INDUSTRIAL OPTIMISATION WITH MULTIOBJECTIVE BAYESIAN METHODS AND OPENFOAM

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Keywords: *Bayesian Optimisation, Industrial Applications, Meshing*

Introduction

Design optimisation often requires optimising multiple (and often conflicting) objectives simultaneously. As an example, a heat exchanger design will attempt to maximise the heat transfer while minimising the pressure drop across the system. In such cases there will be a range of solutions, the Pareto set, which represents a trade-off between the design objectives. Genetic Algorithms perform well in exploring the design space and determining the Pareto set, but typically require thousands of function evaluations, which is impractical with CFD even with modern computing power. An alternative is to use Bayesian Optimisation methods which iteratively seek to improve an approximation of the cost function for the system. Bayesian optimisation operates on two functions, an Objective function which is the approximation to the true cost function, and an Acquisition function which identifies the best location for the next sample. Note that this is not necessarily at the optimum solution but may indicate a location in parameter space to investigate to improve the overall quality of the objective function. Bayesian optimisation has been proved to be an effective approach to find optimal solutions with the minimum number of direct evaluations of the (expensive) cost function [1], which makes it an ideal choice to use with CFD.

Integration with OpenFOAM

In this work, we demonstrate the application of Bayesian methods to the optimisation of real engineering problems. We have developed a general Machine Learning Optimisation framework in Python with a link to use OpenFOAM through the PyFoam library as the CFD engine (other CFD packages could also be used). On the Optimisation side, we have implemented Genetic Algorithm and Bayesian Optimisation methods in Python into this framework.

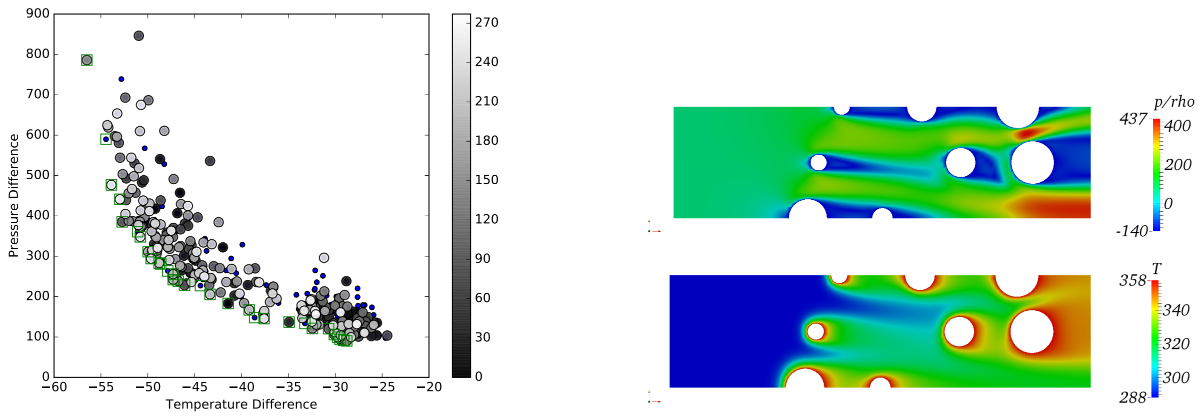

Figure 1: Left; Pareto front for heat exchanger problem. Right; Optimised (non-dominated) solution

Industrial applications

The Bayesian Optimisation algorithms have been applied to a range of including heat exchangers, draft tubes and vortex separators. The heat exchanger case is a 2d heat transfer problem at $Re = 100$, with position and size of the tube surfaces varied through the use of Chebyshev polynomial functions. The problem involves two separate, competing objectives; enhancing heat transfer from the tubes involves increasing the contact area and slowing the flow; whilst reducing the pressure drop would require the exact opposite. The problem has been optimised using both GA and Bayesian approaches, generating a clear Pareto front; a non-dominated solution example is shown in figure 1.

The draft tube is a standard CFD optimisation problem with significant industrial interest. Hydroelectric power generation involves supplying water at high pressure head to a turbine; the water leaving the turbine is then directed through the draft tube back to the natural environment (a river or lake). Optimising the system involves minimising the pressure at the exit from the turbine/entry to the draft tube. The basic geometry (figure 2) known as the Hölleforsen draft tube was originally used for an ERCOFTAC workshop [2] on modelling and optimisation, and has been extensively studied since [3, 4, 5]; there is therefore an extensive literature of experimental and computational results to validate the basic CFD simulations against, as well as a great deal of literature on optimising the design. The problem is complicated by being fully 3d and by the swirling motion at the inlet (from the upstream Kaplan turbine) which has to be included for full acuracy. We have validated our modelling on the base case (figure 2) and then used Bayesian optimisation to find optimal solutions for this important test case.

