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A Machine-Learning-based Surrogate Modeling Methodology for Submodel Integration in the Holistic Railway Digital Twin Platform

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Abstract

A holistic railway infrastructure digital twin (DT) platform is sophisticated and consists of a series of submodels (e.g., turnouts, tracks, vehicles, etc.) that are built through various methodologies and software. However, integrating these submodels into the DT platform is tremendously challenging due to considerable computational complexity, software and interface restrictions. To this end, we designed a machine learning (ML) based surrogate modeling methodology for the submodel integration in the holistic railway infrastructure DT platform and illustrated the methodology through a case study. In this case study, an ML-based surrogate model for multibody simulation of railway vehicle-track dynamics is created, which can replace the railway vehicle-track simulation executed with the Multibody Dynamics (MBD) Simulation commercial software SimPACK. The well-built ML model can accurately and quickly predict the vehicle-track system's dynamic responses to different track irregularities. Besides, the integration process of the ML-based surrogate model into the DT platform through a standardized open-source Functional Mock-up Interface (FMI) is also proposed. The developed surrogate modeling methodology shows great promise owing to its high fidelity, which is verified by the measurement data collected from the Austrian national railway track system. The main contribution of our work lies in the well-built ML-based surrogate modeling methodology for reducing the computation complexity and time of different submodels, which facilitates the unification and integration of different submodels. Furthermore, this approach can also be applied to other submodels and help to build the holistic railway DT platform collaboratively.

Keywords: Surrogate Model, Multibody Dynamics Simulation, Machine Learning, Railway Vehicle-Track System;

1. Introduction

The railway, as a sustainable transportation system, has received considerable attention, especially during the period of the energy crisis. Digital twin (DT) plays a transformative role in building an intelligent, comprehensive, and sustainable railway infrastructure system (RIS) by enhancing its resilience and efficiency, reducing costs, and saving energy [8]. The RIS is complex, and it comprises various subsystems, such as tracks, tunnels, bridges, etc. The majority of current research focuses on the development of DT for individual subsystems, but the comprehensive communication and interaction between various subsystems remain largely unexplored. Zhou, et al. [22] have proposed a DT platform, named Rail for Future Platform (R4F Platform) for seamlessly integrating digital models and data from various subsystems into a large-scale system. In this platform, all these models and related data are split into small clusters, which are defined as assets. These assets are digital representations of different railway subsystems, allowing the users to look into the performance of the subsystems without creating any entities in the real world. However, most of these assets are conventionally composed of detailed mathematical models with considerable complexity, which require a long runtime and enormous computation power. The tremendous computational complexity, together with different software and interface restrictions, makes the integration of these assets into the holistic DT platform extremely challenging.

Surrogate models can provide simplified approaches for mapping the input-output relationships of complicated, computationally demanding mathematical models. Therefore, surrogate modeling methodology is proposed as a practical remedy for the above-mentioned issue. One crucial enabler for surrogate modeling techniques is machine learning (ML), which

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is quite appropriate for predictive analytics. Using simulated data to train models and then deploying these models to design cyber-physical-systems has already been explored in various applications [14, 20, 2, 18]. In this regard, ML-based surrogate modeling methodology promises to be an effective tool in developing a holistic railway DT platform by replacing complex computational models while preserving their high fidelity.

This paper proposes an ML-based surrogate modeling methodology for the submodel integration in the holistic railway DT platform. We use railway vehicle–track dynamics analysis as an example to showcase our approach. The railway vehicle–track system is one of the crucial subsystems for a stable holistic RIS. Understanding vehicle–track dynamics is critical for maintaining good running stability and reliable ride quality. However, railway vehicle–track is an intricate system: the interplay of various sub-parts, such as the rail-wheel interaction, track irregularities, bogies, couplings, and other moving parts, determines its performance. Therefore, building virtual representations for the complex vehicle–track dynamics system is rather challenging. Multibody Dynamics (MBD) Simulation has been employed to analyze and understand the vehicle–track dynamics. Nevertheless, most MBD simulations are complex mathematical models with significant computing demand, and this demand normally obstructs rapid data exchange between different models. Besides, due to the respective requirements of different software and interfaces, it is complicated to directly integrate MBD simulations from various resources into one holistic railway DT platform. In this work, it is shown that with the ML-based surrogate modeling methodology, the computational complexity of MBD simulation executed with the commercial software SimPACK can be reduced without compromising its fidelity. The integration process of the surrogate model into the holistic railway DT Platform is also illustrated.

