### FAST CFD FOR SHAPE AND FLOW PARAMETERIZATION WITH META-MODELS BUILT ON HIGH-ORDER DERIVATIVES. APPLICATIONS TO FAST DESIGN

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#### Abstract

The design of new geometries for one aerodynamic conception leads to difficulties of CPU costs when discrete methods are used (one configuration). *Strategies* per run of simplification must be chosen either to restrict the number of calculations, or to limit the CPU time associated with each run. The approach proposed here consists in associating two strategies: using a meta-model and adjusting the limits of the parameters domain. A continuous database is so built of which size varies according to the number of parameters.

The meta-model is based on high-order derivatives of flow variables  $(Turb'Opty^{TM})$ solver). These are obtained by automatic differentiation of the discretized averaged Navier-Stokes 3D equations around a reference solution. The equations are therefore like those of conventional solvers (like SC/Tetra, Fluent, Star CD), but the unknown factors are here the derivatives of order 1, 2, ..., N of the field with respect to the parameters of operation or shape. These successive derivatives are stored in a database and their exploitation makes it possible to instantaneously obtain the new fields corresponding solution to the configurations sought by the user.

The limits of the exploration domain depend on the derivatives order, the possible evaluation of the coupled terms, imposed constraints and physical high non-linearities. A continuous database can then be explored directly or coupled with other physics solvers, as well as with optimization tools.

Some simplified applications show the validity of this approach. As an illustration, the database is coupled with a multi-objective Genetic Algorithm (GA) in order to solve large scale global optimization problems.

It was found that high-order reconstruction leads to a drastic reduction in the number of design iterations, shortens the design cycle, lowers the cost and improves the quality.

# 1 General introduction on optimization in aerodynamics

Design in aeronautics is quite challenging due to the large parameter space to be explored. Using high fidelity CFD to resolve multi-objectives demands optimization problems large computing resources, numerous software licenses, hardware for massive parallelism and significant human power. Under stringent time scales and costs, advanced optimization techniques are therefore needed to achieve a practical design.

The ideal data for a designer is the set of optimal points, defined as the Pareto frontier, in order to find the compromise that best fits the application.

The classical industrial optimization approach is to minimize a pseudo-objective function, which is a weighted sum of each single objective, with a gradient-based method [1] [2]. By operating this way, the designer only finds a single point

of the Pareto front determined by the weights given to each objective. Therefore, he has to run multiple optimizations with different sets of weights to get the entire Pareto front. Besides, when the Pareto front features a concave zone, the optimizer is not able to find optimal solutions in this particular zone. An additional drawback is that the obtained optimum is local, therefore its quality strongly depends on the chosen baseline. Gradient-based optimization supported by the adjoint approach is more efficient when the number of design variables is large [3] [4]. However, the adjoint equation depends on the objective function, so that changing the objectives is not quite flexible. To summarize, gradient-based methods are not very efficient for solving multi-modal and multiobjective optimization problems. One can also point out that they have a high level of coupling between the search and the evaluation.

An interesting alternative to gradient-based methods is the family of meta-model assisted Evolutionary Algorithms [5]. We focus here on Genetic Algorithms (GA) [6] such as SPEA2, NSGA2. GAs are global algorithms that are uncoupled with the objective evaluation process. Moreover, they handle multi-objective optimization problems quite well. Their drawback is the very large number of required objective evaluations. Even if these evaluations can be easily distributed on a computer cluster, the process is still slow and implying to buy as many CFD software licenses as computer nodes. One way of alleviating this computational burden is by using a meta-model, which are described in the following section.

### 2 Meta-Model

A major issue in CFD is the prohibitive simulation time required to get an accurate flow solution: some problems can require weeks of computation on high-performance computers, as well as Gigabytes of storage memory. On the other hand, multi-objective optimization techniques always require the evaluation of numerous candidate solutions in order to build the Pareto-optimal frontier, and become therefore out-of-reach if a single CFD simulation is expensive. Based on approximation theory, meta-models address this challenge by quickly evaluating the objective functions for any given set of parameters, only using a sample database and some mathematical analytical functions. Optimization algorithms, such as the costly evolutionary ones, will then evaluate the candidates without calling the CFD solver but the meta-model, which "engenders" a substitute for the desired design point. We underline here that the meta-model building procedure is completely independent from the choice of the optimization algorithm. Besides drastically saving CPU time, the approximation process of the meta-models also allow the designer to have access to the smoothed continuous objectives space and thus really apprehend the sensitivity of the parameters over a large domain. In other words, the benefit of the meta-models is twofold: they give engineers a better perception of the physical issues while they offer optimization algorithms an efficient way to locate the Pareto-optimal frontier when several concurrent objectives are targeted by the designer.

