Accelerating CFD-Driven Symbolic Turbulence Modeling with Multi-Objective Bayesian Optimization

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Prediksi Cepat Sistem Fluida Nonlinear: Pendekatan Machine Learning berbasis Fourier Neural Autoencoder

Abstract

Developing CFD-consistent turbulence models using gene-expression programming (GEP) typically requires thousands of CFD evaluations. This study integrates multi-objective Bayesian optimization (MOBO) with GEP to select promising symbolic model candidates.

A Gaussian process surrogate and acquisition functions efficiently guide the approximation of the Pareto front. Two natural-convection cases demonstrate the framework. For vertical natural convection, the number of CFD evaluations beyond initialization is reduced by approximately 95% while maintaining solution quality.

The framework enables more computationally efficient development of turbulence closures for RANS.

Keywords: CFD, turbulence closure, GEP, Bayesian optimization, RANS.

Introduction

Reynolds-averaged Navier–Stokes (RANS) simulations are widely used in engineering, but their accuracy depends strongly on turbulence closure models. Conventional closures may struggle with complex flows and turbulent heat transfer.

Gene-expression programming produces interpretable mathematical expressions. However, directly evaluating candidate models through CFD makes training computationally expensive.

This study aims to accelerate CFD-driven symbolic turbulence model discovery without compromising multi-objective solution quality, using uncertainty-aware adaptive sampling.

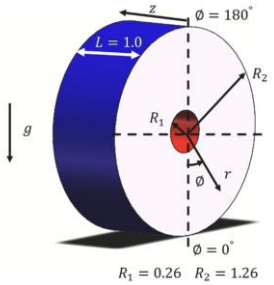


Figure 1. The depiction of Concentric Horizontal Annulus, which becomes the main application of this study

Research Method

1. GEP generates candidate symbolic expressions for turbulence closure corrections.
2. Candidates are mapped to scalar features and modeled using Gaussian process regression.
3. MOBO selects candidates using expected improvement or expected hypervolume improvement (EHVI).
4. Only selected candidates undergo CFD evaluation; the results update the surrogate and Pareto front.

Discussion & Result

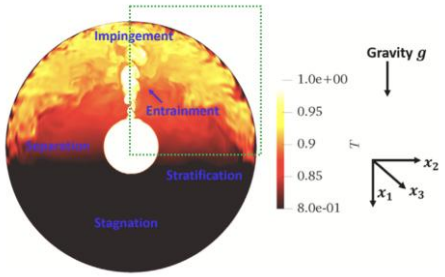


Figure 2. An example of DNS simulation from the Concentric horizontal annulus test case

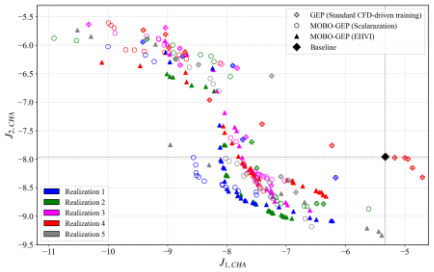


Figure 3. Pareto front discovered by the proposed algorithm

- Test cases: (i) vertical natural convection (VNC), with velocity and temperature profile objectives; and (ii) concentric horizontal annulus (CHA), with velocity profile objectives at two angular locations.
- The developed models correct Reynolds stresses and/or turbulent heat fluxes in RANS simulations. Predictions are evaluated against direct numerical simulation (DNS) data.
- MOBO separates inexpensive symbolic candidate exploration from costly CFD evaluations, allocating the computational budget to the most promising models.

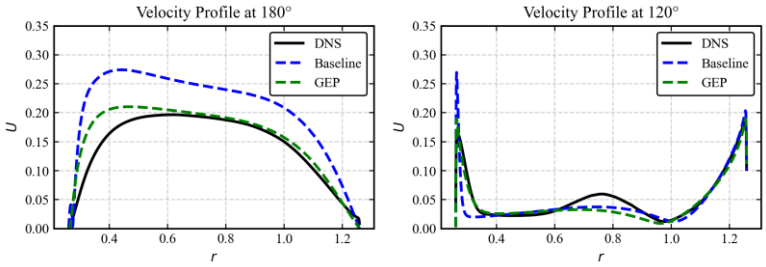


Figure 4. Comparison of DNS, baseline RANS, and model discovered by GEP. The result clearly shows that the profile obtained from GEP is close to DNS.

Conclusion

- Integrating MOBO with GEP enables the development of interpretable turbulence closure expressions using substantially fewer CFD evaluations.
- The proposed discrete candidate-based approach uses Gaussian processes to guide model selection and improve multi-objective search efficiency.
- Results from two natural-convection cases demonstrate the potential to accelerate RANS turbulence model development under limited computational budgets.
- The ITB–University of Melbourne collaboration advances scientific machine learning for fluid modeling.