle-ductile transition, predicting fracture toughness in tungsten across a range of temperatures – consistent with the experimental findings of Gumbsch.

Keywords: data-driven, dislocations, plasticity, effective temperature, strain rate.

A Convolutional Neural Network Trained on CT-Based Finite Element Simulations for Bone Strength Prediction

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Bone fracture is a prevalent health issue among the elderly worldwide. Bone strength, along with fall-induced impact force, is a key determinant in assessing fracture risk and guiding treatment decisions. Clinicians rely on CT images to evaluate bone strength, but the relationship between CT-derived information and bone strength is highly complex. This complexity arises from the multiphase composition of bone, nonlinear material behavior of the phase materials, and intricate multiscale microstructural organization. Conventional bone mineral density (BMD)-based approaches fail to capture these complexities, making them unreliable and inaccurate for evaluating bone strength. Finite element (FE) modeling based on CT images provides a powerful alternative for bone strength estimation. However, it remains impractical for clinical use due to several challenges: the computational process is time-consuming, even with high-performance computing resources, which are often unavailable in clinical settings; and clinicians lack the specialized training required for FE simulations, making widespread adoption infeasible given their already extensive medical education. To bridge this gap, we are developing a convolutional neural network (CNN) trained on FE simulation results and validated through *in vitro* bone mechanical testing. This AI-driven approach aims to provide clinicians with an efficient and accessible tool for rapid and accurate bone strength assessment, eliminating the need for direct FE simulations while maintaining predictive accuracy.

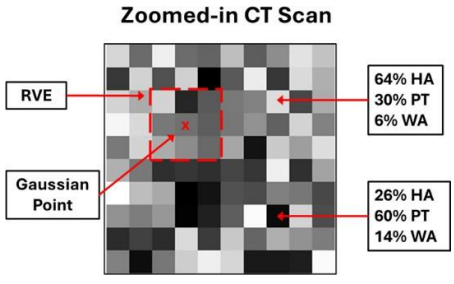

Figure 1 Information that can be extracted from bone CT scan for strength simulation.

Bone is a composite biomaterial composed of inorganic minerals (IM), organic proteins (OP), and water (WA). IM primarily regulates bone rigidity, OP governs flexibility, and WA facilitates smooth stress transition. The relative proportions of these components determine key material properties such as elastic modulus, yield stress, ultimate stress, and toughness. However, their distribution within bone is highly heterogeneous, leading to variations in voxel intensities expressed in Hounsfield Units or grayscale in CT images. An example of such a zoomed-in CT image is shown in Figure 1. Each voxel in the CT scan contains different amounts of IM, OP, and WA, which are reflected in voxel intensity.

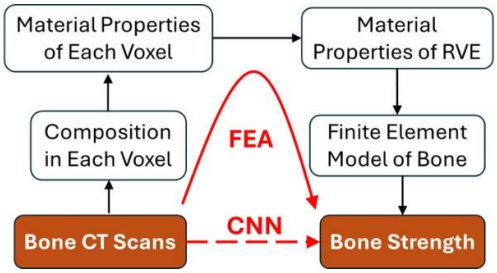

Figure 2 Framework for predicting bone strength from CT scans using convolutional neural network (CNN) trained on FEA results.

To predict bone strength at the organ level using finite element analysis (FEA), several steps are required, as illustrated in Figure 2. First, the composition of each voxel in the CT scan is determined based on voxel intensity using a basis material decomposition algorithm [1], which reflects the varying amounts of inorganic minerals (IM), organic proteins (OP), and water (WA). Using this compositional information, the material properties of each voxel, such as elastic modulus and yield stress, are simulated using the microstructure-free finite element modeling (MF-FEM) approach [2]. Next, the material properties at a Gaussian integration point within an element are predicted from a representative volume element (RVE), which consists of multiple voxels and is essential for calculating the element stiffness matrices. Finally, by solving the finite element equations of the bone model, constructed from its CT scan dataset and subjected to appropriate boundary conditions, the bone strength can be determined. This simulation accounts for the complex material heterogeneity and microstructural organization of the bone, ensuring an accurate prediction of its mechanical behavior and strength.

Although the FEA process for determining bone strength from CT scans is

complex, once validated by *in vitro* testing data, the FEA results can be used to train a convolutional neural network (CNN), as shown in Figure 2. The FEA-derived bone strength serves as a reference for CNN training, enabling rapid and accurate bone strength estimation from CT images while bypassing the computationally intensive finite element modeling process. Once trained, the CNN can predict bone strength directly from a CT scan, allowing clinicians to obtain reliable bone strength assessments without requiring any expertise in FEA.

Keywords: Bone Strength; Fracture; Computed Tomography (CT); Convolutional Neural Network (CNN); Finite Element Simulation.

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Tailored Data Fusion Methodology for Drilling Engineering and Its Applications in Drilling Anomaly Diagnosis

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The oil and gas drilling industry entails the utilization of data sourced from diverse formats across various systems and platforms. Such heterogeneity presents considerable obstacles to the effective diagnosis of anomalies and the facilitation of efficient decision-making. This paper endeavors to elucidate a tailored data fusion technology specifically designed for applications within oil and gas drilling. The primary objective of this technology is to mitigate interoperability challenges inherent in disparate types of drilling-related data, thereby furnishing a cohesive and precise depiction of the drilling process.

A bespoke data fusion methodology has been devised to amalgamate all pertinent drilling- related data, thereby furnishing quantifiable decision-making assistance in drilling applications. Initially, an overview of the sources, formats, and typologies of commonly employed drilling data is provided, accompanied by the proposition of classification criteria serving as the foundational basis for data fusion endeavors. Subsequently, a comprehensive examination of four distinct tiers of data fusion methodologies is conducted, encompassing direct fusion, feature fusion, model fusion, and decision fusion, each strategically aligned with the diverse requisites inherent in various engineering applications. Furthermore, the application of fused information in practical decision-making processes is demonstrated through the utilization of the aforementioned methodology in the realm of drilling anomaly detection and diagnosis.

Following the proposed data fusion methodology, the major problems for data fusion in drilling applications are unrevealed and classified into five categories: data fusion across disparate spatial scales, exemplified by the correlation of properties extracted from core samples with those derived from larger-scale formations; data fusion across varying time scales and temporal misalignments, such as the integration of high-frequency vibration data with low- frequency drilling logs; data fusion within environments characterized by uncertainty and incompleteness, as exemplified by the uncertain nature of downhole conditions; data fusion within scenarios marked by conflicting information, illustrated by inconsistencies between recorded data and feedback provided by engineers; and an examination of the uncertainties inherent in diverse data types, along with their propagation dynamics and subsequent impact on decision-making processes. This analysis is further elucidated through a detailed investigation of a stuck-pipe diagnosis case study, effectively illustrating the practical ramifications of these uncertainties in decision-making contexts.

This endeavor presents to the industry a comprehensive data fusion methodology aimed at integrating information sourced from diverse origins and characterized by heterogeneous formats. Such an approach facilitates a more profound comprehension of the drilling process,thereby establishing a fundamental framework conducive to the broader digitization of drilling operations and the advancement of intelligent drilling

systems tailored to address complex operational scenarios.

Keywords: Data fusion, physics-informed machine learning, drilling, anomaly diagnosis

Classification of Epilepsy MEG data using Artificial Neural Network based on TDA features

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Topological data analysis (TDA) is a statistical method used to reveal the structure of data. In this study, we applied TDA to classify brain neuroimaging data obtained from magnetoencephalography (MEG). Through exploratory data analysis (EDA), we extracted TDA features from the shape of the MEG data. Our findings showed that TDA features connected to Betti curves and persistence landscapes are significant for classifying patient groups.

We developed artificial neural networks (ANNs) that incorporate these TDA features, which include an embedding layer, a gated recurrent unit (GRU) layer, and a fully connected layer. The performance of our model was evaluated, achieving a classification accuracy of 95% or higher for epilepsy patient groups. TDA, as a specialized tool, has great potential for summarizing and clustering data to extract meaningful features, making it a valuable asset in data analysis, neuroscience, and machine learning.

Keywords: artificial neural network (ANN), brain network data, classification, magnetoencephalogrhapy (MEG) signal, topological data analysis (TDA)

Modelling MHD Flows, Heat & Mass Transfer in Liquid Metal Breeders for Fusion Engineering: Past, Present and Future

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In future fusion power reactors (such as TOKAMAKs) liquid metals (LMs) (such as pure lithium (Li) or eutectic lead-lithium (PbLi) alloy) are used as coolants and breeders to breed tritium (T), which is along with another hydrogen isotope deuterium (D) serves as a fusion fuel component. Although D is found naturally, T is not and therefore needs to be produced. Breeding T occurs in a special fusion device surrounding the plasma volume of the reactor called "blanket". Another important function of the blanket is to convert plasma energy in the form of energetic neutrons into heat. To provide required breeding ratios and power conversion, the LM breeder circulates in blanket conduits at velocities from < 1 mm/s to several m/s (depending on the blanket concept). The most promising blanket concepts are those utilizing the PbLi breeder, such as: Dual Coolant Lead Lithium (DCLL), Self Cooled Lead Lithium (SCLL), Water Cooled Lead Lithium (WCLL) and Helium Cooled Lead Lithium (HCLL) blankets. Being electrically conducting, the flowing LM in a blanket experience strong magnetohydrodynamic (MHD) effects due to the electromagnetic interaction with the plasma confining magnetic field (5-10 T). Along with strong MHD effects, heat and mass transfer processes associated with transport of T and corrosion products in the LM breeder are among the feasibility issues of a fusion blanket.

Modelling MHD flows and transport processes in the LM breeder in fusion breeding/cooling applications is nowadays the most effective technology to assess and improve existing blanket concepts and to design new blankets. Several efforts on the development of integrated modelling tools and blanket Digital Twinning are underway all over the world. The centerline of these efforts is the Computational Magnetohydrodynamics (CMHD), which compared to the traditional Computational Fluid Dynamics (CFD) is a relatively new computational discipline that addresses LM MHD flows and associated transport processes in a blanket via high-fidelity computations in complex-geometry, multi-material computational domains representing various blanket concepts and designs. From the very first computations of MHD flows dated back to late 1960s, it was observed that the computational time increases dramatically with the Hartmann number *Ha* (*Ha* squared is the

ratio between electromagnetic and viscose forces). Since that time, the progress in the CMHD computations is measured using *Ha* as the main metrics. Other metrics are the Reynolds (the ratio between inertial and viscous forces) and Grashof (the ratio between buoyancy and viscous forces) numbers. Despite the tremendous CMHD progress over the last two decades showing significant improvements in the high *Ha* computations, the full blanket modelling in most of the published computations is still limited to *Ha*, *Re* and *Gr* significantly lower than the targeted numbers in the top blanket designs of *Ha*, *Re*~10^6, and *Gr*~10^{12}.

All present CMHD codes used in computations for fusion LM applications can be subdivided into three major groups. The first group is comprised of customized commercial multi-purpose CFD codes with a built-in or user-defined MHD module. Three typical examples of such codes are FLUENT (now a part of ANSYS), CFX (also a part of ANSYS), and COMSOL. Another code that can be added to this group is OpenFOAM, an open-source multi-purpose CFD toolbox with a built-in electromagnetic module. The second group includes massive "home-made" solvers, which are specially developed for MHD applications. Among such codes are "HIMAG" (USA) and an MHD code called "MHD-UCAS" (China). The third group is represented by research codes, which are typically limited to a special type of MHD flows and/or relatively simple flow geometries.

Most of the blanket studies in the US have been performed using the HIMAG (HyPerComp Incompressible MHD solver for Arbitrary Geometry) code, which was developed by a small US business company HyPerComp Inc and the University of California, Los Angeles (UCLA) under the DOE support in the early 2000's. The HIMAG code is unsteady, 3D, parallel, finite-volume code that can use both unstructured and structured meshes. The code includes a wide array of advanced physical models relevant to fusion blanket conditions, including MHD flow and heat & mass transfer. It provides accurate conservation properties when multiple materials (solid and liquid) are present for both closed-duct and open-surface flows. In recent years, the HIMAG code has increased greatly in scope, following extensive interactions with General Fusion (Canada) and Oak Ridge National Laboratory (USA), and is now able to model flows driven by pulsed currents and transient magnetic fields.

Two successful examples of the application of CMHD tools to the blanket analyses representing state-of-the-art in the field are demonstrated in

this paper for the DCLL blanket, where PbLi is used as a breeder and coolant of the breeding zone, reduced activation ferritic/martensitic (RAFM) steel as a structural material, and helium (He) gas as a coolant of the blanket first wall (FW) and internal steel structure. One example is integrated modelling using HIMAG and research codes to access feasibility of the DCLL blanket concept for a very high applied magnetic field up to 20 T, which is envisaged in the modern compact fusion reactor designs. The second example shows the 3D modelling of the entire PbLi blanket at high Ha~10^4 and Gr~10^{12} using the MHD-UCAS code. These unique computations are first of the kind, where the entire full-geometry blanket system with realistic parameters are fully resolved. The computed results suggest that many conclusions from the earlier blanket studies for separate blanket sub-components and lower flow parameters need to be revisited.

Keywords: computational MHD, fusion engineering, breeding blanket, integrated modelling

Feature Engineering for Roller Bearing Fault Detection: Time and Frequency Domain Analysis

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This paper focuses on fault diagnosis of roller bearings using vibration signal analysis, based on a raw dataset (bearing run-to-failure test) provided by the Center for Intelligent Maintenance Systems (IMS). The study categorizes the progression of bearing damage into five stages, analyzing vibration signals in the time domain using three key methods: Root Mean Square (RMS), Crest Factor, and Kurtosis. Results indicate that Crest Factor analysis of the horizontal vibration signals show a more pronounced increase in vibration levels over time, distinguishing the Useful Life, Wear, and Failure stages more effectively than the other methods. Additionally, in the frequency domain, the study assesses bearing damage by calculating the average FFT amplitude of the vibration signals for each period, with a focus on the characteristic Ball Spin Frequency (BSF). It was found that the 6^{th} harmonic (839.10 Hz) of the horizontal vibration signals provided the clearest indication of roller defect severity. This study identifies the most effective feature engineering approaches for vibration data.

Keywords: fault diagnosis, vibration signal analysis, remaining useful life

A Hybrid Deep Ritz Method for the Numerical Solution of the Monge-Amp`ere Optimal Transport Problem

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Abstract: In optimal transport theory, the objective is to map two probability distributions while min- imizing some costs, in order to model the transport of a material from one location to another. The Monge-Amp`ere optimal transport problem is a model problem that arises when modeling such a mapping. It relies on the Monge-Amp`ere equation, which is the prototypical example of so-called fully nonlinear partial differential equations.

We propose a numerical method to approximate smooth, convex solutions to this Monge-Amp`ere equation that is built on a least-squares formulation of the partial differential equation. An iterative scheme allows to decouple the nonlinear and variational components of the problem. The framework introduced in [1] leads to the solution of two subproblems at each iteration: a local, nonlinear, optimization problem that can be solved pointwise with mathematical programming techniques, and a linear variational problem of biharmonic type that has been solved historically with finite element methods.

In this work, we use the Deep Ritz method [2] to solve the linear variational problem instead of using finite element methods. The resulting hybrid method allows to take advantage of the neural networks to solve linear problems, while keeping optimal optimization techniques to solve for the nonlinear character of the problem.

Unlike Physics-Informed Neural Networks (PINNs) [3], the Deep Ritz approach preserves the variational structure of the problem and does not impose additional regularity conditions on the input data. The convexity of the solution is enforced by using Input Convex Neural Networks (ICNNs) [4]. Furthermore, unlike PINNs, the Deep Ritz method allows to maintain a better control over the approximation error, for instance in the H^2-norm.

Numerical experiments in two or three dimensions of space show the effectiveness of the approach through applications to the classical Dirichlet problem for the Monge-Amp`ere equation, and to the optimal transport problem. We highlight the potential of the method to obtain accurate solutions with controlled error in only a few iterations. We compare the method with the original finite element based method and the PINNs approach. Conclusions show that the hybrid approach can be efficient in certain situations. As time allows, we extend the results to other fully nonlinear equations, such as, e.g., the mean curvature (Minkowski) problem.

Keywords: Fully nonlinear PDEs, Hybrid methods, Optimal transport, Deep Ritz method, Input convex Neural Networks, Least-squares algorithm

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* Presenting author

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Digital Models for Optimizing Energy Production from Municipal Waste through Gasification and Pyrolysis

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Introduction

The objective of this study is to develop a flexible, portable, durable, and expandable technology solution for efficiently transforming communal waste into valuable energy forms, particularly combustible gases or liquids. The research focuses on two systems: a gasification facility (primary facility) and a small pyrolysis unit (secondary facility). Both systems are underpinned by data from real experimental facilities and are simulated using symbolic regression models suitable for various testing and optimization purposes to find the best-fit mathematical models for a given dataset.

The appropriate software has been developed. It also offers sustainable waste management solutions to municipalities and local communities through the use or sale of the (electricity) energy produced.

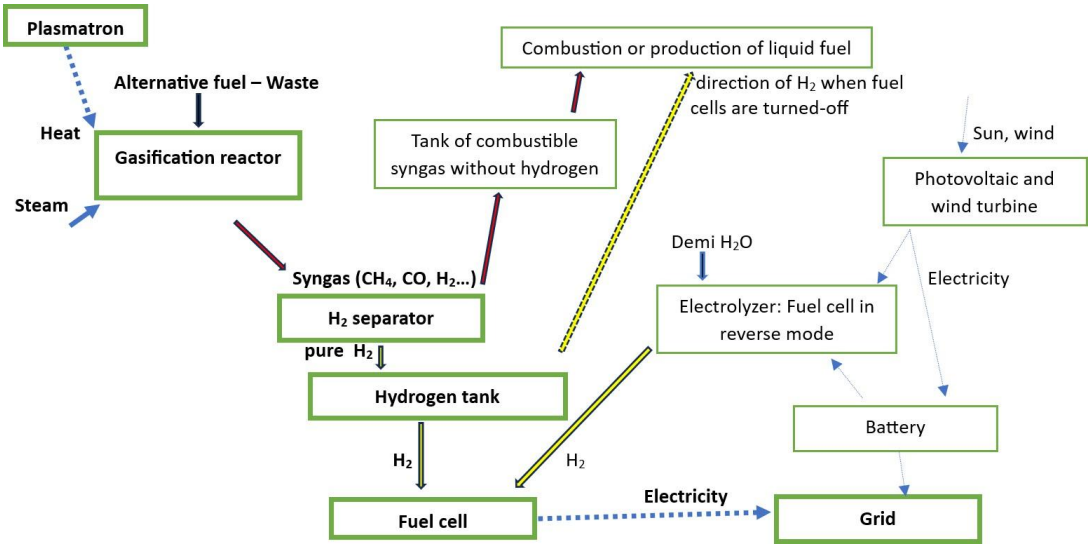
Waste-to-Energy Experimental Facilities — Models of the System

Gasification occurs in the presence of ambient air, whereas the pyrolysis reactor operates in the absence of air. The temperature in both facilities is the main driving factor. In gasification, it is set to maximize hydrogen production from syngas, while in the pyrolysis facility, it is set to maximize liquid fuel production.

