24th IACM Computational Fluids Conference (CFC 2027)
March 12-15, 2027, Yokohama, Japan

BIG SCIENCE IN COMPUTATIONAL FLUID DYNAMICS: CAN MACHINE LEARNING AND QUANTUM COMPUTING PUSH OUR KNOWLEDGE?

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Key words: quantum computing, machine learning, big science, turbulence closures, physics-informed, rare events, multi-physics

ABSTRACT

Independently, machine learning [1] [2] [3] [4]and quantum computing [5] [6] [7] [8]have revolutionised, or at least proposed to, several paradigms in the realm of CFD, suggesting speed-ups enabling quantitatively new applications and regimes to be explored.
However, the adoption of machine learning to unlock research questions qualitatively impossible to address within the realm of traditional computational methods is in its infancy, as applications targeting what could be classified as big science questions emerge, enabling fundamental understandings of the laws behind the behaviour of fluids in specific conditions [9]. These explorations have possibly lagged behind in the realm of quantum computing, as the shortening and limitations of quantum hardware have hindered broad scope numerical explorations so far, making assessments of computational capabilities much more first-principled. In this workshop, we plan to gather contributions and encourage discussions about the interplay of these two technologies in addressing such questions, as well as selected examples illustrating the recent progress in their separate application.
We expect the symposium speakers to touch at least some of the following, tentative relevant sub-thematics.

i) **Turbulence closures**. Can we address this inverse problem, plagued by non-uniqueness, hidden variables, and multi-regime physics even in scenarios with sparse, biased data [10]? Which flow regimes do we expect to be most challenging for the novel techniques explored in this symposium? Bayesian and probabilistic turbulence closure with physical constraints are a starting point, and quantum-enhanced sampling for posterior exploration might possibly be a complement.

ii) **Scientific inference for PDEs** in CFD: beyond physics-informed paradigms. The idea here is to move further away from “solving faster a known model” into “what is the governing physics of an unknown regime”? The inverse problems might involve: unknown forcings, constitutive laws, boundary/initial conditions... Hybrid quantum–classical variational inference for PDE-constrained problems have been proposed [11], and physics informed paradigms have reaped some success in this area [12]. What comes next?

iii) **Rare events in fluids**: quantum-ML for tails, transitions, and extremes Here the rationale is that extreme events are (close to) measure-zero in simulations, but can dominate risk in real scenarios, and disrupt the accuracy guarantees of the numerics. Predicting, detecting, and characterizing such transitions (laminar→turbulent, blow-up events like unstable singularities, rogue waves analogs, intermittency) is thus an important task [13], often relying on statistics and heuristics.

iv) **Multi-physics CFD** as a grand inverse problem: condensation, phase change, reactive flows, multi-physics closures and phase transition kinetics can in principle be understood also as an inference problem [14] [15], as they sit at boundaries where key governing physics becomes uncertain, and data acquisition for model validation is indirect (e.g., nucleation, interfacial transport, reaction mechanisms). Key applicative areas could span constitutive relations under constraints (thermodynamics, entropy production), pa rameter/posterior exploration in stiff chemical kinetics / phase changes, multi-fidelity and multi-scale assimilation, regime classification from sparse sampling

REFERENCES

[1] S. L. Brunton, B. R. Noack, and P. Koumoutsakos, "Machine Learning for Fluid Mechanics," *Annu. Rev. Fluid Mech.*, vol. 52, no. Volume 52, 2020, pp. 477–508, 2020, doi: https://doi.org/10.1146/annurev-fluid-010719-060214.

[2] M. Raissi, P. Perdikaris, and G. E. Karniadakis, "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations," *J. Comput. Phys.*, vol. 378, pp. 686–707, Feb. 2019, doi: 10.1016/j.jcp.2018.10.045.

[3] F. De Avila Belbute-Peres, T. D. Economon, and J. Z. Kolter, "Combining differentiable PDE solvers and graph neural networks for fluid flow prediction," *37th International Conference on Machine Learning, ICML 2020*, vol. PartF16814, pp. 2380–2389, 2020.

[4] D. Kochkov, J. A. Smith, A. Alieva, Q. Wang, M. P. Brenner, and S. Hoyer, "Machine learning–accelerated computational fluid dynamics," *Proc. Natl. Acad. Sci. U. S. A.*, vol. 118, no. 21, p. e2101784118, May 2021, doi: 10.1073/PNAS.2101784118;WGROUP:STRING:PUBLICATION.

[5] B. Ljubomir, "Quantum algorithm for the Navier-Stokes equations by using the streamfunction-vorticity formulation and the lattice Boltzmann method," *International Journal of Quantum Information*, vol. 20, no. 2, pp. 1–20, 2022, doi: 10.1142/S0219749921500398.

[6] O. Kyriienko, A. E. Paine, and V. E. Elfving, "Solving nonlinear differential equations with differentiable quantum circuits," *Phys. Rev. A (Coll. Park).*, vol. 103, no. 5, pp. 1–22, 2021, doi: 10.1103/PhysRevA.103.052416.

[7] X. Li *et al.*, "Potential quantum advantage for simulation of fluid dynamics," no. 7, pp. 1–23, 2023, [Online]. Available: http://arxiv.org/abs/2303.16550

[8] C. Sanavio, R. Scatamacchia, C. de Falco, and S. Succi, "Three Carleman routes to the quantum simulation of classical fluids," *Physics of Fluids*, vol. 36, no. 5, p. 57143, 2024, doi: 10.1063/5.0204955.

[9] Y. Wang *et al.*, "Discovery of Unstable Singularities," Sep. 2025, Accessed: Nov. 17, 2025. [Online]. Available: https://arxiv.org/pdf/2509.14185

[10] A. Beck and M. Kurz, "A perspective on machine learning methods in turbulence modeling," *GAMM-Mitteilungen*, vol. 44, no. 1, p. e202100002, Mar. 2021, doi: 10.1002/GAMM.202100002.

[11] N. Heim, A. Ghosh, O. Kyriienko, and V. E. Elfving, "Quantum Model-Discovery," pp. 1–19, 2021, [Online]. Available: http://arxiv.org/abs/2111.06376

[12] Y. Sun, U. Sengupta, and M. Juniper, "Physics-informed Deep Learning for simultaneous Surrogate Modelling and PDE-constrained Optimization," *Comput. Methods Appl. Mech. Eng.*, vol. 411, pp. 1–26, Jun. 2023, doi: 10.1016/J.CMA.2023.116042.

[13] L. Wang, "Discovering phase transitions with unsupervised learning," *Phys. Rev. B*, vol. 94, no. 19, 2016, doi: 10.1103/PhysRevB.94.195105.

[14] O. Hennigh *et al.*, "NVIDIA SimNet™: An AI-Accelerated Multi-Physics Simulation Framework," *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, vol. 12746 LNCS, pp. 447–461, 2021, doi: 10.1007/978-3-030-77977-1_36/COVER.

[15] H.-K. Noh, C. Won, J. Lee, S. Choi, S. Lee, and J. H. Lim, "Physics-informed machine learning: technological trends in turbulence flow, topology optimization, and convergence enhancement with temporal causality consideration," *JMST Advances 2025 7:1*, vol. 7, no. 1, pp. 113–124, May 2025, doi: 10.1007/S42791-025-00101-8.

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