Developement of Digital Twins of Scientific Equipment and Systems for MegaScience-class Installations.

Denis Zhigalov
Master Student.
Department of Computer Technologies,
Novosibirsk State University.
email: d.zhigalov@g.nsu.ru

Stanislav Shakirow
Scientific Advisor.
Ph.D. in Physics and Mathematics,
Associate Professor,
Department of Computer Technologies,
Novosibirsk State University.
Acting Director of the Tecnological
Design Institute of Scientific
Instrument Engineering of the
Siberian Branch of the RAS.
email: shakirov@tdisie.nsc.ru

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Abstract

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1 Introduction

In the realm of MegaScience-class installations, the concept of digital twins has emerged as a transformative technology, offering unprecedented opportunities for enhancing the design, operation, and maintenance of scientific equipment and systems. A digital twin is a virtual representation of a physical asset that enables real-time prediction, optimization, monitoring, controlling, and improved decision making in scientific equipment and systems [1]. This technology is not just a theoretical construct but a practical tool that has been increasingly applied in various fields, including manufacturing, healthcare, and now, in scientific research facilities.

The development of digital twins for scientific equipment and systems involves creating a framework that provides monitoring and evaluation capabilities for equipment involved in manufacturing and experiments [2]. This framework is crucial for MegaScience-class installations, where the complexity and scale of equipment and experiments demand precise and real-time monitoring for optimal performance and safety.

Moreover, digital twins serve as a new normal form for solving problems in a changing context, such as in the case of product quality monitoring, as highlighted by Zhang et al. (2020) in their study on a product quality monitor model with the digital twin model [3]. This adaptability is particularly valuable in the dynamic environment of MegaScience installations, where equipment and systems must consistently operate at peak efficiency under varying conditions.

The integration of computational models, sensors, learning, real-time analysis, diagnosis, and prognosis in digital twins supports engineering decisions related to specific assets [4]. This comprehensive approach is essential for the intricate and high-stakes nature of scientific research, where even minor miscalculations or malfunctions can lead to significant setbacks.

In summary, the development of digital twins for scientific equipment and systems in MegaScience-class installations represents a significant leap forward in the management and operation of complex scientific infrastructure. By leveraging the power of virtual modeling, real-time data analysis, and predictive capabilities, digital twins offer a pathway to more efficient, reliable, and advanced scientific research.

2 Literature Review

In the evolving landscape of mega-science projects, the integration of digital infrastructure and remote access capabilities has become increasingly crucial. A seminal paper in this domain is [5], which offers a comprehensive analysis of the role and implementation of digital twins and digital traces in mega-science facilities. This paper is instrumental in understanding the shift towards remote accessibility in scientific research, particularly in the context of large-scale, international scientific collaborations.

Balyakin et al. emphasize the necessity of minimizing the physical presence of researchers at scientific facilities, a concept exemplified by the Borexino project's use of an independent data collection system. This approach not only facilitates remote data acquisition but also significantly reduces the logistical and financial burdens associated with travel to these facilities. The paper further delves into the development of appropriate digital infrastructure, highlighting the need for new digital elements such as data centers and advanced processing algorithms. This infrastructure is crucial for the seamless integration of mega-science installations into existing e-Infrastructure, thereby enhancing the efficiency and scope of scientific research.

Moreover, the paper discusses the legal and methodological frameworks required to support the operation of scientific facilities in remote access mode. This aspect is critical in addressing the challenges posed by data security, intellectual property rights, and the nuances of international scientific cooperation. The authors also underscore the importance of engineering personnel in maintaining and ensuring the functionality of remote access modes, pointing to the need for specialized skills and resources in this area.

A key contribution of this paper is its exploration of the concept of e-Infrastructure, particularly its emergence and evolution within the European Union. The European Open Science Cloud (EOSC) and the Go FAIR initiative are presented as pivotal developments in this field, demonstrating the EU's commitment to digitalizing scientific research and fostering a more interconnected scientific community. The paper posits that while natural sciences are the initial beneficiaries of e-Infrastructure, its most significant impacts are likely to be seen in the field of humanities, necessitating the development of new assessment methods and legal solutions.