2. Related Work

DTs in railway: A holistic railway DT platform consists of various subsystems. Each subsystem may have its own specific tool, interface, and software license. Current research mainly focuses on the development of DT for individual subsystems. For example, Kampczyk et al. [10] used DT to monitor the status of railway turnout subsystems. They used cyclic data from an established DT model to study and verify the health situation of railway turnouts. Kaewunruen et al. [9] utilized a digitalization tool called Building Information Modelling (BIM) for the DTs of the railway, which aims to improve the railway's sustainability and resilience. The BIM produces good results in terms of cost-effectiveness and ideal schedule, assisting in reducing unforeseen consumption throughout the life cycle of the railway infrastructure. By evaluating the electric current waveform and magnitude, Zhang et al. [21] also established a DT-based framework for the real-time detection and monitoring of the health status of railway point machines. However, these reports only focus on the railway subsystems, the integration of DT into a holistic railways DT system remains unsolved yet.

Railway vehicle-track dynamics: In the last decade, research has been focused on improving stability, curve guiding, riding comfort, and other performance indicators of the railway vehicle-track dynamic system [19, 7]. The dynamic performance of a rail vehicle is determined by the vibration during the operation, which is primarily caused by track irregularities. Track irregularities, also called track geometric irregularities, are deviations in the track geometry, which primarily result from construction flaws, the sun kink due to hot weather, and the rail wear in service [13]. The MBD simulation is an eminent tool for engineers to analyze and examine the kinematic and dynamic motion of the railway vehicle-track system caused by track irregularities. With MBD simulation, virtual 3D models can be constructed and utilized to predict and visualize the motion, coupling forces, and stresses of the rail vehicle-track system. For example, Pombo et al. [13] designed a multibody formulation-based computational model, which utilized the data acquired directly from track-recording vehicles to simulate the track irregularities and the dynamic responses of the wheelset. Abdullah, et al. [1] constructed a computer simulation model of a railway vehicle using the ADAMS/Rail MBD package to simulate sophisticated, realistic railway vehicle-track systems, which may help to explore their dynamic response to curve and straight track inputs. However, the simulation time is rather long. Besides, due to the software restrictions, the proposed model might not fulfill the interactivity requirement of the holistic railway DT platform.

Surrogate modeling: Surrogate modeling methodology works as a substitute that can map the input-output relationships of complicated, computationally demanding mathematical models. It has already been successfully applied in many use cases. Zhu et al. [23] proposed a simulation-based optimization framework using a surrogate model for the operation optimization of a Cryogenics Natural Gas Liquids recovery unit. Wahid et al. [3] used radial basis functions as a surrogate model to optimize the performance of a process at a natural-gas liquefaction facility using a single mixed refrigerant. Despite the fact that tremendous research has been done on surrogate modeling, applying this methodology to DT systems is still in its infancy. Till now, few studies have been done on applying surrogate modeling methods in DT systems [4], not to mention the holistic railway DT system.

