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Coupling Bayesian Optimisation with CFD for Multiphysics Optimisation

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Extended Abstract

Over the past decades Computational Fluid Dynamics has developed ever more accurate methods and is now able to accurately model flow and multiphysics problems in a range of industries. Ever increasing computer power opens the door to using CFD as a key tool in virtual design, with new designs being accurately simulated to test their properties, maybe as part of a human-centered design loop. The next level of simulation would be to automate this design loop, with the human designer setting the design parameters and stepping back to let the computer develop a (or a range of) solutions. The two main approaches to optimisation are gradient based optimisation and evolutionary optimisation. Gradient based methods such as Adjoint Optimisation are efficient but have the potential to find local rather than global optimal solutions, and require a significant level of effort to find the gradient in the first place, for any new physics in the problem. Evolutionary optimisation methods such as genetic algorithms only require the evaluation of the objective function and can efficiently explore the whole of objective space and find the global optimum. GA's do however require the objective function to be evaluated tens of thousands of times, which is impractical if this requires the evaluation of a CFD model each time. However this can be replaced by a surrogate model; a simple mathematical function (such as radial basis function or gaussian process) which can be trained on a limited number of CFD runs, and which can then be repeatedly evaluated to provide the cost function.

Bayesian Optimisation is a development of evolutionary methods where the focus is on the development of the surrogate model. We start with a coarse grained surrogate for the cost function (the objective function) which is iteratively refined in tandem with the optimisation, via an acquisition function which identifies the best location for the next CFD simulation – this might be either to explore the objective space (reduce high variance regions away from the global optimum) or to improve our knowledge of the global optimum. Bayesian Optimisation is thus a form of sparse data machine learning in which the algorithm learns the salient features of the cost function from a minimal number of expensive CFD evaluations.

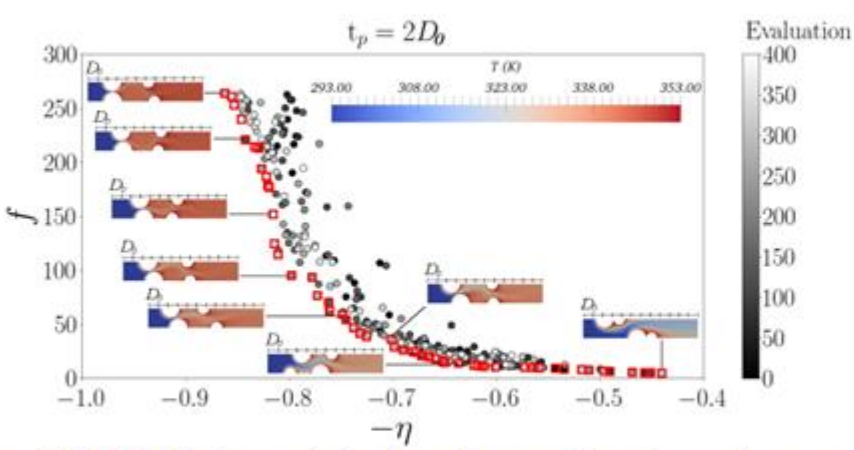

Figure 1: Multiobjective optimisation of a cross-flow heat exchanger using Bayesian methods[1]

In Exeter we have been working on integrating Bayesian Optimisation methods with CFD for a number of years. I will present a number of exemplar multiobjective optimisation cases, ranging from simple “proof of concept” challenges (eg optimisation of a cross flow heat exchanger[1], see Fig 1) to industrial problems such as the Holleforsen-Kaplan draft tube[2] and optimisation of particle separation for a vortex separator. Key challenges in using Bayesian Optimisation with CFD include automatic mesh generation and use of parallel HPC resources, so running the Bayesian evaluations in parallel[3]. The results demonstrate that Bayesian Optimisation is a powerful tool that can generate optimal solutions for high cost, complex flow problems with a range of multiphysics and is even mature enough to provide patentable IP for industry.

References

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