UNIVERSITY OF Southampton
School of Engineering Sciences

Response surface method based design optimisation CFMS (AP3) Work Package 14.4B

UTC for Computational Engineering

Chris Brooks, Alexander Forrester and Andy Keane, CEDG, School of Engineering Sciences
Shahrokh Shahpar, Rolls-Royce plc.

Introduction

Expensive 3D Computational Fluid Dynamics (CFD) solvers are finding increasing use in the design process for aerospace components. The objective of this work item is the development of improved surrogate model based optimisation methods using design space reduction, parallel multi-objective, multi-fidelity and Hermite response surface models (RSMs).

The work presented here has been undertaken using funding from the Centre for Fluid Mechanics Simulation, which is a British consortium of government and industry partners which aims to transform design processes for aerospace, marine, automotive and other industries through the use of innovative computer-based simulation systems.

NASA compressor rotor 37 3D geometry optimisation test case

The NASA rotor 37 is a transonic rotor for which experimental and CFD analysis has been reported in detail. The rotor is representative of the complex three-dimensional viscous flow structures common to transonic blading, such as three-dimensional shock structures and secondary flows. The Rolls-Royce SOPHY system has been used to generate CFD data for the NASA rotor for the purposes of validating the RSM and optimisation methods developed within this work item, see Fig1. The single-point optimization problem considered is to maximise isentropic efficiency, η, of the rotor subject to constraints on pressure ratio, *PR*, and mass flow, *m*. The rotor geometry was parameterised using the engineering parameters defined in the PADRAM rapid meshing tool. A total of 28 variables were used to define the geometry.

Efficient construction of Kriging RSMs

Kriging is a spatial prediction method that has become a popular method of generating inexpensive surrogate models of potentially complex, expensive aerodynamic and structural models. In order to mitigate the cost of Kriging hyperparameter tuning for large samples and high problem dimensions a gradient-based optimisation of the likelihood function is used here. The derivatives of the likelihood function are efficiently obtained via reverse algorithmic differentiation of the original function. In this manner the derivatives are obtained at a computational cost of around 2-3 times the standard likelihood function call, whilst remaining independent of the number of hyperparameters involved.

The effectiveness of the adjoint gradient based hyperparameter tuning is demonstrated by building a Krig from the NASA rotor 37 test case. Two hyperparameter tuning strategies are implemented: in the first, a GA is applied using 130 generations of population size 100, and in the second, a GA is run for an initial 1000 iterations before four SQP searches are undertaken from cluster centroids. Up to 1000 calls to the adjoint likelihood are permitted for each SQP search (costing around 2-3 standard likelihood function calls). Convergence histories for each strategy are shown in Fig2. The hybrid strategy is shown to efficiently converge to solutions, whilst the GA shows a slow convergence. The hybrid strategy produces the most accurate RSMs in each case.

Having obtained suitable Kriging RSMs for objective and constraints, it is possible to undertake design optimisation using the Constrained Generalised Expected Improvement (CGEI) figure of merit. The optimisation strategy is to obtain a total of 30 update points per iteration by

- maximising the CGEI for g=1 and g=2 (10 updates)
- maximising the Krig error for each response (15 updates)
- searching the original problem using the Krig RSMs (5 updates)

After seven iterations of 30 update points the best design found improved efficiency over the datum by 2.23%, whilst pressure ratio was maintained at -0.18%, and mass flow maintained at +0.197%. The optimised geometry is compared with the datum in Fig 3. The radial profile of efficiency presented in Fig 4. demonstrates that efficiency is either maintained or improved over the radius.

Gradient enhanced cokriging RSMs

If gradient information is available, it can be used to enhance the global accuracy of the response surface. Gradient information from CFD simulations is usually obtained either from finite differencing or from adjoint solutions. To demonstrate the effect upon prediction accuracy of varying the number of included derivatives, a series of cokriging models were built based on 10 sample points from the Branin function, with derivative information removed point by point from the cokrig construction. The correlation of predictions with a 400 point validation DoE is shown in Fig. 5, indicating the improvement in accuracy as derivative information is added.

