Robust design applications with modeFRONTIER, applying NODESIM-CFD tools

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Abstract:

This paper illustrates how the Multi-Objective Design Environment modeFRONTIER can be efficiently used as a Robust Design computational environment, integrating, in addition to the existing ones, the technologies developed during NODESIM-CFD project.

modeFRONTIER is a tool that allows the coupling of any CAE tool or in-house code in a distributed computational environment, giving to the designer several solutions, such as the possibility to define the parameterisation of any computational system and to run automatically series of design simulations, optimising the specified objectives, performing statistical analysis, define Response Surface methodologies, and perform Design under Uncertainties (Robust Design) analysis. Concerning the last ones, during NODESIM-CFD project the Polynomial Chaos methodology, developed with the help of University of Trieste, have been integrated in the software to improve the accuracy and efficiency of the Robust Design.

Aeronautic test cases have been prepared and reported in this paper, using the CFD code FINE/HEXA from NUMECA: the compulsory Rotor37 test case for a Robust Design Analysis of an axial compressor rotor under inlet total pressure uncertainty, the compulsory RAE2822 test case and a shape optimisation of the same RAE2822 airfoil, through Bezier curves, under the three uncertainties of Mach number, angle of attack and thickness.

1. Introduction- General overview about modeFRONTIER environment

modeFRONTIER[1] is a multi-objective design environment software that allows the integration of any commercial CAE tool or in-house code (including CAD, FEM, CFD, Matlab, etc..) into a common environment, in order to run automatically a series of designs, proposed by the available optimisation algorithms, until the defined objectives are satisfied.
In this modular environment, each component of the optimisation, including input variables, input files, scripts to run the commercial software, script to run processes on remote machines, output files, output variables and objectives/constraints, is defined as a node to be connected to the other components in the available workflow.
In this way, the complete logic flow from CAD parameterisation to performances evaluation is defined by the user, that can select among several available optimisation algorithms, accordingly to the defined objectives; they include Genetic Algorithms[2], Evolutionary Algorithms, Game

Strategies[3], Gradient-based Methodologies, Response Surfaces and Robust Design Optimisation, as well as main DOE (Design Of Experiments) algorithms (Sobol, Factorials, Latin Square, Montecarlo, D-Optimal, etc.).

These algorithms drive automatic series of simulations, allowing when available distributed and parallel computations to fully exploit the computational resources, until the objectives are met.

In addition, the influence of all the parameters in the process can be analysed in detail by the use of statistical analysis (correlation matrix, t-Student, ANOVA, etc.) and Response Surface Methods (Kriging, Neural Networks, Radial Basis Functions, SVD, Parametric, Gaussian, etc.), that can be also used to reduce the number of computations required in the optimisation, allowing an extrapolation of the results.

A dedicated module of modeFRONTIER is dedicated to Robust Design or Design under Uncertainties, and it has been enriched, through NODESIM-CFD project, of new tools to improve its efficiency. Next section will describe the available tools of modeFRONTIER for Robust Design, and further the test cases applications will be presented.

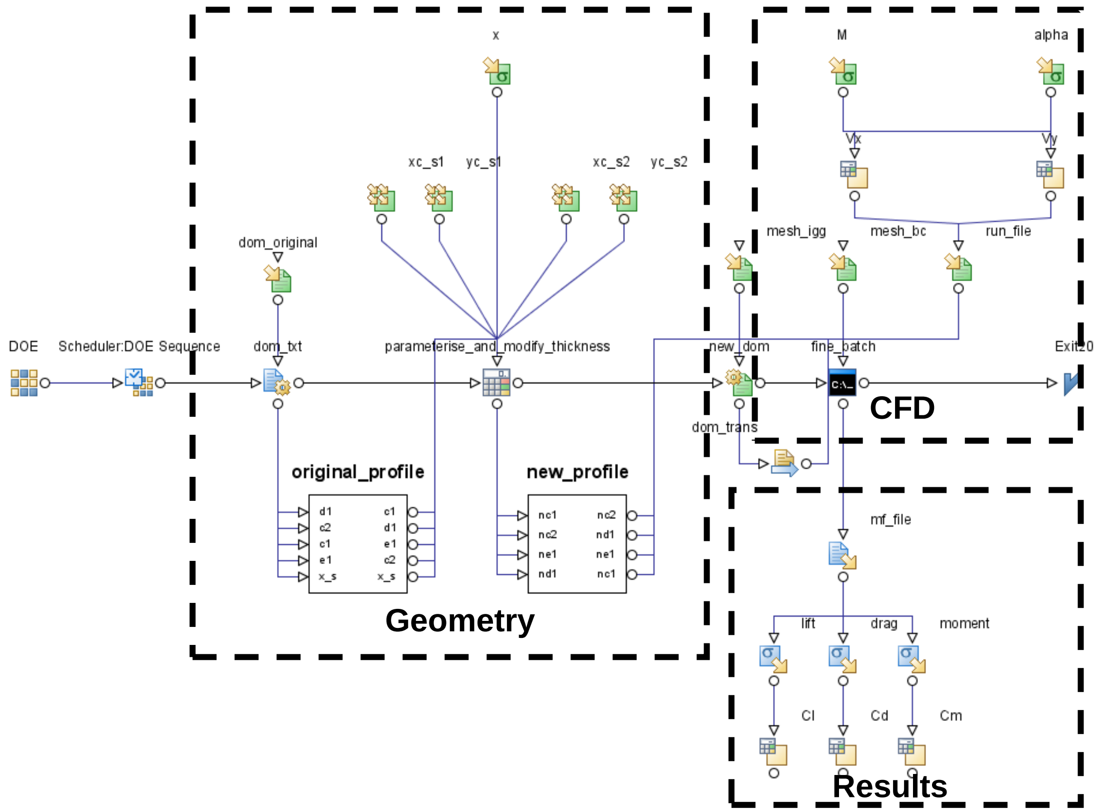

Fig.1 Example of modeFRONTIER workflow for CAE integration (used for NODESIM-CFD aeronautic test case)

