Towards an Automated AI Based Simulation Framework in Aerospace Engineering

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Abstract

In the aerospace industry, there is an increasing inclination to replace costly and time-consuming prototyping with computer simulations. These simulations are characterized by their complexity and the necessity of not only a proper physical representation, but also the capacity to meet time-to-solution expectations. Numerous specialized software packages have been developed in recent years, incorporating a range of numerical techniques. However, the majority of these packages are designed to address specific problems such as structural mechanics or computational fluid dynamics problems. Real-world applications, however, are more involved and require the consideration of coupling approaches, which allow the combination of available tools to realize complex and interdisciplinary simulations, involving not only multi-scales, but also multi-physics. In this regard, supercomputing systems are indispensable, as they allow the realization of complex problems. The main question persist, how to enhance the efficiency of computations beyond the scaling with increased computational resources. Hererby, machine learning has the potential to play a pivotal role by not only reducing the computation but also allow for predicting the numerical solutions that do not necessitate extensive hours of computing time on supercomputing systems. This, in turn, has the effect of significantly reducing the time to solution, which is an important factor from the industrial perspective. However, it is important to ensure the reproducibility and reliability of the predicted results for critical decision-making processes. The processes involved in such an approach are complex and data-driven. The incorporation of this approach requires not only the software itself, but also data, batching, preprocessing, and other related components, to utilize the training and validation of the machine learning algorithm. In this context, provenance emerges as a crucial element in the documentation of the entire process, from the initial configuration of a simulation to the prediction of results and the identification of the ultimate solution. In this work our goal is the utilization and integration of existing powerful tools in a framework, that enables accurate and efficient workflows for complex simulations in an automated manner. Moreover, the central aim is to facilitate complex simulations by making sustainable use of available software packages, without in-depth knowledge of the underlying algorithm.

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CCS Concepts

• **Computing methodologies → Massively parallel and high-performance simulations**; **Massively parallel algorithms**; **Machine learning**; • **Applied computing → Aerospace**.

Keywords

CFD, Multi-scale, Multi-physics, Coupled problems, Machine learning, Provenance, HPC, Sustainability

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1 Introduction

In recent years, advances in the numerical simulation have been witnessed across various disciplines, including the development of novel techniques to allow for real-world applications, such as those related to aircraft turbines. However, the majority of these software packages are primarily designed to address specific problems, including structural or incompressible fluid solvers [3, 6]. It is important to acknowledge that real-world applications are inherently complex, involving multi-scales and physics that have to be considered. In the case of e.g. a turbine, we have the rotating blades (structural mechanics), the flow field (fluid dynamics), and the sound generation (aeroacoustics) that needs to be taken into account. Simulating all these different physical phenomena with a single solver is not only difficult, but also costly, even on modern supercomputers. Consequently, there have been developments towards the integration of dedicated tools and simulation environments [1, 2, 7], deploying advanced software capabilities, including the utilization of multiple solvers to address complex, multi-scale, and multi-physics problems. This approach enables the execution of complex simulations by coupling different solvers, hence enhancing efficiency. Due to the recent advancements in this domain, the potential implementation of even more sophisticated techniques has become more important. Machine learning (ML) has emerged as a pivotal element in this context. Although coupling different solvers can help to reduce the computational effort and the time to solution expectations, the growing era of AI-based techniques has led to increased attention being given to the incorporation of ML methods. The integration of ML techniques in the field of numerical simulations has shown to offer numerous advantages, including enhanced efficiency and the potential to achieve comparable results as classical numerical simulations [10, 11]. However, it is important to acknowledge the lack of reliability of these results, given the inherent complexities of the ML methodologies employed. These methodologies can be seen as a 'black box', in that the underlying decision-making processes used for prediction are not transparent to be trusted. There are approaches for explainable AI trying to make AI predictions more suitable for safety critical applications. But these approaches are still in development. Instead of using XAI we believe for a real understanding of the underlying simulation process, the understanding of the data and its flow is important. Consequently, provenance has gained attention in this field, to address this drawback, by tracking the workflow and collecting required information [4, 5, 8, 9]. This enables not only a transparent workflow, but also one that is reproducible and reliable for even critical decision-making. The software and strategies previously refered to, have been demonstrated to enhance the efficiency of numerical simulations. In addition, provenance frameworks have been developed to facilitate the documentation of simulation processes. However, as of our knowledge, there has been no framework that combines available tools with each other in an automated manner, to allow for **(i)** a sustainable use of availabe tools and **(ii)** efficient combination of different solvers to enable complex simulations and **(iii)** transparent, reproducible and reliable outcomes. The objective of this work is to propose a framework that allows enhanced accessibility and utilization of various solvers and their underlying methodologies, without in-depth knowledge of the underlying code and its development process.

2 An automated framework for large and complex simulations

The availability of software packages is considerably high, with each dedicated to solving specific problems efficiently. While each have their strengths and weaknesses, they address specific problems to be solved. The objective of this work is to establish an automated framework, where multiple solvers can be used to enable large and complex simulations, not necessitating in-depth familiarity with the underlying algorithm. This allows researchers to utilize solvers available, despite their inherent complexity and their lack of knowledge of the underlying developed code. Though the user is required to have at least a solid knowledge of the simulation field to interpret the outcomes. The framework is meant to coordinate the interaction between the user and the underlying model. Based on the problem to be solved, the user provides information about the simulation that needs to be executed to the framework. The framework utilizes large language models (LLMs), where source code analysis and documentation analysis are taken into account. According to the received information, the model will suggest after a comprehensive analysis of different solvers, which solver or solvers to use (source code analysis) and generates the specific setup and interface if needed to connect them (source code generation). The suggestion is based on the available information or best practice experiences. This will require special techniques using AI models specifically LLMs, that will allow better understanding of the code and its generation. Is the solver or solver combination chosen, the LLM will first generate a configuration file with the settings required to execute the simulation. The user has here the option to either accept the suggestion or provide further information. In the latter case, the underlying model will be able to reconfigure the settings for the simulation in order to provide an appropriate configuration file that can be executed on a supercomputing system. In Fig. 1 the basic principle of the framework is depicted. The input is the user-provided information about the simulation. This information is directed to the LLM (referred to as a 'Black box' in Fig.1) that analyzes available softwares and identifies the suitable tools, while generating the required interface, in case multiple tools are needed to address the problem. Moreover, the configuration file is generated to facilitate its execution. Provenance is utilized at all stages of the framework, to keep record of decisions that have been made.

