

Enhancing and Developing the Practical Optimisation Capabilities and Intelligence of Automatic Design Software

Timoleon Kipouros*,

Cambridge University, Cambridge CB2 1PZ, United Kingdom

Tom Peachey†, David Abramson‡

Monash University, Clayton, VIC 3800, Australia

and A. Mark Savill§

Cranfield University, Cranfield MK43 0AL, United Kingdom

In the modern engineering design cycle the use of computational tools becomes a necessity. The complexity of the engineering systems under consideration for design increases dramatically as the demands for advanced and innovative design concepts and engineering products is expanding. At the same time the advancements in the available technology in terms of computational resources and power, as well as the intelligence of the design software, accommodate these demands and make them a viable approach towards the challenge of real-world engineering problems. This class of design optimisation problems is by nature multi-disciplinary. In the present work we establish enhanced optimisation capabilities within the Nimrod/O tool for massively distributed execution of computational tasks through cluster and computational grid resources, and develop the potential to combine and benefit from all the possible available technological advancements, both software and hardware. We develop the interface between a Free Form Deformation geometry management in-house code with the 2D airfoil aerodynamic efficiency evaluation tool XFOIL, and the well established multi-objective heuristic optimisation algorithm NSGA-II. A simple airfoil design problem has been defined to demonstrate the functionality of the design system, but also to accommodate a framework for future developments and testing with other state-of-the-art optimisation algorithms such as the Multi-Objective Genetic Algorithm (MOGA) and the Multi-Objective Tabu Search (MOTS) techniques. Ultimately, heavily computationally expensive industrial design cases can be realised within the presented framework that could not be investigated before.

I. Introduction

COMPUTATIONAL Engineering and e-Science are strongly related disciplines that need to emerge together and produce suitable technology that supports the demands of advanced industrial design tasks. In e-Science, computational tools and methodologies are continuously developed and explored in order to identify and suggest solutions to highly challenging problems. This is particularly true in modern engineering. In energy and power and propulsion sciences, for example, these applications can expand from the fine geometrical modifications of turbomachinery blade components or aircraft wings to whole engine and whole aircraft conceptual and detail design. The primary objective is always to improve the efficiency of these machines, and at the same time to develop a more sustainable operation within the environmental conditions, and satisfy strict regulations and constraints that combine aerodynamic, structural, aeroacoustical, cost, or

*Research Associate, Cambridge Engineering Design Centre, Member.

†Researcher, Faculty of Information Technology.

‡Professor, Faculty of Information Technology.

§Professor, Power and Propulsion Sciences Group, Department of Power and Propulsion, Senior Member.

manufacturing characteristics. Furthermore, new methodologies and technologies can be explored with these design tools and systems that could not have been investigated before.

Apart from the fact that the complexity of the optimisation problems explodes when the number of design variables and objective functions increases, moreover, the different hard and soft constraints that should be considered in order to maintain practicality of the new design configurations, test the strengths of the optimisation algorithms to their limits.

In this paper we develop and expand the optimisation functionalities of a platform that can efficiently manage the simultaneous execution of computational tasks through cluster and grid environments. This is a very important development that combines the merits in the fields of both e-Science and Engineering.

Only when such capability exists can engineers exploit and consider difficult design problems that require substantial computational resources due to the size of the design space, the size of the design problem, and the computational cost for the evaluation of the critical metrics of each discipline.

Normally, many design systems developed by engineers exhibit powerful capabilities for tackling complex, non-linear, and discontinuous problems, but with weaknesses in the ease of use and expansion of applicability. On the other hand, design systems developed by computer scientists often integrate very powerful computational infrastructure, but with limited emphasis on the suitability for practical engineering problems.

In the following Sections we present a description of the software development, as well as analyses of the results, in order to highlight the benefits of such a system and identify future directions for research exploration and exploitation. It should be highlighted here that the main objective of this work and the optimisations executed is not to produce optimum 2D airfoil shape designs, but to address the need for such computational design tools that facilitate flexible and efficient execution of computationally demanding design cases. In addition, we would like to highlight the importance of being able to assess and select the most suitable optimisation technique for a given real-world design problem. In the present example, we consider the deployment of two leading and state-of-the-art optimisation algorithms; NSGA-II⁴ and MOTS.⁵

II. Technical Description of the Software

In order to define an aerodynamic benchmark test case we deployed the Free-Form Deformation (FFD) technique¹⁰ as a 2D airfoil geometry management capability. The scheme is based on trivariate Bernstein polynomials and can express global or local geometrical deformations. We then couple this in-house implementation of the FFD parameterisation functionality with a quick and reliable flow evaluation tool, Xfoil, for the prediction of the lift, drag and moment coefficients. Xfoil is a freeware code developed and described by Drela¹¹ for the design and analysis of subsonic airfoils, which deploys a linear-vorticity stream function panel method coupled with a two-equation lagged dissipation integral boundary layer formulation and a Karman-Tsien correction for compressibility effects. The force coefficients are calculated via the momentum deficit in the wake. Reliable predictions can be obtained in the presence of attached flows and even small separated regions, in a fraction of the time required by a Navier-Stokes solver (about a minute for a complete lift curve), making it ideal for the realistic representation of aerodynamic design problems and demonstration of the capabilities of the developed computational design tool.