2. Robust Design tools in modeFRONTIER

This section describes the tools for Robust Design (Design Under Uncertainties) available in modeFRONTIER. Different analysis typologies can be performed in this environment.
One possibility is to perform a single DOE (Design of Experiments) specifying the uncertainty distribution of all the input parameters, and after the automatic execution of the designs, post-processing charts can be used to analyse in detail the distribution results.
A different approach, common in industrial practice, is to perform a Robust Design Optimisation. The optimisation algorithm, normally used for deterministic problems, can be applied also defining uncertainties on input variables: in this case, a sampling strategy is automatically adopted by the algorithm, that computes for each candidate solution the mean and standard deviation of the responses, obtained from a set of sample points corresponding to the specified uncertainties distribution. Objectives and constraints can therefore be defined on the response distributions (for instance, maximise average performance, and minimise its standard deviation).
The latter approach, can be combined with Response Surfaces (the responses of the system are extrapolated through a metamodel trained on the available database), in order to reduce the overall time needed to perform a Robust Design Optimisation.

We analyse now in detail the different sampling methodologies available in modeFRONTIER.
Basically, three algorithms can be selected: Montecarlo, Latin Hypercube and Polynomial Chaos [6].
More precisely, only the first two can be actually considered as sampling algorithms, while the PC, that has been developed in modeFRONTIER during NODESIM project, with the collaboration of University of Trieste, is an algorithm to be used in the response distribution analysis, to have a more accurate and efficient computation of the distribution parameters.
Montecarlo is the simplest sampling methodologies, and is just based on a random definition of sample points. From a random sequence of points defined by a uniform probability, the sample points are obtained by the projection of the former points onto a Gaussian Cumulative Distribution (defined as uncertainty of the input variable). The process can be extended to a case with a generic number of variables. It is possible to prove that the statistical moments, and as a result the mean and the standard deviation, of a random sample converge to the exact moments of the full distribution as the inverse of squared N, where N is the sample size.
A more efficient sampling methodology, in the sense that the convergence of the random sample to the exact full distribution is more rapid, and in particular proportional to the inverse of N, is **Latin Hypercube**. In this case, if a LH is composed of N points, and every variable is divided in N strata with equal probability (the same portion of area under the Gaussian distribution), every single stratum will be occupied by exactly one point. Latin hypercube sampling has been designed specifically to produce better accuracy than Monte Carlo in uncertainty quantification.
Polynomial Chaos methodology consists essentially in expanding the uncertain variables in a suitable series and then determine analytically (and thus exactly) the statistical moments of the

truncated expansion. The expansion itself is referred to as the "chaos", while the maximum degree of the expansion is called the "chaos order".
As a result, it can be proved that the estimate of the statistical moments converge to true values at exponential rate, i.e., the error in the estimates scales as e^{-N}, where N is the sample size.
More precisely, the function f(x) can be expressed as a series of orthogonal Hermite polynomial (if uncertainties have a normal distribution), so that

$$f(x) := \sum_{i=0}^{k} \alpha_i p_i(x).$$

It follows that the statistical moments, and in particular mean and standard deviation, can be expressed by a simplified expression, that is respectively:

$$\langle y^1 \rangle = \alpha_0$$

$$\langle y^2 \rangle = \sum_{i=0}^{k} \alpha_i^2 \|p_i(x)\|^2$$

Using normalised Hermite polynomial, the expression can be simplified further (norms are equal to 1).
In the case of multiple variables, assuming they are independently distributed, it is possible to write multivariate chaos considering the tensorial products of the univariate polynomials corresponding to the distributions of every single variable, generalising the above expressions.
To define the requested moments is thus just required to determine the Polynomial coefficients, and to do this, in the case of d variables and expansion of order k, the minimum number of requested samples is:

$$\binom{k+d}{d} = \frac{(k+d)!}{k!d!}.$$

In practical cases, it is necessary to arrest the expansion at a certain order, and the values for mean and standard deviation, exact for the truncated chaos, will be an approximation of the true mean and standard deviation. If the stochastic distribution of the uncertain variables is different, a different series of polynomial is used: for instance, in case of Beta distribution, Jacobi polynomials are used.

In modeFRONTIER, when a DOE or Optimisation sequence has been run (or alternatively experimental data are imported), the results can be analysed in the post-processing panel (Design Space).
Several tools can be used by the user to analyse the results of his analysis, including Correlation Matrix or Student Charts (to find which are the variables most influencing in the process), Interaction Effect Matrix (to keep into account also the interaction between variables in the effects), SOM or Self Organising Maps, as well as Clustering Anlaysis (particularly useful to find local correlations when the number of variables is high). Among the tools explicitly

dedicated to Robust Design Analysis, all the most relevant statistical information are summarised in the Distribution Fitting tool (fig.2), developed by ESTECO during NODESIM-CFD project. It consists in four charts, that corresponds to Probability Distribution Chart, Cumulative Distribution Chart, Quantile-quantile plot, and Distribution table with fitting details. The basic idea of the tool, is to perform an internal optimisation, in which the input variables are the parameters of 11 main Statistical Distributions, and the objective is the maximisation of Kolmogorov Smirnov (KS) coefficient, in order to find the Statistical Distribution that better approximate the given database. The KS test is computed in function of the highest distance, in Cumulative Distribution Function, from a database point and a Statistical curve point.
The % value of optimised KS test (being 100% the Statistical Distribution itself) is reported in the table, as well as other statistical tests (LL is Normalised Likelihood function), and the optimal values of the Statistical Distributions.