-Gasification Facility – Primary Facility

The primary facility features a plasma torch, gasification reactor, hydrogen separator and tank, fuel cells, and connections to the electric grid and batteries, with additional links to photovoltaics and wind turbines. Additionally, hydrogen can be produced from water in an electrolyzer.

[a] Presenting Author



Gasification occurs under stoichiometric conditions. The resulting gas mixture, mainly composed of hydrogen, methane, carbon monoxide, carbon dioxide, and nitrogen, varies depending on the waste type and plasma temperature. The facility includes a combustion unit as an alternative process, which operates only when the main process is turned off. The facility is optimized for hydrogen production.

-Small Pyrolysis – Secondary Facility

The small pyrolysis unit primarily produces pyrolysis oil. It is designed to process 2-5 kg of waste per hour, yielding outputs such as char, liquid fuel, and gases.

Software Tool

An in-house developed software tool, written in Python, simulates both facilities. The software uses machine learning methods, including symbolic regression and polynomial regression, to model the processes. The software enables optimization of the facilities, providing a sustainable solution for waste management in municipalities and offering additional income through the use or sale of produced energy. The software can be found at: https://shinyenet.vsb.cz/,

Conclusion

The integration of gasification and pyrolysis processes, along with the use of symbolic regression models to simulate and optimize these processes, provides a comprehensive approach to transforming municipal waste into valuable energy forms, enhancing the sustainability and efficiency of waste management systems.

The developed software can simulate mobile, compact, and robust waste-to-energy facilities, useful for planning, development, management, and optimization of waste management. The software allows for the modeling of various scenarios, such as loss of functionality due to technical failure, and offers sustainable waste management solutions to municipalities.

Keywords: Fuel cells; Hydrogen; Pyrolysis; Symbolic regression; Syngas; Software;

Waste- to-gas

Prediction of the stereoselective C/O migration of boronic compounds inside a nanoreactor using machine learning

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Stereoselectivity is a critical factor in organic synthesis, especially in pharmaceutical contexts, where the spatial arrangement of molecules can significantly influence biological activity. In this study, we combine nanotechnology and machine learning to predict the stereoselectivity of boron compounds within carbon nanotube (CNT) nanoreactors. Leveraging density functional theory (DFT) and ONIOM methods, we provide fast and accurate calculations of the energies of boron compounds in CNTs, offering insight into the transition states influenced by steric hindrance and electrostatic effects. The reaction dynamics are further refined using a chiral vector (13,0) for the CNT, ensuring enhanced precision in our model's predictions. Additionally, this work explores the impact of different structural configurations on reaction outcomes and applies mechanistic learning to predict both the occurrence and stereoselectivity of these reactions. By utilizing a comprehensive dataset of material properties, we develop a machine learning model capable of accurately predicting stereoselective outcomes. Optimization strategies are employed to further enhance the model's performance, demonstrating its applicability to complex chemical systems. Our findings have profound implications for organic synthesis, particularly in drug development, where stereoselectivity is crucial. This research underscores the transformative potential of machine learning in advancing stereoselective chemical synthesis, with broader applications in materials science and nanotechnology.

Keywords: Boronic Compounds, Stereoselectivity, Machine Learning, Carbon Nanotube, DFT Calculation

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AI-Based Quantitative Characterization of Bone Components Using Simulated and Real-World DECT Noise Patterns

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Bone is often considered a composite biomaterial consisting of inorganic minerals (IM), organic proteins (OP), and water (WA), each playing a crucial role in achieving both mechanical and biological functionalities. The inorganic mineral phase, primarily hydroxyapatite, provides rigidity and load-bearing capacity, serving as the primary component that enables bones to withstand compressive stress. The organic matrix, mainly composed of collagen and other proteins, imparts flexibility and toughness, acting as the primary component that allows bones to resist fractures by dissipating energy under tensile stress. Water plays a vital role in maintaining bone hydration, facilitating ion transport, and influencing viscoelastic properties. The interplay among these three components is fundamental to bone mechanical behavior and biological function.

Quantitative characterization of bone components is essential for evaluating bone health, understanding the etiology of various bone diseases, and predicting fracture risk. The relative proportions of inorganic minerals, organic proteins, and water directly influence bone mechanical properties, such as stiffness, strength, and toughness. Deviations from the normal composition are often associated with pathological conditions, including osteoporosis, osteomalacia, and brittle bone disease, which compromise bone integrity and increase susceptibility to fractures. Accurate quantification of these components enables clinicians and researchers to detect early-stage bone deterioration, monitor disease progression, and assess the effectiveness of therapeutic interventions. Moreover, integrating compositional analysis with biomechanical models enhances the ability to predict fracture risk beyond conventional bone mineral density (BMD) measurements, offering a more reliable assessment of bone health.

Dual-energy computed tomography (DECT) based material decomposition[1] is a promising non-invasive technique for quantitatively characterizing bone

components. However, a key challenge arises from the highly similar X-ray linear attenuation coefficients of organic proteins and water, resulting in a flattened triangular distribution of CT intensities for the three phantoms in the low- vs. high-energy voxel intensity coordinate plane, as shown in Figure 1(a). This issue is further compounded by CT noise, which causes the bone intensity point (BN) to drift outside the expected triangular region. Consequently, solving the decomposition equations in Figure 1(b) can produce unrealistic values, including negative values or values greater than 1, which are physically meaningless since the volume fractions of bone components should always range between 0 and 1.

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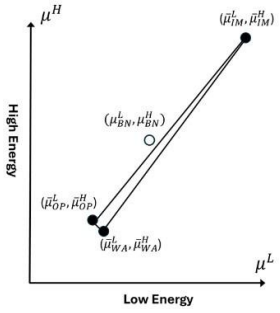
[a] Presenting Author



(a)

$$v_{IM}\,\bar{\mu}^L_{IM} + v_{OP}\,\bar{\mu}^L_{OP} + v_{WA}\,\bar{\mu}^L_{WA} = \mu^L_{BN}$$
$$v_{IM}\,\bar{\mu}^H_{IM} + v_{OP}\,\bar{\mu}^H_{OP} + v_{WA}\,\bar{\mu}^H_{WA} = \mu^H_{BN}$$
$$v_{IM} + v_{OP} + v_{WA} = 1$$

$\bar{\mu}^L_{IM}, \bar{\mu}^L_{OP}, \bar{\mu}^L_{WA}$ – Phantom intensities at low energy
$\bar{\mu}^H_{IM}, \bar{\mu}^H_{OP}, \bar{\mu}^H_{WA}$ – Phantom intensities at high energy
v_{IM}, v_{OP}, v_{WA} – Volume fractions of bone

(b)

Figure 1 Challenges faced by conventional algorithms in quantitatively characterizing bone components.

The proposed AI-based quantitative characterization of bone composition (Figure 2) integrates DECT simulation with an artificial neural network (ANN) trained on both simulated and real-world CT noise patterns. As shown in Figure 2, the method begins with the generation of training data, where DECT simulations are performed using the linear attenuation coefficients of bone components and their prescribed volume fractions. To enhance realism, noise patterns extracted from real-world CT scans are incorporated into the simulations, generating synthetic low-energy and high-energy CT images. These images serve as input for the ANN, which is trained to predict the volume fractions of bone components. The ANN training process iteratively refines its model to minimize errors, leveraging a validation step where the characterized volume fractions are compared against the prescribed values. Ultimately, the trained ANN enables robust and accurate decomposition of bone composition components from DECT scans, overcoming challenges associated with CT noise and the similarity in attenuation properties of organic

proteins and water.

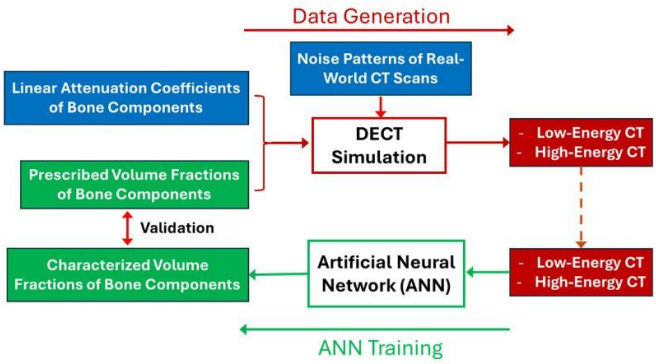


Figure 2 Workflow of AI-based quantitative characterization of bone composition, integrating DECT simulations with real-world CT noise patterns for ANN training and validation.

Keywords: Bone Components; X-Ray Linear Attenuation Coefficient; Volume Fraction; Artificial Neural Network (CNN); DECT Simulation.

Reference

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Fast Alignment of Heterogeneous Images in Sliced Wasserstein Distance

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Image alignment is a central task in computer vision with diverse applications across many fields of engineering. In many applications, the images being compared may be diffeomorphic or drawn from different underlying distributions. For these *heterogeneous* images, standard correlation methods often fail to provide meaningful alignments as they are sensitive to deformations in the images.

In this work, we present a fast algorithm for aligning heterogeneous images based on optimal transport. Our approach combines the speed of fast Fourier methods with sliced probability metrics and allows us to efficiently compute the alignment between two $L \times L$ images using the sliced 2-Wasserstein distance in $O(L^2 \log L)$ operations. We show that our method is robust to translations, rotations and deformations in the images. Our method has the potential to improve engineering applications that rely on computer vision.

Keywords: Image alignment, Optimal transport, Computer vision

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[a] Presenting Author

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Energy Flow Forecasting using LightGBM

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Abstract: Accurate forecasting is a critical issue for energy transactions, grid stability, and operational planning since energy is necessary for both economic growth and the transition to low-carbon sectors. Energy management in Europe is made more complex by changing regulations, the integration of renewable energy, and market dynamics. To maintain energy security, stabilise prices, and balance supply, interconnectors such as the 140-kilometer NEMO Link between Belgium (BE) and Great Britain (GB) are essential. However, the complex or even stochastic nature of the features governing supply, demand, and transmission limitations make energy transaction forecasting particularly difficult.

Energy systems are frequently analyzed using classical statistical tools (CST), such as trend analysis, cor- relations, and causal relationships. However, when working with complex temporal connections and a large number of variables, these methods could not always offer enough insights [1]. In this context, machine learn- ing (ML) methods, particularly Gradient Boosting Decision Trees (GBDT), offer practical tools for feature selection and time series forecasting. Among GBDT algorithms, LightGBM [2] has emerged as a promising candidate due to its computational efficiency, ability to handle large datasets, and integrated feature selection process. For an initial analysis, LightGBM is particularly useful for identifying key features that influence energy flow, providing a structured approach to feature selection that enhances model interpretability and predictive accuracy. Its ability to rank feature importance allows analysts to identify the most influential variables, enhancing model efficiency and generalization.

To improve energy trading strategies, cost stability, and grid reliability, this work focuses on developing a 48-hour-ahead energy flow forecasting strategy for the NEMO Link using collected market, environmental, and capacity data. To do this, we used datasets covering the period of January 2021 to June 2022 with hourly measurements of 41 variables, provided by N-SIDE[1] with the help of the Cenaero research centre.[2] Data preprocessing was first achieved to capture temporal dependencies. Then, time-lagged features at 1-hour, 2-hour, 1-day, 2-day, and 1-week intervals were incorporated, with an additional 1-month lag for the target variable, yielding 245 features. The feature selection was based on LightGBM feature importance scores, with a threshold $\Gamma = 18$ to retain the top 33 most relevant features, balancing predictive accuracy and model efficiency. Fig.1 illustrates the dataset split; 80% of the data was used for training and 20% for validation. Positive values indicate exports from BE to GB, while negative values represent imports from GB to BE. Flow fluctuations are typically influenced by market demand, supply conditions, and transmission capacity.

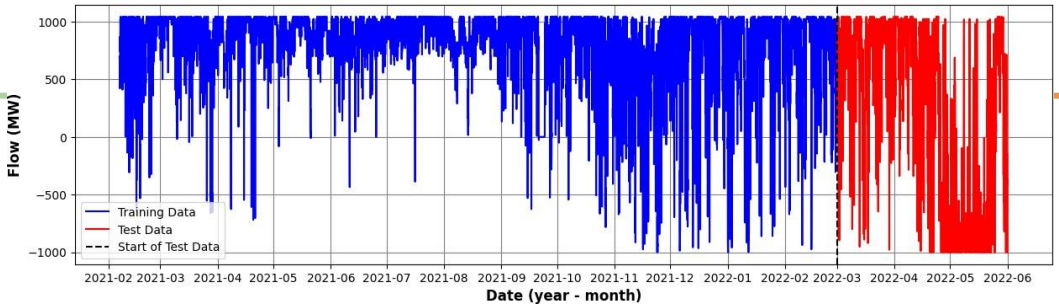

Figure 1: Output flow training (blue) and testing (red) data.

[1]N-SIDE is a global company with offices in Belgium, the USA, and Japan, which develops software solutions for complex challenges involving time series. This study was conducted in collaboration with its Belgian office.

[2]Cenaero is a Belgian non-profit applied research centre supporting the TRAIL grand challenge[3].

[3]Trusted AI Labs (TRAIL) is a Belgian initiative uniting universities and research centers in the Walloon and Brussels regions to advance AI research and innovation.

A LightGBM model was trained for forecasting, utilizing its histogram-based gradient calculation and leaf- wise tree growth to improve efficiency and predictive performance. Hyperparameter tuning was achieved using the Optuna framework. A systematic search across the hyperparameter space was conducted to select, for instance, the number of trees and learning rate, with cross-validation ensuring optimal selection.

Given a data set $(x_i, y_i)_{i=1}^{N}$, where x represents input features, y the target variable, and N is the number
of samples, the objective is to estimate a function $F(x)$ that minimizes the expected loss function:

$$F^* = \arg\min_F \mathbf{E}_{x,y}[L(y, F(x))]$$

To forecast the next 48 hours with the trained model, a recursive multi-step approach was considered. Fig.2 illustrates the performance of a 48-hour-ahead recursive multi-step forecasting approach, where the model predicts each future step sequentially using prior forecasts as inputs. The predicted values are compared with actual energy flow measurements on unseen data, effectively serving as a time series cross-validation method, and a 95% confidence interval (CI) is provided to quantify the uncertainty. This validation process ensures the model's consistency and generalization ability when forecasting multiple steps ahead. The findings demonstrate consistent prediction performance, with actual values typically staying within the CI boundaries. The LightGBM model is a valuable tool for operational planning in energy trading and grid management, as evidenced by its attained root mean square error (RMSE) of 169 MW, which indicates that it accurately captures fluctuations in energy flow.

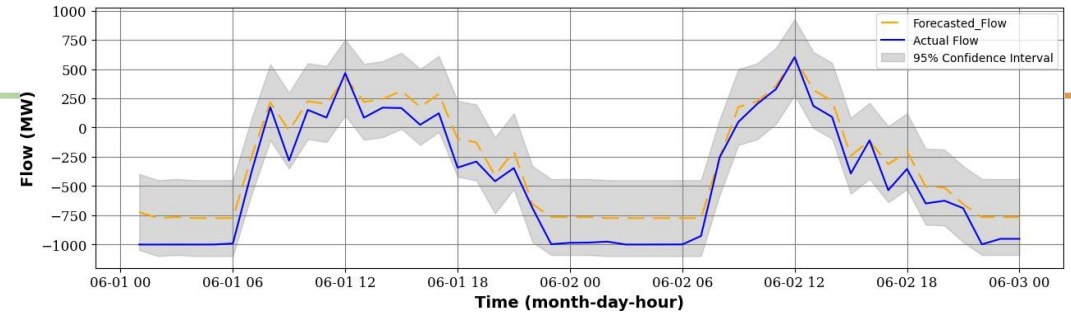

Figure 2: The forecasted target for 48 hours ahead with 95% CI.

This study underscores the importance of energy forecasting in addressing contemporary energy challenges and demonstrates that LightGBM provides a valuable tool for high-dimensional time series forecasting due to its effective feature selection and capability to capture key temporal dependencies. As part of our ongoing research, we aim to develop and compare alternative forecasting models, including Long Short-Term Mem- ory (LSTM) networks and conventional time series models such as Autoregressive Moving Average model with eXogenous inputs (ARMAX). This will allow us to assess the role of nonlinearity, model complexity, prediction accuracy, and interpretability in energy forecasting.

The authors express their gratitude to the TRAIL-ARIAC initiative for its financial support.

Keywords: Energy Forecasting, Time Series Forecasting, Machine Learning.

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* Presenting author

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Autonomous robots in On-demand food deliveries: an Agent-Based Simulation

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Last-mile delivery (LMD) is the delivery of products ordered online to the final customers. This logistics process is very critical from both the efficiency and the effectiveness perspectives, due to small order dimension, geographically dispersed destination, and very stringent service level requirements. These criticalities are even more severe if considering the ODFD (On-Demand Food Delivery), i.e., the delivery of freshly prepared meals to customers' home from restaurants, enabled by the use of online platforms. Delivery lead times are very short, as the meals must typically be delivered very quickly from the moment they are ready – often within 15 minutes – and punctuality is key – since customers expect their order to arrive in the selected time-window. ODFD delivery operations are therefore much more complex than those for non-food e-commerce parcels, where a rather conventional Vehicle Routing Problem (VRP) has to be solved. In the ODFD case, the underlying problem is a variant of the dynamic Pickup and Delivery Problem (PDP), with rigid precedence constraints to be respected for pickups and deliveries, and with the points of origin being a large number of dispersed restaurants.

To mitigate the complexities of last-mile delivery (LMD), several innovative autonomous solutions have been deployed. Among them, autonomous robots are being employed in the ODFD to pick up orders from restaurants and deliver them to a single final customer, since their characteristics and features well align to the peculiarities of the associated delivery problem.

The present research addresses delivery robots for food delivery under the logistics perspective, investigating operational and economic performances. More specifically, the aim is to explore the relevant parameters affecting the operational results of the application of this technology and to study their impact on two key metrics for the industry: *Order Cycle Time* (the total time required for delivery from the moment the order is issued) and *Lateness* (the delay incurred by the robot in arriving at the pickup point compared to the scheduled time).

The adopted methodology combines interviews with practitioners (to both collect data and validate the outcome of the research) with an agent-based simulation (first applied to a base case scenario, and then complemented with sensitivity analyses on relevant variables).