The objective functions were defined as follows:

$$F(C_L) = -\frac{C_L}{C_{L,datum}} \quad (1)$$

$$F(C_D) = \frac{C_D}{C_{D,datum}} \quad (2)$$

where datum parameters used for the NACA0012 airfoil section.

Figure 1 illustrates the stages during the aerodynamic shape optimisation process of a 2D airfoil section. The Free Form Deformation (FFD) parameterisation technique¹⁰ applies the modifications with respect to a reference datum geometry. In our test problem we consider fixed position of the leading and trailing edges, in order to secure fixed chord length of the airfoil and angle of attack between all the new candidate design configurations that will be explored during the optimisation. The eight design parameters that describe our benchmark optimisation study correspond to the horizontal and vertical movement of the FFD control points, as presented in Fig. 2

For each new design vector received in the FFD stage the corresponding modified geometry is expressed in x-y coordinates. This definition of airfoil geometries is appropriate for Xfoil⁷ evaluation, which is the

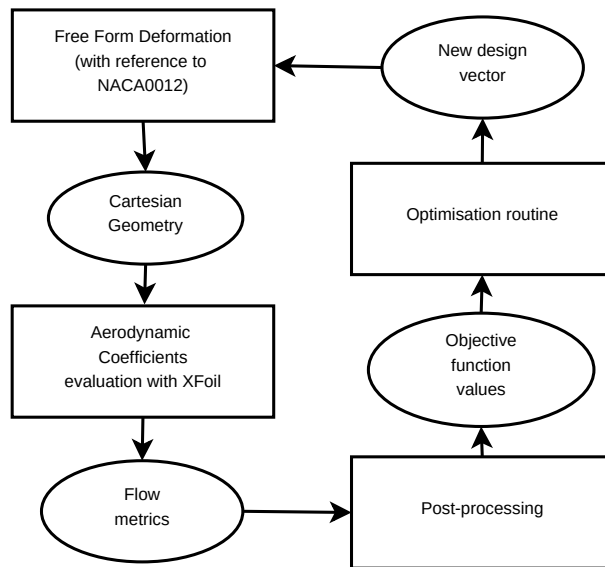


Figure 1. The flow diagram for the traditional shape optimisation process

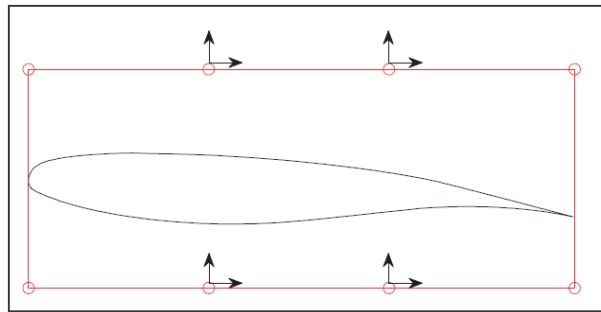


Figure 2. The design parameters that describe the benchmark 2D shape aerodynamic optimisation

following stage in the process as shown in Fig 1. Once the aerodynamic coefficients are calculated, they are post-processed, in order to assign the corresponding values to the objective functions that describe the optimisation problem, and then this information is provided to the optimisation routine where it will be assessed. Then the optimiser will allow to continue the process by suggesting new candidate designs for exploration.

The optimisation algorithms have been integrated as functions within the Nimrod/O framework,^{1,2,3} Nimrod/O (part of the Nimrod toolkit) allows a user to run an arbitrary computational model as the core of a non-linear optimisation process. Nimrod/O allows a user to specify the domain and type of parameters to the model, and also a specification of which output variables are to be minimised or maximised. Accordingly, a user can formulate a question like: what parameter settings will minimise the model output?. Nimrod/O currently employs a number of built-in single-objective optimisation algorithms, including BFGS, Simplex, Divide and Conquer and Simulated Annealing. Jobs can be executed on a variety of platforms, including distributed clusters and Computational Grid resources. We have now expanded these capabilities and the toolkit facilitates the multi-objective NSGA-II⁴ and MOTS⁵ algorithms. Previously, an interface of external advanced optimisation algorithms with Nimrod/O has been developed by Riley *et al.*⁶ and extended by Ferraro *et al.*⁷ The communication between the job dispatcher (Nimrod) and the optimisation tools has been established via pipes. Since these techniques are not available as an option for automatic selection through the Nimrod portal, it is required a built-in interface of additional optimisation methodologies.