Model Integration: In the last few decades, methodologies and software for integration, exchange, storage, deployment, and visualization of different models are prevalent. Functional Mock-up Interface (FMI), for example, is a standardized open-source interface that can be used to integrate different models. Fang et al. [6] has successfully developed an FMI-based integration methodology for different aero-engine digital simulations based on AMESim. Pazold et al. [12] applied FMI to integrate heating, ventilation and air conditioning submodels. However, these studies mainly focus on using FMI for integrating regular numerical models. The problems of immense computational complexity of the model and long calculation time remain unsolved. Combining FMI with surrogate modeling methodologies can be a solution to this challenge. Besides, in order to build, test and deploy the surrogate models continuously, pipeline technology has been employed as an automation server [17]. Moreover, an open-source relational database management system is usually integrated with the pipeline technology, which is then used to efficiently and continuously store, update, and archive simulation results as adapted data located in a database [5].

Despite extensive work on different railway DT subsystems and model integration, storage, and deployment methodologies, there is no systematic study for simplifying and integrating different submodels to build a holistic railway DT platform. It is urgent to unify the interfaces of various simulation tools, reduce the vast model computational complexity of different DT subsystems, and find a proper way to integrate them into a holistic railway DT platform. The present work aims to fill the gap.

3. Design Process

In this section, we will introduce an ML-based surrogate modeling methodology for replacing the railway vehicle-track MBD model as a use case. In subsection 3.1, we will briefly introduce the MBD model for railway vehicle-track dynamics analysis. In subsection 3.2, the general development process of ML-based surrogate modeling methodology will be demonstrated. Then we will analyze and validate the surrogate model with the dataset generated from MBD Model and the measurement dataset collected from the ÖBB-Infrastructure AG (Infrastructure Manager of Austrian Federal Railways) track system in subsection 3.3. In the end, the integration process of the submodel into the holistic railway DT platform will be briefly discussed in subsection 3.4.

3.1. MBD Model of the railway vehicle-track dynamics

The interaction between the wheels and the track determines the dynamic behavior of railway vehicles. The geometry irregularities of the track can result in large dynamic forces on the vehicles, which can damage the vehicle wheels, leading to derailments in the worst cases. Therefore, understanding vehicle-track dynamics is important for the RIS. The commercial software SimPACK, which can provide a reliable way to understand the dynamic forces acting on the track elements and the vehicles, is used to build the MBD model. SimPACK can generate different types of track irregularities using the Power Spectral Density (PSD) function, which describes the frequency-specific power distribution of the track excitation. The track excitation will be deployed to the predefined track. Normally, the calculation of the PSD is based on the relevant regulations (commonly known as the ERRI B176 [15]), which are established from various parameters measured by the European railway operators. In the end, the irregularity data can be utilized as the input for the MBD model. The calculated forces on the wheelset can be extracted from the MBD Model as outputs.

3.2. Development process of ML-based surrogate modeling methodology

Figure 1 presents an overview of the development process of the ML-based surrogate modeling methodology. First, in the MBD model, the basic subvariables, such as track length, velocity, and vehicle mass, will be defined. After that, the PSD functions will be created based on practical requirements (frequency and amplitude, etc.) in SimPACK. Accordingly, the track excitation will be generated, and its related parameter will also be defined (frequency interval type, start and end distance, etc.) (Step 1). In Step 2, different types of track irregularities are created by the corresponding track excitation based on the actual demands (e.g., vertical, lateral, cross-level track irregularities or any of their combinations). These irregularities work correspondingly together to determine the forces on the wheelset. Then, the MBD model will be run with a solver implemented through a SODASRT integration method in SimPACK. After the simulation is done, the dynamic responses, i.e., the sum of wheelset forces, will be collected from the post-processing software SimPACK-Post as output data in Step 3. Finally, different types of track irregularities as input data and the wheelset forces as output data will be sent to the ML model for further ML training and testing.

In the ML Model, all the input and output data from the MBD Model will be firstly processed in Step 4. To reduce the computation complexity, all the input data (i.e., different track irregularities) and the corresponding output data (i.e., wheelset forces) will be equally divided into multiple datasets. Then, these datasets will be randomly split into two groups: one group for network training and the other group for network testing. After that, the input datasets will be normalized and standardized. The purpose of normalization is to make the data homogeneous across all different track irregularity dimensions, which helps to improve the data quality. Standardization means putting various features of all types of input data on the same scale. In other words, standardized data may be described as rescaling the characteristics of the input data so that their mean is 0 and the standard deviation is 1. After normalization and standardization, the datasets will be fed to the ML Network for training and testing.