### 2.1 The General approach

There is a broad variety of meta-model Response techniques such as Surface Methodology, Artificial Neural Network (ANN) [7], Radial Basis Functions [8] or Kriging [9] (reference [10] presents a good survey of these different techniques). The main drawback of all these meta-models is that the parameters space has to be scarcely sampled while each point corresponds to a high-fidelity CFD solution. This step is crucial as the resulting transfer function from the input to the output of the meta-model strongly depends on which sample CFD points have been brought to it. Although these latter points can be chosen at random, Design of Experiments [11] is the most popular method to discretize the parameters space while preserving the maximum of information. Note that for every sampling methods, the number of CFD computations required to fill the sample database grows exponentially with respect to the number of design parameters. If each of these methods have their own advantages and

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disadvantages regarding the complexity of internal setting parameters. robustness, efficiency or accuracy, it can be said that using any of them is a complex and critical task for the engineer. For example, when using ANN, the set of already evaluated design points needs to be divided by the user into some training and test sets. The latter set contains the samples needed to evaluate the capability of the ANN to predict unknown points different from the training set. Usually, one tries to stop the ANN procedure when the error on the test samples is no longer decreasing, to avoid over-learning.

The meta-model approach presented in the following is fairly different since we do not sample the parameter space to build the meta-model: a single design point is used, which is the reference design point.

### 2.2 Turb'Opty<sup>TM</sup> and Turb'Post<sup>TM</sup>

In the meta-model described here, the flow field for a given set of parameters is approached using high-order derivatives of the discretized flow variables with respect to the design parameters at the reference point. This parametrization method could be viewed as a high-order extension of the first- and secondorder sensitivity equations methods described in references [12], [13], and [14] by Pelletier et al., where the method is applied to standard but complex cases. However, here the derivatives are not computed analytically but thanks to direct mode Automatic Differentiation (AD) of Turb'Flow<sup>TM</sup>, a Reynolds-averaged Navier-Stokes flow solver based on the finite-volume method (see [15] for an example of AD tools applied to a CFD industrial code). This AD methodology is similar to the one commonly used in the adjoint-state method in order to evaluate the first-order derivative, except that reverse mode is used in that latter case. By also generating the high-order derivatives. Turb'Opty<sup>TM</sup> [16] makes possible the highly accurate parametrization of the flow field in the region neighboring the reference design point. Indeed, the derivatives being discretized over the fluid mesh, the generation of a complete flow field is performed for any given design

parameters with Turb'Post<sup>TM</sup> using Taylor Series expansion or some other functions such as Fourier series [17]. As shown in Fig. 1, the meta-model consists in the combination of both Turb'Opty<sup>TM</sup> and Turb'Post<sup>TM</sup>: the former generates the derivatives database once, then the latter constructs as many flow fields as required by the designer or the optimization tool, each of these evaluations being almost instantaneous. We note that the derivatives can be either with respect to operation or shape parameters.

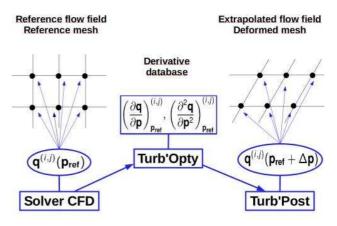


Fig. 1 Diagram of the parametrization process

Another advantage of this meta-model is that the complete flow fields are generated for each design points so that objectives can be defined in an independent step, unlike most other metamodels, which require a new training process when an objective is changed or a new one is introduced. The meta-model can be generated first by the CFD engineers and the objectives formulated later by the designers, with a total freedom. Also, new parameters can be introduced afterwards, and combined with the old ones, without having to start from scratch. Regarding the computational cost of the method, Turb'Opty<sup>TM</sup> implies linear system resolutions such as the ones resulting from the adjoint-state method, while Turb'Post<sup>TM</sup> cost is not significant.

We now give an example of application, with a standard CFD case.

#### **3 Validation example: the NLR 7301 twoelement airfoil**

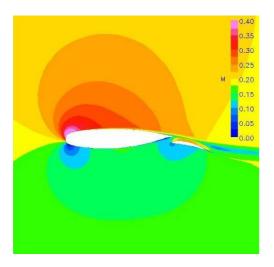
The geometry is the 2D NLR 7301 airfoil/flap configuration [18]. Freestream Mach number is

M=0.185, chord Reynolds number is 2.51  $10^6$  and far-field pressure is 101227 Pa. The parametrization is done with respect to the angle of attack  $\alpha$ , with unchanging boundary conditions. Results are compared with experimental data and reference computations (see [19] and [20]).