Multi-fidelity CoKriging RSMs

Simulations can often be run at different levels of fidelity, where an accurate dataset is obtained from an expensive, slow code, and a less accurate dataset from a cheaper, fast code. In this work, a correction process between cheap and expensive data is obtained by using cokriging. The NASA rotor 37 problem was run at two levels of fidelity: a coarse mesh of 240k nodes and the datum fine mesh of 540k nodes. The coarse mesh data was sampled at the 280 training DoE points, whilst a random subset of 28 fine mesh data was used.

The correlation between predictions and validation data are shown in Fig. 6, where the coarse mesh data is shown to underpredict the values of the fine mesh responses (green), but the correlation between them is quite good since the scatter is low. By combining the datasets, the fine mesh data is predicted with greater accuracy (red) than simply Kriging the 28 fine mesh data points alone (purple).

Future work

- Work is currently focussed on building the current methods into the SOFT optimisation software.
- Further assessment of gradient enhanced and multi-fidelity RSMs is planned, including application to the NASA rotor 37 optimisation.
- Work has started on multi-objective optimisation based on extensions to the Expected Improvement figure of merit.
- Research into the use of penalty and augmented Lagrangian merit functions within Expected Improvement, to allow better exploration of nonlinear constraint functions.
- Investigation into design variable transformations.

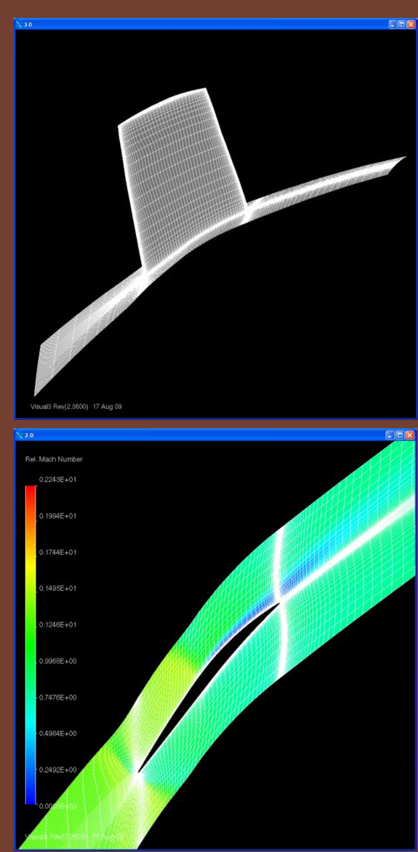

Fig1. Baseline NASA37 geometry (540k nodes) and flow solution at 50% radius.