The ML network we used in this study is a nonlinear autoregressive network with exogenous inputs (NARX), which is a recurrent dynamic neural architecture. It is one type of feed-forward time delay neural networks (TDNN) and is commonly used in time series data prediction. Time series data is a sequence of data points that are generally measured across time intervals of uniform length. The outputs, sum forces of the railway wheelset, are time series data. At the timestep t, the output dynamic behavior at the current state $y(t)$ is not only dependent on the current input status $x(t)$, but also on the last n input statuses $x(t-1), x(t-2), \ldots, x(t-n)$ and last u output statuses $y(t-1), y(t-2), \ldots, y(t-u)$. Therefore, the NARX network (see equation 1), in which the value of the output data $y(t)$ in the current state is regressed on previous values of the output data and the current and previous values of an exogenous input data, shows promising qualities for these dynamic system predictions. The landscape of the NARX model utilized in this paper is presented in Step 5.

$$\begin{aligned} y(t) = f(&x(t), x(t-1), x(t-2), \cdots, x(t-n), \\ &y(t-1), y(t-2), \cdots, y(t-u)) \end{aligned} \tag{1}$$

The optimization algorithm applied in this model is the Levenberg-Marquardt algorithm. For regular networks, in which the number of the weights is under a few hundred, the Levenberg-Marquardt algorithm has the fastest convergence speed in function approximation problems [11]. Furthermore, with this algorithm, the squared errors and weights may be continuously reduced before reaching the optimum combination for the best-performing network so that overtraining can