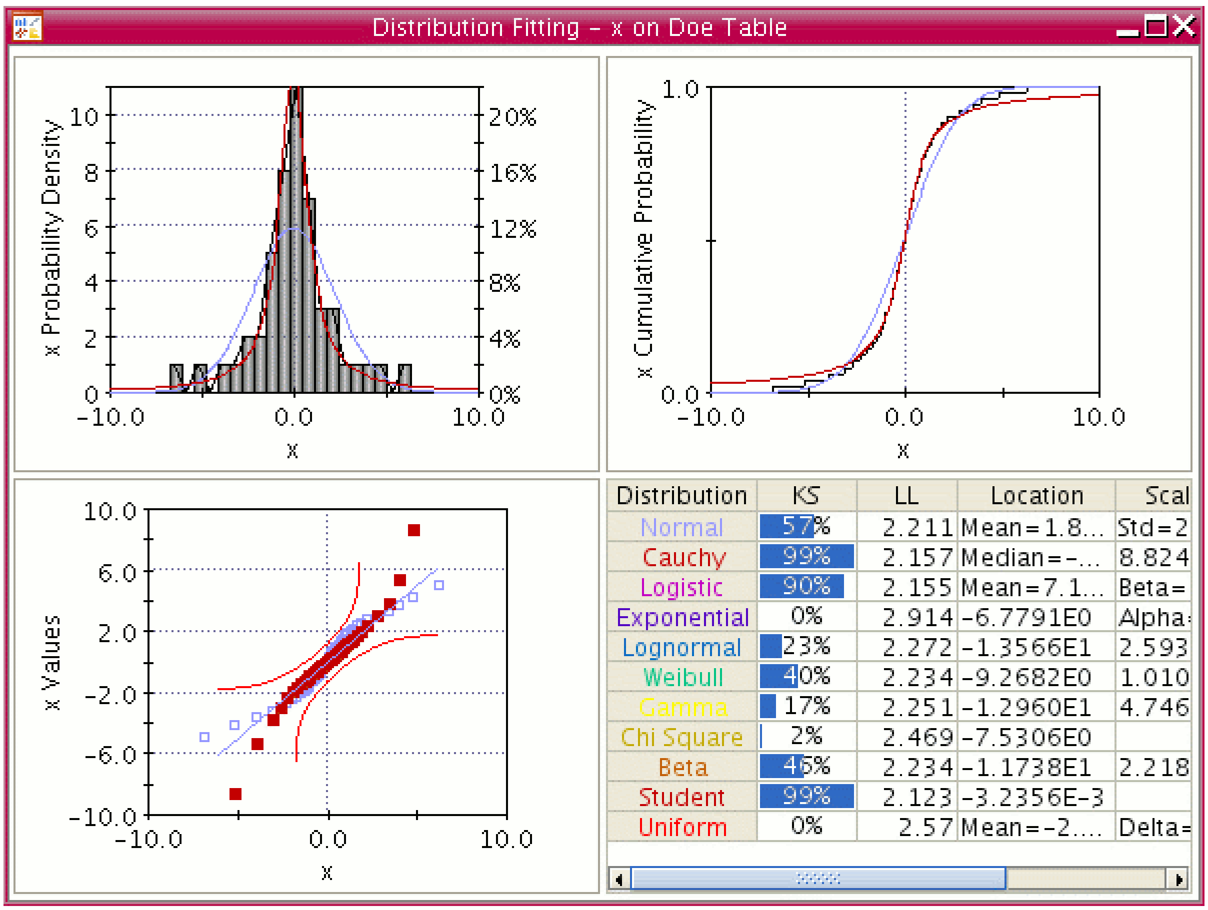

Fig.2 Distribution Fitting tool in modeFRONTIER

In next sections we are going to present the application of modeFRONTIER Robust Design tools for the proposed test cases.

3. Application of Robust Design Tools of modeFRONTIER for ROTOR37 Test Case

The first application we present is related to an axial compressor rotor test case: the Rotor 37 [4]. The CFD model of the Rotor has been provided to ESTECO by NUMECA, using the CFD code FINE/XA [5] (fig.3, left). The mesh is built up by 567,296 cells; full Turbulent Navier-Stokes equations are used, with the Spalart-Allmaras turbulence model.

Six different running points are considered, each one given by a different outlet static pressure, as specified by the test case. For each running point, the stochastic uncertain variable is the inlet total pressure: from the standard or most likely input profile *m* (fig.3, right) a symmetric Beta distribution (minimum value equal to 95% *m* and maximum value equal to 105% *m*, with *a* and *b* coefficients equal to 4) is considered.