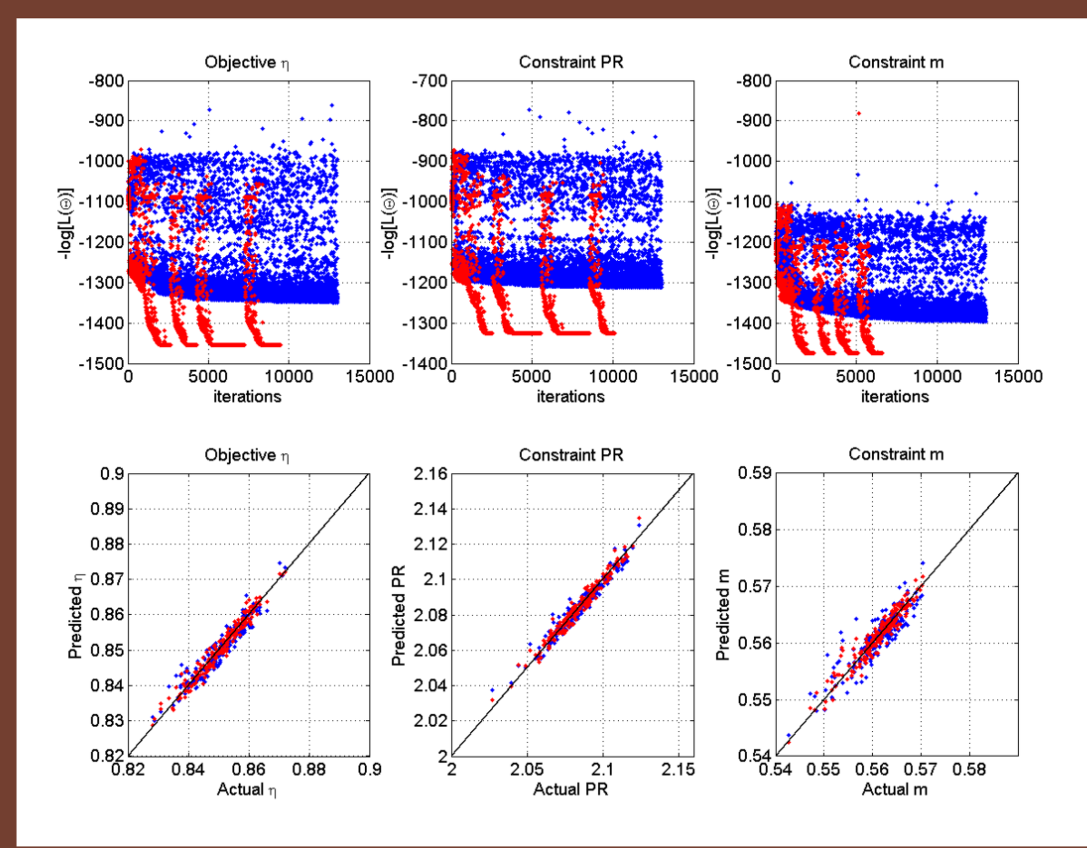

Fig 2. Hyperparameter tuning log-likelihood converge and correlation with validation data for each response. Red is GA_SQP strategy and blue is GA strategy.