The results of the simulations show how the performances of the delivery system are strongly affected by different elements, among which the density of the delivery destinations (customer orders) as well as of the points of origin (restaurants). Furthermore, they proved the negative effects generated by significant peaks during the day – typically lunch/dinner time – which, if not properly met, lead to high order cycle times (and a higher number of required robots). Accordingly, efforts could be made to integrate multiple shops/restaurants into the platform, considering the possibility of including pharmacies or supermarkets, which could both increase the density and smoothen the distribution of requests.

The analysis on the area and the robots speed confirmed the significance of the application sites for the success of the initiative. The effects on order cycle time are not only related to the increase/decrease in lateness, but also to the average travel time between restaurant and customer. Given the impact of the route network on travel time, selecting the proper location for the deployment of the technology is the most crucial factor. Limited traffic and road crossings as well as flexibility in routes are important elements to look for when selecting the deployment area. In this respect, university campuses and protected neighborhoods are promising examples for the application due to the restricted area, high density of potential customers and traffic restricted routes. Regulations and infrastructures may play a crucial role in moderating or enhancing such factors.

Based on the above, the present research contributes from both an academic and a managerial perspective. Considering academia, it advances extant literature around autonomous solutions in last-mile delivery for the ODFD business by investigating the impact of several factors on relevant performance indicators. Considering industry, it offers practical suggestions for a successful deployment of this innovative delivery solution for ODFD.

Keywords: Food delivery; robots; logistics; e-commerce

S-mileSys platform as a sustainable development solution for local authorities and freighters

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In recent years, the field of logistics and transport systems has witnessed the rapid development of tools designed to support the organization of freight deliveries in cities and metropolitan areas. One outcome of these research efforts is the S-mileSys platform—developed under the international project "Smart platform to integrate different freight transport means, manage and foster first and last mile in supply chains (S-mile)." The project focuses on the challenges of the so-called "first" and "last mile" in supply chains, i.e., short-distance segments near the point of dispatch or delivery. By leveraging data analytics and advanced ICT solutions, S-mileSys aims to optimize logistics processes while simultaneously promoting **environmental protection**, sustainable energy management, and innovative applications in **civil engineering** and **structural engineering**.

The platform's design ensures that all key stakeholder groups—local authorities, freight carriers, and clients—gain practical benefits. Such an approach highlights how discovering the impact of modelling and data-driven insights can bring about not only smoother logistics operations but also improved **urban infrastructure planning**, **reduced social costs**, and **enhanced quality of life**. The S-mileSys platform was designed with three key user groups in mind:

1. **Local authorities**– They gain access s to freight traffic data, making it easier to make informed decisions on route planning, infrastructure management, and the implementation of environmentally friendly transport solutions.
2. **Freight carriers** – They can use dedicated planning and management tools to optimize fleets, routes, and schedules, thereby reducing costs, delivery times, and environmental impacts.
3. **Clients commissioning freight transport** – Through the platform's marketplace component (the S-mile Market Tool), they can quickly find carriers offering services in a given area, simplifying the process of locating service providers and concluding shipping contracts.

A central component of the platform is the **S-mile Transport Planner Tool**, which enables comprehensive planning of freight deliveries by accounting for variable road conditions, available infrastructure, and multiple priorities (e.g., time, cost, emissions). Its optimization algorithms allow for routes that **minimize negative environmental impact**, while consolidating different orders—both pick-ups and drop-offs—into a single run. Moreover, the platform uses GIS-based tools (including Open Street Maps) for a more precise representation of road networks (road parameters, dimensional constraints, infrastructure status). This setup allows S-mileSys to suggest and modify vehicle routes in real time based on emerging issues or changing conditions.

Below is a summary of the key S-mileSys tools:

1. **S-mile Market Tool** – A freight exchange platform that integrates client demand with carrier offers.
2. **S-mile Freighter Tool** – A module for carriers, supporting route monitoring, vehicle parameters tracking, and order updates, as well as driver-dispatcher communication.
3. **S-mile Transport Planner Tool** – The system's core component, enabling automatic route planning based on economic and environmental (emissions, noise) criteria.
4. **S-mile Fleet Management Tool** – An extension for transport companies, assisting in fleet efficiency analysis and the generation of cost reports, factoring in fuel consumption, driver hours, etc.
5. **S-mile Simulation Tool** – A module primarily for public institutions and environmental agencies, allowing simulations of transport policy variants (e.g., road charges, low- emission zones, parking plans) and evaluation of their socio-economic and environmental effects.
6. **S-mile Visualizer Tool** – A visualization utility for assessing real-time road network conditions, aiding local authorities in ongoing supervision and long-term infrastructure planning.

The S-mile project aligns with the **smart city** vision, in which ICT solutions serve to:

- Collect and **analyze data** on key factors shaping urban freight transport,
- Make better use of existing infrastructure while introducing new solutions **to reduce CO_2 emissions,**
- Support informed decision-making by local communities and administrative authorities.

Wider implementation of the system can contribute to enhanced freight delivery efficiency, greater transparency in logistics services, and reduced pollution and noise in cities. S-mileSys demonstrates that by involving various stakeholders—public administration, transport companies, and service recipients—one can create a platform that balances economic objectives (lower transport costs), environmental goals (reduced emissions), and social considerations (less intrusive transport).

The S-mileSys platform exemplifies how integrated ICT and data-driven solutions can tackle urban freight challenges. By delivering concrete benefits to local authorities, freight carriers, and clients alike, it demonstrates the feasibility of **balancing economic growth with environmental protection and social well-being**. Moreover, the system's capacity to discover the impact of modelling fosters deeper collaboration across Civil Engineering, structural engineering, and energy management, forging pathways toward a genuinely sustainable urban future.

Keywords: data analytics; environmental protection; energy management; first and last mile

ETPlanner approach for more environment-friendly and energy-efficient sustainable transport systems

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Sustainable development should be based on identification of needs, take the limited natural resources into account, and initiate technological development. The choices made by the travelling population, pertaining to how one travels, by what means of transport, by which transfer routes etc., globally translate into the negative impact of transport which takes diverse forms, primarily that of the emission of harmful substances, noise and the resulting traffic obstructions caused by congestion. In line with the European Union guidelines, minimisation of the negative environmental impact of transport cannot be pursued through mobility limiting, but rather through efficient utilisation of natural resources. The task of improving transport systems towards sustainable mobility requires adequate information transfer as well as systems capable of supporting integration of operations and synergy of modelling and data analytics. As part of the international project implemented under the ERA-NET CoFund Electric Mobility Europe Programme "Electric travelling – platform to support the implementation of electromobility in Smart Cities based on ICT applications," a tool was prepared with prospects to evolve towards supporting both the process of **fostering specific behaviour patterns among the travelling population and local authorities in making decisions on the changes to transport systems**. The present research has been financed from the means of the National Centre for Research and Development.

People who daily travel often do not consider alternative ways to reach a specific destination. They tend to use but the same travelling mode they originally chose, and it is frequently a passenger car. It should be noted that such a conduct may be founded on diverse grounds, yet the most typical of them include a habit and lack of full information on alternative travelling modes and environmental impact. With regard to transport systems, the flow of information has become particularly important. The tool designed by the authors, i.e. **ETPlanner**, successfully fills the functional and methodological gap related to how data are acquired and processed, as well as to the integration of diverse traveling modes and promotion of eco-friendly solutions by increasing the environmental awareness of the travelling population (which will bring finally **environmental protection**).

The planner provides **routing capabilities using 11 modes**, which ultimately boils down to the user receiving a comprehensive collation of travelling options, including the relevant parameters, **based on four criteria: distance, time, cost, and environmental impact.** Such information can change the manner in which one travels by fine tuning one's previous behaviour patterns (e.g. using the Park&Ride system or urban bikes and e-cars rental services).

What proves particularly important is that the data taken into consideration while planning travels be up to date. The ETPlanner has been built as much as possible on open sources, which makes it a universal tool suitable for implementation at virtually any place in the world (laboratory tests have been performed for more than a dozen cities and regions). It can be **integrated with the ITS** currently deployed across the given city, since it is ready to dynamically process such data as, for instance, information about the congestion at individual transport network sections, the current availability of vehicles in the car-sharing and bike- sharing systems, including specification of locations and rental costs, up-to-date information about the availability of electric car charging stations, including their parameters.

The tool prepared by the authors is also integrated with **a heuristic approach**, which has made it possible to extend the scope of its applications. It features two types of heuristic concepts, either addressing individual transport network sections or using a matrix-based perspective (separately for different travelling modes). In both these cases, the selection of points considered critical to the given means of transport triggers a dynamic change of the route planned while it is being defined. Such a methodology allows local authorities to impose some pressure on the travelling population in terms of the distribution of traffic flows across the transport network (which may lead to congestion reduction and improved performance of collective transport) as well as the breakdown into means of transport.

The travel planning tool **archives the queries submitted by users**, thus providing additional possibilities of analysing their potential travelling needs as well as adapting the existing transport system (including currently suppressed traffic) to these needs. In parallel to the operations performed by the ETPlanner server, a database of queries is being built, where besides the travelling motivation (home, work, school, shopping, business, recreation, etc.) also user-defined parameters are stored, and these include e.g. the origin/destination points (geographic coordinates), the travel beginning time, the chosen travelling mode, the route optimisation criterion and the information on the declared acceptable walking or cycling distance. The set of queries characterising the **travelling population's needs** becomes a big database, making it possible to monitor the behaviour patterns and habits people display.

Travelling preferences exert a significant influence on how transport systems operate, and by that means, when perceived from a global perspective, also on how cities and regions function. In order to attain an adequate modal split of traffic (with the emphasis put on eco- friendly solutions), all the foregoing preferences need to be intentionally moulded. This can be achieved through various organisational, legal and infrastructural activities. On the other hand, mobility-related needs must be taken into account while introducing changes. It is the only way to orient them towards sustainable development. With extended features, as described in the paper, the ETPlanner can support local authorities in their efforts to solve decision making problems as well as to tackle regular urban traffic management problems on a daily basis. Described approach may well be applied in the future through data standardisation and unification towards

globally endorsed ITS standards.

Keywords: Environmental protection, Sustainable transport system, Electromobility, Transport needs, Travels modelling, Data analytics, Holistic approach for urban travel planning

Cointegration approach in vibration-based misalignment detection in rotating machinery

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Rotating machines are a fundamental type of mechanical equipment and serve as key components in a wide range of industrial applications. Without early detection, misalignment problems in rotor shaft systems can escalate, leading to excessive vibration, increased friction, heightened heat generation, and elevated noise levels. These issues can ultimately result in costly repairs, unexpected operational downtime, and hazardous situations.

The cointegration method has been continuously developed as an effective approach to structural health monitoring (SHM) problems. Rotating machines, being structures subjected to changing and dynamic environments, exhibit non-stationary dynamics. This study aims to apply cointegration to support fault detection within one of the most challenging condition monitoring techniques—vibration measurements. Two approaches are proposed: (1) unit root testing using Augmented Dickey-Fuller (ADF) test of vibration time series before and after cointegration and (2) analysis of cointegration residuals obtained from the cointegration process of vibration time series.

The proposed methods were validated using experimental data obtained from a laboratory test bench comprising a motor, gearbox, and hydraulic gear pump, with and without simulated misalignment of varying severity. The results demonstrate that the proposed method can effectively detect faults and assess their severity. Additionally, the cointegration residuals have been shown to serve as a damage-sensitive feature, highlighting the potential of the cointegration approach in vibration-based condition monitoring.

Keywords:

Structural health monitoring, condition based maintenance, cointegration analysis, time series

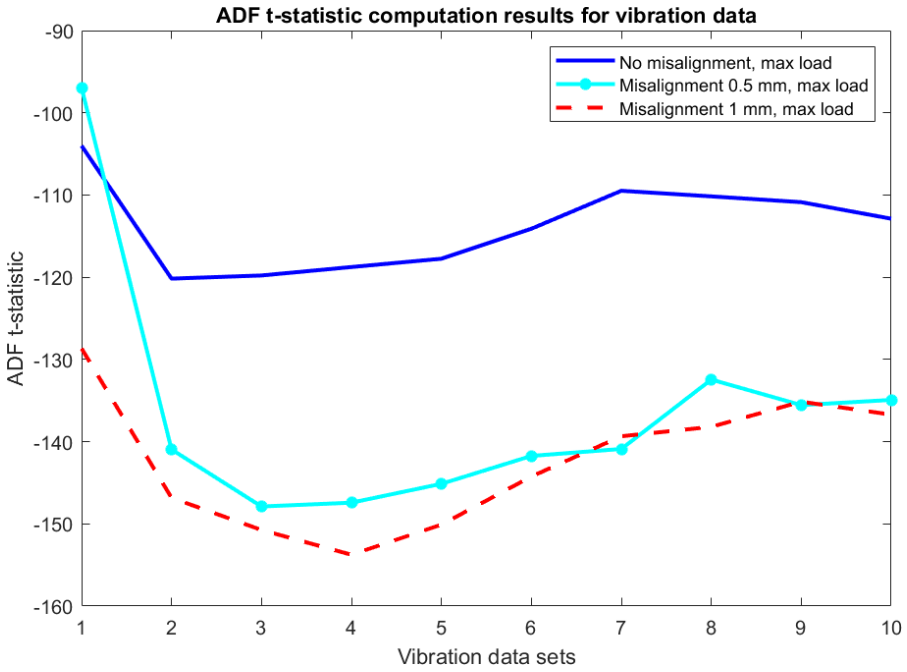

Figure 1 ADF t-statistic computation results for vibration data

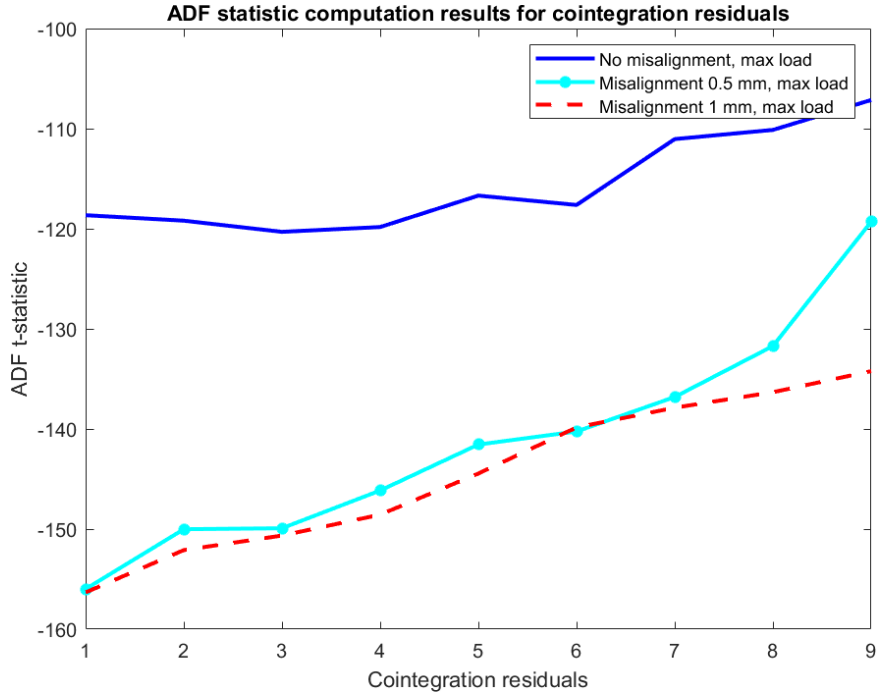

Figure 2 ADF t-statistic computation results for cointegration residuals from different projection cases

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Exploring an Engineering problem with uncertainty in an interdisciplinary journey on the Web

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Abstract: We present the study of a system of nonlinear ordinary differential equations (ODEs), and our objective is to tackle the problem under these complementary perspectives: (*i*) preliminarily, solving the IVP system of ODEs numerically; (*ii*) exploring the solution by imposing random variation on the initial values (IVs), subjected to Gaussian distributions; and (*iii*) providing a constructed, free web page for the consequent dynamic verification of our results by the reader.

The study interlaces modeling and data analysis in an interdisciplinary context, combining a question in Engineering, its mathematical resolution, and its computational and operational research approaches, with a glance at Artificial Intelligence (AI).

The IVs are subjected to random variation, in order to assess the effect of the uncertainty on the quality of the results. Indeed, the IVs are data that can be inaccurate in contrast to the admittedly rigorous mathematical methods. Our problem is related to manufacturing, emanates from Chemical Engineering, and is treated in its mathematical nature, for greater generality.

If the data depend on a practical operation, this may introduce errors, all the more so if the operation is repetitive, hasty, such as in an industrial environment. The problem stems from chemical kinetics, and is adapted from the kinetics of an arbitrary "autocatalytic" reaction, suggested by AI.

The problem was chosen merely because the above mentioned reactions are typically described by nonlinear systems of ODEs that require numerical integration, which facilitates to solve most problems by nonspecial- ists, such as practicing engineers.

Regarding methodology, the study has two stages: (*i*) in a preparatory stage, we present the numerical resolution of the ODEs; and (*ii*) in the main stage, Monte Carlo simulation is applied to the said resolution under random variation of the IVs, in order to assess the effect of that variation under a certain criterion.

STAGE 1: the system of nonlinear ODEs is solved numerically by means of the Python procedure 'solve ivp', allowing to use any of its methods (such as Runge-Kutta). The (free) languages chosen are: PHP to construct the web page; Python for computing, embedded in the web page; and 'gnuplot' (instead of the usual Python module 'matplotlib') as a graphical utility, adopted, once more, for generality, because it is easily called from languages (C, Fortran, etc.) without graphical capabilities.

Although this text is only an abstract of a full description, the result in this stage and the second — according to our Web strategy— can be seen in reference [2] (M. Casquilho, 2025. Explore ODEs, uncertainty), which contains a link to the computation, with all of its results.

STAGE 2; the criterion (among many) was to examine the behavior of the maximum of $y(t)$, one of $x(t)$, $y(t)$, $z(t)$, for the best instant, t^*, found in the previous stage. The maximum is attained only if the IVs are the correct ones, otherwise $y(t^*)$ will oscillate around the true value. How much it oscillates is the result
of the study. The value of $y(t^*)$ will oscillate around the true maximum, as the evolution of the functions is affected by the perturbed IVs. These IVs are each made Gaussian, with μ its true

value and $\sigma = c_v\mu$. Values of c_v, such as 0.5%, 1%, 2%, 5%, 10%, reveal expected increasing distance from the true maximum. The statistical behavior of this value approaches Gaussians, finding their parameters being out of our scope. Interestingly, a finer analysis from extensive Monte Carlo runs negates this impression, by showing a slight positive skewness.

The computations led to qualitative variability in the results, which would, without the proposed procedure, be quantitatively unpredictable.

Providing a Web route to verify our results is meant to be one of the novelties in the study. The web page can be used with our default data or other supplied by a user. This mode of operation is also a gateway for the desired link between academia and industry.