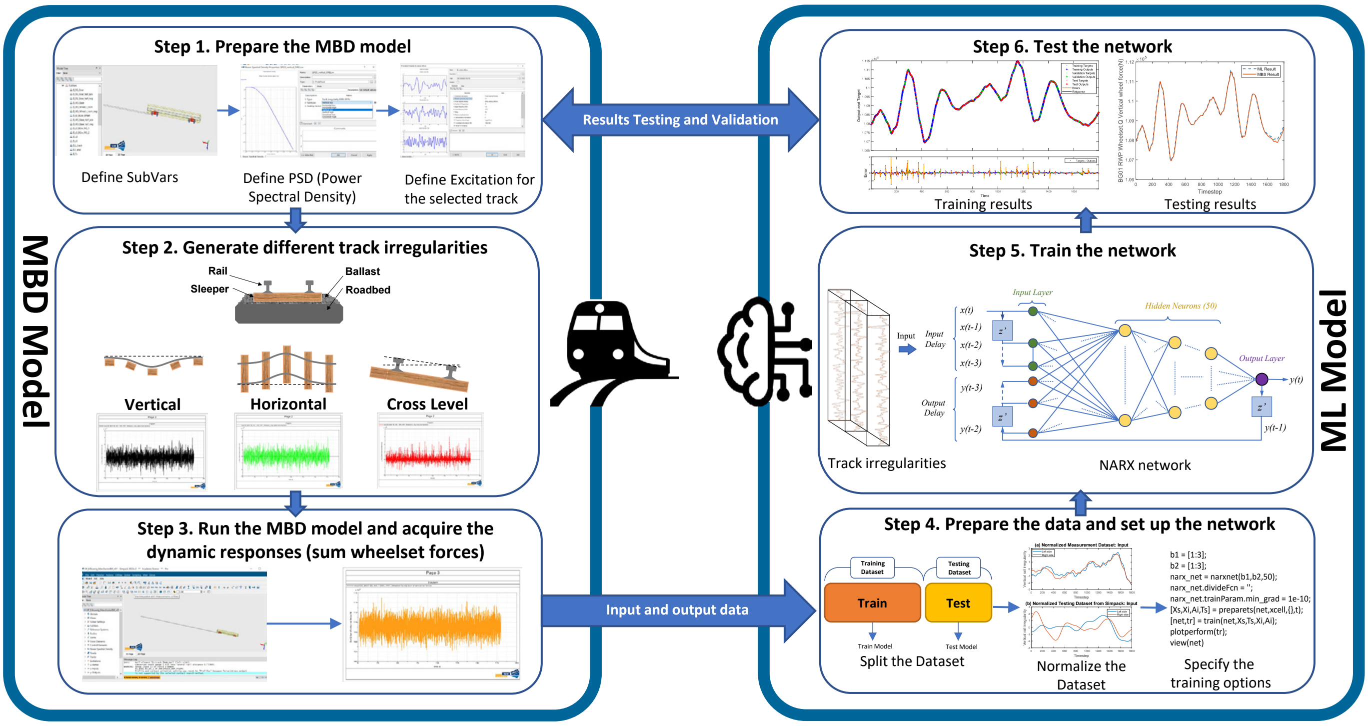

Fig. 1. Landscape of the ML-based surrogate modeling methodology

be avoided. During training, the number of neurons and delays needs to be determined from experimental iterations. The network's performance is evaluated using the normalized Root Mean Square Error (RMSE). After the training process is done, the testing datasets will be applied to the well-trained ML model to evaluate the performance (Step 6). Finally, for validation, measurement data will be applied to both the MBD Model and the ML Model as input. The results from both models will be compared to validate the fidelity of the ML-based surrogate model.

3.3. *Case study: building, testing and validation*

We build an MBD model to simulate the railway vehicle-track dynamics, which is based on the Manchester Benchmarks Passenger Vehicle. The parameters of the MBD model are derived from realistic situation, as presented in Table 1.

Table 1. Parameters of the MBD model

Name	Value	Unit
Track Length	5	km
Velocity	100	km/h
Vehicle Mass (include passengers)	31032	kg
Simulation Time	180	s
Sampling Rate	2000	Hz

The reliability and fidelity of surrogate models are of great importance. A well-built surrogate model should ensure the integrity of the original resources and the reliability of the optimization, prediction and feasibility evaluation. Therefore, it is a vital task to validate the trained ML Model properly. In this study, the measurement data from the Austrian national railway track system are employed for the final validation of the fidelity of the ML-based surrogate model. Due to the measurement restrictions, only the vertical track irregularities are obtained. These measured vertical track irregularities are composed of two dimensions, i.e., irregularities from the left-side track and right-side track. In line with the measurement data, two-dimensional input datasets are created following Step 1-3 in Figure 1. The vertical wheelset forces were extracted from SimPACK-Post as the output data.

The data were equally divided into 200 datasets. Each dataset consists of 2-dimensional input, i.e., 2×1800 Input Data (equals 25 m) and 1×1800 Output Dataset. Then, 200 datasets were randomly split into two groups: 120 datasets for network training and another 80 for network testing. Plenty of experiments were carried out to acquire the best-performing ML Model. In the final developed network, we defined the hidden layers with 50 neurons, target time series $y(t)$ with three feedback delays, and external input $x(t)$ with three feedback delays. The accuracy and suitability of the methodology presented here are demonstrated through the comparison of the MBD simulation results against ML Model prediction results. The normalized RMSE, one of the most commonly used measurements for evaluating the quality of predictions, is used to assess the comparison results. The normalized RMSE was calculated by dividing the RMSE by the range of the simulated output data from the MBD model: Normalized RMSE = RMSE / (max value – min value) [16]. This produces a value between 0% and 100%, where values closer to 0% represent better fitting models. In this use case, the normalized RMSE value is considered acceptable when it is below 10% (based on the expectations of the industry partners), which indicates that the predictions are within the deviation range.

