∂'Alembert
Institut Jean le Rond d'Alembert

Sci-Fi-Turbo

Two PhD Positions open within project
Sci-Fi-Turbo HORIZON CL5
SCALE-RESOLVING SIMULATIONS FOR INNOVATIONS IN TURBOMACHINERY DESIGN

Contacts

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Location : Sorbonne Université, Pierre et Marie Curie Campus, 4 Place Jussieu, 75005, PARIS, France
Profile of the successful candidate : Master in Fluid Mechanics or Applied Mathematics, taste for multidisciplinary research, proved skills in scientific computing. (python, Fortran or C++, MPI would be appreciated)
How to apply: please send the following information to P. Cinnella: CV, motivation letter, references.
Duration: three years
Starting date : January/February 2024.
Salary : fully funded positions, partial refunding of local mobility fees

Context

The design of next-generation aero engines requires integrating high-order scale-resolving simulations (SRS) and optimization methodologies into standard industrial workflows. Future engine concepts require opening up the design space and solving complex design problems out of reach for today's standard industrial design processes within the required timeframe. In the frame of the Horizon cluster 5 collaborative project **Sci-Fi-Turbo** we seek filling this urgent need by exploiting opportunities in three foundation technologies: High-performance computing, high-order numerical methods, and AI/ML. The combination is used to implement and demonstrate key advancements in turbomachinery design.

Participants

Sci-Fi-Turbo is led by the German Center for aerospace research DLR (Cologne) and includes partners such as GE-Germany, ANSYS, Sorbonne University, Imperial College, University of Melbourne, CINECA, University of Braunshweig, Chalmers.

POSITION1

Objective: On-the-fly data-driven turbulence models for high-fidelity aerodynamic design

Industrial turbomachinery design processes rely on second-order finite-volume (U)RANS solvers. The required step change in predictive capability required however the introduction of high-order accurate and SRS approaches in the design process. Nevertheless, the current maturity of HPC-capable, high-order SRS solvers for turbomachinery applications is not sufficient for use in standard industrial design workflows. Only a very small number of SRS can be performed during an optimisation, because of their high computational cost. To mitigate that, we plan to exploit high-fidelity SRS data to train and machine-learning-augmented RANS models, and more specifically open-box data-driven models based on symbolic identification algorithms [1,2], to provide accuracy levels that are close to SRS, at least within the vicinity of the training set.
The objectives of the PhD work are: achieving computationally efficient and automatised model training, to enable “on the fly” retraining during optimisation, if needed; ensuring numerical robustness of the data-driven models, which must meet strict convergence criteria to avoid uncertainties associated with solution errors; developing data-driven models that are generalisable over a sufficiently large subregion of the parameters space, and to avoid catastrophic extrapolation errors or the need for too frequent retraining. To tackle these challenges, the data-driven approaches will be constrained to ensure well-behaved models (invariance, symmetries, realisability). In addition, we will investigate generalisation criteria, e.g., based on the Malahanobis distance or PAC-Bayes bounds [3,4]. Such criteria will be used to measure the model predictive reliability and trigger retraining if needed.

Work plan

The PhD work will be distributed over three years. She/He is expected to work in tight interaction with other team members (permanent staff, PhD and postoc involved in Sci-Fi-Turbo) and to participate to project activities: interactions with other partners, participation to progress meetings, writing of reports. She/He is also expected to participate to dissemination activities through the participation in international conferences and writing of papers.

The tentative program is as follows.

- Bibliography on machine-learning-augmented turbulence models and generalization criteria. Collection of training and validation data (including data generated within the Sci-Fi-Turbo consortium) and generation of additional SRS databases if needed. Investigation of computationally efficient and fully automatic training techniques.
- Investigation of optimality criteria for training data. Training of data-driven RANS model and assessment on a variety of test cases. Investigation of generalization capabilities and estimation of predictive uncertainties. Definition of suitable extrapolation measures and criteria for retraining. Definition of an automatic workflow.
- Application of the workflow to Sci-Fi-Turbo compressor configurations and extensive validation. Integration within multi-fidelity optimization algorithms developed by PhD2 and application to the design of a compressor blade.