In sum, we studied a system of ODEs describing the dynamics in a Chemical Engineering problem, to assess its behavior under uncertainty in the IVs of the ODEs. This was achieved by Monte Carlo simulation, combining Engineering, Mathematics (with Statistics and Operational Research), Computing, and an aid from Artificial Intelligence, and resulting in a constructed, dynamic web page.

We have since long adopted the Web as a computing medium, using terms such as "web-computing" (ref- erences to our work in 2011–2024), although this preference seems rare in the literature (an exception by Ponce's academic website). Regarding journal articles, the presence of links to computing web pages is rare. Programs sometimes are offered in repositories in languages unknown to the reader. We have advocated our mode of sharing and promoting connectivity, which itself simultaneously protects the authors' own labor.

The accommodation to the Web does not fare without its perils. In fortuitous articles with links for verifi- cation, the links land on extinct addresses. If we recall *verba volant, scripta manent*, any article or similar invoking links to direct computations must survive, maintaining its value, even if the linked addresses disap- pear. In the present and other articles, we comply with this principle by inserting all the related information. The advantage of the Web as the computing medium is the possibility offered for the user to confirm the results shown and try other data. This opening is friendly and has the handy advantage of immediacy.

Keywords: modeling; web computing; ordinary differential equations; Monte Carlo simulation; Engineering.

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Porosity prediction in porous layer electrodes of lithium-ion batteries via Machine learning on Laser Speckle Photometry data

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Keywords: porosity, Laser Speckle Photometry (LSP), prediction, machine learning, electrode

Recent years have focused increasingly on the electrification of transportation, particularly in passenger vehicles, energy storage systems and renewable energies [1]. In the automotive industry, car manufacturers continuously work to enhance vehicle performance and offer competitive products with improved attributes. The battery industry aims to improve battery parameters such as gravimetric and volumetric energy densities. Achieving these improvements requires high-quality electrodes with suitable electrochemical, mechanical, and other quality- related parameters. Our research focuses on evaluating one of these quality parameters, thereby contributing to the production of high-quality electrodes suitable for meeting competitive industry demands. By implementing a nondestructive inspection method in the production process, we aim to improve cost efficiency and product quality.

In production the electrodes, the rolling in the calendaring process leads into a change in the surface topography and, at the same time, to a change in the thermal properties of the coating material due to the compaction of the porous coating. These two properties could be determined using Laser Speckle Photometry (LSP) [2]. This contactless, fast, direct, optical method could be transferred to test LIB coatings.

Therefore, the data acquisition was performed using LSP. The LSP technique comprises three main components: an illuminating laser, an excitation laser, and a camera, enabling high- speed local focus on the inspected surface. For reference, the porosity of the coating was determined by measuring the thickness using the stamp and computer tomography (CT) in the laboratory. Data obtained from the LSP were processed to analyze correlations in dynamic changes of electrode porous-layer topography during thermal excitation. The data was encoded into parameters representing characteristic changes, which were subsequently used as inputs for the Deep Learning model. These input parameters combine quasi-time-related values and cumulative optical changes. In total, eight input parameters were employed—four time-related and four optically related—to represent dynamic changes of surface expansion.

A regression model with eight inputs and two outputs was developed. One output represents porosity, while the other represents the thickness of the porous layer in the scanning area. The model architecture consists of convolutional and fully connected

layers; convolutional layers process quasi-visual inputs, and fully connected layers handle time-series inputs. At an intermediate stage, branches merge into one fully connected layer and subsequently split into two branches: one focused on porosity and the other on thickness. This design allows the model to emphasize data features most relevant to each output.

A total of 911 measurements were collected for experimentation. Twenty-one training iterations were performed, with data splits ranging from 60-40 to 85-15 for training and testing, respectively. Our model achieved an average error of 2.52% for porosity prediction on test data, with a standard deviation of 1.94%. These results confirm the possibility of LSP hardware and software solution for nondestructive porosity inspection of thin layers based on visual surface data of LSP.

Our results demonstrate the feasibility of applying LSP hardware and software solution for inline battery electrode inspection within manufacturing processes [3]. Due to the nondestructive nature of the proposed method, it significantly contributes to smarter, more economical, and higher-quality production and reduction of production waste. In the course specific challenges such as focusing issues on hardware setup and high sensitivity in visual data streams were addressed and successfully mitigated.

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Declaration of Interest:

The authors declare that patent application covering certain aspects of the research reported in this manuscript is currently being prepared.

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Enhancing tribological material characterization and design optimization using Artificial Neural Networks

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In recent decades, polymer-based composites have been widely utilized in tribological applications due to their lightweight nature, self-lubricating properties, and high damping capacity. To accommodate the increasing specific loads associated with compact system designs, these materials are frequently reinforced with fibers and supplemented with internal lubricants or submicron-sized particles to enhance their tribological performance.

The characterization of tribological materials is inherently labor-intensive and time-consuming, requiring comprehensive evaluation across diverse material compositions and load conditions to meet the demands of various working environments. To address this challenge, we employed Artificial Neural Networks (ANNs) as an advanced and efficient approach to improve the evaluation process. With their ability to learn and predict complex relationships, ANNs enable faster analysis and provide deeper insights into the correlation between material composition and tribological behavior under specific conditions, thereby accelerating material optimization. Furthermore, ANNs facilitate systematic comparisons between different formulations, allowing for a more holistic assessment of both production costs and tribological performance. This approach not only aids in selecting cost-effective material solutions but also ensures that essential friction and wear requirements are met. By transitioning from traditional empirical methods to a more systematic strategy, this work provides valuable support and a novel perspective for the development and application of polymer-based tribological composites. Our findings demonstrate that the integration of ANNs into tribological research significantly expedites the characterization process while exhibiting strong predictive capabilities, ultimately enabling a more efficient and cost-effective approach to designing high-performance tribological materials.

Keywords: Artificial Neural Networks, Polymer-based Composites, Tribological Characterization, Performance Prediction, Composite Design

Smart Autonomous Ship Navigation: Combining Automated Route Planning and Model Predictive Control for Collision Avoidance

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Autonomous ship navigation presents significant challenges due to the complex and dynamic nature of maritime environments. Unlike land-based autonomous vehicles, which operate on structured road networks, autonomous ships must navigate unstructured open waters where traffic patterns are less predictable, and environmental factors such as wind, currents, and waves introduce additional uncertainties. Additionally, ensuring safe and efficient navigation requires compliance with the International Regulations for Preventing Collisions at Sea (COLREGs), which govern maneuvering protocols in multi-vessel encounters. Traditional rule-based or heuristic methods for collision avoidance often struggle to adapt to rapidly changing maritime scenarios, resulting in suboptimal route planning and inefficient evasive maneuvers. Consequently, there is a growing need for advanced decision-making frameworks that integrate automated route planning with real-time control strategies to enhance safety, efficiency, and regulatory compliance in autonomous maritime navigation.

This research presents a novel two-stage planning and control framework for autonomous ship navigation based on Model Predictive Control (MPC). The proposed approach consists of an initial route planning phase followed by dynamic waypoint tracking, integrating real-time MPC optimization of vessel trajectories while accounting for multi-vessel interactions, environmental constraints, and navigational safety. Furthermore, it ensures compliance with COLREGs.

In the first stage, global route planning is performed using search-based algorithms (e.g., A* and Theta*) to construct an optimal path represented by a series of waypoints. This precomputed trajectory serves as a high-level navigation plan, guiding the vessel toward its destination while avoiding static obstacles such as coastlines and restricted zones.

In the second stage, real-time dynamic tracking of the planned waypoints is executed using an MPC-based control system. When the vessel is in open waters and no other ships or obstacles are detected within the predictive horizon, it follows the trajectory in a straight-line manner toward the next waypoint. However, when other vessels enter the predictive horizon, the MPC controller activates, dynamically adjusting the trajectory to avoid collisions while adhering to COLREGs. By continuously solving an optimization problem over a receding time horizon, the system ensures that navigational decisions remain adaptive to dynamic environments, including changing traffic densities. This guarantees a balance between safety, efficiency, and regulatory compliance in complex maritime environments.

A MATLAB-based simulator has been developed to model various maritime scenarios involving multiple ships with different speeds and courses. The MPC framework predicts future vessel states within the predictive horizon based on real-time sensor inputs, such as the Automatic Identification System (AIS), and dynamically adjusts steering commands to minimize collision risk while optimizing route efficiency.

Simulation results demonstrate the effectiveness of the proposed MPC-based approach in integrating route planning with proactive collision avoidance. Compared to conventional heuristic-based methods, the proposed system significantly reduces unnecessary course alterations, leading to lower energy consumption and improved voyage planning. The framework is adaptable to various ship types and operational conditions, making it a promising solution for real-world autonomous maritime navigation.

Future work will focus on integrating real-world sensor data, refining the cost function for enhanced decision-making under uncertainty, and validating the approach in physical autonomous vessels. Additionally, the framework will be extended to multi-agent scenarios where multiple autonomous vessels operate concurrently, requiring cooperative and non- cooperative maneuvering strategies. Future research will also incorporate machine learning techniques to enhance environmental perception and decision-making in complex maritime conditions.

Keywords: Maritime Navigation, Autonomous Ships, Automated Route Planning, Collision Avoidance, COLREGs, Model Predictive Control, MATLAB Simulation

AI-Driven Analysis of User Interactions in Parametric CAD Systems

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To remain competitive in a highly globalized market, industrial companies must adopt rigorous design and production processes. These processes must be both efficient and adaptable, and enable rapid design iterations and modifications to meet the demand for new and updated products while maintaining high-quality standards. Reducing 'Time to Market (TTM)' is critical to allow companies to respond swiftly to industry needs, optimize costs, and expand their market share. In this context, advanced 3D CAD modeling tools, particularly those based on parametric associative technologies, are instrumental for boosting productivity, ensuring design precision, enabling simulations under real-world conditions, and facilitating interdisciplinary collaboration.

To be truly effective, the 3D models created with these tools must meet specific requirements to achieve their goals. Models should clearly convey the design intent of the parts they represent, allowing modifications and updates without compromising integrity. They must also establish precise geometric relationships and constraints to ensure changes propagate consistently and without errors. Additionally, models must be reusable across various contexts and applications, i.e., adaptable to new projects without requiring complete redesigns, while also being resource-efficient to avoid unnecessary complexity that could negatively impact regeneration and processing speeds. It has been shown that the adoption and systematic application of formal parametric modeling methodologies like Horizontal, Explicit Reference, and Resilient, in the design process have a positive impact on achieving the previous objectives, particularly when compared to other non-structured modeling approaches. These studies also highlight the importance of parametric CAD methodologies in general, to meet expected standards of quality, reuse, and model adaptability.

An increasing number of companies, particularly those embracing the Model-Based Enterprise (MBE) paradigm, are beginning to consider the role of CAD quality in their approaches to modeling. However, significant resources must be allocated to master these methodologies and also evaluate the quality of the models produced. Typically, models are reviewed and assessed by experts or peers at the end of the design phase. Findings are then sent back to design teams for revisions and updates, of necessary. Similarly, in educational contexts, instructors regularly evaluate the modeling quality and procedure of the models created by students. In both cases (industrial and academic), implementing a continuous supervision model within the

organization could significantly enhance the evaluation process, instead of relying on feedback from subsequent design stages. This approach, however, would require considerable human resources for supervision tasks, potentially making it financially unsustainable.

This research introduces an automated supervision system for CAD quality assessment that reduces reliance on specialized personnel. The system, an expert tool based on Artificial Intelligence (AI) technology, supervises the design process and evaluates the quality of parametric 3D CAD models and the correct application of formal methodologies.

Although parametric CAD applications can generate some metadata and log basic information about the user's actions during a work session, accessing and analyzing this data relies on the proprietary Application Programming Interface (API) libraries provided by the CAD vendors. These libraries are notoriously complex, poorly documented, application-dependent, and generally incompatible with each other. Moreover, access to modeling operation sequences is often limited or non-existent.

The proposed system analyzes images from video data captured directly from the computer screen in real time, while the user operates the CAD system. It extracts information using artificial intelligence techniques, specifically a real-time object detection model based on YOLO (You Only Look Once), which employs a Convolutional Neural Network (CNN). The Neural Network must be trained once for each 3D CAD application where design analysis is required, resulting in an AI model. In this study, models were trained for the major 3D CAD applications. The training process is straightforward, does not require advanced programming knowledge, and is consistent across all CAD applications, overcoming the major challenge of working with different APIs.

The developed system extracts and identifies any visual elements visible on the screen from the video signal (icons, icon states, messages, symbols, etc.) and stores each event in a Temporal Database (TDB). Additionally, an initial version of a neural network was trained to analyze these temporal event sequences, providing an automated evaluation of key aspects related to the accuracy and quality of the modeling process. This neural network operates as an advanced analysis layer, independent of specific applications, and relies solely on common information from the temporal event sequences.

The preliminary validation of the system involved comparing assessments of models with different levels of complexity, conducted both by experts and through automated methods.

Keywords: 3D parametric CAD, Artificial Intelligence, Neural Networks, Automated Analysis

Probability Mass Function based Divergence Guided Focal Loss for a Multi-Head Multi-Task Neural Network

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Encouraged by the sustainability benefits, many industrial manufacturers adopted carbon fiber (CF) materials as a standard material for the components manufacturing across various domains. However, these materials are likely to reach their end-of-life in the upcoming years. To enhance the optimal usage of resources and reduce the CO2 emissions many companies are looking to extract, reprocess and reuse these end-of-life CFs at an industrial scale. During the manufacturing process of virgin or recycled CF material (CFM), several unwanted defects can be introduced, which may consequently result in the reduced strength of the manufactured end-component. Thus, the inspection of the CFM prior to final component production represents an essential quality control step.

Computing the depth of a scene using multi-directional light sources with a single camera is photometric stereo. This method is widely used for CF quality control as it facilitates the computation of fiber orientations at each location of the CFM. Inspecting CFM images for quality control using deep learning introduces several challenges and distributional shift is among them. Global, local and self-attention based mechanisms try to mitigate these issues and improve the classification results. However, these methods might either not 1). improve the overall accuracy much, 2). increase resource consumption or 3). reduce the inference speed due to complex self-attention mechanism. Thus, making the inspection system more counterproductive in an industrial production environment. Hence to minimize these issues, custom lightweight multi-head convolutional neural networks are preferred in industrial environment.

This paper addresses the issue of improving accuracy of a multi head classifier though adaptive focus parameter (γ) in focal loss besides attention mechanism. This γ value is computed by the similarity metric using Jensen-Shannon divergence between each head's output i.e. the probability mass function (PMF). This paper demonstrates the efficacy of the proposed method through extensive benchmarks performed on publicly available dataset and prior state of the art works. To estimate the improved accuracy, prior state-of-the-art architecture was extended with attention mechanisms to obtain multi-head architecture, and the proposed method was tested. Several ablation studies were also conducted with Kullback- Leibler divergence, Total Variation (TV) distance, Hellinger distance and Wasserstein distance to determine the optimal metric. The proposed method outperformed the current state of the art by more than 5%.

Keywords: Probability mass function, probabilistic divergence, Jensen-Shannon divergence, Kullback-Leibler divergence, total variation (TV) distance, Hellinger distance and Wasserstein distance, multi-head neural network, multi-task neural network, class activation maps, and global attention mechanisms.

SEMF: Supervised Expectation-Maximization Framework for Predicting Intervals

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Abstract: This work introduces the Supervised Expectation-Maximization Framework (SEMF), a versa- tile and model-agnostic approach for generating prediction intervals in datasets with complete or missing data. SEMF extends the Expectation-Maximization algorithm, traditionally used in unsupervised learning, to a supervised context, leveraging latent variable modeling for uncertainty estimation. Extensive empirical evaluations across 11 tabular datasets show that SEMF often achieves narrower normalized prediction in- tervals and higher coverage rates than traditional quantile regression methods. Furthermore, SEMF can be integrated with machine learning models like gradient-boosted trees and neural networks, highlighting its practical applicability. The results indicate that SEMF enhances uncertainty quantification, particularly in scenarios with complete data.

Keywords: Supervised learning, Expectation-Maximization, Prediction intervals, Uncertainty quantification

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Evaluation of data pre- and post-processing strategies for MOSFET

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ANN modeling application

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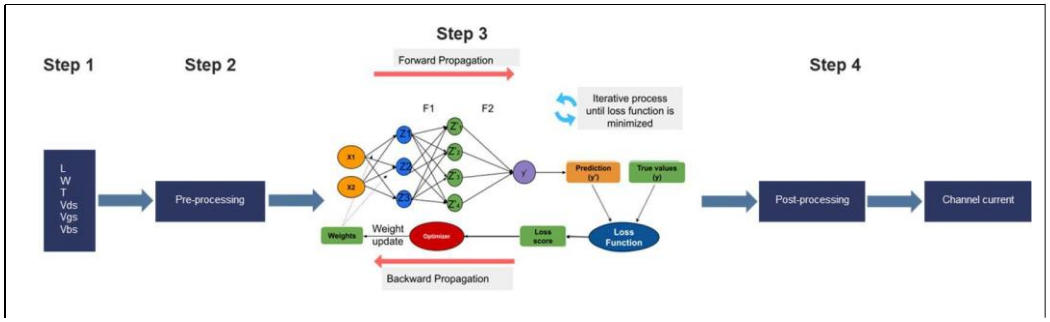
Over the past years, the number of submitted articles studying MOSFET modeling with artificial neural networks (ANNs) has increased within the microelectronics research community. However, many recent works tend to replicate previous approaches. Most studies follow a similar framework: starting from a physics-based model, generating data, applying pre- and post-processing (PPP), training an ANN with a tailored loss function, and presenting results. However, previous works often lack details on key choices, such as data processing techniques and the implementation of the loss function. In our work, we aim to address these ambiguities by providing a deeper insight of these aspects. Additionally, we will highlight the regions where the ANN model still struggles to achieve accurate predictions. Our objective is to guide future research and offer a structured approach for further improvements.

Keywords: Artificial neural networks, Compact model, Device modeling

Methodology and Preliminary Results

As illustrated in **Figure 1,** the development process of an artificial neural network (ANN) model for modelling the MOSFET channel current follows a workflow that is widely utilised in contemporary research. This serves as the baseline in multiple studies [1] and it is used in our work with particular emphasis for the



analysis of critical steps in the modelling process. In our study, we use simulation data of FD-SOI transistor generated from the standard compact model L-UTSOI [2]. Our dataset is a complete set of channel curent (I_{ds}) under six parameters: gate, drain and bulk voltages (V_{gs}, V_{ds} and V_{bs}), gate length and width (L and W), and temperature (T).