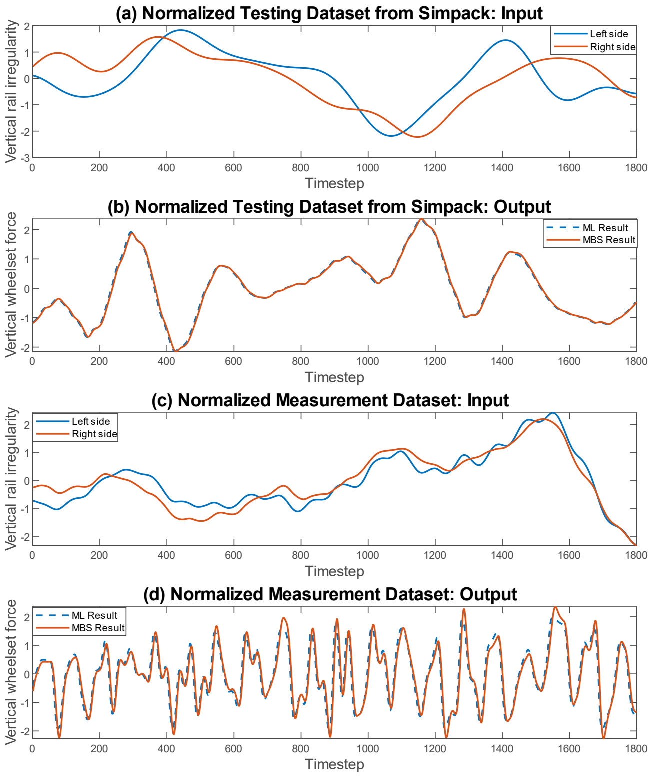

Fig. 2. Comparison between the output of MBD simulation (MBS) and ML surrogate model. The input datasets are either the testing dataset (upper two panels) or the measurement dataset (lower two panels).

Considering the data security of the Austrian railway system, all the presented data are normalized (with center 0 and standard deviation 1). Figure 2 (a) shows the normalized testing input dataset of the irregularities of the left and right tracks generated from MBD simulation for 1800 timesteps. Figure 2 (b) shows the normalized simulated output data from the MBD model and the predicted results of the ML-based surrogate model. It can be seen that the predicted results are in perfect coincidence with the simulation results from MBD Model. The corresponding normalized RMSE value between the two results is 0.48%, which indicates the ML-based surrogate model can perfectly replicate the MBD model with high precision. Then, we used the measurement datasets provided by the Austrian national railway track system to prove the fidelity of the ML surrogate model. Figure 2 (c) shows the irregularities of the left and right tracks that are measured from a 25 m long track in a part of the Austrian railway system. The fluctuation in these data is much higher than that of the PSD-generated ones (Figure 2 (a)). Even in this case, the prediction results of the ML-based surrogate model are also in good coincidence with the simulation results from MBD Model. The corresponding normalized RMSE value between both results is 3.52%, which is much lower than the 10% deviation threshold (Figure 2 (d)). Both comparisons allow us to conclude that the developed ML-based surrogate modeling methodology is not only qualitatively but also quantitatively correct. Moreover, the computing speed is significantly improved using the ML-based surrogate model. In our use case, for a 5 km long railway, with the ML-based surrogate model, it only takes about 8 seconds to finish the calculation, in stark contrast with 30 minutes required for the MBD simulation. Apart from the two-dimensional input measurement data, one-dimensional (vertical track irregularities) and three-dimensional (vertical, horizontal, and cross-level track irregularities) input data generated from the SimPACK have also been successfully applied in building respective ML-based surrogate model following steps in Fig.1, which proves the reliability and validity of the proposed methodology.

