ADVANCING SIMULATION CAPABILITIES AT EUROPEAN XFEL: A MULTIDISCIPLINARY APPROACH

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Abstract

At European XFEL, computational techniques such as finite element analysis (FEA) and computational fluid dynamics (CFD) are widely applied in various scientific and engineering fields, such as damage simulation due to heat load, bleaching effect study of gas attenuator, optimization of fluid cooling system for detectors and characterization of liquid sheet jets for sample delivery system. Without being constrained by experimental conditions, the multiphysics and multiscale models in simulation could virtually replicate the interaction process of XFEL beam with different materials, taking into consideration heat transfer, structural deformation and phase transition. In this contribution, to gain comprehensive insights into the fluid behaviors of the detector cooling system, as well as the performance of reduced order modelling solvers, parametric studies are conducted using CFD simulation code. Furthermore, a realistic simulation requires a secured process of Verification and Validation (V&V) of the computational model. Specific guides and standards need to be followed to ensure the credibility and accuracy of the simulation results. Besides following the FAIR principle (Findable, Accessible, Interoperable, and Reusable), a smart simulation data management system using machine learning algorithm is under construction. Moreover, the large amount of data from the simulations in the past can be utilized to train the machine learning model, which can be used for simulation results prediction without running further simulations. Further AI and machine learning tools are going to be employed to set up generative design workflow and digital twin scheme for the beamline components, serving as a new safety constraint for monitoring and optimizing of the facility operation.

VERIFICATION, VALIDATION AND UNCERTAINTY QUANTIFICATION

The goal of setting up a systematic verification, validation and uncertainty quantification (VVUQ) for all simulations is to build a common agreement based on corresponding ISO standard [1–3] regarding the reliability of simulation results. This topic is increasingly important when many models could be reused for new applications. As an example, to characterize the thickness change of the CVD diamond of the spectrometer, simulation results using various numerical methods are compared in Fig. 1. It shows that the divergence between these methods is obvious. Without having possibility to validate with experimental results, it is important to execute a VVUQ process. The comparison shows that the element using convective coordinates which include the 2nd order bending moment is the most precise and efficient computational model. But since the elements in commercial code are only based on Cartesian coordinates, finer meshing is needed for a precise results [4]. Therefore, a standard workflow is essential, to ensure the credibility of the simulation models and results as following: (a) Purpose and Scope (b) Model Development (c) Verification and

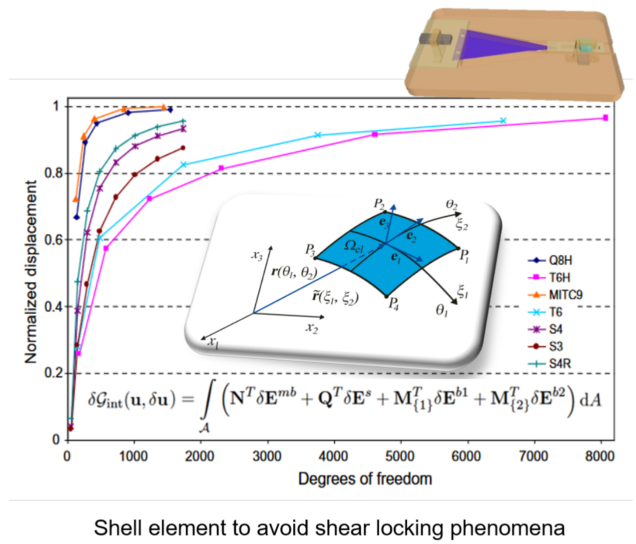

Figure 1: Characterization of thickness change of bending crystal.

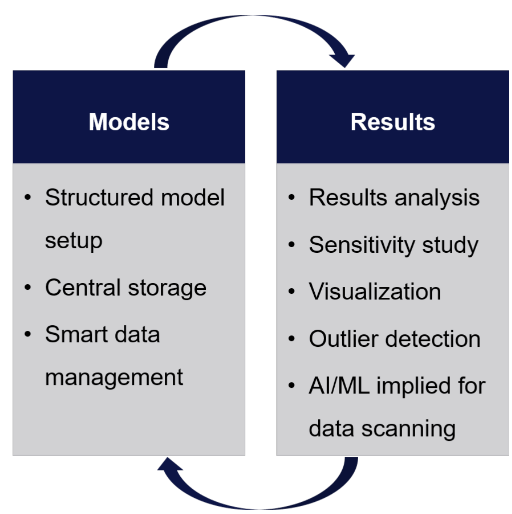

Figure 2: Simulation data management Scheme.

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Pulse energy [mJ]	Photon Energy [keV]	power [W]	FWHM [mm]	simulation results [°C]	AI predicted [°C]
1.87	10	5.05	0.2	29.34	30.77
1.56	12	4.21	0.19	26.23	27.94
1.34	14	3.61	0.18	24.90	24.99
1.17	16	3.16	0.17	24.13	23.46
1.04	18	2.81	0.17	23.60	23.04
0.94	20	2.53	0.16	23.41	22.63

Figure 3: Simulation results prediction.

Validation (d) Uncertainty Quantification (e) Credibility Assessment. For each term there are key points that need to be clarified, communicated and documented.

APPLICATION OF AI AND MACHINE LEARNING IN SIMULATION

Accompanied with the development of artificial intelligence and machine learning algorithm, as well as the interaction of natural language with machine language, the mode of simulation is being revolutionized. In the following subsections, some first applications of AI and ML tools in the field of simulation at European XFEL are briefly introduced.

Simulation Data Management (SDM) System

A systematic data management for the large amount of simulation data has been for long time a crucial subject in the research facilities [5]. To improve the current situation, two main categories are being reconstructed in SDM, see Fig. 2. Using ML algorithm, it is possible to scan the models and results in very short time on the central storage, automatically accomplish the sensitivity analysis, outlier detection and visualization functions.

