Accelerating Design Exploration and Optimization with Surrogate Physics Models

Background

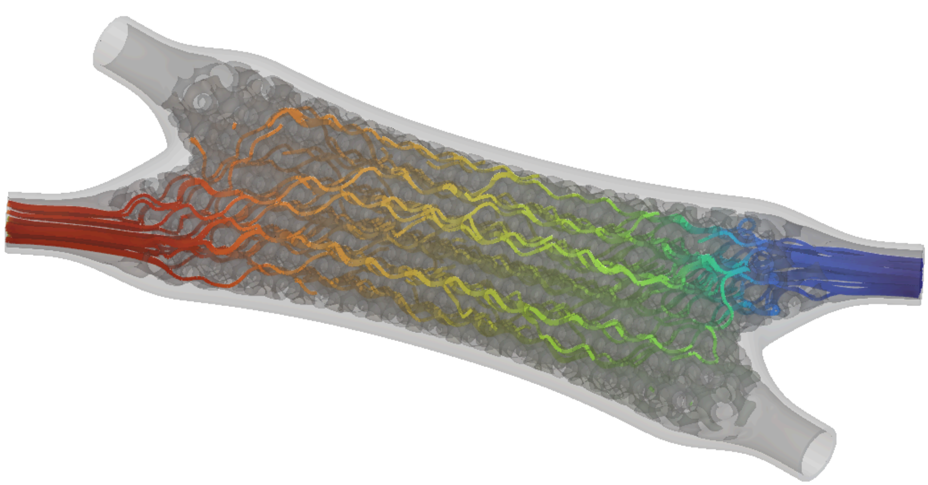
When optimizing a complex part, each iteration takes a long time, both due to geometry generation and simulation compute time. One approach is to sample the design space and use machine learning to train a surrogate physics model from high-quality simulation data. Unlike generic black-box ML models, this surrogate is grounded in the parameter space of interest and reflects the governing physics captured by the simulations. This allows for quicker iteration and trustworthy inverse design approaches.

Problem Statement

Using the data set from a heat exchanger, train a surrogate model capable of predicting pressure drop, core surface area, and mass properties given input lattice cell size in the X-direction and Y/Z-direction. Once your model is trained, use inverse design to specify the optimal lattice cell size to minimize pressure drop and mass while maximizing the surface area. The value of a surrogate model is measured in both accuracy and speed, so you will also be evaluated on how long it takes for your model to generate a prediction given input parameters.

Generating Additional Data

We have also provided the nTop file of the parameterized heat exchanger design. It is not required, but you are welcome to generate additional data for training or evaluating your model using nTop Fluids (you can request a free nTop EDU License here). Your license will include access to nTop Automate, which allows you to run your nTop notebook through a script (example Python file also provided). You are not required to generate additional data, but doing so could help you when training your model for inverse design.



Submission

Your submission should be shared as a zip file containing the model so it can be run on the judge's computer. The judge should be able to input a set of parameters and receive a prediction for pressure drop, surface area, and mass of the part for a given set of input parameters (Cell Size X, Cell Size Y/Z). Your model should also be capable of predicting an optimal set of parameters given the scoring criteria below using inverse design (input parameters can be specified up to 6 significant figures). Please also provide a short description (~5 sentences) of your training approach and why you chose the method that you did along with any relevant visualizations of your model performance.

Evaluation

The data set and evaluation inputs will fall within the following ranges

- 7mm < Cell Size X < 15mm
- 7mm < Cell Size Y/Z < 15mm

Submissions will be scored as follows:

- How closely does your model predict the pressure drop of a specified cell size compared to simulation results in nTop Fluids and how long does the prediction take?
    - Score = 1/(RMSE of Pressure Drop prediction compared to simulation result over 3 input parameter combinations) - Time to generate prediction (in s)
- How optimal is the design predicted by your model ?
    - Score = HEX Surface Area (in mm^2) - Part Mass (in kg) * 10 - Pressure Drop (in Pa) * 1500