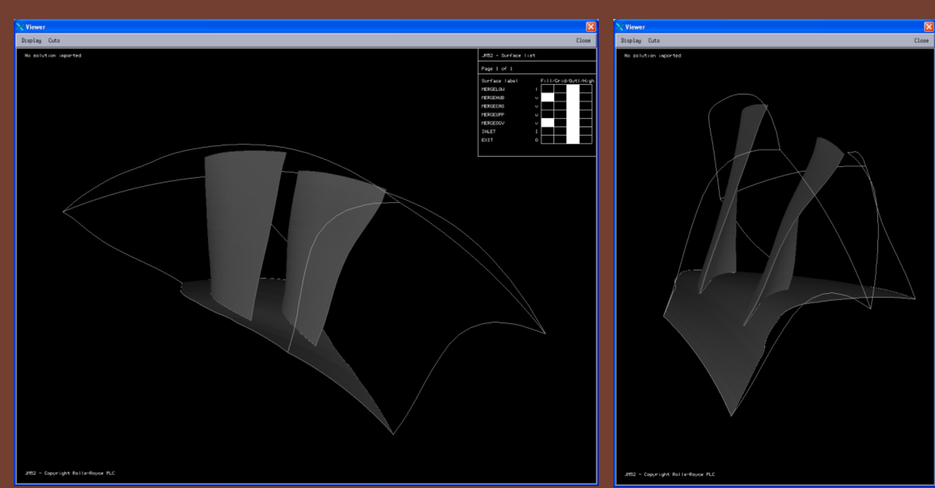

Fig 3. Optimised (right-hand blade) and datum geometries

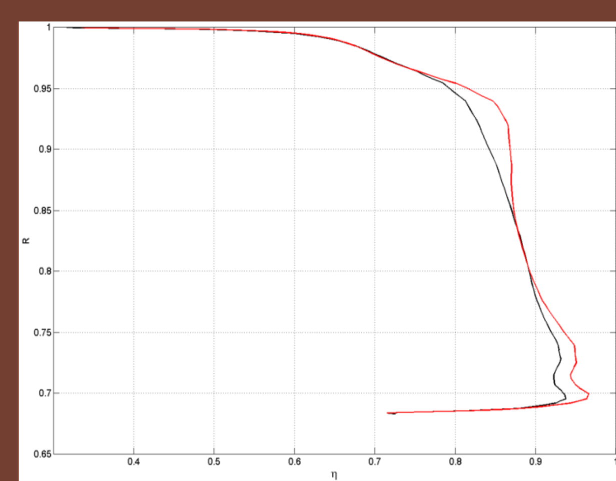

Fig 4. Radial profiles of efficiency for optimised and datum geometries.

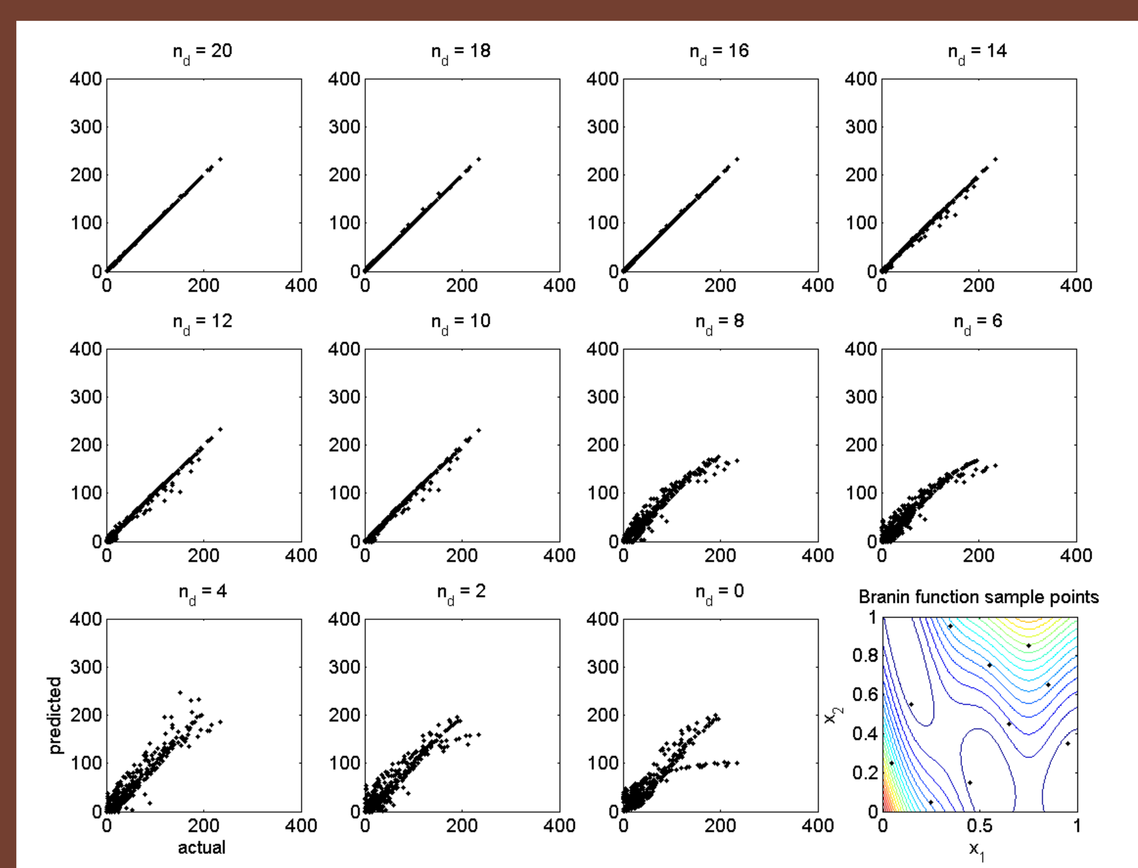

Fig 5. Correlation of cokrig prediction with validation data for increasing number of directional derivatives of 2D Branin function.

