Predictive Preprocessing of CFD Solver Parameters Using Random Forest and Bayesian Optimization

***Emil Barciś*[1] *Krzysztof Rojek*[1]**

[1]Częstochowa University of Technology, Faculty of Computer Science and Artificial Intelligence

emil.barcis@pcz.pl, krzysztof.rojek@pcz.pl

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This study presents a preprocessing framework designed to predict optimal SU2 solver parameters based on physical conditions (Mach number, Angle of Attack) and mesh features for NACA0012 airfoil simulations. The primary objective is to automate hyperparameter selection to ensure simulation convergence and minimize computational iterations [1, 2].

To eliminate human bias and predefined heuristics in the selection process, a baseline dataset of 1,000 unguided configurations was generated using Latin Hypercube Sampling (LHS) [3]. Evaluation of this dataset resulted in a baseline convergence rate of 34.8%. To improve selection prior to solver execution, a Random Forest (RF) classifier was trained as a surrogate model to evaluate the convergence probability of a given complete configuration [4].

To identify optimal solver settings, the RF evaluator was coupled with two search algorithms: a Sequential Random Search (SRS)—which iteratively samples the parameter space until the surrogate predicts convergence—and Bayesian Optimization (BO) [5]. The implementation of the RF-BO preprocessing approach increased the convergence rate to approximately 93% while reducing the average number of required simulation iterations.

To verify generalization, the models were tested on out-of-sample datasets generated with different random seeds, representing unseen physical and topological combinations. The surrogate-guided configurations maintained consistent convergence and acceleration metrics, confirming the viability of the automated preprocessing method.

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