The very popular and widely known Non-dominated Sorting Genetic Algorithm - II (NSGA-II) has been initially integrated within this interface. The functionalities of the algorithm have not been modified and used as initially defined and presented in Deb *et al.*⁴

The authors express particular interest to the aerodynamic design optimisation problems, and hence, the Multi-Objective Tabu Search (MOTS) technique has been integrated within the Nimrod toolkit too. This method has been implemented by Jaeggi *et al.*⁵ and proved to be extremely beneficial in shape optimisation and aerodynamic design^{8,9}

```

parameter x1 float range from -0.3 to 0.3
parameter x2 float range from -0.3 to 0.3
parameter x3 float range from -0.3 to 0.3
parameter x4 float range from -0.3 to 0.3
parameter x5 float range from -0.3 to 0.3
parameter x6 float range from -0.3 to 0.3
parameter x7 float range from -0.3 to 0.3
parameter x8 float range from -0.3 to 0.3

results 2

task main
  copy ffd-xfoil-multi node:ffd-xfoil-multi
  copy datum node:datum
  copy xfoil.def node:xfoil.def
  node:execute ./ffd-xfoil-multi $x1 $x2 $x3 $x4 $x5 $x6 $x7 $x8
  copy node:exp_result output.$jobname
endtask

method nsgaii
  starts 1
    seed 0.3
    popsize 120
    ngenerations 50
    pcrossover 0.9
    pmutation 0.5
    crossoverindex 10
    mutationindex 20
    tolerance 0.000
    on error ignore
  endstarts
end method

method mots
  starts 1
    starting points specified
    (0 0 0 0 0 0 0 0)
    nstm 15
    nregions 4
    intensify 15
    diversify 25
    restart 45
    stepsize 0.07
    stepsizerf 0.5
    nsample 8
    nevaluations 6000
    tolerance 0.000
    on error ignore
  endstarts
endmethod

```

Figure 3. Schedule file for the simultaneous execution of the two optimisation processes using Nimrod/O
 Figure 3 describes the definition of the whole design investigation for Nimrod/O execution. There are

four distinct blocks that comprise the schedule file. In the top block the design space is defined, as well as the type of each design parameter. The *results* property expresses the number of objective functions considered for this optimisation study. The following block describes the execution of the evaluation tool. In this case, we have combined the FFD parameterisation and Xfoil evaluation in a single operation. This task is copied and executed to all the compute nodes that are assigned to work for this job. These compute nodes can be part of heterogeneous or even geographically distributed clusters. In the last two blocks the optimisation methods are selected and all their critical parameters are assigned. With this schedule file, both optimisations will be executed simultaneously, and also the same database is used as it is enriched from both optimisation tasks.

III. Results and Analyses

The benchmark aerodynamic design optimisation of the NACA0012 section has been defined by maximising the lift coefficient and minimising the drag coefficient subject to hard geometrical constraints of the thickness at 25% and 50% of the chord, in order to satisfy structural requirements that secure a minimum available space to accommodate the two main spars that support the wing. 6,000 objective function evaluations have been allowed with each optimisation algorithm. In NSGA-II the population size was set to 120 and the optimisation operation evolved for 50 generations. The produced trade-off surfaces are presented in Figs. 4 and 5 for different levels of flexibility to the geometry management. The limits of variability of the 8 design parameters have been defined accordingly, which effectively allow larger changes to the values of the control points of the FFD technique, and hence larger geometry modifications.

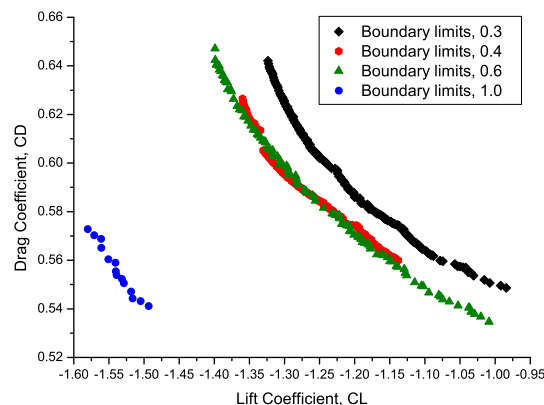


Figure 4. Simulation Results - MOTS (the boundary limits correspond to the range of variability for each design parameter)

It is clear that for wider range of variability the optimisation algorithms can reveal significantly improved design configurations. In particular, Fig. 4 shows that the MOTS algorithm can reveal a continuously dominant Pareto set as the design parameter boundary limits increase, but also a wider spread of the trade-off surface. Only in the final test case, where the largest variability of the design parameters is considered, the Pareto front significantly fully dominates the earlier optima identified, apart from a small region of the extreme lowest Drag Coefficient objective function. It is expected though that this region of the objective function space will be explored as well, once a higher number of evaluations is allowed.