Figure 1 : The Process of Developing a Compact ANN Model for MOSFET Channel Current

The next step after data preparation is PPP (Steps 2 and 4 in our workflow). For post-processing, an established way to improve the physicality of the model [3]

is to predict the logarithm of the conductance $y = \ln(I_{ds}/V_{ds})$ rather than direclty I_{ds} [1], [3]. In the state of the art, choices in PPP steps are often not supported by performance metrics, although their motivations are discussed. In our work, we systematically benchmark the impact on these metrics of three PPP strategies: 1) a ln transformation applied on W and L inputs 2) input normalizations amongst four formulations and 3) (**Table 1**) introduction of W and L scalings into the output post-processing.

In Step 3, two key aspects need to be discussed: the model architecture, and the optimization algorithm along with the loss function. For the proposed ANN model, we used a 6-15-15-15-1 architecture, comprising 601 parameters, to effectively capture the relationships within our dataset. All neurons have a tanh activation function appart from the last one that has an identity activation function. Regarding the loss function, we implement a composite one [1], composed of 4 mean squared error (MSE) terms. $Loss = MSE(y) + A \cdot MSE(e^{y}) + B \cdot MSE(\partial y/\partial Vds) + C \cdot MSE(\partial y/\partial Vgs)$, each term ensuring accuracy across both sub-threshold and saturation regions (1st and 2nd terms) and on the monotonicity of the model with respect to V_{ds} and V_{gs} (3rd and 4th terms) , improving training stability [3]. To determine the coefficients, [3] suggest to increment each loss term during successive trainings and adjusting the coefficient so that the magnitude of the new loss term is comparable to the previous global loss. In our work we evaluate the benefit of this loss implementation conducting an ablation study, summarized in **Table 2**, Additionally, we assess an alternative approach where coefficients are computed at the begining of the training to equalize the contribution of each loss term. The iterative loss method achieves the best accuracy.

Conclusion

This study developed an ANN-based model for FD-SOI transistor modeling, aiming to address key challenges in data preprocessing, model architecture, and loss function design. By providing a deeper insight into these aspects, we were able to clarify some ambiguities that were previously unexplored. While our approach shows improvements, some limitations remain in specific input regions, (***Figure* 2**). In the final paper, we will focus on refining these areas to further improve the model's accuracy and robustness, offering clear guidance for future

research.

Table 1 : Comparison of RMSE for Different y Relative to I_{ds}

Model	RMSE _ Ids	RMSE _ log(Ids)
1 : $y = \log(I_{ds} + V_{ds} * g_{ds})$	2.03e-5	9.68e-2
2 : $y = \log(I_{ds} + V_{ds} * g_{ds})$	9.00e-6	6.02e-2
3 : $y = \log(I_{ds} + V_{ds})$	2.50e-5	1.14e-1
4 : $y = \log(I_{ds} + V_{ds})$	1.61e-5	7.98e-2

Table 2: Ablation Study: Impact of Loss Function

Loss composition per Model	$MSE(y)$	$MSE(e^y)$	$MSE\left(\frac{\partial y}{\partial V_{ds}}\right)$	$MSE\left(\frac{\partial y}{\partial V_{gs}}\right)$
1 term	2.72e-3	2.73e-3	1.87e-2	1.01e-1
2 terms / A = 100	1.13e-3	1.91.e-6	9.41e-3	5.89e-2
3 terms / A = 100 & B = 0.15	8.72e-4	1.52.e-6	4.32e-3	4.77e-2
4 terms / A = 100 & B = 0.15 & C = 0.02	8.70e-4	1.83.e-6	4.10e-3	3.47e-2

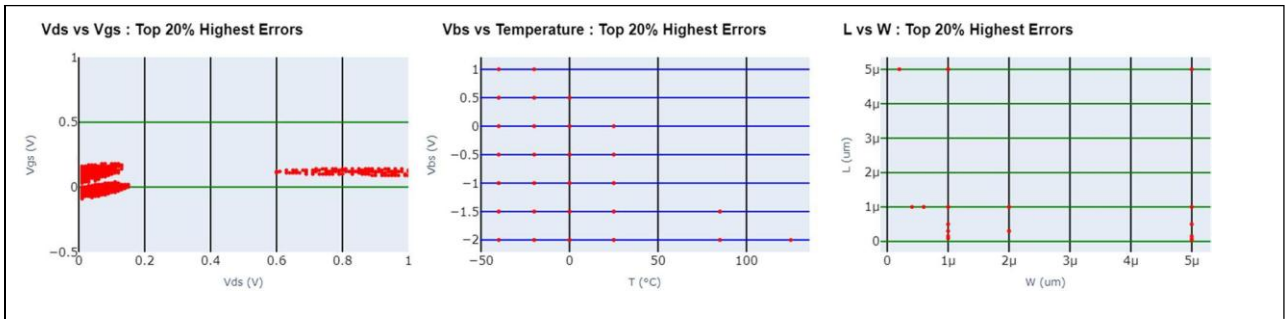


Figure 2: Distribution of Top 20% Errors in the Test Set Across Input Features

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Analysis of the Results of an Experimental Campaign on Tire-Road Dry and Wet Friction Conducted with the British Pendulum Evo Bench

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Abstract:

Friction at the tire-road interface is a fundamental aspect of vehicle safety, handling, and braking perfor- mance. Ensuring sufficient friction is essential for both high-performance and passenger vehicles, as it directly influences stability and rideability. Friction results from a combination of various factors, including the vis- coelastic properties of the tire compound, road surface characteristics, contact pressure, temperature, and sliding velocity [1]. Over the years, numerous studies have focused on frictional behavior in dry conditions, with findings indicating that the interaction forces between the tire and the road surface are mainly due to an adhesive and hysteretic contribution related to the viscoelastic properties of the rubber compound and the roughness of the counter surface. Various theories have been developed to better understand the underlying physical mechanisms [2, 3]. While the mechanisms governing wet friction remain less understood, existing studies indicate that frictional interactions in the presence of water are influenced by additional complex effects, such as hydrodynamic lift, viscous shear, and the capacity of the tread pattern to evacuate water [4, 5, 6]. Despite extensive research efforts, existing studies do not converge toward a single comprehensive model capable of describing wet friction mechanisms, leaving gaps in our understanding of which contribu- tions are dominant. However, they all agree that wet conditions lead to a significant reduction in friction, posing a serious risk to vehicle passengers.

This study positions itself within this research landscape by systematically analyzing the frictional behavior of rubber specimens under both dry and wet conditions, with the aim of investigating the differences between these two scenarios. Overall, the objective is to provide a quantitative evaluation of the key influencing factors in the physics governing tire-road friction in both conditions.

To achieve this, an extensive experimental campaign was conducted using the British Pendulum EVOlved, a specialized test apparatus designed to analyze the frictional behavior of rubber materials sliding on a controlled counter-surface. The device functions by releasing a rigid arm from a predetermined height, causing a rubber specimen mounted at its end to impact and slide over the test surface. A triaxial load cell continuously records longitudinal, lateral, and normal forces, enabling a comprehensive characterization of the interaction dynamics. An encoder measures the velocity of the rigid arm, which is controlled by adjusting the pendulum's release height, allowing for a systematic investigation of the sliding velocity of the rubber compound on the counter surface and, hence, the velocity-dependent friction effects.

A key feature of this study is the systematic variation of experimental parameters to assess their influence on frictional forces. In particular, tests were conducted on two different asphalt-like surfaces, each characterized by roughness scans to highlight their differences. The role of rubber viscoelasticity was investigated by testing seven different specimens with distinct viscoelastic properties, evaluated with the VESevo innovative device. Temperature effects were analyzed by preheating the rubber samples with a heat gun to a target temperature before each test, ensuring precise thermal conditions. Contact pressure was adjusted by varying the preload of the pendulum arm's internal spring, providing insight into pressure-dependent friction effects. Since normal force plays a crucial role in friction performance, controlling this parameter allowed for a deeper

investigation of its impact, particularly in comparing dry and wet conditions.

A major focus of this work is the direct comparison between dry and wet frictional behavior under the same testing conditions. The wet condition was simulated through a controlled application of water on the test surface, ensuring a uniform water film. The contact pressure was found to play a crucial role in differentiating the behavior between dry and wet conditions, influencing the overall frictional response.

To ensure the robustness of the findings, each test configuration was repeated multiple times, and an average normal and longitudinal force curve was computed for each set of parameters. The force evolution over time followed a characteristic trend, best described using a novel double-exponential fitting model. This new methodology accurately captured three key parameters: peak magnitude, peak location, and the width of the force response. Once extracted, these parameters were interpolated across the dataset, allowing us to evaluate the forces and, hence, the frictional behavior beyond the tested cases.

This setup allowed us to isolate the effects of sliding velocity, temperature, contact pressure, and rubber properties on frictional forces while minimizing external variations. The analysis revealed several key findings: the evaluated friction coefficient exhibited a strong dependence on velocity and temperature, showing a parabolic trend [7, 8]; the presence of water significantly modified the force response, leading to an expected reduction in friction. However, this reduction was not uniform across all conditions, as material properties and surface characteristics played a crucial role in determining the extent of friction loss. Additionally, the relationship between contact pressure and friction differed considerably in wet versus dry scenarios: wet tests showed more complex variations.

The comprehensive dataset and subsequent analysis provided new insights into the evolution of friction across different sliding speeds, temperatures, rubber materials, and contact pressures, enabling a deeper understanding of dry and wet friction behaviors and their differences. By systematically quantifying these effects, this study contributes to a more refined comprehension of the physical phenomena governing tire-road interaction.

Future research will focus on developing predictive models that incorporate the experimental findings, aiming to improve tire-road interaction simulations and road safety.

Keywords: tire-road interaction, friction, wet contact, innovative friction tester

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On the vehicle performance optimization: a methodology to predict tire behavior through viscoleastic analysis

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Abstract: Motorsport represents one of the most advanced domains for testing and enhancing vehicle performance, where even marginal gains can determine the outcome of a competition. Consequently, contin- uous optimization of vehicle performance is pursued across all subsystems, including aerodynamics, chassis setup and tires [1]. Among these, tire research has gained considerable attention in recent years due to the complex and highly nonlinear behavior of tires, as well as their fundamental role as the sole contact interface between the vehicle and the road surface [2]. Rather than being passive components, tires actively regulate the transmission of forces essential for acceleration, braking and handling, ultimately constrain- ing the vehicle's performance capabilities. Regardless of advancements in aerodynamic efficiency or engine power, the vehicle's overall performance is inherently dependent on the tire's ability to generate and main- tain grip. This aspect is particularly critical in motorsport, where extreme operating conditions and highly competitive environments further amplify the influence of tire performance. In this context, a comprehensive understanding of tire behavior becomes essential for optimizing overall performance. Although tires of the same nominal compound are expected to perform similarly, subtle variations in their characteristics—such as those arising from manufacturing tolerances, thermal conditions or usage history—can lead to significant differences in performance. These variations impact key factors, including grip, wear and handling, which in turn affect the vehicle's competitive advantage.

The dynamic behavior of a race vehicle is intrinsically linked to the viscoelastic properties of the tire tread material, which govern its interaction with the road surface. These properties are influenced by two primary mechanisms: (i) the chemical adhesion between rubber molecules and the road surface, and (ii) the mechan- ical interlocking between the tread and road asperities [3]. Understanding and quantifying these viscoelastic properties are therefore crucial for predicting tire performance and, consequently, vehicle behavior under dynamic conditions. This study aims to investigate tire viscoelastic properties and assess their influence on the maximum achievable

longitudinal and lateral acceleration of a race vehicle. The analysis is conducted using the VESevo device, which enables non-destructive characterization of viscoelastic materials [4]. This methodology provides two complementary approaches to evaluating tire viscoelasticity. The first involves measuring and analyzing the storage modulus and loss factor as functions of temperature, which offer insights into the thermal dependence of the material's elastic and dissipative characteristics. The second approach involves the calculation of two viscoelastic indices at room temperature: the Adhesive Viscoelastic Index (AVI), which quantifies the adhesive properties of the rubber compound, and the Hysteresis Viscoelastic In- dex (HVI), which characterizes its energy dissipation behavior due to hysteresis. The ability to characterize viscoelastic properties in a non-destructive manner enables repeated testing on the same tires, allowing foran in-depth evaluation of performance evolution as a function of wear and mileage.

The findings of this study provide a comprehensive viscoelastic characterization of the tires, shedding light on how these properties evolve with tire usage and identifying correlations between viscoelastic behavior and on-track performance. By analyzing these relationships, this research aims to determine which viscoelastic characteristics contribute most significantly to enhanced performance. Ultimately, a novel methodology has been developed to evaluate tire viscoelastic properties, establish correlations with wear, and predict the maximum potential acceleration of a race vehicle as tire mileage increases. This approach offers valuable insights for optimizing tire selection, usage strategies and overall vehicle performance in competitive racing environments.

Further advancements in this research will focus on expanding the available dataset to enhance the robust- ness and reliability of the identified correlations between tire viscoelastic properties and vehicle performance. By incorporating a broader range of test samples, particularly those with very high mileage, it will be possi- ble to refine the predictive model and improve its accuracy in capturing the evolution of tire behavior over extended usage periods.

Keywords: measurements; vehicle dynamics; viscoelastic material; race strategy; tire analisys; race methodologies; performance evaluation; predictive model

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Developing a Chatbot for MBSE Models using Knowledge Graphs and Large Language Models

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In recent decades, the development of automobiles has become increasingly complex due to the integration of software and electronics and growing customer demands for functionality. Simultaneously, stricter regulations for regarding functional safety further complicate product development. As a result, engineers face challenges in managing the rising number of interdependencies between systems and ensuring compliance with evolving safety regulations. To address this increasing complexity, establishing digital models of the system following the idea of Model-Based Systems Engineering (MBSE) during product development has emerged as a key strategy. MBSE helps manage complexity through formalization, ensuring unambiguity in system representations. It enables traceability of development artefacts and provides a single source of truth, meaning all information about the system is centralized and accessible.

Despite these advantages, several significant challenges impede the efficient utilization of MBSE. MBSE models are intrinsically complex. The effective utilization of these models necessitates a workforce with specialized systems engineering expertise. However, a notable deficit in such expertise constitutes a significant barrier. The process of acquiring these advanced competencies requires substantial investments in both training and time, which further exacerbates the challenge. Consequently, these factors impede the broader adoption of MBSE, as the long-term benefits are frequently perceived to be outweighed by the initial costs.

To address these issues, we propose the development of an interactive chatbot that enables engineers to effectively query MBSE models, making the information more accessible and easier to understand. By simplifying interaction with MBSE models, the chatbot reduces the need for extensive training and lowers the barrier for workforce skill development. For example, engineers could ask questions like "What are the functional requirements for the battery?" or "Which components are necessary for function X?" Such queries help users quickly obtain specific information without navigating complex models, thereby demonstrating tangible short-term benefits and facilitating organizational acceptance.

However, integrating MBSE models directly with large language models (LLMs) poses technical challenges. The structured nature and extensive size of these models can exceed the context window of LLMs, making direct interpretation impractical and resulting in context that is not necessary to answer a certain question making this approach inefficient. To overcome this, our methodology involves the transformation

of a SysMLv2 MBSE model into a knowledge graph – a structured representation that facilitates efficient querying and reasoning. The knowledge graph captures the rich relationships and semantics within the system model in a format more accessible to LLMs. By abstracting the complex syntax of SysMLv2 into interconnected entities and relationships, the knowledge graph mitigates incompatibility issues. Building upon this knowledge graph, we implement a Retrieval-Augmented Generation (RAG) approach. Retrieval Augmented Generation is a method that enhances the output of large language models by integrating relevant external information retrieved from knowledge sources into the generative process. The use of a knowledge graph enhances the chatbot's ability to interpret and reason over the system model data, improving the quality and relevance of the responses.

In this paper, we present this methodology using a case study of a battery electric powertrain, modeling the abstraction levels of requirements, functions, logical architectures, and product structures (RFLP). We also provide examples of chat interactions as a proof-of-concept to demonstrate the effectiveness of our approach. Furthermore, we offer an outlook on potential use cases and applications that will be explored in future research.

Keywords: Model-based Systems Engineering, Knowledge Graphs, LLM, RAG, SysMLv2, RFLP

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Design of a reduced-order model of suspension constraints for real-time applications

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Abstract: The automotive industry is increasingly advancing its level of automation, progressively moving towards autonomous driving and smart mobility solutions, driven by the development of Advanced Driver Assistance Systems (ADAS) [1]. In this scenario, virtual sensing techniques play a crucial role by enabling the estimation of unmeasurable quantities using commonly available on-board measurements [2]. In particular, a critical aspect of real-time vehicle stability and drivability control lies in the estimation of tire kinematics and dynamics, particularly slip and the forces exchanged with the road. In this regard, the suspension system, with its inherent constraints, plays a decisive role in influencing wheel alignment under various loading and steering conditions [3], but in the current state of the art it is not explicitly integrated into virtual sensing logic, except through multibody modeling approaches [4], which are computationally intensive and typically customized for the specific geometry being modeled.

This paper presents a simplified and highly computationally efficient approach to model suspension kinematics, aiming to accurately reproduce wheel camber and toe angles as functions of wheel displacement and steering angle. The proposed method relies on extremely efficient and continuous polynomial functions, whose differentiability is crucial for integration into model-based estimators. Furthermore, to make the approach suitable for on-board auto-tuning applications that enable real-time parameterization of the model [5], monotonic relationships between the model's coefficients and the key geometric parameters influencing suspension kinematics have been included within the formulation.

The development and validation process of the proposed approach can be divided into three phases: a sensitivity analysis, conducted to identify the key geometrical parameters—such as the lengths of the rigid elements and the angles between them; a data collection designed for the identification of the model parameters, performed through an optimization algorithm; finally, the model validation on an additional data-set to mitigate the risk of overfitting. In each of these phases, a multibody model has been employed to generate the simulation data used as references. The simulations consisted of vertical wheel displacements under static conditions, with a constant steering angle, repeated for different steering angles and varying suspension geometries.

In the sensitivity analysis, a preliminary set of simulations has been conducted to identify the geometric parameters that most significantly influence the kinematic quantities of interest. In this phase, the simulations have been repeated by varying a single parameter at a time, applying different percentage changes, and observing the corresponding variations in the toe and camber curves with respect to wheel displacement, compared to the initial geometric configuration.

The described selection phase has been crucial in reducing the number of simulations required to build the dataset employed for the model parametrization, performed by varying only the most influential parameters on suspension kinematics. The simulation set has been designed by fixing a range of variation for the aforementioned geometries and steering angles, and including both

single and combined variations of these parameters to make the optimization process as robust as possible.

Following the identification and accuracy verification with respect to the tuning dataset, the model has been validated on an additional set of simulations conducted with different parameters compared to the previous data-set, applying random variations even to parameters excluded from the optimization process. This further validation showed a good level of accuracy in matching the reference data, particularly for the camber-displacement curves. For the toe-displacement curves, which exhibited more nonlinear variations with the suspension geometries, the accuracy tends to decrease.

