Postdoc Position

Physics-constrained deep network augmentation of turbulence models

Contacts

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Location : Sorbonne Université, Pierre et Marie Curie Campus, 4 Place Jussieu, 75005, PARIS, France

Profile of the successful candidate : PhD in Fluid Mechanics, Applied Mathematics or Computer science, taste for multidisciplinary research, proved skills in scientific computing

How to apply: please send the following information to P. Cinnella: CV, motivation letter, references.

Duration: two years

Starting date : flexible, preferably september 2023.

Salary : fully funded positions, partial refunding of local mobility fees

Context

Numerical simulation of fluids plays an essential role in modeling complex physical phenomena in domains ranging from climate to aerodynamics. Fluid flows are well described by Navier-Stokes equations, but solving these equations at all scales remains extremely complex in many situations and only an averaged solution supplemented by a turbulence model is simulated in practice. Unfortunately turbulence models present important weaknesses (Xiao and Cinnella, 2019). The increased availability of large amounts of high fidelity data and the recent development and deployment of powerful machine learning methods has motivated a surge of recent work for using machine learning in the context of computational fluid dynamics (CFD), and specifically turbulence modelling (Durasaimy et al., 2019). Combining powerful statistical techniques and model-based methods leads to an entirely new perspective for CFD. From the machine learning (ML) side, modeling complex dynamical systems and combining model-based and data-based approaches is the topic of active new research directions. With the aim of fostering progress in the understanding, modeling and design of turbulent flows the **Sorbonne Institute of Computating and Data Science** (ISCD) has funded the **LearnFluidS** (Machine-LEARNing for FLUID Simulations) projet team: a well-balanced team of researchers well-known in the fields of CFD, Deep Learning, numerical analysis and turbulence modeling.

Our aim is to develop the interplay between Deep Learning (DL) and CFD in order to improve turbulence modeling and to challenge state of the art ML techniques.

Participants

The project team **LearnFluidS** promotes **the development of recent machine learning advances in the field of computational fluid dynamics**. Until very recently these two domains were completely separated and this is only during the last few years, thanks to the considerable advances of Deep Learning and the increased availability of simulation data, that researchers from both fields started to cooperate. The project gathers specialists from the two disciplines involved in the thesis topic: fluid dynamics at **Institut Jean Le Rond ∂'Alembert** (Institute of theoretical, computational and experimental mechanics) and machine learning at **ISIR** (Institute of intelligent systems and robotics). ∂'Alembert has a recognized expertise in CFD, turbulence modelling and in the development of machine-learned RANS models using sparse formal identification techniques. The Machine Learning team at ISIR is well known for its expertise in Deep Learning. The team develops interdisplinary research on dynamical systems involving cooperation with maths and climate specialists.

Objective: Combining CFD models and Deep Learning for predicting turbulence

Our objective is to improve traditional CFD models, both in terms of complexity and of accuracy of the predictions, with the addition of ML components. Recent progresses, and the generalized use of automatic differentiation both for differentiable solvers and DL algorithms have paved the road to the integration of DL techniques and ODE/PDE solvers. In the ML community, a starting point for such investigations was the Neural ODE paper (Chen 2018) that promoted the use of ODE solvers for ML problems.

We advocate for this research the use of DL modules for complementing CFD solvers, in the spirit of (Le Guen 2021) who introduced a principled approach (APHYNITY, Augment incomplete PHYsical models for ideNtIfying and forecasTing complex dYnamics) however still limited to basic PDEs. In our new context, we will analyze how to model unclosed terms in the RANS equations. This approach can be seen as a generalization of classical closure models. In order to make easier this theoretical analysis, the approach will be first developed for a scalar surrogate of the Navier-Stokes equations, namely, the nonlinear Burgers' equation, which has been widely used in the literature as a simplified ansatz for Navier-Stokes turbulence, and two-dimensional homogeneous isotropic turbulence. Both internal (within the PDE) and external (on the PDE outputs) corrections will be investigated. The system will be trained using different strategies, e.g., end to end with the DL modules and the numerical solvers using high-fidelity data, gradient-free ensemble variational methods, and reinforcement learning, and assessed in terms of accuracy, training cost, and robustness.

