

CONVERGENCE OF ARTIFICIAL INTELLIGENCE AND HIGH-PERFORMANCE COMPUTING FOR COMPUTATIONAL FLUID DYNAMICS (AI + HPC4CFD PT. 5)

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Abstract. The rapid advancement of accelerator technologies, especially their integration in large-scale HPC systems in the form of GPUs, together with the emergence of practically usable AI architectures, such as transformers or physics-informed neural networks, continues to revolutionize science and industry. As a consequence, AI technologies are now used in almost every area. Their integration into workflows to automate and accelerate processes, and their ability to uncover new, unseen relations in huge datasets have elevated them to become key components of strategic agendas of many scientific disciplines and industrial sectors. In addition, the new player on the market "agentic AI" facilitates, e.g., autonomous workflows, AI-AI interactions, automatic model selection, or optimization, and unites the worlds of domain and data sciences, AI, and HPC.

In the field of engineering, AI technologies are used to develop new models for CFD, e.g., reduced-order models, surrogates, and closure models aiming at efficiently representing complex physics that are otherwise expensive to compute. Furthermore, reinforcement learning is employed for flow control applications, while receiving feedback from CFD solvers after an action, and emerging physical AI approaches enable closed-loop interaction with real-world systems. The quality of these methods depends on the quantity and accuracy of the training data, as well as the physical constraints imposed. Modular HPC systems are required to create and process high-fidelity simulation data, and to deal with the demands of complex and intertwined simulations and AI data processing workflows towards foundation and multi-modal models and their application for CFD. Agentic AI is expected to massively advance CFD workflow management with automatic data retrieval, CFD-simulation- and AI-methods selection, model fine-tuning, or interpretation of results.

This mini-symposium aims at continuing the successful 2022 – 2025 AI+HPC4CFD mini-symposia. It gathers experts in the fields of development and application of parallel CFD methods incorporating novel AI methods, and pure AI method and workflow developers contributing to the fields of CFD and HPC alike. It offers a platform for discussion and exchange in the context of the convergence of AI and HPC with respect to parallel CFD methods using the power of future computing systems and agent-based workflows.

Topics of interest for this mini-symposium include, but are not limited to:

1. Physics-informed/-aware architectures for, e.g., efficient flow field predictions
2. (Federated) AI technologies for accelerating CFD workflows on HPC machines
3. Agentic AI for, e.g., autonomous CFD workflows, user-simulation interaction, optimization, or result interpretation
4. Physical AI and closed-loop interaction with real-world systems
5. Optimization and flow control using, e.g., reinforcement learning techniques
6. Foundational and multi-modal models for CFD
7. Super-resolution, AI-based turbulence, surrogate modeling
8. Benchmarking neural network architectures for CFD applications
9. General neural network architectures to predict flow quantities (also temporally) for a wide set of applications, e.g., in combustion, aerodynamics, bio-fluid mechanics, or further engineering applications

Short bio of the organizers



Dr. Andreas Lintermann is the leader of the Simulation and Data Lab "Fluids & Solids Engineering" at the Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich. He was coordinating the European CoE RAISE and leads/co-leads JSC's activities in various national and international projects, e.g., in EuroCC3, SPECTRUM, HANAMI, RI-SCALE, AIRIS, TwinRISE, or nxtAIM. He is involved in the Industry Relations Team of the institute. His research focuses on HPC, modular supercomputing, AI, bio-fluidmechanis, lattice-Boltzmann methods, high-scaling meshing methods, and efficient multi-physics coupling strategies.



Since 2005, Dr. Guillaume Houzeaux has led the "Physical and Numerical Modeling" team at the Barcelona Supercomputing Center in Spain. He is a key architect of the Alya HPC simulation code, which is applied in fields such as aeronautics, combustion, wind energy, and biomedicine. His research is centered on High Performance Computational Mechanics, with a particular focus on high-performance computing with applications in biomedicine. This involves physical modelling, mathematical algorithms, adaptive mesh refinement, code development following a CI/CD methodology and code optimization, all driven by the objective of efficient use of parallel resources.



Dr. Mario Rüttgers is a visiting professor in "Energy Process Innovation Convergence" and a member of the "Data-Driven Fluid Engineering" (DDFE) laboratory at Inha University, with a Walter Benjamin stipend from the German Research Association (DFG). Before, he was a member of the Simulation and Data Lab "Fluids & Solids Engineering" at JSC. In 2024, he received his Ph.D. degree at the Institute of Aerodynamics and Chair of Fluid Mechanics, RWTH Aachen University. His research focuses on combining computational fluid dynamics and machine learning techniques.



Dr. Christian Lagemann is a Postdoctoral Research Fellow at the Machine Learning & Statistics department at the German Center for Neurodegenerative Diseases and leads its HPC AI section since 2025. His research focuses on the application of artificial intelligence to dynamic systems, with interests in deep learning based surrogate modeling, reinforcement learning and data-driven discovery of complex real-world systems. He holds a Habilitation in Artificial Intelligence in Fluid Mechanics and a Ph.D. in Mechanical Engineering from RWTH Aachen University.



Dr. Corentin Lapeyre is a Strategic Research Collaboration Manager at NVIDIA, where he empowers scientists to achieve breakthrough discoveries through accelerated computing and AI. With a background in computational physics, Corentin earned his PhD from Toulouse INP in 2015, specializing in massively parallel simulations of thermoacoustics in aircraft engines. In 2018, he founded the AI for Science team at CER-FACS, and for 6 years he spearheaded the application of data-driven techniques to complex modeling and simulation challenges across aerospace, energy engineering, and geoscience applications.



Makoto Tsubokura is a professor of computational fluid dynamics at the Graduate School of System Informatics, Kobe University since 2015, and the leader of the Complex Unified Simulation Research Team at the Center of Computational Science, RIKEN since 2012. After earning a Ph.D. from the University of Tokyo in 1997, he first became a lecturer at the Tokyo Institute of Technology in 1999, then an associate professor at the University of Electro-Communications in 2003, then at Hokkaido University in 2007. He specializes in research and development of mathematical modeling and simulation algorithms for thermal fluids in turbulent state, and their expansion to massively parallel environment on high-end supercomputers.