In summary, "Digital Twins vs Digital Trace in Megascience Projects" by Balyakin et al. is a foundational paper that provides valuable insights into the digital transformation of mega-science facilities. It not only addresses the technical and infrastructural aspects of this transformation but also considers the broader implications for scientific research, policy, and international collaboration. The paper's exploration of digital twins and digital traces offers a nuanced understanding of modern data processing techniques, making it a crucial reference for researchers and policymakers involved in the planning and operation of large-scale scientific installations.

3 Research Setup

3.1 The Siberian Ring Source of Photons (SKIF) and the Development of its Digital Twin

The Siberian Ring Source of Photons (SKIF) represents a significant advancement in the field of synchrotron radiation sources. As a 4+ generation synchrotron with six research workstations, SKIF generates synchrotron radiation with a power density of 92 kW/mrad², making it a key research tool in physics and scientific research [6, 7]. This 3-GeV electron energy SR source, developed in Novosibirsk, is designed to provide a new level of capabilities for scientific experiments, particularly in the fields of materials science and physics [8, 9].

The development of a digital twin for SKIF offers numerous benefits, enhancing the facility's operational efficiency and research capabilities. A digital twin, in this context, is a virtual representation that mirrors the physical attributes and dynamics of SKIF, allowing for real-time monitoring, simulation, and optimization of the facility's performance. This technology is particularly beneficial in complying with the precise requirements for the mutual positioning of electromagnetic axes of the elements during installation, which is crucial for the optimal functioning of SKIF [10].

One specific component of SKIF that is of particular interest is the diamond window. This component is essential in the facility's operation, serving as a robust and transparent medium for synchrotron radiation. The development of a digital twin for the diamond window involves creating a detailed virtual model that can simulate its behavior under various operational conditions. This model can predict how the diamond window will react to different radiation intensities, thermal loads, and mechanical stresses, thereby aiding in its design, testing, and maintenance.

The digital twin of the diamond window allows for the efficient modeling and testing of new control opportunities, improving the operation and longevity of this critical component. It enables the simulation of temperature, stress, and strain distribution within the diamond window, ensuring that it can withstand the intense conditions of SKIF without degradation [6]. Additionally, the digital twin can be used to study the impact of different cooling strategies on the diamond window, optimizing its thermal management and ensuring its performance remains consistent.

In summary, the development of a digital twin for the Siberian Ring Source of Photons (SKIF), particularly for its diamond window, represents a significant step forward in the digitalization of scientific research facilities. This technology not only enhances the operational efficiency and research capabilities of SKIF but also serves as a model for other mega-science-class installations looking to leverage the benefits of digital twin technology.

4 Methodology

4.1 Utilizing COMSOL Multiphysics for Simulating the Diamond Window in SKIF

COMSOL Multiphysics is a versatile and powerful engineering software package widely used for simulating physical phenomena across various domains. It is particularly adept at modeling heat and stress fields in materials, making it an ideal tool for simulating components like the diamond window in the Siberian Ring Source of Photons (SKIF) [11, 12]. COMSOL provides a comprehensive environment for finite element analysis, allowing researchers to create detailed models of complex systems and materials.

In the context of SKIF, COMSOL Multiphysics is employed to simulate the heat and stress fields of the diamond window and its cooling system. The diamond window, a critical component in synchrotron radiation sources, must withstand extreme thermal and mechanical stresses during operation. By using COMSOL, we can accurately predict how the diamond window will behave under various conditions, such as different ray positions and cooling water flow rates. This simulation includes assessing the temperature distribution, thermal stresses, and potential deformation of the diamond window, ensuring its reliability and performance in the SKIF facility.

However, one limitation of COMSOL Multiphysics is its inability to run simulations in real-time. To address this, we use COMSOL to pre-generate heat and stress data for a set of different parameters. This pre-generated data is then integrated into the digital twin of the diamond window. The digital twin, a virtual representation of the diamond window, uses this data to predict the window's behavior under various operational scenarios. This approach allows for rapid and accurate assessment of the diamond window's performance without the need for real-time simulation, making it a practical solution for monitoring and optimizing the component's operation in SKIF.