In conclusion, since the error remains within an acceptable range, the model demonstrates good reliability and robustness, especially considering its simple formulation and the non-customized approach for which it was designed. In fact, its parameters are not optimized for a single configuration but for a wide domain,which consists of a fundamental requirement for auto-tuning applications in scenarios where, lacking accurate suspension system information, it is necessary to recognize the system's parameters during the real-time estimation process.

Keywords: suspension modelling, constrained systems, kinematics, vehicle state estimator, computational efficiency

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Scalable Data-Driven Allergenic Pollen Forecasting for Enhanced Allergy Risk Management

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Airborne allergenic pollen is a significant environmental factor affecting public health, triggering allergic rhinitis and asthma in millions worldwide. Accurate forecasting is essential for mitigating health risks, yet traditional chemical transport models (CTMs) struggle with uncertainties in meteorological inputs, pollen emissions, and species distribution. Recent advances in machine learning (ML) offer a promising alternative, leveraging data-driven techniques to enhance forecast accuracy. However, ML-based pollen forecasting remains underutilized, particularly in regions with sparse monitoring infrastructure.

This study presents a scalable ensemble ML methodology for multi-day forecasting of airborne pollen concentrations, focusing on two of Europe's most allergenic taxa—birch (*Betula*) and grasses (*Poaceae*). The approach integrates four top-performing ML algorithms— Random Forest, Extremely Randomized Trees, Extreme Gradient Boosting, and Light Gradient Boosting Machine—to improve predictive accuracy and robustness. Models were trained on historical pollen data (2006–2022) from Wrocław, Poland, incorporating meteorological and phenological predictors derived from the Weather Research & Forecasting (WRF) model, as well as pollen concentrations with various time lags. Performance was rigorously evaluated through nested leave-year-out cross-validation and tested on independent data from 2023–2024. Additionally, the models were assessed at other locations in Poland (Szczecin, Łódź, and Kraków), demonstrating their broader applicability. The methodology was further tested under varying conditions of local pollen data availability, including scenarios where local observations were missing. Results indicate that the ensemble models

consistently outperform individual ML algorithms and remain reliable for up to five days, even in the absence of local lagged pollen data. Forecast interpretability analysis highlights key predictors, such as meteorological factors (temperature, wind dynamics, humidity, solar radiation), phenological indicators (growing degree days), and lagged pollen concentrations, which played a dominant role in short-term predictions.

This research underscores the potential of ensemble ML models for operational pollen forecasting, offering a data-driven alternative to traditional numerical approaches. As real-time pollen monitoring technologies continue to develop, integrating automated detection systems with ML-based forecasting could further enhance prediction accuracy. The proposed methodology provides a foundation for future advancements in AI-driven environmental health applications, enabling more effective management of pollen-related allergies in regions with sparse monitoring infrastructure.

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Autoencoder-Based Deep Learning Model for CFD Urban Airflow Prediction

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Abstract: Urban Air Mobility (UAM) is emerging as a key solution to modern transportation challenges, integrating Unmanned Aerial Vehicles (UAVs) into complex urban environments. However, the viability of UAV operations depends on the ability to predict urban airflow dynamics in real time, as turbulent flows and wind gusts can significantly affect flight stability. Traditional numerical simulations, such as Computational Fluid Dynamics (CFD), provide detailed insights but are computationally expensive, limiting their use for real-time applications. To address this challenge, we propose a data-driven model capable of rapidly predicting urban wind fields, which can be integrated into UAV flight planning systems.

This study develops a deep learning framework that combines convolutional autoencoders (CAE) and deep neural networks (DNN) to reconstruct flow fields efficiently. A CFD database is generated by simulating air- flow within a circular domain containing central obstacles that mimic urban buildings. Two key parameters, wind speed and wind direction, are parametrized to generate a dataset with different flow conditions. The resulting flow fields are then encoded into a low-dimensional latent space using the CAE, capturing essential aerodynamic features. A DNN is subsequently trained to predict this compressed representation based on wind magnitude and direction, enabling the rapid inference of new flow scenarios without requiring full CFD simulations. The predicted embedding is then decoded to reconstruct the corresponding flow field.

By leveraging nonlinear feature extraction, this approach could offer an alternative to classical reduced- order modeling techniques such as proper orthogonal decomposition (POD). The accuracy of the proposed model is evaluated against POD-based methods to assess its effectiveness in preserving flow structures and computational efficiency. This work demonstrates the feasibility of deep learning for real-time urban airflow prediction, paving the way for its integration into UAV navigation systems.

Keywords: Computational Fluid Dynamics, Data-Driven Models, Autoencoders, Deep Neuronal Networks

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* Presenting author

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Composite Bayesian Optimisation of Materials and Structures

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Meeting growing industrial demands requires the rapid development of materials with enhanced mechanical properties. With tighter technological constraints and limited time for material exploration, simulation-based design has become increasingly valuable. Advances in high-performance computing and numerical modeling enable cost-effective, flexible, and fully automated material discovery. However, efficient optimisation techniques, such as Bayesian optimisation, are essential for quickly identifying optimal materials.

This work presents a composite Bayesian optimisation framework, which has been applied for both parameter identification via curve fitting [1], as well as structural and material analysis and design [2]. By leveraging the compositional nature of the objective function, our approach significantly reduces the number of required experiments and outperforms state-of- the-art optimisers. Its probabilistic foundation allows for uncertainty modeling, making it well- suited for optimising stochastic objective functions. We also introduce piglot [3], an open- source Python package for derivative-free optimisation, and demonstrate the framework through applications such as parameter identification in a crystallographic-slip model, beam cross-section design, and stochastic polycrystalline microstructure optimisation. Our results show that the composite Bayesian optimisation framework is a powerful tool for material and structural design, enabling the rapid development of advanced materials with superior properties in a completely unsupervised manner.

Keywords: Bayesian optimisation, multi-scale modelling, material design

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https://doi.org/10.21105/joss.06652

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Advancing Degradation Modeling in PEM Water Electrolysis with Physics-Informed Machine Learning

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Accurate degradation modeling is crucial for enhancing operational efficiency and extending the lifespan of proton exchange membrane water electrolysis (PEMWE) systems. By effectively predicting degradation trends, optimized maintenance strategies can be developed, significantly lowering operational costs. Machine learning (ML) has emerged as a promising approach for predictive tasks, as it can benefit from the increasing amount of available data to address the limitations of traditional physical models, which arise from an incomplete understanding of complex degradation processes.

Previous analyses of a proposed data-driven degradation modeling matrix highlight this ML potential and present a modeling concept demonstrating the feasibility of predicting future polarization curves from discrete operational data [1]. This capability provides valuable state- of-health (SOH) insights that are typically inaccessible during normal operations. However, using artificial neural networks (ANN) based solely on the provided training data unveils a limitation: if test data deviates from the training data distribution, the ANN struggles to accurately predict polarization curves at low current densities, compromising physical plausibility. This issue emphasizes the potential of physics-informed machine learning (PIML), where domain knowledge is integrated into the modeling process to ensure compliance with established scientific principles [2]. Considering the known logarithmic nature of activation losses, embedding such physical knowledge in this exemplary case is a natural extension toward better prediction accuracy and increased reliability. Therefore, this study systematically investigates and evaluates the applicability and effectiveness of selected PIML approaches (see Figure 1) within practically relevant modeling scenarios, paving the way for innovative modeling solutions in the field of systems prognostics and health management.

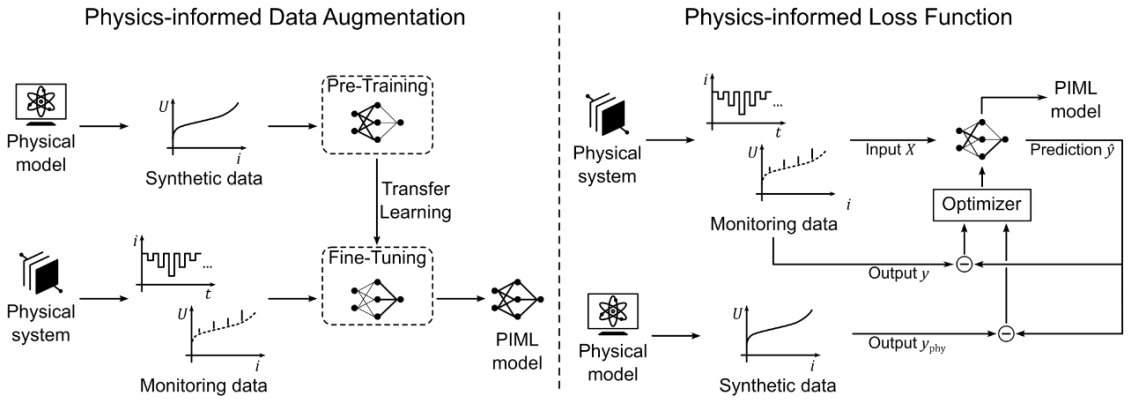

Figure 1: Exemplary selection of the investigated physics-informed machine learning (PIML) approaches for embedding physical knowledge into the modelling process, according to Ref. [3].

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Keywords: Proton exchange membrane water electrolysis (PEMWE), Prognostics and health management (PHM), Physics-informed machine learning (PIML)

Improvement of Wave Height Prediction Based on a Spatio-Temporal Deep Learning Model with Time-Series Decomposition

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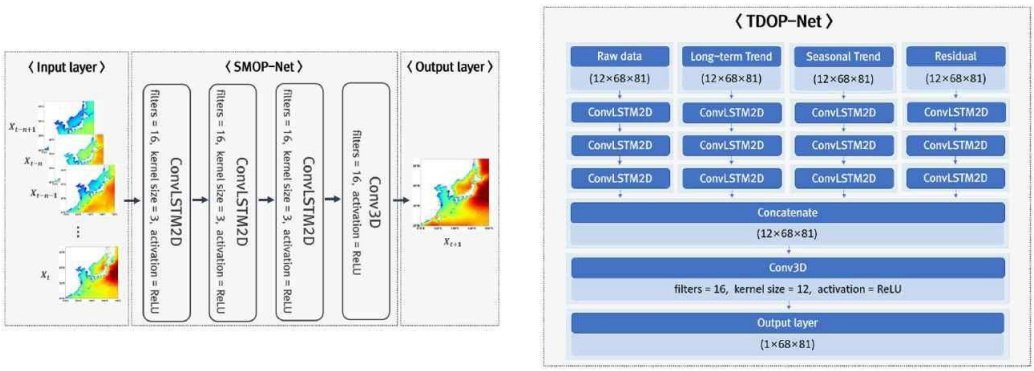
ABSTRACT

Advancements in artificial intelligence (AI) have improved oceanic time-series predictions across various marine variables. However, existing studies often focus on long-term temporal forecasting, neglecting spatial features. This study proposes a spatio-temporal deep learning model, trained with ERA5 reanalysis data, to enhance Significnat Wave Height (SWH) forecasts around the Korean Peninsula. A new model, the Time-series Decomposition-based Ocean Prediction Network (TDOP-Net), integrates time-series decomposition into input data, significantly improving prediction accuracy. By decomposing wave height data into long-term trends, seasonal patterns, and residual components, TDOP-Net outperforms conventional deep learning models, particularly in nearshore areas. Performance evaluation across multiple maritime regions, including the Yellow Sea (YS), East China Sea (ECS), East Sea (ES), and the Adjacent Sea of Korea (ASK), confirms its effectiveness.

METHOD

The study employs Convolutional Long Short-Term Memory (ConvLSTM) networks to capture spatio-temporal dependencies. A baseline model, the Simple Ocean Prediction Network (SMOP-Net), is developed and enhanced with time-series decomposition techniques in TDOP-Net.



(a) SMOP-Net **(b) TDOP-Net**

Figure 1. Structure of the deep learning model: (a) SMOP-Net, and (b) TDOP-Net.

[a] Presenting Author

The decomposition method extracts distinct temporal components, each serving as an independent input channel. Model training uses ERA5 SWH data (2016–2020), with 2021 data for testing. Performance is assessed using Relative Root Mean Squared Error (RRMSE), Relative Mean Absolute Error (RMAE), and Correlation Coefficient (Corr).

RESULTS

TDOP-Net significantly enhances forecast accuracy. Compared to SMOP-Net, it achieves a 1–7% reduction in RRMSE, a 15–29% decrease in RMAE, and a 0.01–0.04 improvement in Corr. The greatest improvements occur in nearshore areas rather than offshore areas. Time-series decomposition proves especially beneficial for longer lead times, mitigating cumulative error effects. Among sub-regions, the Yellow Sea exhibits the highest accuracy gains despite its complex basin characteristics.

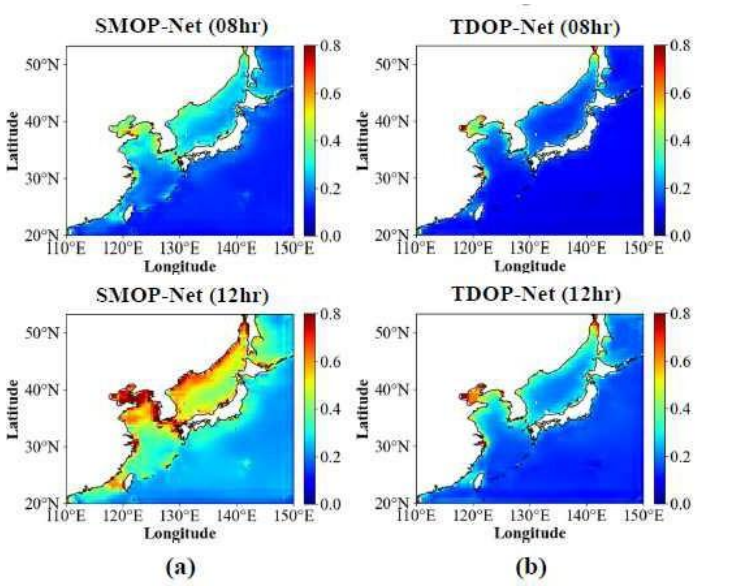


Figure 2. Spatial maps of RMAE with increasing forecast lead time (8 and 12 hours):
(a) SMOP-Net, (b) TDOP-Net.

CONCLUSION

This study demonstrates that integrating time-series decomposition with deep learning significantly improves wave height predictions, particularly in nearshore environments. TDOP- Net's approach can be extended to other oceanic and meteorological variables, such as sea surface temperature and wind patterns. By advancing AI-driven marine science applications, this study contributes to operational oceanography, disaster mitigation, and coastal management strategies.

Keywords: Spatio-temporal deep learning, ConvLSTM, Time-series

decomposition, Significant wave height prediction, ERA5 reanalysis data.

HOW DOES AI HELP DEVELOP EoS FOR PURE LIQUIDS AND MIXTURES?

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The search for a suitable and accurate model relating the state variables pressure-density-temperature (p-ρ-T) is essential to improve calculations in scientific research and industrial applications. The most well-known and widely used equations of state (EoS), such as Van der Waals, Redlich-Kwong, Peng-Robinson, etc., and the more recent ones, such as SAFT, PCA, and other parametric equations [1,2], have also been used. However, its predictive capacity is almost always limited to specific pure compounds or solutions, and especially in the liquid phase. Recent advances in machine learning (ML), a branch of artificial intelligence (AI) have provided powerful tools that can improve the accuracy of EoS by capturing complex relationships integrating experimental data. An extensive work has been done to find the AI answer to define a relationship between state variables using the ML tool, which incorporates polynomial feature expansion (PFE) and artificial neural networks (ANN) to obtain density estimates for each situation of p and T, with high accuracy in the case of pure liquids and/or liquid mixtures. The proposed framework comprises three phases (see scheme in Figure 1) which are commented below:

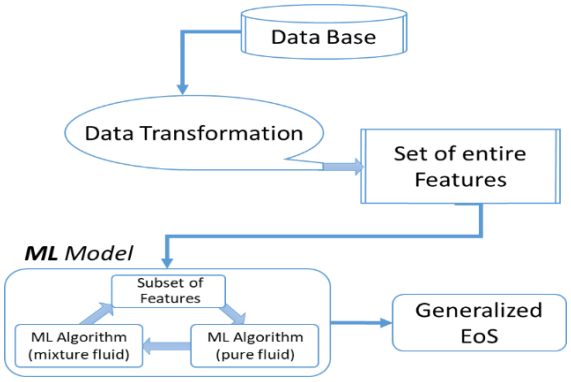

Figure 1. Sequence of tasks carried out in the ML process

• Data collection and preprocessing: Several experimental data sets with density measurements of compounds of different nature, such as alkanes, alcohols, and esters under different T and p conditions were collected from literature A statistical analyses allowed to assess the distribution and variability of the data.

• Feature analysis and model development: Polynomial expressions as a function of p and T were developed to observe nonlinear dependencies. A sequential feature selection algorithm was used to optimize the inclusion of variables, ensure the model robustness and minimize over-fitting.

• Artificial neural network training: A multilayer perceptron (MLP) model was implemented with an input layer defined by the selected features, optimized hidden layers,

and an output layer predicting fluid density, ρ. The network, using the RPROP optimization algorithm was trained, with a percentage data partition of, respectively, 60-20-20, for training, validation, and testing. Early stopping techniques were incorporated to improve the generalization. After carrying out the above phases, the ANN gives us as a final result the following parametric expression, explicitly for density:

$$\rho(p,T) = \sum_{i=1}^{2} a_i T^i \; p^1 + \sum_{i=1}^{2} b_i p^i \; T^1 + \sum_{i=1}^{2} \left(c_i T^i + d_i p^i \right)$$

For mixtures, an extended formulation, incorporating composition-dependent variables was achieved allowing the model to accurately predict density variations at different mixture proportions.

Comparison with other EoS. The predictive capability of the ML-derived EoS was evaluated against the following four models, widely used for liquid-phase density estimation. (i) The modified Tamman-Tait EoS: a temperature-dependent empirical formulation incorporating logarithmic pressure terms. (ii) The Rackett-Tait EoS: a hybrid approach incorporating the Rackett equation as a reference state for liquid density [3]. (iii) The MTS EoS: a modified Toscani-Szwarc equation extended by an additional exponential correction term [4]. (iv) The Sanchez-Valle et al. EoS: a polynomial-based model incorporating pressure-temperature dependencies [5].

Individual comparisons showed superior performance of the ML-based EoS, with significantly lower mean absolute percentage deviation (MAPD) across different fluid classes. For pure substances, the proposed model showed a 25–50% reduction in MAPD compared to traditional EoS models. For mixtures, the composition-based formulation showed up to 40% higher accuracy than other models.