However, when the geometrical flexibility exceeds a threshold the NSGA-II algorithm struggles to satisfy the hard geometrical constraints and cannot express any progress in the exploration of the design space (Fig. 5). Apart from that, a random generation of the initial population contains a high fraction of aerodynamically infeasible designs, and hence it is very difficult for any Genetic Algorithms type optimisation method to perform competitively in shape aerodynamic optimisation cases.

Figure 6 highlights the fact that for the same extent of the design parameter boundary limits, the population based algorithm benefits from its global search characteristics and produces a trade-off that fully dominates the one produced with a Tabu Search exploration. However, it has to be noted that the

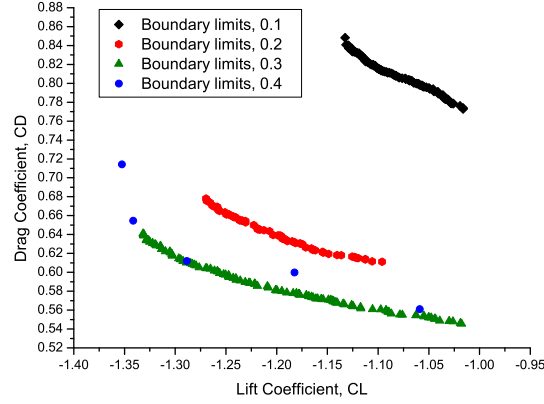


Figure 5. Simulation Results - NSGA-II (the boundary limits correspond to the range of variability for each design parameter)

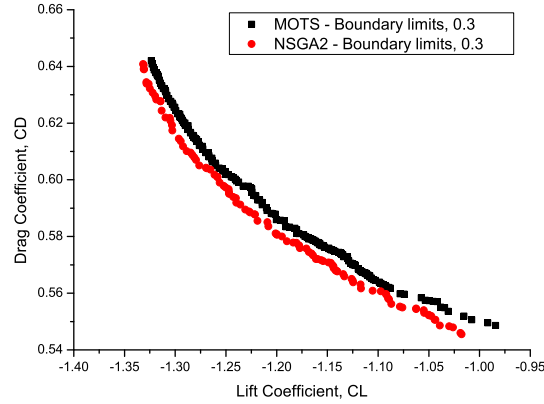


Figure 6. Comparison between MOTS and NSGA-II

optimisation level between the two Pareto fronts is very similar, and quite remarkably the diversity of the trade-offs is very similar as well. There is only an issue with the richness of the final Pareto front for all the population based algorithms, as implicitly, a maximum size is set once the number of individuals within a population is fixed. In contrast, there is no limit assigned to the size of the Pareto front in MOTS.

IV. Conclusions

The paper describes additions to the Nimrod/O optimisation suite. We have demonstrated through a benchmark aerodynamic design case that it is possible to easily explore and investigate the performance of various optimisation techniques, and hence being able to identify and select the most suitable algorithm. Even further, depending on the requirements of the design problem each time, the selection of the optimisation technique can change when the boundaries of the design space change. Hence, it is not always the physical nature of the problem under investigation that controls this choice. In the case of a limited design space, the evolutionary based optimisation algorithms outperform the local-based Tabu Search, even though naturally the latter technique can tackle much more successfully aerodynamic design problems.

Advanced engineering design tools are now available through the Nimrod Portal toolkit and accessible to a wider community of engineers that do not have the technical expertise required to manually configure, execute, and monitor such complex computational design systems and processes. At the same time, more

computational resources from different geographical locations can be combined and deployed to a particular computational design problem. As a result, academic collaborations are possible and equally, industrial companies can benefit from all their resources available.

Moreover, experimentation and development of new optimisation methodologies is now easier than ever, and global optimisation techniques can be hybridised with intelligent local search mechanisms that can reveal a wide range of alternative solutions to engineering problems that are inherently difficult and highly complex.

Apart from the practical industrial interest to this technological advancement, engineering optimisation theory and principles can now be taught in University level easier than ever before. At the same time, Information Technology and e-Sciences can enjoy the merits and progress further towards more efficient management of massively all-level-parallel computations.

Furthermore, the whole software development can be expanded even more and integrate it within Nimrod/OK,¹² where the automation of scientific processes is managed through workflows. The clear advantages of such software are the flexibility to describe, construct and analyse complex engineering design systems, but most importantly the various search methods available within Nimrod/OK can be combined in novel ways and hence define and explore new avenues in computational engineering design research.

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