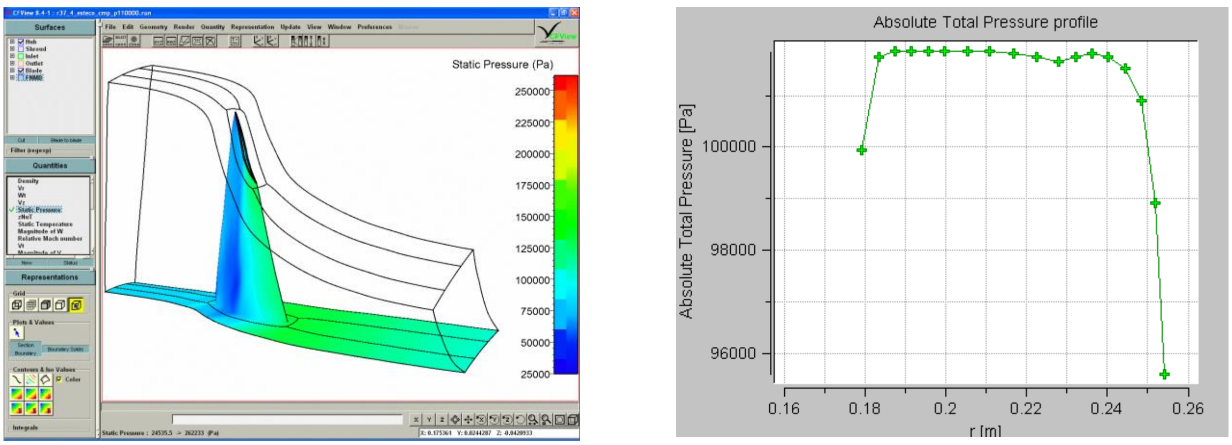

Fig.3 Rotor 37 CFD model by FINE/HEXA (left) and standard input pressure profile (right)

This means that we need to compute, for each running point, the mean and standard deviation of the distributions relative to the performance parameters, i.e mass flow rate, efficiency and total pressure ratio.

A workflow is built in mF (fig.4), for the automatic run of the Robust Analysis.

The stochastic variable in this case is *pt_in*, i.e. the factor that multiplies the inlet total pressure, whose standard value is 1, and whose Beta distribution is defined as indicated above.

This parameter is linked to a Calculator node, that receives also the pressure profile vector (*inp_p*), extracted from the original profile file. The node just contains the expression to multiply this vector for the *pt_in* parameter, extracting in this way the modified pressure profile vector *n_inp_p*, that is inserted in the original FINE *.run* file, in place of the standard vector profile.

Note that in this file also the output static pressure variable, *p_out*, is inserted in the corresponding location: this parameter will be different for each one of the six running points, that will be just run as a different DOE (Design Of Experiments) point specified in the DOE node.

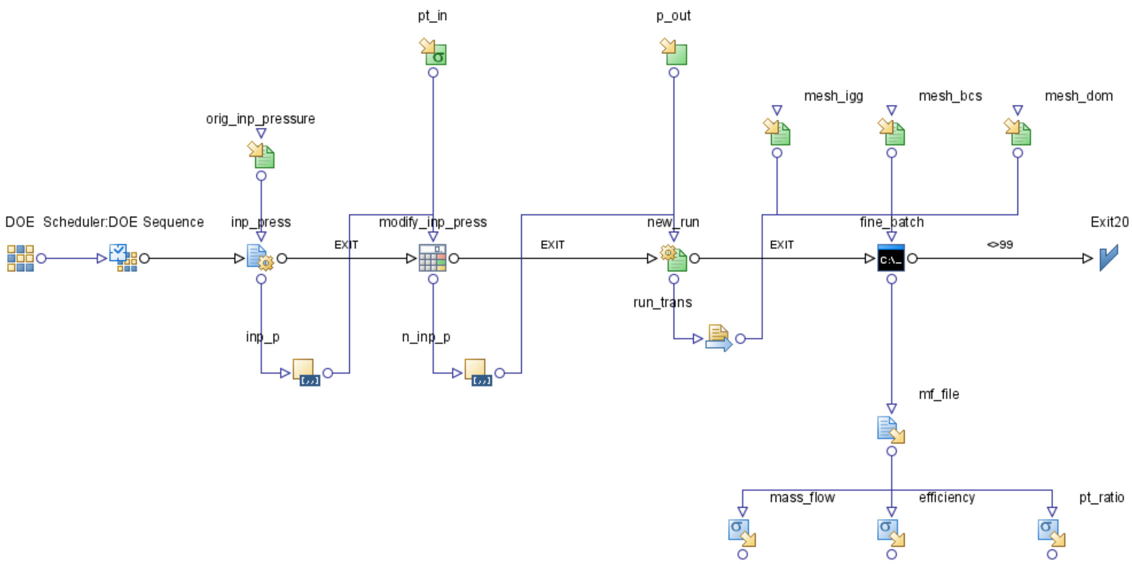

Fig.4 modeFRONTIER workflow for Rotor 37 test case

The remaining part of the workflow consists in a DOS node that is used to run FINE/HEXA in batch and from the *.mf* output file node the three performance parameters are extracted.
For each one of the 6 running points (the value of the output pressure is specified by the user in the DOE node), we need to specify how many sampling points will be run by mF, and which algorithm will be used to define them.
To improve the efficiency of the sampling analysis, we decided to use the Polynomial Chaos expansion [6], order 1, selecting only 3 design samples. This because the relationship of performances vs input total pressure is pretty linear, and Polynomial Chaos methodology has been proved to be very efficient in these cases.
Fig.5 here below reports the results for each running point, indicating the mean and the standard deviation for each one of the three performance parameters, as are obtained by the Polynomial Chaos expansion (Robust Design Table in mF).