Simulation Results Prediction

AI/ML tools could be used in simulation for the results prediction based on the input data [6]. As an example, the interaction of X-ray laser beam with B4C component for shutters at European XFEL are show in Fig. 3. Hundreds of input data, such as photon energy, pulse energy, beam size, penetration depth are used to train the model. Using layer wise neural network of machine learning code, the temperature profile could be precisely predicted without running further simulations.

Generative Design

AI and ML could be implied not only in the data management system, but also during the complete life cycle of engineering design. In the conventional design workflow, simulation is used to be a bottle neck in the design iteration loop, see Fig. 4. Using AI driven generative design, it is possible to get an optimized solution in relative short time, see Fig. 5. Different from topology optimization, generative design doesn't start from an existing design. Based on the defined targets that need to be fulfilled, e.g. minimize the temperature gradient, set the maximum allowed flow velocity below 1 $\mathrm{m\,s^{-1}}$, etc., the ML algorithm will generate several hundreds of conceptual design and layer wise find the optimized solution based on simulation with reduced order models.

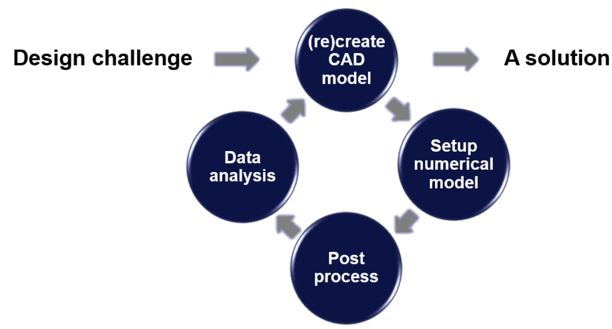

Figure 4: Conventional design workflow.

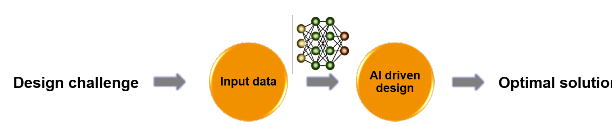

Figure 5: Generative design workflow.

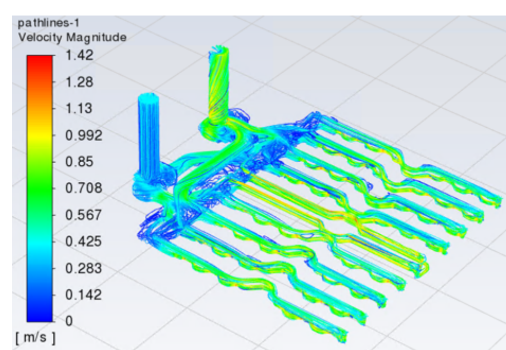

Figure 6: CFD simulation of detector cooling component using ANSYS Fluent.

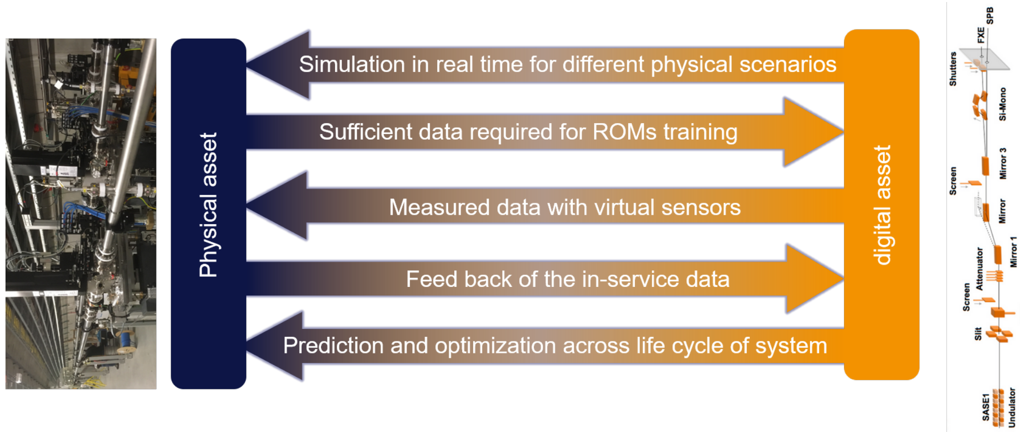

Figure 7: Diagram of digital twin.

Reduced Order Modelling (ROM) and Digital Twin

Reduced order modelling [7] offers opportunity for an efficient, in real time simulation, by reducing the number of equations that need to be solved significantly without losing main features of the system. ML algorithm enhanced the ROM by data driven optimization in reducing the model orders. It is specifically used for CFD simulations and complex system, in which millions of variables need to be solved. Figure 6 presents a cooling element for detectors. Using ROM with ML algorithm integrated in the solver, the computing time reduced from 4 hours to 5 seconds, without losing accuracy of the results.

The real time simulation capability of ROM enables the implementation of digital twin for either single device or assembly of the beamline, see Fig. 7. In a digital twin system, parametric study with hundreds of scenarios could be simulated in real time, and the optimized setup will be transferred to the physical asset, vice versa the measured data from physical sensors will feedback the performance of the device to the virtual system. Through communicating with each other synchronously, the digital replica will accompany the physical asset during the whole life cycle of the components.

CONCLUSION

In this contribution, a multidisciplinary approach of simulation at the European XFEL [8, 9] has been presented . Verification and validation workflow ensure the credibility of simulation results. With the aid of AI/ML tools, data management and simulation results prediction is under developing gradually. Looking forward, generative design and digital twin with implied generative AI model will reshape the world of simulation [10].

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