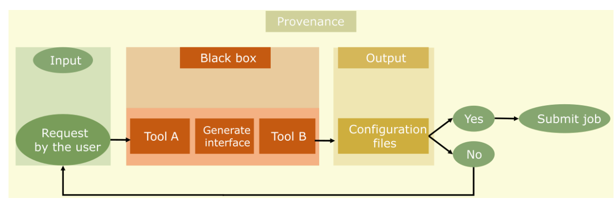

Figure 1: Workflow of an automated framework to run complex simulations without in-depth familiarity of the underlying algorithm. The input information (the request) is provided by the user. The automated framework does a comprehensive investigation of the available solvers (Black box) and provides a configuration file that can be executed (Yes) or can be adjusted (No) by providing additional information to the framework. The final configuration will be submitted to a supercomputing system (Submit job).

3 Conclusion

In this work we propose the idea of an automated framework used to enable complex multi-scale, multi-physics and coupled simulations in the domain of aerospace engineering. The main focus of this framework is the utilization of available tools, that have been developed for specific problems, which allow for their sustainable use for different numerical problems. Moreover, this approach allows their combination based on the technical intention of the user and its interpretation by an LLM. The advantage of the framework is its capability to use tools without necessitating a comprehensive understanding of the underlying code and its development process by the user. Instead, the methodology employed and the results obtained from the simulation are of significance.

References

[1] R. Ahrem, P. Post, B. Steckel, and K. Wolf. 2001. MpCCI A tool for coupling CFD with other disciplines. In *5th World Conference in Applied Fluid Dynamics. Simulation and Visualisation 2001 Conference; SIM 2001. Proceedings of the Conference.* Springer Berlin Heidelberg, Berlin, Heidelberg.

[2] Hans-Joachim Bungartz, Florian Lindner, Miriam Mehl, Klaudius Scheufele, Alexander Shukaev, and Benjamin Uekermann. 2016. Partitioned Fluid-Structure-Acoustics Interaction on Distributed Data – Coupling via preCICE. In *Software for Exa-scale Computing – SPPEXA 2013-2015*, Hans-Joachim Bungartz, Philipp Neumann, and E. Wolfgang Nagel (Eds.). Springer Berlin Heidelberg.

[3] Hans-Joachim Bungartz, Miriam Mehl, and Schäfer Michael. 2010. *Fluid structure interaction II.* Springer.

[4] Nils Hoffmann and Neda Ebrahimi Pour. 2024. A low overhead approach for automatically tracking provenance in machine learning workflows. In *9th IEEE European Symposium on Security and Privacy Workshops, Euro S and PW 2024 (9th IEEE European Symposium on Security and Privacy (Euro&SP)).* IEEE Computer Society Conference Publishing Services, 567–573. https://elib.dlr.de/205258/

[5] Matteo Interlandi, Kshitij Shah, Sai Deep Tetali, Muhammad Ali Gulzar, Seunghyun Yoo, Miryung Kim, Todd D. Millstein, and Tyson Condie. 2015. Titian: Data Provenance Support in Spark. *Proceedings of the VLDB Endowment International Conference on Very Large Data Bases* 9 (2015), 216 – 227. https://api.semanticscholar.org/CorpusID:8433820

[6] G. Link, M. Kaltenbacher, M. Breuer, and M. Döllinger. 2009. A 2D finite-element scheme for fluid-solid-acoustic interactions and its application to human phonation. *Computer Methods in Applied Mechanics and Engineering* 198, 41-44 (2009), 3321–3334.

[7] Kannan Masilamani, Adam Büchner, Simon Ehrmanntraut, Sebastian Gottfried, Lars Reimer, and Arthur Stück. 2024. A Scalable MDAO Framework Approach Enabling Nested Solution Algorithms for Static Aeroelastic Coupling Scenarios. In *AIAA AVIATION FORUM AND ASCEND 2024 (AIAA AVIATION FORUM AND ASCEND 2024).* https://elib.dlr.de/210810/

[8] Arnab Phani, Benjamin Rath, and Matthias Boehm. 2021. LIMA: Fine-grained Lineage Tracing and Reuse in Machine Learning Systems. In *Proceedings of the 2021 International Conference on Management of Data (SIGMOD '21)* (Virtual Event, China). ACM, 14. doi:10.1145/3448016.3452788

[9] Fotis Psallidas and Eugene Wu. 2018. Smoke: fine-grained lineage at interactive speed. *Proc. VLDB Endow.* 11, 6 (feb 2018), 719–732. doi:10.14778/3199517.3199522

[10] Amin Totounferoush, Neda Ebrahimi Pour, Sabine Roller, and Miriam Mehl. 2021. Parallel Machine Learning of Partial Differential Equations. In *2021 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW).* 698–703. doi:10.1109/IPDPSW52791.2021.00106

[11] Ricardo Vinuesa and Steven L. Brunton. 2022. Enhancing Computational Fluid Dynamics with Machine Learning. *Nature Computational Science* 2, 6 (2022), 358–366. doi:10.1038/s43588-022-00264-7