Conclusions. This work presents the results obtained by using ML to obtain an accurate relationship of state variables. The results support the proposal and show that AI is able to define expressions of canonical variables that improve the predictive capacity of other EoS when applied to liquids, both for pure compounds and mixtures. By leveraging PFE and ANN architectures, the proposed framework efficiently captures complex p-ρ-T relationships while maintaining high generalization capabilities. The results highlight the transformative potential of ML in the modeling of thermodynamic properties. Future research will explore alternative ML architectures, including Gaussian processes and Bayesian neural networks, to further refine model interpretability and improve predictive performance.

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Knowledge Distillation: Enhancing Neural Network Compression with Integrated Gradients

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Abstract: Efficient deployment of deep neural networks on resource-constrained devices demands advanced compression techniques that preserve accuracy and interpretability. This paper proposes a machine learn- ing framework that augments knowledge distillation (KD) with Integrated Gradients (IG), an attribution method, to optimize the compression of convolutional neural networks. We introduce a novel data augmen- tation strategy where IG maps, precomputed from a teacher model, are overlaid onto training images to guide a compact student model toward critical feature representations. This approach leverages the teachers decision-making insights, enhancing the students ability to replicate complex patterns with reduced param- eters. Experiments on CIFAR-10 demonstrate the efficacy of our method: a student model, compressed 4.1-fold from the MobileNet-V2 teacher, achieves 92.5% classification accuracy, surpassing the baseline stu- dents 91.4% and traditional KD approaches, while reducing inference latency from 140 ms to 13 ms–a tenfold speedup. We perform hyperparameter optimization for efficient learning. Comprehensive ablation studies dissect the contributions of KD and IG, revealing synergistic effects that boost both performance and model explainability. Our methods emphasis on feature-level guidance via IG distinguishes it from conventional KD, offering a data-driven solution for mining transferable knowledge in neural architectures. This work contributes to machine learning by providing a scalable, interpretable compression technique, ideal for edge computing applications where efficiency and transparency are paramount. (A first draft of the full article will within a day be available in arXiv.)

Keywords: model compression, knowledge distillation, integrated gradients, deep learning, explainable ai

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* Presenting author

Evaluating a Large Language Model for Automated Assessment of Bradykinesia in Parkinsons Disease

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Abstract:

Background: Parkinsons disease (PD), a progressive neurodegenerative condition, affects 11.77 million individuals globally, as reported by the Global Burden of Disease Study 2021, contributing 89.59 disability- adjusted life years per 100,000 inhabitants [1]. A hallmark of PD, bradykinesia, manifests as delayed move- ment initiation and execution, measurable via the Movement Disorder Society-Sponsored Revision of the Unified Parkinsons Disease Rating Scale (MDS-UPDRS) Finger Tapping (FT) test [2]. This test evalu- ates speed, amplitude, and rhythm, traditionally scored by clinical neurologists–a process that is resource- intensive and prone to subjective variation seen in studies of intra-rater reliability [3]. Recent advancements in general-purpose large language models (LLMs), which increasingly excel in analytical tasks, suggest their use for scoring or interpretation, making it essential to evaluate them as tools for UPDRS assessments.

Objective: This research investigates the efficacy of ChatGPT-4 (version: gpt-4-turbo-2024-04-09), a general-purpose LLM, in scoring FT tests for PD patients. It compares the models performance, using varied input configurations, against that of expert neurologists.

Methods: Video data from 53 FT tests were collected from 16 PD patients using smartphones (720p/240FPS). Two neurologists independently scored the videos to establish baseline scores and assess human inter-rater re- liability. In parallel, ChatGPT-4 conducted 10 independent evaluations per video, leveraging time-series data of finger and thumb trajectories derived from CoTracker (https://co-tracker.github.io/) and guided by MDS-UPDRS FT criteria. Four experimental conditions tested the model: (Exp A) analysis of a 10-second video segment starting 2.99.4 seconds (mean 4.0 s) post-initiation of the movement; (Exp B) integration of Python-based extrema detection for tapping features; (Exp C) evaluation of the first 10 taps to capture early movement patterns; and (Exp D) incorporation of four low-performance examples from Exp C with neurologist scores to enable few-shot learning.

Results: In Exp D, ChatGPT-4 achieved an intra-rater reliability of 0.45 (Intraclass Correlation Coefficient, ICC(2,1)), exceeding the neurologists inter-rater reliability of 0.37, demonstrating its consistency potential. Performance varied across experiments: Exp A yielded a Wasserstein Distance (WD) of 1.22, ICC(2,1) of 0.05, and accuracy of 18.2%, resembling random guessing; Exp B improved to WD 0.79, ICC(2,1) 0.16, and accuracy 22.7% with feature detection; Exp C, focusing on initial taps, reached WD 0.58, ICC(2,1) 0.21, and accuracy 50.0%; and Exp D, with few-shot learning, recorded WD 0.63, ICC(2,1) 0.45, and accuracy 61.1% excluding the four examples. The models inter-rater reliability with neurologists in Exp D (ICC(3,k) = 0.85) outperformed all but one neurologist benchmarks from prior studies [4, 5, 6].

Conclusion: Incorporating example-based inputs with chain-of-thought instructions markedly enhanced ChatGPT-4's reliability and accuracy, aligning its performance with that of clinical experts. While these initial findings show the promise of LLMs, when paired with tailored computational frameworks, as trans- formative tools for engineering-driven medical diagnostics, further research is essential to determine whether this approach is a feasible path for automated

scoring. Caution should be exercised when comparing per- formance metrics, as current metrics and study designs vary widely, and large-scale comparative studies are needed to provide definitive answers. Nonetheless, to the best of our knowledge, this study represents the first attempt to use an LLM directly for UPDRS scoring.

Keywords: Parkinsons disease, bradykinesia, finger-tapping assessment, large language models, ChatGPT- 4, computational methods, reliability analysis, engineering applications* Presenting author

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Multivariate LSTM-Based Time Series Forecasting for Battery Cycling Analysis with Crossed Attention Mechanisms

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In the context of the accelerating next industrial revolution propelled by modeling, data analytics, and AI across fields such as aerospace, construction, energy, transportation, manufacturing and materials, the energy transition remains a major challenge for our future. Within this broad shift, energy transition remains a critical priority, especially given the intermittent nature of renewable energy sources like batteries. Batteries serve as the indispensable element for power generation and transition, ensuring a stable and consistent energy supply.

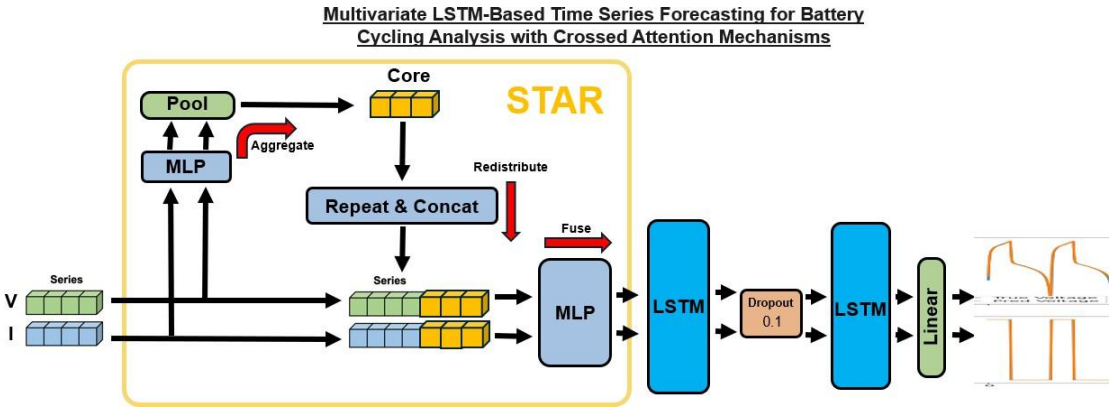
However, battery technology itself, especially lithium-ion batteries, presents significant challenges. Changes in temperature, charging protocols, usage patterns, and overall battery chemistry all affect battery performance, lifetime, and safety. Characterizing these electrochemical processes often requires time-consuming and labor-intensive testing under controlled conditions. Such protocols can significantly delay innovation, increase costs, and limit the widespread adoption of cutting-edge battery systems.

To address these constraints, our research focuses on modeling electrochemical profile prediction using long short-term memory (LSTM) networks. We also propose a variant of LSTM enhanced by the STAR (attention) mechanism. By accurately predicting battery behavior, these data-driven approaches aim to reduce testing time and resource consumption. Ultimately, integrating advanced AI into the battery development and evaluation process can accelerate innovation, reduce production costs, and promote more sustainable energy solutions.

We exploited an open-source dataset provided by the Toyota laboratory, including measurements of voltage, current and the number of charge-discharge cycles. These data show that voltage and the current clearly have seasonality but as the number of cycles increase, the duration of a seasonality decreases, so we have nonstationary data. There is a lot of missing data due to the cycler crash. Tests were performed on the cell during the cycling, so it changes the cycling condition for one cycle. The data were acquired without a constant time step, so we interpolated the data to have one.

Once the pre-processing phase was complete, we trained a network consisting of three LSTM layers and an output fully connected layer. We then inserted the STAR module before the LSTM^{b} component to leverage more of the information in the input

data. Several hyperparameters were tested—such as different input sequence sizes (initially 90, matching our dataset's timestep, then larger values), the number of LSTM layers, the number of neurons per layer, and the number of STAR cores—to determine the optimal configuration. As a result, we achieved a mean squared error (MSE) of 0.001 on the test set, indicating the model's ability to capture curve deformation and cycle time evolution.



[b] Figure: On the left, the two series are first processed by an MLP, then aggregated (Pool) to extract a "Core" representation. This representation is then combined (Repeat & Concat) with the raw series to form the block. A "Fuse" mechanism via MLP reintegrates the information before passing it on to a first LSTM layer. A Dropout regularization module (0.1) precedes a second LSTM layer, and the final output is produced by a Linear layer, responsible for generating the prediction of voltage and current curves (shown on the right).

However, for longer-term predictions (more than 90 cycles), the predicted length of each cycle begins to deviate, even when attention is included. At this stage, the main limitation of our model is that some parts of the cycle are unstable, which reduces the overall accuracy and clarity. To address this issue, we plan to train a larger model using multiple CSV datasets to obtain a wider range of information and ultimately improve prediction performance.

Keywords: Deep Learning, Times Series, Machine Learning, Forecasting, Energy

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Data driven model using VAE to fasten phase field model for lithiation simulation of a LFP particle

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Phase-field (PF) modeling is a powerful approach for simulating lithiation dynamics in cathode materials, effectively capturing phase evolution and spatial localization driven by reaction-diffusion processes [1]. In this study, we employ a PF model to simulate the phase transition of $FePO_4$ (FP) into $LiFePO_4$ (LFP) within an individual LFP particle. This model provides critical insights into the local distribution of lithiation dynamics by generating high- resolution image datasets of phase transformations at the particle level. However, the physics- based nature of the model requires a large set of parameters, making it computationally intensive and time-consuming. Future work aims to optimize computational efficiency while maintaining model accuracy.

This number of parameters makes it harder to see the sensibility of the parameter, a way to easily see the impact of the change in the parameter, projecting the data into a latent space using a Variational Auto Encoder (VAE). Projecting the data into a lower dimension space allows us to have a global view of the simulation, and an advantage of using VAE is the construction of a structured latent space. We observe that images from simulation close to each other are still close when we project them into the latent space. Because of this characteristic, we can see the impact of each parameter. For this purpose, we trained a VAE algorithm using simulated image datasets generated with a large range of parameters.

The first step was to choose which parameter we want to see the sensibility, the first parameter is the nucleation point, it is the starting point of the lithiation process, the second parameter is the speed of the reaction, and the last parameter is the direction of the lithiation, this direction is represented by a ration between dx and dy.

The second step is to choose the grid of parameters: the minimum, the maximum and the step for each parameter, a first small study gave us insight about the sensibility of each parameter, which allows us to have an idea of the sensibility function for each parameter. Based on this we choose a grid and simulate all the combinations of three main parameters we choose.

In the end we have our dataset to train the VAE, our model consists of two layers of convolution and max pooling, a latent space of size 16 and two layers of transpose convolution for the decoder. Once trained we can observe that the starting and the ending point of each simulation is close but their trajectories in the latent space are different, and each simulation with close parameters are close to each other.

To optimize our network we try different number of kernel in the convolution layer, to adjust the dimension of the latent space we choose the lowest number of dimension which give us a high quality reconstruction, we change from convolution layer with dimension reduction to max pooling, we try to add upscale instead of transpose convolution but it result in lower quality reconstruction.

Finally with this dense latent space we are able to generate simulation between parameters. To try the capability of the generation of our model we encode and decode

a test dataset and compare the generated one with the input,We achieve on a test dataset a MSE of 2,2169 * 10^{-3}. To go further we will add a LSTM in the latent space to predict the entire simulation [2], and then reconstruct it with the decoder. For now our model still has problems with the start and the end of the simulation because they are the part with the biggest difference. To solve this we plan to improve our data augmentation by adding rotation and translation.

To conclude we train a VAE with a grid of parameter in order to see the impact of each parameter and at the end we obtain a model able to generate new simulation with parameter we did not train our model with with a MSE of 2,2169 * 10^{-3}, To encode and decode 2000 images it takes less than 10 seconds compared to PF where it takes 30 minutes for one simulation of 2000 images. So it fastens the generations by a factor of 180.

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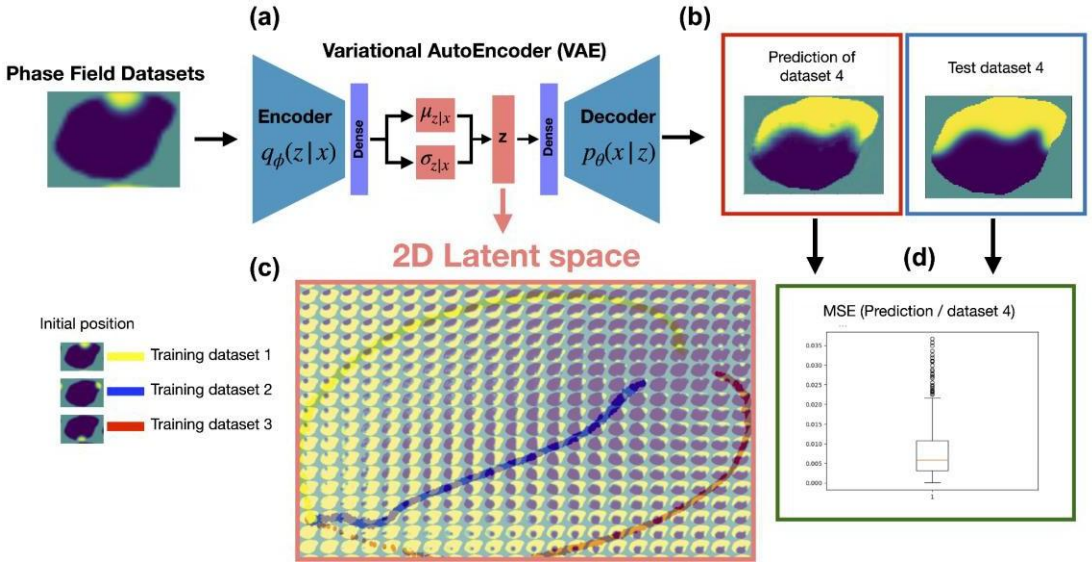

Figure 1: a) Schema of the VAE structure. b) The image on the left is generated based on the image on the right. c) Visualisation of a grid generated using a 2D latent space trained with 3 different nucleation points. d) Boxplot corresponding of the MSE on the test dataset, we encode and decode the images and compute the MSE between the input and the output

Keywords: Deep Learning, 2D Images, Energy, Simulation, Time series

Performance Comparison of Three Control Algorithms for Mixed Mode Ventilation in Apartments and Small Offices

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Residential space heating accounts for 18% of GHG emissions in the European Union and ventilation is one of the main actions driving energy demand. In the past two decades, most European Countries have adopted standards requiring measures that reduce ventilation related energy consumption, such as mechanical heat recovery ventilation (HRV), for dwellings and tertiary buildings. Mechanical ventilation usually requires sizable investments and can be difficult to implement in existing buildings. An often-overlooked alternative to constant flux mechanical ventilation is natural demand controlled ventilation, which, instead of recovering the energy contained in the exchanged air, dynamically adjusts ventilation rates according to the demand of fresh air. Mixed mode or hybrid ventilation consists of a strategic combination of natural ventilation via operable windows or vents and mechanical assistance to maintain indoor air quality and thermal comfort in an energy-efficient manner. By adapting to changing occupancy levels and outdoor conditions, such systems can potentially reduce heating and cooling loads while promoting a healthier indoor environment with low investment. However, the effectiveness of mixed mode ventilation hinges on the control approach that manages both mechanical and natural components. This paper provides an overview of three different algorithms designed for mixed mode ventilation in apartments and small offices.

The first control strategy follows a traditional rule-based system, which defines specific thresholds for activating or deactivating ventilation modes. The inputs include measured indoor temperature, humidity, and CO_2 concentration, supplemented by known occupancy schedules in the case of offices and external weather conditions. Whenever a trigger parameter, such as CO_2 or temperature, crosses the pre-defined set point, the algorithm opens the windows or starts/stops extraction ventilation, or both. Although easy to implement and transparent, rule- based control may not adequately handle abrupt or non-routine occupancy patterns, which may lead to instances of either over-ventilation (unnecessary energy use) or under-ventilation (deteriorating air quality).

The second control strategy relies on window operation curves based on human preference and outdoor temperature. The defined set of curves reflects observed preferences based on past studies in which building occupants performed certain ventilation actions based on current indoor and outdoor conditions. Instead of static thresholds, the control system looks up a preference curve to determine the degree of aperture of windows and the working regime of the mechanical ventilation. Adopting

statistically obtained preferences in window opening should lead to higher satisfaction (thermal comfort) and better acceptance of automated control, which is challenging in automated building management systems. However, these preferences can vary widely among different individuals or climates. To adjust for this, a family of curves was tested, obtained through displacement of the original preference curves.

The third control strategy presents an innovative hierarchical multi-agent system (HMAS) based on learning agents that uses two different policies. One policy is used by a single top- level agent that behaves like a manager and gives a long-term goal to others, i.e., this policy takes an observation and gives a goal. The second policy is used by all the other agents, taken observations, and goals to gives actions. This policy is a fully shared parameter one, allowing coordination and scalability in the HMAS. The policies are trained simultaneously with a Proximal Policy Optimization (PPO) Deep Reinforcement Learning (DRL) algorithm. The observation space takes data from the indoor environment (e.g., CO_2, humidity, temperature, volatile organic compounds) alongside external weather data and occupant schedules. The action space considers the possibilities of the different ventilation modes for the exhaust fan system and the grade of aperture of windows in the south facade. The optimization process uses a reward function for all the agents that guide the HMAS to improve thermal comfort, indoor air quality (IAQ), and energy demand. This reward function has two terms, one for all the comfort aspects and the other for the energy demand. Both terms are normalized to take values between 0 and -1. A ponderation factor is used to give more importance to one over the other. In this work, the reward used by the manager considers that the energy demand accounts for only 1% of the total reward. The goal transmitted to the low-level agents directly affects the ponderation factor, indicating that for a period, comfort is more important than the use of energy, or bise versa.

