Understanding CNN-Based Shape Optimization for Thermo-Hydraulic Efficiency Using Explainable Deep Learning

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Abstract. Numerical simulations can be a bottleneck for computational fluid dynamics (CFD) based optimization. To address this, we developed a convolutional neural network (CNN) surrogate model to predict thermo-hydraulic performance in structured channels under a laminar flow regime [1]. Our model targets are the total drag and net heat transfer rate, characterized using the non-dimensional parameters drag coefficient C_f and Stanton number St respectively. The significant speed-up from the CNN model is then utilized with particle swarm optimization (PSO) to explore the high-dimensional parameter space of structured channel geometry for three different objective functions: minimizing C_f, maximizing St, and maximizing the overall thermo-hydraulic efficiency described by the ratio of St/C_f [2]. This extended abstract focuses on understanding the optimized geometries obtained from the CNN-PSO approach using the explainable deep learning (XAI) tool, SHapley Additive Explanations (SHAP) [3].

Keywords: Convolutional neural networks· Particle swarm optimization· Explainable deep learning.

1 Introduction

In the field of engineering, optimizing the shape and topology of heat transfer devices holds immense significance, spanning from electronic cooling applications to power generation sectors. However, the efficacy of CFD-based optimization approaches is often hindered by the significant computational time required for numerical simulations. These simulations can vary from a few seconds to several weeks to achieve converged solutions, posing a significant bottleneck. To address these challenges, we leverage surrogate modelling with machine learning (ML).

For the design of a surrogate ML model, we considered a generic heat exchanger, which can be conceptualized as an internal flow between structured walls (refer Fig. 1). Although an analytical solution exists for laminar flow between flat walls, numerical simulations are necessary to determine the thermo-hydraulic performance of internal flows if wall structuring is present. We aim to design an ML model capable of predicting the thermo-hydraulic behaviour of such systems if an arbitrary structure of a channel wall is given as an input.

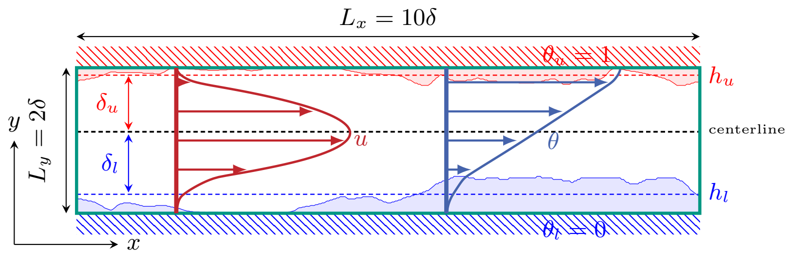


Fig. 1: Laminar channel flow with imposed wall structuring [1, 2].

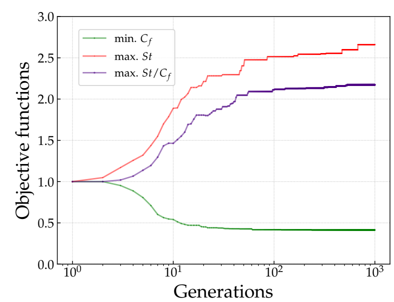


Fig. 2: Evolution of the three objective functions over 1000 generations [2].

For this purpose, we selected CNN due to its inherent ability to handle grid-like data. The regression CNN uses a standard architecture with convolutional, activation, max-pooling, and fully connected layers. Training hyperparameters are detailed in our paper [1]. To train the CNN model we generated approximately 10,000 labelled structures. The dataset was generated using the spectral solver SIMSON [5]. The global quantities of interest, drag coefficient C_f and Stanton number St are obtained by solving the incompressible Navier-Stokes equation and the scalar transport equation for temperature. After training, the CNN model accurately predicted C_f and St values in under 100 ms per input geometry, significantly faster than numerical simulations, which take approximately 20-30 minutes per channel geometry (refer [1] for hardware details).

We then combined the CNN-based ML model with PSO to explore the high-dimensional parameter space of structured channel geometry for three different objective functions: min. C_f, max. St, and max. St/C_f [2]. These three distinct PSOs are run with the same initial population of particles (which translates into the same initial geometry) to enable a consistent comparison of the results. The evolution of the corresponding three objective functions is shown in Fig. 2. Our study showed that min. C_f leads to the trivial solution of a flat channel. In contrast, the St-maximized geometry achieves nearly a 250% increase in heat transfer, while the St/C_f -maximized geometry achieves a 15% improvement in overall efficiency compared to the reference flat channel geometry. The mean velocity and temperature for these optimised geometries are shown in Fig. 3. This extended abstract focuses on understanding the optimized geometries obtained from the CNN-PSO approach using the XAI tool called SHAP [3], that can be used for classical statistical models as well as complex ML models [4].