As explained in the previous section, one reference design point needs to be simulated first, in order to build the derivative database.

#### 3.1 Reference flow field, angle of attack $\alpha$ =6°

The reference flow field is evaluated with Turb'Flow<sup>TM</sup> for the angle of attack  $\alpha=6^{\circ}$ . Jameson's centered convective scheme along with Kok's turbulence model are used in the computation (see Fig. 2 for the Mach number around the airfoil).



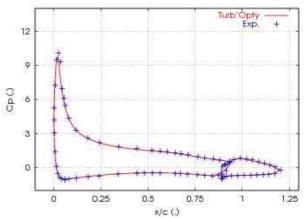


The calculated wall pressure coefficient agrees well with experimental data, both on the airfoil and flap. Also, the calculated lift coefficient is 2.372 while the measured one is 2.4. Thus, this aerodynamic field is shown to be good enough to be used in Turb'Opty<sup>TM</sup>.

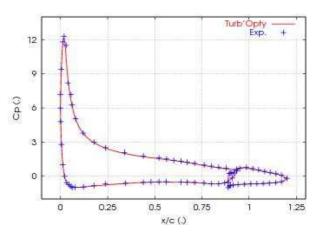
#### 3.2 Extrapolated flow fields

Using the reference solution at  $\alpha=6^{\circ}$ , first- and second-order derivatives of the flow field, with respect to  $\alpha$ , are computed by Turb'Opty<sup>TM</sup>. Afterwards, a flow field corresponding to any value of angle of attack can be generated by Turb'Post<sup>TM</sup>, and some local and global flow

coefficients can then be evaluated from that extrapolated field. For example, Fig. 3 and Fig. 4 show the wall pressure coefficients at  $\alpha$ =10° and  $\alpha$ =13° compared to experimental data. We observe on both figures that plus signs (experimental data) are almost matching with the solid curve (numerical results from Turb'Opty<sup>TM/</sup> Turb'Post<sup>TM</sup>).



**Fig. 3** Wall pressure coefficient, angle of attack  $\alpha = 10^{\circ}$  (ref.  $\alpha = 6^{\circ}$ )



**Fig. 4** Wall pressure coefficient, angle of attack  $\alpha$ =13° (ref.  $\alpha$ =6°)

In Fig. 5, the lift coefficient is evaluated for an angle of attack spanning the interval 0° to 16°. We observe that the error between the results from Turb'Opty<sup>TM</sup> and experimental data remains small over a large domain of the parameter  $\alpha$ , where the error is actually close to the one measured at the reference point  $\alpha=6^{\circ}$ . If experiments show that massive stall occurs suddenly when  $\alpha$  reaches about 15°, the drop of lift coefficient is not correctly evaluated either

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on the extrapolated flow field or on the solution issued from Turb'Flow<sup>TM</sup> at  $\alpha$ =16°. However, both solvers predict a large flow separation on suction side before the main body trailing edge, as shown on Fig. 6 (Turb'Opty<sup>TM</sup> results). This highly non-linear flow feature seems to be unpredicted by RANS simulations, as reported by Abalakin et al. [20].

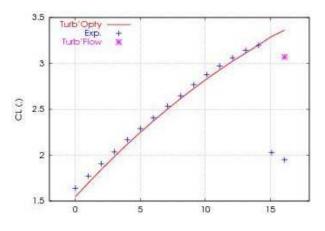


Fig. 5 Lift coefficient with respect to angle of attack (ref.  $\alpha=6^{\circ}$ )

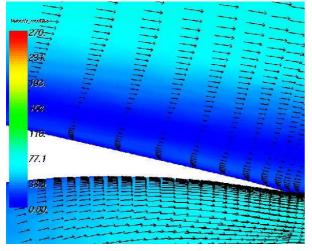


Fig. 6 Velocity modulus and velocity vectors extrapolated at  $\alpha=16^{\circ}$  (ref.  $\alpha=6^{\circ}$ )

We now look at an optimization example.