To compare the three approaches, a digital twin of a small office in Zarautz, in northern Spain, was set up and modelled using EnergyPlus. This small office is part of the SMA(i)RT project and is fitted with a controllable exhaust ventilation device and motorized window openings. A monitoring campaign was deployed in through 2024 in the real office. In the digital twin, simulation parameters were defined according to the national Spanish regulations CTE DB HE and RITE. The performance assessment for these three strategies was done using key indicators such as the indoor temperature range, CO_2 levels (used as a general IAQ proxy), ventilation energy usage, and energy demand for heating.

This piece of research has allowed to compare the performance of three control approaches using simulation. In the future and after implementing some adjustments based on what was learned with these simulations, the three control alternatives could be implemented in the SMAI(i)RT pilot and tested in real-life conditions in a small office currently in use.

Keywords: Residential Ventilation, Mixed-mode Ventilation, Heat Recovery Ventilation (HRV), Energy Efficiency, Building Automation, Building Management Systems, Building Simulation

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Data-driven Approaches with Bayesian Physics-Informed Neural Networks in Neurodegenerative Disease Biotechnology

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Abstract: Bioengineering and biotechnology play a crucial role in research related to neurodegenerative diseases. They provide innovative approaches for early detection, treatment, and understanding of the mechanisms behind these diseases. This includes the use of biomaterials, gene editing, and bioengineered extracellular vesicles. As a result, new hopes have emerged for treating conditions like Alzheimer's disease. Currently, an estimated 55 million people worldwide are living with dementia, with Alzheimer's disease being the most common form. This number is projected to rise to 139 million by 2050. Alzheimer's is particularly challenging to address due to its gradual and progressive nature, impacting memory, thinking, and eventually the ability to perform basic tasks. This creates significant challenges for both individuals affected by the disease and their caregivers.

Biotechnological research in this area requires the development of novel data-driven mathematical models that can aid in understanding and developing therapies for Alzheimer's disease, particularly those targeting amyloid-beta plaques using monoclonal antibodies, with the goal of slowing or even halting the progression of Alzheimer's disease (AD) [1, 2, 3]. The foundation for developing such models in this study is based on the characteristics of this complex neurodegenerative disorder, which include the accumulation of amyloid- beta ($A\beta$) and phosphorylated tau (p-tau) proteins. This accumulation leads to cognitive decline, which can be measured using the Alzheimer's Disease Assessment Scale (ADAS) score. In the first part of this contribution, we developed and analyzed data-driven models based on differential equations to describe the progression of AD by incorporating the dynamics of $A\beta$, p-tau, and the ADAS score. These models provided valuable insights into the interactions between $A\beta$ and p-tau, illustrating their roles in the progression of the disease.

To ensure accurate model calibration, we utilize Bayesian inference and Physics-Informed Neural Networks (PINNs) for parameter estimation based on data from the Alzheimer's Disease Neuroimaging Initiative (ADNI). The data-driven Bayesian approach allows for uncertainty quantification, which enhances confi- dence in model predictions. Meanwhile, the PINN framework harnesses neural networks to capture complex nonlinear dynamics directly from the data. These complementary methodologies improve the predictive power of our models, providing a reliable framework for understanding the progression of Alzheimer's dis- ease.

In the second part of this contribution, we applied an optimal control strategy to assess the effectiveness of an anti-tau drug in reducing phosphorylated tau (p-tau) accumulation and its impact on cognitive decline. Our simulations demonstrated that optimal drug administration significantly lowers p-tau concentration in the brain, which aligns with clinical observations. However, the effect on the ADAS score remains limited over extended treatment periods, indicating that cognitive improvements do not necessarily result from biomarker reductions alone. Additionally, our in silico trials highlight the importance of early intervention in neurodegenerative disorders and provide valuable insights into the timing of anti-tau therapeutic strategies. Furthermore, prolonged use of the medication does not eliminate associated side effects, underscoring the need for personalized treatment strategies.

The developed approach, which combines PINNs with a Bayesian framework, integrates Artificial Intelligence (AI) in a significant way. This method provides a natural means to quantify uncertainty in predictions and model parameters, particularly in situations where understanding confidence in decisions is crucial—such as diagnosing diseases by updating the probability of a

condition based on new test results and analyzing brain imaging data like MRI and PET scans to identify patterns associated with AD. However, it is important to note that most AI models require rigorous validation before being used in clinical settings, which can cur- rently still be time-consuming and costly. Nevertheless, as AI technology evolves alongside large datasets, its role in modelling neurodegenerative diseases presents new opportunities to improve patient outcomes, including early detection, personalized treatment, and a better understanding of disease mechanisms. Future developments of our work will focus on exploring multi-target therapeutic strategies that integrate interven- tions aimed at Aβ and tau proteins, along with optimized dosing regimens to improve clinical outcomes. Based on our current findings, we conclude that combining mechanistic modelling, data-driven parameter estimation, and control-based therapeutic optimization offers a powerful framework for advancing precision medicine in the context of AD and other neurodegenerative diseases.

Keywords: Data-driven models, Universal function approximators, Scientific machine learning, Mechanisms of Alzheimer's disease, Optimal control strategy, Bioengineering and Biotechnology

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Long-Term Hydrological Drought Modeling of Lake Nuntași-Tuzla

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According to Romania's national implementation report of the UN Convention to Combat Desertification (UNCCD), prepared by the Ministry of Waters, Forests, and Environmental Protection in 2000, the most drought-affected areas are in southeastern Romania, including Dobrogea, the eastern Romanian Plain, southern Oltenia, and the central Moldavian Plateau. Several lakes in the region mentioned before have recently dried up. In October 2020, Lake Iezer in Călărași County, covering about 400 hectares, dried completely. Similarly, Lake Nuntași-Tuzla in Dobrogea dried up in August 2020. Understanding the parameters describing drought is crucial for water resource management. These parameters fall into two categories: indicators and indices. Drought indicators include variables such as precipitation, temperature, river flow, groundwater and lake levels, soil moisture, etc. Drought indices, on the other hand, provide numerical representations of drought severity, using climatic or hydrometeorological data to assess drought location, severity, and duration.

In this context, a study was conducted on drought hydrological indices in the Nuntași-Tuzla Lake, Dobrogea, Romania, using different models. The data were sourced from the National Meteorological Agency (ANM) and the National Institute of Hydrology and Water Management (INHGA). The results show: (i) until the year 2000, there were no periods of hydrological drought due to supplementation of river flows either by increasing the base flow, as a result of water infiltration from irrigation and the rise of the groundwater level, or even by discharging water from irrigation systems at the end of the irrigation season, (ii) it took 10 years from the reduction in the operation of irrigation systems, and 4 years from their complete shutdown, for the groundwater body (BH) to start reacting and for hydrological droughts to appear, culminated in the complete drying up of Lake Nutași-Tuzla in August 2020.

Keywords: drought indices, hydrological drought, model, Nuntasi-Tuzla Lake, Romania

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Bridging Data and Diagnostics:A Review on Integrating Trend Monitoring and Change Point Detection for Wind Turbines

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Wind turbines undergo severe operation challenges due to their complex mechanical and electrical systems, harsh environmental conditions, and costly maintenance. Effective Structural Health Monitoring (SHM) is extremely necessary for fault detection at an early stage, downtime minimization, and maintenance strategy optimization. Traditional fault detection methods, based on either Trend Monitoring (TM) or Change Point Detection (CPD), have limitations when used individually—TM excels at identifying the type of fault that has occurred but is weak at specifying its occurrence time, whereas CPD detects faults' occurrence time precisely but not their type.

This review critically evaluates the synthesis of TM and CPD methods for comprehensive fault diagnosis in wind turbines by reviewing available literature, highlighting the complementary strengths and weaknesses of popularly utilized TM methods (Fast Fourier Transform, Wavelet Transform, Hilbert-Huang Transform, Empirical Mode Decomposition) and CPD techniques (Bayesian Online Change Point Detection, Kullback-Leibler Divergence, Cumulative Sum). The synthesis of both methods is demonstrated to yield increased diagnostic accuracy by taking advantage of TM's high-resolution fault characterization and CPD's high- precision fault timing.

Finally, the optimal TM-CPD combinations are established in relation to fault type (sudden vs. gradual), real-time vs. historical analysis, sensitivity, accuracy, computational efficiency, and operating environments. A case study of simulated blade failure illustrates the effectiveness of this hybrid approach in detecting both gradual fatigue and sudden structural cracks, verifying its feasibility.

A case study on wind turbine blades fault diagnosis based on dataset analysis illustrates how the integration of TM and CPD enhances early fault detection by coupling TM's detailed characterization of vibration and frequency changes with CPD's precise statistical validation of fault onset.

Keywords: Structural Health Monitoring; Trend Monitoring; Change Point Detection; Wind Turbines

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Flood-Prone Area Modeling Using the GIS and AHP Methods in the Voinesti Catchment

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The main objective of this paper is to identify the flood-prone area in the Voinesti River basin, using GIS and AHP (Analytic Hierarchy Process) methods. Voinesti catchment is located Dâmboviţa County, within the Dâmbovița watershed, a primary tributary of the Danube, in the southern region of the Curvature Carpathians. It is crossed by the Muret River and its tributaries. According to FAO 2003, the basin features preluvosol, characterized by podzolization, colluvium, and stagnogleying processes, varying in intensity. Land use consists of forests and permanent natural meadows. Flood-prone areas identification is based on various factors related to hydrography, relief, soil, vegetation, and precipitation. To conduct a spatial analysis that integrates factors of different natures, the method used is based on Weighted Overlay, a component of spatial modeling that employs the Multicriteria Evaluation (MCE) method, integrated within GIS. Weighted Overlay is a technique used for suitability modeling. Assigning weights to each factor in the overlay process is done using the Analytic Hierarchy Process (AHP), which is a Multi-Criteria Decision Analysis (MCDA) method. The results show that the most exposed areas are found along the river valley; the flood-prone areas are located at low altitudes and gentle slopes near the basin outlet. The methodology used can be regarded as a qualitative approach to identifying flood-prone areas rather than a quantitative tool for precisely delineating them.

Keywords: flood-prone area, GIS, AHL, Voinesti Romania

Open-loop Nash equilibrium in computational game

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Abstract: In the last ten years we observe an enormous interest in applying AI techniques to video games (see review articles [1], [2]). The typical methodologies originated from deep learning are: neural networks models using supervised learning, unsupervised learning, reinforced learning and evolutionary approaches, hybrid learning approaches (see [4], [5], [3]).It should be noted that reinforcement learning has roots in dynamic programming and it is called, within the control community, as adaptive/approximate dynamic programming. That means it uses mathematical tools (see [2]). In mathematics we have also game theory tools for cooperative games as well as for non-cooperative games. The cooperative games (collaboration of two players) is developed in [3]. In the paper we consider a possibility to apply the non-cooperative differential game tools with a finite decision horizon for a video game with two players. This type of game is an invaluable tool to describe the interactions and strategies in the model of fighting two agents in computer game. As an example of video game we use Street Fighter 2: Champion Edition, a classic 1992 production released by Capcom. The goal is finding optimal strategy for these fighting game. In it, the player takes on a role of a chosen martial artist champion to compete with other contestants in a massive fighting tournament. The choice of this game was made because of the relatively small complexity of the system, which makes it easier to present when it comes to mathematization of the strategies. We assume that the game is playing on flat bounded domain and it consists of a series of sparring one vs one in constrained two-dimensional space.

Keywords: differential game, computational game, dual dynamic approach, dual open-loop Nash equilibrium

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Structured Inputs for NLP-based automatic Testcase-generation in Mechatronic MBSE Verification

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With rising competition around the world, there is a constant shift in the industry to reduce costs in development projects [1]. A major issue in technical development projects is faulty requirements management, which has been identified as the main reason for project failure in approximately 24.1% of cases [2]. Therefore, the incorrect tracking of requirements can cause financial harm to the developer. To mitigate this risk, it is necessary to define suitable verification and validation (V&V) measures already during the formulation of requirements [3]. Test cases play a central role in this context: they systematically capture the relevant boundary conditions and states of a subsystem that must be considered during requirements verification. Within function-oriented model-based systems engineering (MBSE), test cases serve as the bridge between the requirements and the system by defining the attributes to be verified in order to satisfy one or more requirements.

Currently, requirements are usually described in natural language. The creation of test cases from requirements for mechatronic systems is mostly performed manually [4]. As every requirement must be verified by a testcase, the manual creation of testcases for mechatronic systems is associated with significant time and resource expenditure. A potential solution lies in the use of artificial intelligence applications, particularly through natural language processing (NLP). The automated generation of test cases based on natural language requirements and MBSE system models could significantly accelerate this process while simultaneously improving quality.

The IEEE Standard 829-2008 defines a test case as a set of inputs, execution conditions, and expected results to verify compliance with specific requirements [5]. Automated test case generation is already common in computer science, often with a model-to-test approach using activity and state diagrams [6][7][8]. However, mechatronic MBSE models differ significantly from the discrete actionflow-based MBSE models in computer science, as they incorporate physical behavior, matter and energy flows, and complex domain-specific simulations [9][10][11]. Current AI-based tools focusing on mechatronic systems can generate test cases from textual requirements (requirement-to-test) but often lack contextual understanding and detail of the physical interdependencies of mechatronic systems, resulting in simplified outputs, paraphrased the initial requirement [12].

To fulfill the definition of test cases for mechatronic systems stated above, two key research gaps need to be addressed. First, it must be defined which input information is needed for an AI-agent to generate test cases for each type of requirement—functional, performance, resource, and interaction [13,14]. Second, it must be determined which AI approach is suitable for processing the input information in a way that enables the consistent generation of valid test cases.

To address these gaps, this work proposes a structured approach for test case generation. A test case must specify the scope of the subsystem under consideration, the target variable to be investigated, the boundary conditions and system inputs, as well as the expected outcome. Using requirements for a water pump as an example, it is shown that the relationships between information elements within and across requirement types are crucial to identifying the relevant content for test case construction.

Various AI methods are evaluated for test case generation, ranging from prompting with contextual information and similarity-based retrieval using embeddings to a graph-based retrieval approach. A structured approach is derived to enable consistent test case generation.

In the future, the chosen approach shall be implemented to a rule- and retrieval-based AI toolchain for automated test case generation and integration into MBSE models for V&V across the product lifecycle.

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Keywords: MBSE, NLP, Test Case Generation

Graph Neural Network Assisted Gauss Quadrature for Isogeometric Analysis: Application to Contact Problems

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Abstract:

Isogeometric analysis (IGA) is a computational method for solving partial differential equations (PDEs). It utilizes non-uniform rational B-splines (NURBS) to define the geometry and approximate the solution field [1]. One crucial aspect of IGA for linear-elastic problems is calculating the element stiffness matrix. The Gauss quadrature rule is commonly employed to perform the numerical integration required to compute the stiffness matrix [1]. The accuracy of the computed element stiffness matrix in IGA depends on the number of Gauss quadrature points (GQPs) used for numerical integration. Deformed elements typically require higher values of Gauss quadrature points to capture the material's behavior compared to undeformed elements accurately [2]. However, using larger values of the GQPs increases computational costs. Therefore, finding optimal values for the GQPs that balance accuracy and computational efficiency when computing the stiffness matrix is important. Recent developments in computational mechanics have seen a surge in the integration of machine learning approaches, demonstrating a trend toward utilizing advanced computational tools for more effective problem-solving and analysis [3]. One such approach involves the use of graph neural networks (GNNs) [4]. GNNs are a class of deep learning methods designed to extract insights and make predictions from data structured as graphs. In our study, we applied a GNN to predict the values of Gauss quadrature points. Specifically, our GNN model takes NURBS elements as input and predicts the optimal values for the GQPs from the set of $\{4, 5, 6, 7, 8, 9\}$. The model's overall accuracy on the training and testing data are 96% and 80%, respectively. This approach allows us to determine the appropriate quadrature points efficiently for accurately computing the element stiffness matrix in IGA. The model is validated through the solution of a benchmark contact problem: ironing problem. The model cuts the computational cost by 20% by adaptively selecting the GQPs in each loading step, while maintaining the error less than 1%.

Keywords: Graph neural network, Isogeometric analysis, Gauss quadrature rule, Contact mechanics

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Waste Tire Valorization: Innovative Process Design and Machine Learning-based Component Prediction Model

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As a major contributor to "black pollution," the increasing number of discarded tires poses significant environmental challenges, particularly in terms of eco-friendly disposal. Waste tire pyrolysis has emerged as a promising solution, transforming waste tires into valuable resources such as energy and chemical feedstocks. However, recent studies have identified gaps in the focus on exhaust gas treatment and efficient waste heat recovery in current pyrolysis technologies. Moreover, the composition of pyrolysis oil, a key product of this process, varies depending on the type of tire and operating conditions, which complicates its application in energy production and chemical industries. Accurate prediction of pyrolysis oil composition is crucial for optimizing its use and improving the overall efficiency of the process. Thus, this study aims to address these challenges by developing an integrated process and a prediction model to better manage and utilize waste tire pyrolysis products.

To achieve this, this study designed an integrated process that combines waste tire pyrolysis with combined cooling, heat, and power (CCHP) system, a Steam Rankine Cycle (SRC), desalination, and an MEA-based carbon capture system. This integrated process was simulated to generate data on the composition of pyrolysis oil from different types of waste tires. Based on the simulation data, a Gradient Boosting Decision Tree (GBDT) model was developed to predict the composition proportions of aromatic, aliphatic, and other compounds in waste tire pyrolysis oil. Key input variables for the prediction model were selected using XGBoost feature importance and Cramer's V correlation analysis. The designed process was evaluated by technic and economic analysis and energy analysis. The prediction model's performance was validated against 13 other models, including those from the Decision Tree, BPNN, SVM, and HDMR series.

The performance evaluation of the integrated process demonstrates energy and exergy efficiencies of 49.75% and 49.69%, respectively. A techno-economic analysis revealed that government subsidies of at least $38.18 per ton of waste tires would be required to enhance the process's economic viability. The prediction model also showed strong performance, with over 60% of the test samples yielding a relative error percentage (REP) of less than 30%. Overall, integrating the simulation process with a machine learning-based prediction model provides a valuable tool for optimizing waste tire pyrolysis, contributing to the sustainable development of waste tire management and resource recovery.

Keywords: Waste tire pyrolysis; low carbon integrated process; prediction model; machine learning; simulation and modeling