Results

ID	M	CATEGORY	efficiency.MEAN	efficiency.STDEV	mass_flow.MEAN	mass_flow.STDEV	pt_ratio.MEAN	pt_ratio.STDEV
0		RNDDOE	8.5911E-1	9.6243E-4	2.0877E1	3.8027E-1	1.9428E0	9.7112E-3
1		RNDDOE	8.6542E-1	6.9679E-4	2.0834E1	3.9226E-1	2.0147E0	1.5365E-2
2		RNDDOE	8.6675E-1	2.9277E-5	2.0786E1	4.2073E-1	2.0481E0	1.7981E-2
3		RNDDOE	8.6664E-1	9.5411E-4	2.0667E1	4.4837E-1	2.0901E0	1.7406E-2
4		RNDDOE	8.6435E-1	3.4425E-3	2.0541E1	5.2150E-1	2.1089E0	1.5023E-2
5		RNDDOE	8.6377E-1	3.2239E-3	2.0507E1	5.2973E-1	2.1124E0	1.4636E-2

Fig.5 Rotor 37 test case results

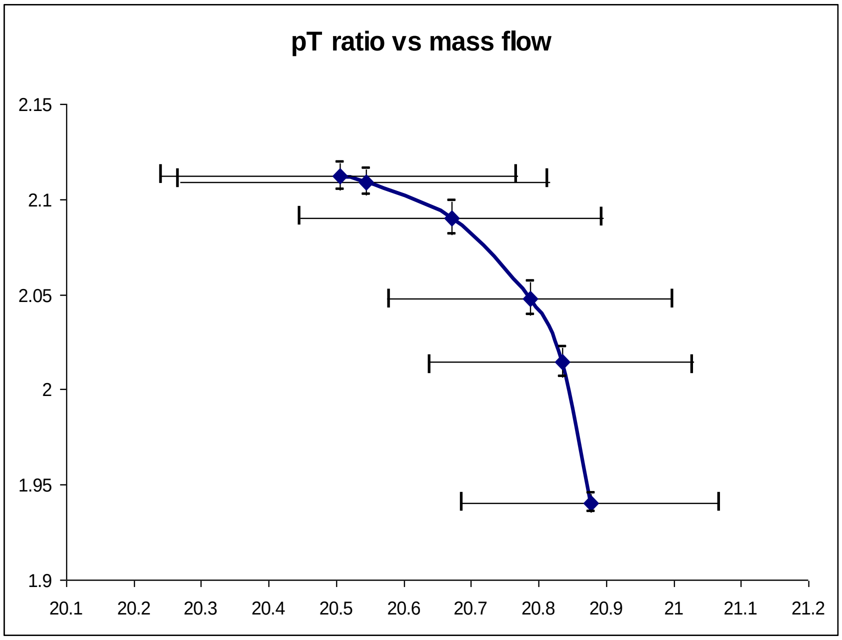

Fig.6 Pressure ratio vs Mass flow chart

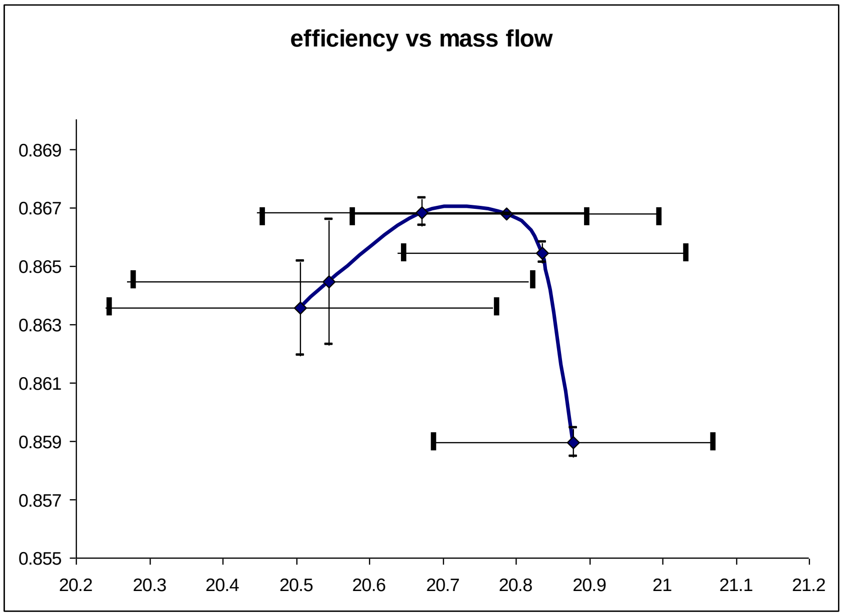

Fig.7 Efficiency vs Mass flow chart

Figures 6 and 7 report instead respectively pressure ratio vs mass flow and efficiency versus mass flow charts, relatively to the simulated six running points. The error bars reports +/- σ/2 values (where σ is the standard deviation) computed for each running point.
Uncertainties of mass flow are much higher than pressure ratio, whilst the lowest are the ones relative to efficiency. We can also note, and it is confirmed by fig.8 below, that the uncertainties are higher for low mass flow rate (high output pressure).
Fig. 8 in fact reports for the three outputs the CoV (coefficient of Variance), computed as the ratio of Standard Deviation with the Average, versus mass flow rate. We can note the different dimension of the three uncertainties, and that, except for pressure ratio, they are higher for lower mass flow.