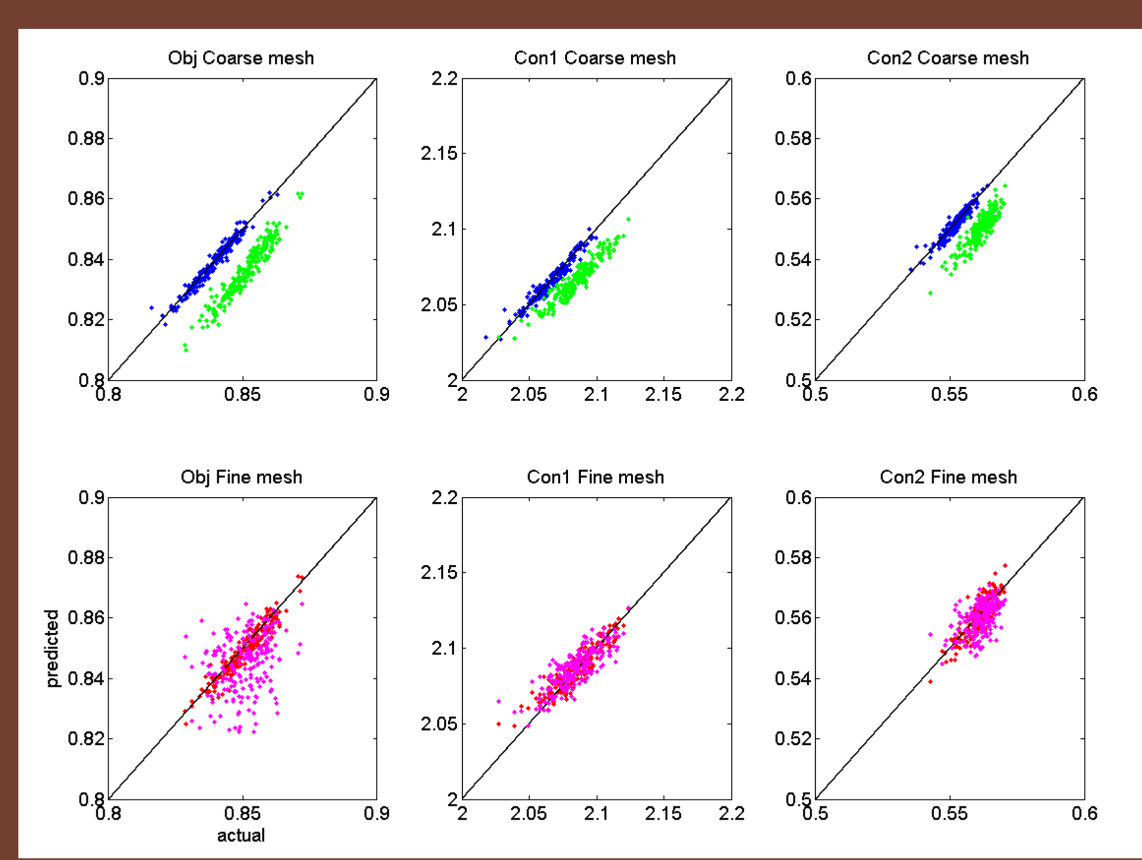

Fig 6. Correlation between predictions and validation data. Blue is coarse mesh prediction vs coarse mesh validation DoE. Green is coarse mesh prediction vs fine mesh validation DoE. Purple is fine mesh prediction vs fine mesh validation DoE. Red is fine mesh multi-fidelity prediction vs fine mesh validation DoE.

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Computational Engineering and Design Group, University of Southampton, SO17 1BJ, UK