3.4. Integration process

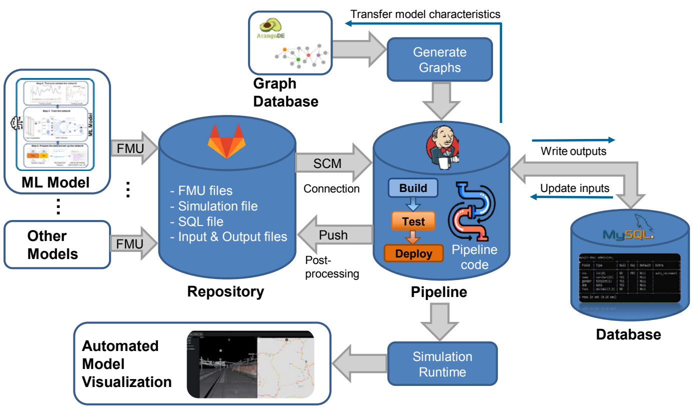

Fig. 3. Landscape of the integration process for the R4F Platform.

The well-built ML-based surrogate model reduces the computation complexity and time significantly. Besides, it may facilitate the unification of submodels built with different software, which may help the submodel to be integrated into the R4F platform more efficiently. Figure 3 demonstrates the integration process of the ML-based surrogate model into the R4F platform. First, the model will be translated into the FMU format (Functional Mock-up Unit, the simulation unit of the FMI), to make it tool-independent and therefore interoperable with other models. Then, the FMU files will be uploaded into a repository (e.g., Gitlab repository), which provides a storage location for their related codes and other files. In the repository, the users are able to design, control and optimize the integration process of the model, and enhance its interoperation with other models. After that, the model will be involved in a simulation pipeline methodology (e.g., Jenkins Pipeline), because the pipeline helps to build, test and deploy the model continuously and automatically. The pipeline is connected to the repository through the Source Code Management (SCM) system, which can be used to track and control changes in the repository. In our case, the integrated model is executed by the pipeline through running a simulation file (e.g., Python file) in a pipeline code that controls the functionality of the pipeline by defining necessary credentials for automatically authorized logins and different stages for step-by-step simulation workflow. Besides, input and output files in the repository get updated simultaneously (e.g. through the "push" command) for the users to check the simulation inputs and results, and then the pipeline gets updated inputs to execute another simulation. As a result, the pipeline can automatically integrate and deliver the model in the platform continuously. Additionally, a database management system (DBMS), e.g., MySQL, will be implemented for storage, exchange, and archiving of the input and output data. Moreover, the inputs and outputs in the database can also be automatically redirected to the visualization interface for the end user through the execution of a query code file by the pipeline after the simulation runtime. Besides, the semantic approach is planned to be involved in the pipeline, so that all characteristics of the integrated model (inputs, outputs, simulation workflow, data and submodel dependencies) can be interconnected and presented through a graph database system, such as ArangoDB. In the end, the visual output of the simulation runtime is expected to be presented for the end user to monitor the whole vehicle-track dynamics and to control it by input parameters through a web-based user interface system.

4. Conclusion and Future Work

In conclusion, the well-built ML-based surrogate model can make quick and precise predictions of the vertical dynamic responses based on different track irregularities. The surrogate model can replace the MBD simulation efficiently and be easily integrated into the holistic railway DT systems, as it has much less computational complexity than the traditional MBD simulation. The calculation efficiency is also greatly improved. For a 5 km long railway, it only takes about 8 seconds for the surrogate model to finish the calculation, a value that is three orders lower than the time needed for the MBD simulation (30 minutes). In addition to computational complexity reduction, the surrogate model also demonstrates great potential in subsystem integration, as it can address the problem referring to different submodels' software and solver restrictions.

Till now, the R4F Platform is still under development. Future studies will be focused on applying the ML-based surrogate model methodology in other railway subsystems beyond the railway vehicle-track system. Besides, more models shall be developed and integrated into this platform to validate the reliability and fidelity of the proposed integration methodology in future publications. Consequently, establishing the above-mentioned ML-based surrogate modeling methodology is a significant part of the R4F research program. It will provide plenty of opportunities for future work, pushing sustainable development of the holistic large-scale railway DT system.

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