Differentiable Computational Fluid Dynamics

Ludger Paehler*, and Jan Hueckelheim†

* Chair of Aerodynamics and Fluid Mechanics
Technical University of Munich (TUM)
Boltzmannstr. 15, 85748 Garching bei Muenchen, Germany
e-mail: ludger.paehler@tum.de, web page: https://www.epc.ed.tum.de/en/aer

† Laboratory for Applied Mathematics, Numerical Software, and Statistics
Argonne National Laboratory
9700 South Cass Avenue, Building 240, 60439 Lemont IL, USA
e-mail :jhuckelheim@anl.gov , web page: https://www.anl.gov/mcs/lans

ABSTRACT

With the ever-faster advances of machine learning-based methods for science and engineering computational fluid dynamicists are including ever more of these differentiable techniques in their computational workflows. Originating from previous advances for adjoint-based methods for computational fluid dynamics [3] differentiable programming, the practice of utilizing gradients of simulations or objective functions for varied applications such as gradient-based optimization, gradient-based sampling approaches like Hamiltonian Monte-Carlo, or in machine learning applications has garnered significant interest in recent years [1]. Going further, some approaches go as far as replacing components of their solver with learned machine learning constructs [2] or learning graph-based surrogate models for their forward simulation [4]. All of these approaches open up a whole array of novel ways to tackle open problems in computational fluid dynamics, while at the same time necessitating new approaches to embed or connect existing computational fluid dynamics workflows with these new algorithmic approaches.

In this minisymposium we will connect computational fluid dynamicists with researchers working at the intersection of these exciting fields to present their recent advances in combining differentiable programming techniques from machine learning and beyond, with their computational fluid dynamics solvers to foster exchange, and present their exciting new applications. This includes, but is not limited to

1. Advances in machine learning-infused computational fluid dynamics
2. Applications of gradient-based techniques in computational fluid dynamics applications
3. Differentiable programming workflows with computational fluid dynamics components

REFERENCES

[1] Vinuesa, R., Brunton, S.L. Enhancing computational fluid dynamics with machine learning. *Nat. Comput. Sci.*, Vol. **2,** pp. 358–366, 2022.

[2] Kochkov, Dmitrii, et al. Machine learning–accelerated computational fluid dynamics. *Proceedings of the National Academy of Sciences*, Vol. **118**(**21**), p. e2101784118, 2021.

[3] Wang, Q. Forward and adjoint sensitivity computation of chaotic dynamical systems. *Journal of Computational Physics*, Vol. **235**, pp.1-13, 2013.

[4] Pfaff, T., Fortunato, M., Sanchez-Gonzalez, A., & Battaglia, P. Learning Mesh-Based Simulation with Graph Networks. *International Conference on Learning Representations*, 2020.