The third example is an actual industrial problem provided by Hydro International; a Vortex Separator for wastewater treatment. Vortex separators use conical plates to encourage the formation of a vortex in the tank; particles in the flow interact with the plate boundary layers and drop out of suspension, collecting at the base of the tank for removal; whilst the cleaned water is removed at the top of the tank. This is the most challenging of the three examples as it involves a 2-stage simulation process, with an initial single phase flow simulation using `simpleFoam` to determine the system hydrodynamics followed by particle tracking to determine the separation. The simulations for this have been validated for the existing geometry and Bayesian optimisation used to determine an optimal design for the plates.

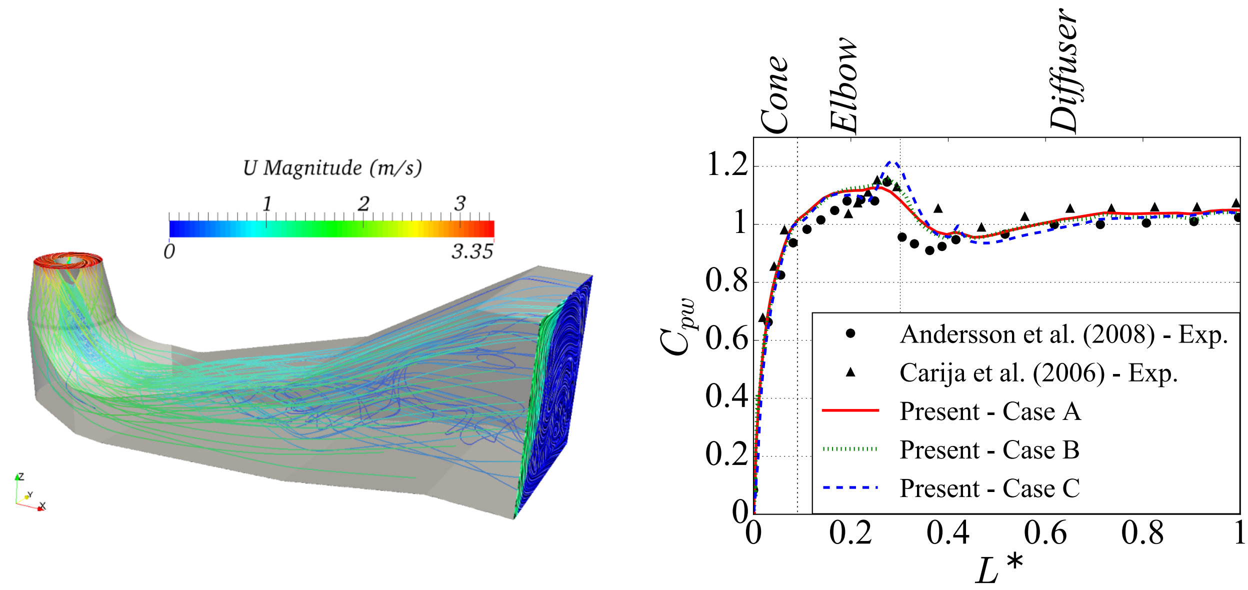

Figure 2: Hölleforsen draft tube; original geometry. Left; streamlines for flow. Right; validation of pressure coefficient along underside of the draft tube.

Mesh optimisation

Development of a high quality mesh is obviously of critical importance for any CFD simulation. However this is a very challenging problem which typically absorbs most of the human effort in developing a CFD model of a problem. This is even true for automated meshers such as `snappyHexMesh` or `cfMesh` which have input parameters controlling the meshing process whose values have to be set, typically through trial and error. This has all the hallmarks of an optimisation problem with several input parameters (the mesher settings) and a limited number of mesh quality parameters such as skewness to be optimised. This problem has been investigated using Genetic Algorithms [6]; here we apply our Bayesian Optimisation techniques to mesh a swirl flow separator using `cfMesh`.

Conclusions

Evolutionary algorithms have benefits for optimisation including their relative simplicity (there is no need to evaluate function derivatives as there is for Adjoint Optimisation) and the fact that they explore the whole of parameter space and reliably identify global optima. However they require the evaluation of 10's of thousands of variants of the design, and this can be prohibitively expensive if each of these evaluations requires a full CFD simulation. Bayesian optimisation iterates improvements in an Objective function which is an approximation to the true cost function, and for which the optimal solution(s) can be found relatively cheaply and easily. This represents a cost-effective optimisation process based on CFD which can realistically be applied to real, complex engineering problems. We have developed a machine learning library in Python for optimisation of flow problems using CFD which integrates well with OpenFOAM; and demonstrate its utility by applying this to optimise three different industrial flow problems. We have also applied the same strategy to optimise the construction of a mesh for a vortex flow separator.

Acknowledgments

The authors thank all those involved in the organisation of OFW13 and to all the contributors that will enrich this event. We acknowledge the funding provided for this project from the EPSRC grant "Data-Driven Surrogate-Assisted Evolutionary Fluid Dynamic Optimisation", EP/M017915/1.

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