In summary, COMSOL Multiphysics plays a crucial role in the development of the digital twin of the diamond window in SKIF. By providing detailed and accurate simulations of heat and stress fields, COMSOL enables us to create a robust and reliable digital twin that enhances the operational efficiency and safety of the SKIF facility.

4.2 Support Vector Regression (SVR) in Simulating Diamond Window Heat and Stress Fields

Support Vector Regression (SVR) is a powerful machine learning method used for regression problems. It is particularly effective in scenarios involving small samples, nonlinearity, and high-dimensional data [13]. SVR has been applied in various fields, including time-series analysis, bioprocesses, and large-scale applications [14].

In the context of simulating the heat and stress fields of the diamond window in the Siberian Ring Source of Photons (SKIF), SVR plays a crucial role. Due to the computational intensity of direct simulations in COMSOL Multiphysics, real-time analysis is not feasible. To overcome this limitation, SVR is employed to train on pre-generated COMSOL data. This approach involves running simulations in COMSOL for a range of parameters, such as different ray positions and cooling water flow rates, to create a dataset that captures the behavior of the diamond window under various conditions.

Once this dataset is established, SVR is used to learn the relationship between the input parameters and the resulting heat and stress fields. The advantage of using SVR in this scenario is its ability to make predictions much faster than a direct COMSOL simulation. The goal is to achieve real-time prediction capabilities, allowing for immediate assessment and adjustment of the diamond window's conditions during SKIF operations.

The application of SVR in predicting physical processes has been demonstrated in various studies. For instance, Lahiri and Ghanta (2008) successfully used SVR to predict the pressure drop of slurry flow in pipelines, showcasing its effectiveness in fluid dynamics [15]. Similarly, Wu, Wei, and Terpenny (2018) applied SVR to predict surface roughness in fused deposition modeling processes, highlighting its utility in manufacturing [16]. These examples underscore the potential of SVR in accurately predicting complex physical phenomena based on historical data.

5 Preliminary Results

5.1 Development of a Python Prototype for Digital Twin Simulation

In the preliminary phase of developing the digital twin for the Siberian Ring Source of Photons (SKIF), a simple prototype has been created. This program is designed to integrate and utilize the pre-generated data from COMSOL Multiphysics simulations, specifically focusing on the heat and stress fields of the diamond window and its cooling system. The core functionalities of this program include:

- Data Integration: The program reads pre-generated COMSOL data and a 3D STL model of the diamond window. This data includes temperature and stress data for each model point for different input parameters.
- User Interface for Parameter Input: The program features a graphical user interface where users can input desired parameters, such as beam position (x, y coordinates) and cooling water flow rate. Additionally, users can select which output parameter (temperature or stress) they wish to visualize.
- Machine Learning Model Training: For each point on the 3D model and for each output value (temperature, stress), the program trains a NuSVR (Nu-Support Vector Regression) model from the scikit-learn library. This machine learning approach allows for predictions of temperature and stress based on input parameters.
- Visualization and Prediction: Based on the inserted input parameters, the program predicts and displays the selected output parameter on the 3D model. This visualization is achieved through color mapping, providing an intuitive understanding of how temperature or stress varies across the diamond window.
- Model Saving and Loading: Recognizing that training machine learning models can be time-consuming, the program is equipped with the capability to save and load trained SVR models.

The development of this program is grounded in Python, a versatile and widely-used programming language known for its readability and extensive support for scientific computing. Python's vast ecosystem of libraries and tools makes it an ideal choice for developing complex simulation and data analysis applications [17].

Scikit-learn, a key library used in this program, is an open-source machine learning library for Python. It provides simple and efficient tools for data mining and data analysis, and it is built on NumPy, SciPy, and matplotlib. Scikit-learn is known for its robustness and ease of use, making it a popular choice for implementing machine learning algorithms, including support vector machines like NuSVR which was used in the described digital twin prototype [18].

In summary, the preliminary results demonstrate the successful integration of COMSOL-generated data with advanced machine learning techniques in Python, facilitated by scikit-learn. This integration forms the foundation of the digital twin's predictive capabilities, enabling accurate simulations of the diamond window's behavior under various operational scenarios.

6 Conclusion

7 References

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