References

[1] Schmelzer, M., Dwight, R. P., & Cinnella, P. (2020). Discovery of algebraic Reynolds-stress models using sparse symbolic regression. *Flow, Turbulence and Combustion*, *104*, 579-603.
[2] 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*, 109047.
[3] Wu, J. L., Wang, J. X., Xiao, H., & Ling, J. (2017). A priori assessment of prediction confidence for data-driven turbulence modeling. *Flow, Turbulence and Combustion*, *99*, 25-46
[4] Alquier, P. (2021). User-friendly introduction to PAC-Bayes bounds. *arXiv preprint arXiv:2110.11216*.

POSITION2

Objective: Adaptive multi-fidelity aerodynamic optimisation using scale-resolving simulations

Industrial turbomachinery design processes rely on second-order finite-volume (U)RANS solvers. The required step change in predictive capability needs the introduction of high-order accurate and SRS approaches in the design process. Nevertheless, the current maturity of HPC-capable, high-order SRS solvers for turbomachinery applications is not sufficient for use in standard industrial design workflows. Only a very small number of SRS can be performed during an optimisation, because of their high computational cost. To mitigate that, we plan to exploit high-fidelity SRS data to train and machine-learning-augmented RANS models (MLA-RANS), and more specifically open-box data-driven models based on symbolic identification algorithms [1,2], to provide accuracy levels that are close to SRS, at least within the vicinity of the training set.
The objective of the PhD work is the development of efficient multi-fidelity optimization algorithms [3,4], combining SRS and MLA-RANS. The automatic optimisation will be driven by evolutionary algorithms, specifically genetic algorithms (GAs) such as NDSAII, or via Bayesian optimisation (BO) approaches. Because of the high number of function evaluations required by the optimization, multi-fidelity surrogate models will be developed to speed-up the process. The latter will fuse together information from MLA-RANS and SRS to achieve designs with SRS-like quality at minimum expense.
The initial surrogate will be based on all available SRS estimates of the cost function plus a suitable number of low-fidelity MLA-RANS estimates. The algorithm will then search for the optimum and periodically adapt the surrogate based on efficient error estimate. An important task of the PhD will be developing suitable error estimates to decide whether to enrich the surrogate through MLA-RANS, SRS, and when MLA-RANS

needs retraining. Various multi-fidelity deep learning surrogates will be explored in conjunction with GAs or BO, together with active learning strategies that progressively enrich the surrogate. Also here, smart strategies will be sought to obtain the best possible surrogate while using a minimal number of SRS and data-driven model retraining. Finally, we will consider optimization strategies accounting for uncertainties due to model choice or to other causes (geometrical tolerances or variable operating conditions).

Work plan

The PhD work will be distributed over three years. She/He is expected to work in tight interaction with other team members (permanent staff, PhD and postdoc involved in Sci-Fi-Turbo) and to participate to project activities: interactions with other partners, participation to progress meetings, writing of reports. She/He is also expected to participate to dissemination activities through the participation in international conferences and writing of papers.

The tentative program is as follows.

- Bibliography on optimisation methods, surrogate models, multi-fidelity methods. Development and assessment of various multi-fidelity optimization algorithms for selected test cases.
- Coupling of the most promising algorithm with SRS and MLA-RANS. Development of suitable active learning strategies. Application to the optimization of Sci-Fi-Turbo compressor configuration. Assessment of the design against SRS and experiments.
- Exploration of efficient techniques for optimisation under uncertainty, and especially model uncertainties. First experiments on test cases. Application to Sci-Fi-Turbo configuration. Assessment of the design against SRS and experiments.

References

[1] Schmelzer, M., Dwight, R. P., & Cinnella, P. (2020). Discovery of algebraic Reynolds-stress models using sparse symbolic regression. *Flow, Turbulence and Combustion*, *104*, 579-603.
[2] 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*, 109047.
[3] Le Gratiet, L. (2013). Bayesian analysis of hierarchical multifidelity codes. *SIAM/ASA Journal on Uncertainty Quantification*, *1*(1), 244-269.
[4] Zhang, Y., Dwight, R. P., Schmelzer, M., Gómez, J. F., Han, Z. H., & Hickel, S. (2021). Customized data-driven RANS closures for bi-fidelity LES–RANS optimization. *Journal of Computational Physics*, *432*, 110153.