# **4** Exploitation example of extrapolated flow fields for optimal design

By coupling Turb'Post<sup>TM</sup> with a GA, the parameter space is thoroughly explored. When the treated problem is "friendly", a single optimization may be enough: the designer just has to choose on the Pareto front the optimal

solution that best suits his industrial specifications. However, some other optimization problems in fluid mechanics can be highly complex: achieving just one optimization loop may not be enough to reach the "perfect" design. To get more insight into the problem, the designer has to run multiple optimizations for which the objectives remain the same, but the active parameters vary from one run to another. By comparing the resulting Pareto fronts, the designer understands the effect of the parameters on the objectives in a better way. To achieve this kind of comparative study with a classical surrogate model such as ANN, the designer has to re-train the metamodel for each choice of parameters. When Turb'Opty<sup>TM</sup>, once the derivative using database has been built, the designer can run optimizations based on any sets of parameters in an efficient way, and also grasp the coupling effects of parameters by activating the second order cross-derivatives of the flow field. Although these cross-derivatives may not be prevailing in some optimization problems, they can make a crucial difference in other cases.

The test case presented here is a 2D low-speed fan profile optimization, which has four objectives:

- maximization of static pressure difference
- maximization of the static efficiency
- minimization of the loss coefficient
- minimization of the torque

The designer can choose to use any sets of parameters among the following:

- stagger angle (C)
- tangent of angle at the leading edge (Tba)
- tangent of angle at the trailing edge (Tbf)
- maximum camber (with respect to the chord) (d)
- position of maximum camber (with respect to the chord) (Xd)

Only two objectives (static pressure difference and static efficiency), are presented in this paper for clarity reasons, which implies that the fronts in Fig. 7 and Fig. 8 are projections. Fig. 7 shows the results of four different optimizations cross-derivatives. without using the The reference solution in the vicinity of which was constructed the derivative database is represented as a green square and referred as "optimA". This reference solution corresponds to a previous optimization, which explains why all the Pareto fronts are close to it. Regarding Fig. 7, three optimizations were performed using a set of only four parameters, while the last one took into account all five parameters. Here, the parameter "Xd" is responsible for the little improvement in the population. Indeed, at fixed static pressure difference, little growth of efficiency is achieved and the same can be said in the other way around. Now, if the designer activates the cross-derivatives and performs the same optimizations as for Fig. 7, he obtains the results shown in Fig. 8. Although Fig. 7 shows that some parameters have no effect on the objectives, Fig. 8 highlights that the best compromises are obtained when all parameters are activated and coupled by the crossderivatives. The comparison of the red, the pink

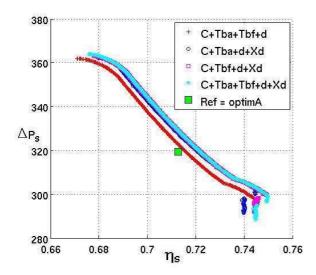


Fig. 7 Pareto fronts, without cross-derivatives

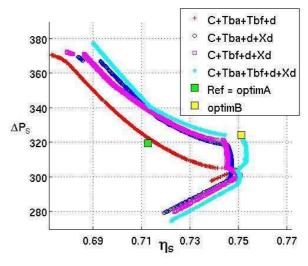


Fig. 8 Pareto fronts, with cross-derivatives

and the blue Pareto front projections shows that all the cross-derivatives involving the parameter "Xd" lead to significant enhancement in the population. Moreover, the cyan Pareto front shows that cross-derivatives projection involving "Tba" and "Tbf" enable to achieve a little more improvement. The optimum referred as "optimB" is an interesting solution: it has maximum efficiency and static pressure difference. Fig. 9 and Fig. 10 show the static pressure field for the design points "optimA" (the reference point) and "optimB" respectively.

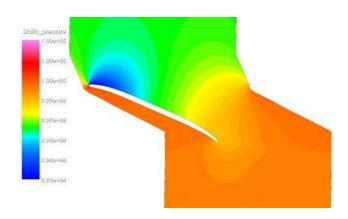


Fig. 9 "optimA" design point, static pressure

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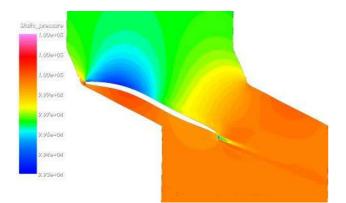


Fig. 10 "optimB" design point, static pressure

#### **5** Conclusion

The authors presented here a meta-model based on high-order derivatives of the discretized flow field with respect to shape or operation parameters. This requires to perform a single CFD simulation, while demonstrating a high level of extensibility and flexibility regarding the definition of parameters and objectives. Once the derivative database has been built, the objective evaluation process for a given design point is almost instantaneous, making GAs optimization algorithm particularly efficient for exploring the parameter space. We have shown an example of the extrapolation technique with the standard NLR 7301 two-element airfoil, and then presented an example of 2D low-speed fan profile optimization using GAs coupled with our meta-model. We found with this analysis that significant improvements can be achieved mainly by changing locally the camber line of the profile.