In order to be useful for CFD applications a learned model must accurately simulate flows outside of the training distribution: operational conditions and environment may vary according to different physical factors thus requiring models to extrapolate to these new conditions. DL could in principle be extremely efficient for learning complex dynamics but they struggle with generalization to out-of-distribution data. We will adopt a new perspective by considering learning dynamical models from multiple environments and propose a new framework leveraging the commonalities and discrepancies among environments. We expect this new setting to be more robust to new distributions than classical empirical risk minimization or robust optimization schemes.

The framework will then be deployed and adapted to the specificity of unsteady RANS simulations. Turbulence model augmentation will be achieved by supplementing classical closure models for which we have prior knowledge with data-driven corrections. The results will be compared with those of data-augmented turbulence models derived by using symbolic regression (Schmelzer et al. 2020, Cherroud et al. 2022) for the flow problems of the NASA Collaborative Testing challenge for data-driven turbulence models (https://turbmodels.larc.nasa.gov/turb-prs2022.html).

References

- Arjovsky M. et al. 2020. Invariant Risk Minimization. *arxiv.org/abs/2002.04692* (2020), 1–31.
- Barber
- Bhattacharya K. et al. 2020, Model reduction and neural networks for para- metric pdes. Preprint arXiv:2005.03180 (2020).
- Chen, R.T.Q. et al., 2018. Neural Ordinary Differential Equations. *NIPS* (2018), 31–60.
- Cherroud S., Merle X., Cinnella P., Gloerfelt X., 2022. Sparse Bayesian Learning of Explicit Algebraic Reynolds-Stress models for turbulent separated flows. International Journal of Heat and Fluid Flow 98(December):109047
- Cherroud S., Merle X., Cinnella P., Gloerfelt X., 2022b. Spatial Model Aggregation (X-MA) of stochastic Explicit Algebraic Reynolds Stress models. 2022 Symposium on Turbulence Modeling: Roadblocks, and the Potential for Machine Learning. Suffolk, VI, July 27-29 2022.
- Duraisamy K., Iaccarino G., and Xiao H., Turbulence modeling in the age of data, Annual Review of Fluid Mechanics 51, 357 (2019).
- Gautier N. et al., 2015 Closed-loop separation control using machine learning. Journal of Fluid Mechanics, 770 (2015), 442–457
- Kochkov, D. et al. 2021. Machine learning accelerated computational fluid dynamics. (2021), 1–13.
- Le Guen V., Yin Y., Dona J., Ayed I., de Bézenac E., Thome N., Gallinari, P. 2021. Augmenting Physical Models with Deep Networks for Complex Dynamics Forecasting. *ICLR* (2021), 1–22.
- Ling Y., Arranz G., Williams E., Lozano-Duran A., 2022. Wall-modeled large-eddy simulation based on building-block flows. Preprint, December 2022. 10.48550/arXiv.2212.05120
- Schmelzer M., Dwight R.P., Cinnella P. 2020, Discovery of Algebraic Reynolds-Stress Models Using Sparse Symbolic Regression. Flow, Turbulence and Combustion 104 (2020), 579–603.
- Sirignano J., MacArt J.F., Freund J.B. 2020. DPM: A deep learning PDE augmentation method with application to large-eddy simulation. *Journal of Computational Physics*. 423, (2020), 109811.
- Um K. et al. 2020. Solver-in-the-Loop: Learning from Differentiable Physics to Interact with Iterative PDE-Solvers. *Neurips* (2020), 1–12.
- Wang R. et al. 2020, Towards physics-informed deep learning for tur- bulent flow prediction, in Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Dis- covery & Data Mining (2020), 1457–1466.
- Willard J.D. et al. 2020. Integrating physics-based modeling with machine learning: A survey. *arXiv* (2020), 1–34.
- Xiao H., Cinnella P. 2019, Quantification of model uncertainty in RANS simulations: A review. Progress in Aerospace Sciences, 108 (2019), 1-31.