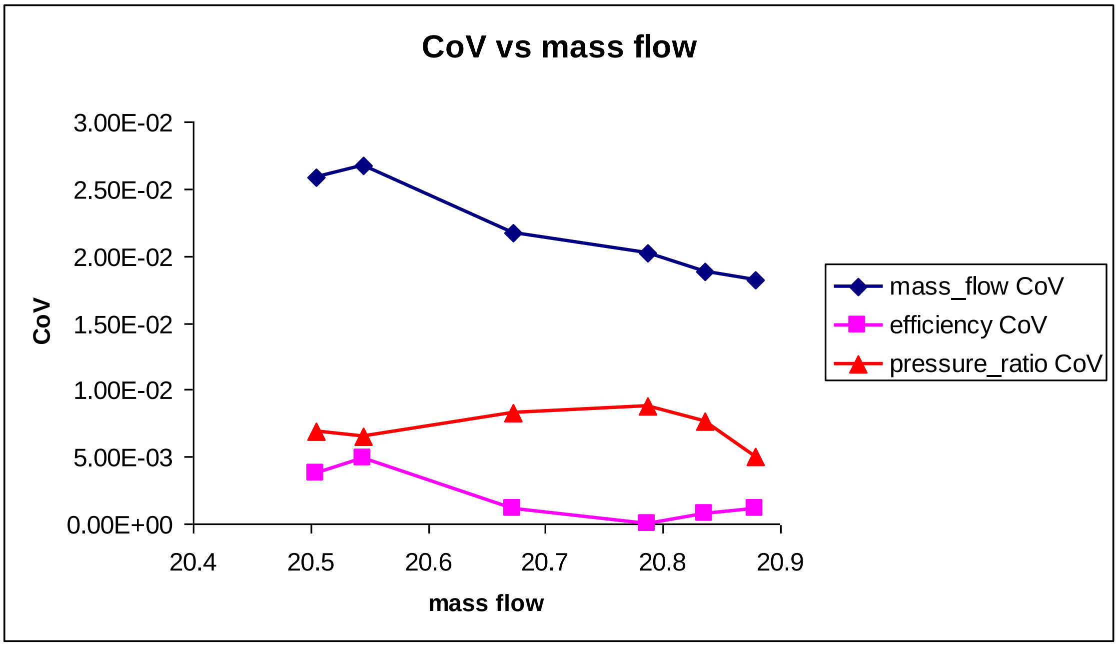

Fig.8 Coefficient of Variance of three outputs vs mass flow

4. **Second Application: RAE 2822 airfoil test case**

The second application we report is the RAE2822 airfoil test case.
The baseline airfoil model is a RAE2822 (fig.9), with nominal Mach number equal to 0.734, and angle of attach equal to 2.79°, defined as the corresponding test case from NODESIM website [4].
Three different analysis are considered:

- Uncertainty on relative thickness, Normal distr. σ =0.005
- Uncertainty on relative thickness, Uniform distr. σ =0.005
- Three uncertainties: thickness (σ =0.005), Mach (σ =0.005), angle (σ =0.1), Normal distr.

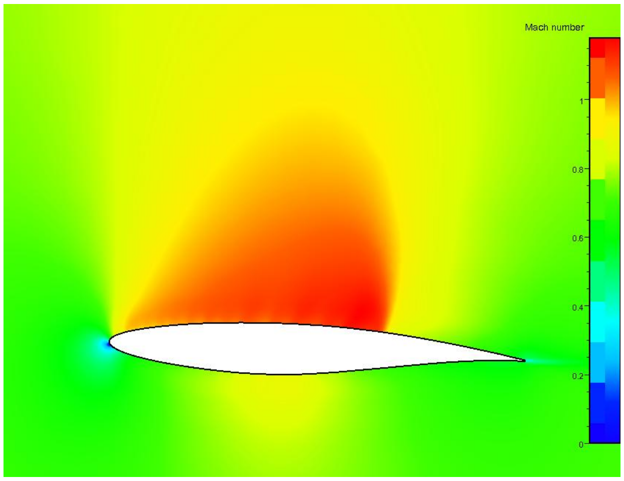

Fig.9 CFD analysis by FINE/HEXA code

Simulations have been performed through FINE/HEXA, with a full turbulent (Spalart-Allmaras model) model of about 30,000 hexahedral cells.
The modeFRONTIER workflow used is the one illustrated in fig.1. Beside the relative thickness variable (that in the calculator node scales all the baseline curve ordinates), also M and alpha (Mach number and Angle of attack) can be defined as stochastic parameters, with their relative distributions, and they are inserted in the workflow directly in the *.run* file (macro file containing specifications for CFD analysis).

At this point, to decide how many samples are needed for the applications, we have performed some tests, computing the performance distributions (drag, lift and momentum coefficients), with different number of samples and methodologies (Latin Hypercube only and Polynomial Chaos).
Fig.10 reports the results of the test, in the case of Normal distribution of three uncertainties: it seems that 12 sample points using Polynomial Chaos gives the best results in terms of accuracy of approximation and cost of simulations, since the relative errors on the standard deviation for all the coefficients is less than 1%. For this reason, we decided to adopt this strategy for the three uncertainty case; after similar results for the cases of single uncertainty, we adopted 5 sample points (order of expansion equal to 4).
Figs.11 show the Statistical Distributions (PDF and CDF) obtained applying the methodologies above defined in the three application case, while table 12 reports the main results of the three cases, and the analysis of the relative influence of the uncertain parameters. In particular, the CoV (coefficient of variance) is reported: it results that the thickness is less influent than the three uncertainties together of about a factor of 5, and the Normal distribution of uncertainty have more effect than the Uniform distribution.
Among the three coefficients, Cd have the highest effect, while Cl the lowest.