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#### References

- [1] G.N. Vanderplaats, "Numerical Optimization Techniques for Engineering Design", *McGraw-Hill*, *New York*, 1984.
- [2] J.C. Vassberg, A. Jameson, "Aerodynamic Shape Optimization": Theoretical Background", VKI Lecture Series on Introduction to Optimization and Multidisciplinary Design, Brussels, 2006.
- [3] A. Jameson, "Optimum Aerodynamic Design Using Control Therory", Computational Fluid Dynamics Review, pp. 495-528, 1995.
- [4] B. Mohammadi, O. Pironneau, "Shape Optimization in Fluid Mechanics", Annual Review of Fluid Mechanics, 2004.
- [5] K. Deb, "Multi-Objective Optimization using Evolutionary Algorithms", *Wiley, New York*, 2001.
- [6] D. Goldberg, "Genetic Algorithms in Search, Optimization and Machine Learning", Addison-Wesley, Stuttgart, 1989.
- [7] B.J.A. Krose and P.P. Van Der Smagt, "An Introduction to Neural Networks", *University of Amsterdam*, 1993.
- [8] N. Dyn, D. Levin and S. Rippa, "Numerical Procedure fir Surface Fitting of Scattered Data by Radial Basis Function", SIAM Journal of Scientific and Statistical Computing, 7:639-659, 1986.
- [9] G. Matheron, "Principles of Geostatistics. Economic Geology", *58:1246-1266*, 1963.
- [10] G. Gary Wang and S. Shan, "Review of Metamodeling Techniques in Support of Engineering Design Optimization", J. Mech. Des., Vol. 129, Issue 4, 370 (11 pages), 2007.
- [11]D.C. Montgomery, "Design and Analysis of Experiments", John Wiley and Sons, New York, 1997.
- [12] J.-N. Mahieu, S. Etienne, D. Pelletier and J. Borggaard, "A Second-Order Sensitivity Equation Method for Laminar Flow", Int. J. Comput. Fluid Dynam., Vol. 19, No. 2, February 2005, 143-157, 2005.
- [13] F. Ilinca, D. Pelletier and J. Borggaard, "A Continuous Second-Order Sensitivity Equation Method for Time-Dependent Incompressible Laminar Flows", Int. J. Numer. Meth. Fluids 2007; 55:565-587, 2007.
- [14] F. Ilinca, D. Pelletier and A. Hay, "First- and Second-Order Sensitivity Equations Methods for Value and Shape Parameters", *Int. J. Numer. Meth. Fluids 2008;* 57:1349-1370, 2008.

- [15] C. H. Bischof, H. M. Bücker, A. Rasch, E. Slusanschi and B. Lang, "Automatic Differentiation of the General-Purpose Computational Fluid Dynamics Package FLUENT", J. Fluids Eng., Vol. 129, No. 5, pp. 652-658, 2007.
- [16] S. Aubert, J. Tournier, M. Rochette, J. Blanche, M. N'Diaye, S. Melen, M. Till and P. Ferrand, "Optimization of a Gas Mixer Using a New Parametric Flow Solver", *Proceedings of the ECCOMAS Computational Fluid Dynamics Conference, Swansea, UK*, 2001.
- [17] L. Soulat, S. Moreau, P. Ferrand, S. Aubert, M. Henner, "Numerical Design and Optimization of a New Casing Treatment for Shrouded Fans", *Proceedings of the 27<sup>th</sup> International Congress of the Aeronautical Sciences, Nice, France, 19-24 September 2010*, 2010.
- [18] J. W. Slater, "NLR Airfoil with Flap", NPARC Alliance Validation Archive, <u>http://www.grc.nasa.gov/WWW/wind/valid/nlrflap/nlr</u> <u>flap.html</u>, 1998.
- [19] B. Van den Berg and B. Oskam, "Boundary Layer Measurements on a Two-Dimensional Wing with Flap and a Comparison with Calculations", AGARD CP-271, Sept. 1979.
- [20] I. Abalakin and B. Koobus, "The Behavior of Two Near-Wall Models for k-ε Prediction of Stall", *INRIA RR-4075: inria-00072558, version 1*, 2000.