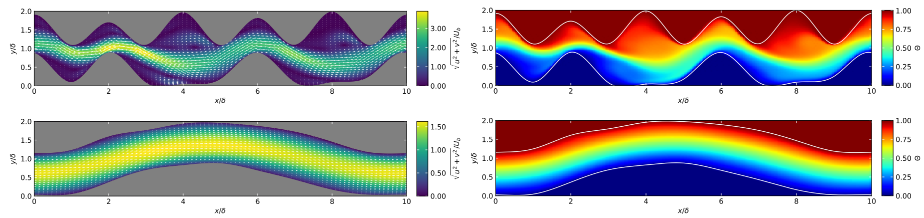
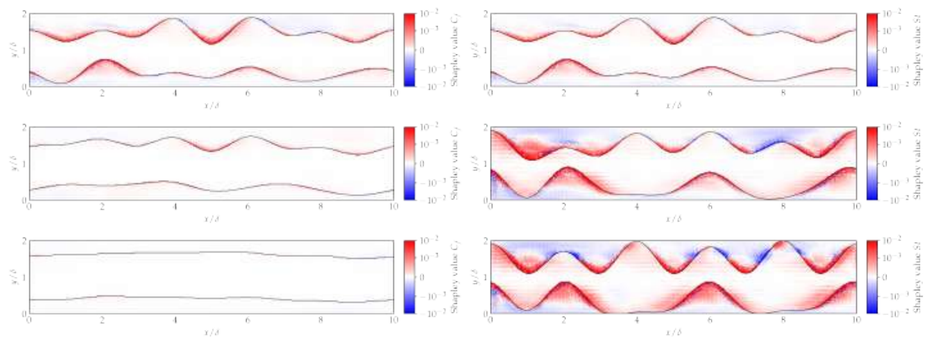


Fig. 3: Mean velocity $|u_i|$ and temperature θ for St- (*top*) and St/C_f-maximized (*bottom*) geometry [2].

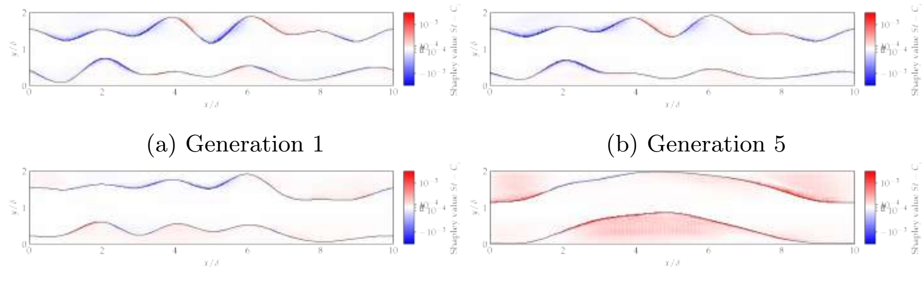


(a) C_f-minimized (b) St-maximized

Fig. 4: The left plots show the local distribution of SHAP values for C_f in the C_f-minimized structure, while the right plots show SHAP values for St in the St-maximized structure. Rows correspond to generations [1, 10, 1000] (refer Fig. 2). A nonlinear color bar is utilized for enhanced visualization; nevertheless, a linear scale is employed within the range of -10^{-3} to 10^{-3} to prevent the plot from diverging near zero.

2 Explainable deep learning (XAI)

For a given structured channel geometry, it is valuable to identify how local geometric features influence the CNN's predictions of total drag and net heat transfer rate (*i.e.* C_f and St). This so-called attribution problem [4] can be addressed by calculating the expected marginal contribution of each pixel in the channel geometry using the SHAP framework [3, 4]. SHAP values thus provide a means to quantify the impact of each pixel, allowing the user to understand how geometric features contribute to the overall predictions. The SHAP values are computed using the CNN model alongside a distribution of background samples. We aim to understand how C_f and St change relative to a flat channel configuration. Hence, we used 90 flat channels located symmetrically or asymmetrically about $y = \delta$ (refer Fig. 1) as background samples. It is important to note that the summation of the SHAP values should be equal to the difference between



(a) Generation 1 (b) Generation 5

(c) Generation 10 (d) Generation 1000

Fig. 5: The local distribution of the difference between the SHAP values, SHAP St - SHAP C_f, for St/C_f-maximized geometry.

Table 1: Shap hypothesis check for the structures.

	$\Sigma(C_f)$	$\Sigma(St)$	$p(C_f)$	$p(St)$	$\langle p(C_f)\rangle$	$\langle p(St)\rangle$
min. C_f	-0.0324	-0.0418	-0.7236	-0.5383	-0.6912	-0.4964
max. St	28.22	37.85	27.53	37.35	-0.6912	-0.4964
max. St/C_f	0.1850	3.64	-0.5062	3.1498	-0.6912	-0.4964

the model prediction for the given structure, denoted as $p(s)$, and the mean prediction derived from the background samples, represented as $\langle p(s)\rangle$. This can be expressed as

$$\text{Sum shap}, \Sigma(s) = p(s) - \langle p(s)\rangle \,, \tag{1}$$

where the scaled mean prediction (i.e. $\langle p(s)\rangle$ value) for C_f and St are obtained as -0.6912 and -0.4964 respectively. Corresponding values for the optimised geometries are tabulated in Table 1.

The local distribution of SHAP values for C_f and St-optimized structures are shown in Fig. 4. Figure 4a demonstrates that any deviation from a flat channel increases C_f. In contrast, Fig. 4b indicates that even though undulations in the wall in general increase St it also depends on the flow physics - like the presence of recirculation regions in the flow domain (refer Fig. 3). SHAP value distribution of St/C_f-maximised structures shown in Fig. 5 also confirms the same.

3 Conclusion and Outlook

Using an explainable deep learning tool called SHAP we analysed the optimized geometries from CNN-augmented particle swarm optimization. The SHAP value analysis (refer Figures 4 and 5) illustrates that SHAP values can act as a measure of sensitivity, suggesting the potential for conducting PSO optimization based on SHAP value-driven sensitivity analysis, rather than explicitly optimizing for C_f or St values. This approach will be investigated in future studies. Additionally, we will explore the relationship between SHAP value distributions and the underlying physics of the problems as the next step in our research.

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Disclosure of Interests. The authors have no competing interests.

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