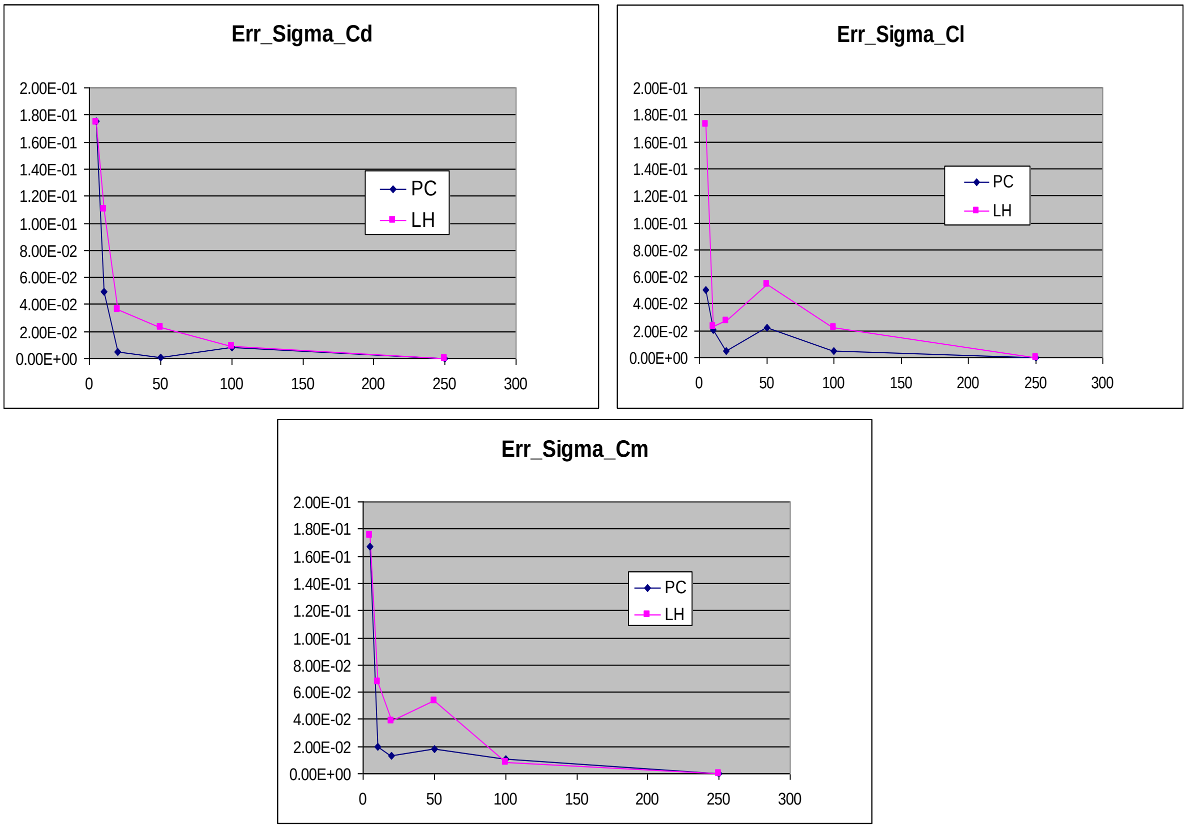

Fig.10 Error% on Standard Deviation for Cd, Cl and Cm vs sample size, for LH and PC sampling methodology

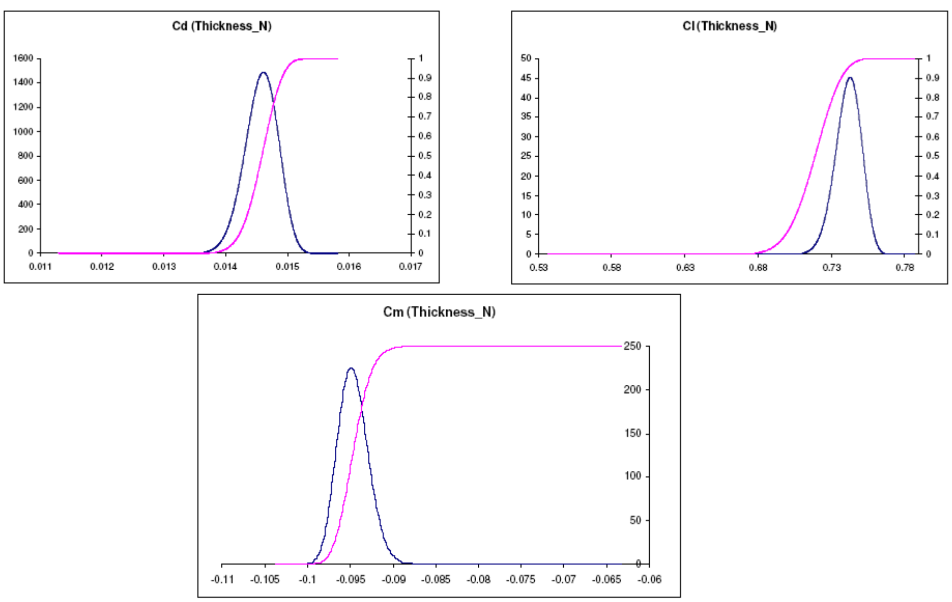

Fig.11a PDF and CDF charts for Cd, Cl, Cm in Normal distribution of thickness uncertainty case

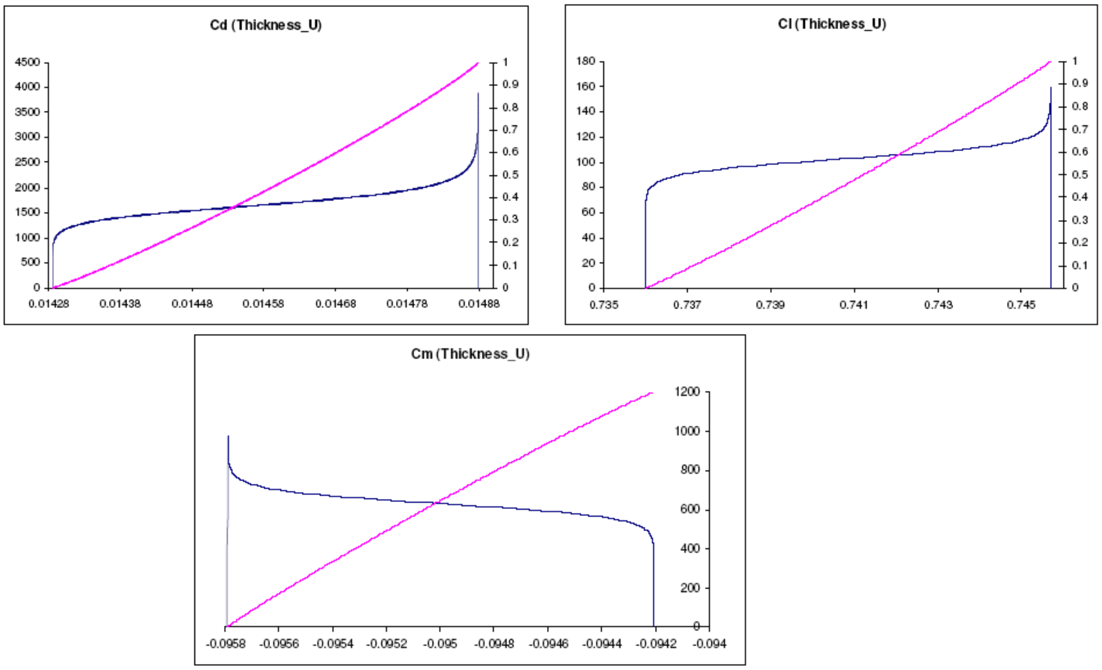

Fig.11b PDF and CDF charts for Cd, Cl, Cm in Uniform distribution of thickness uncertainty case

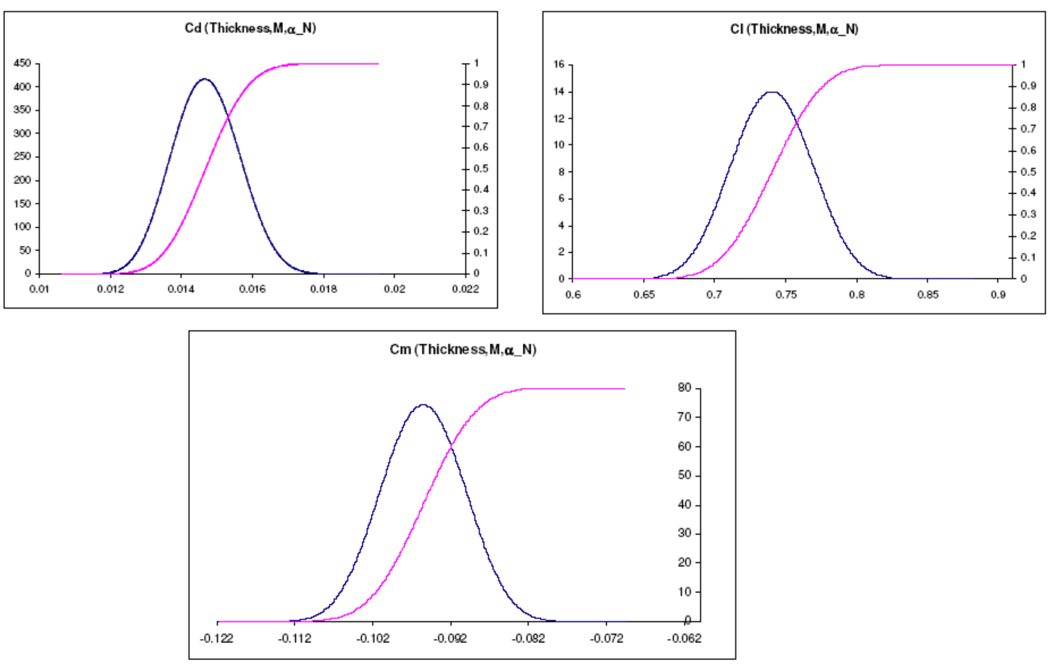

Fig.11c PDF and CDF charts for Cd, Cl, Cm in Normal distribution of three uncertainties case

Uncertainty	Cd: MEAN	Cd: STDEV	Cd: CoV	Cl: MEAN	Cl: STDEV	Cl: CoV	Cm: MEAN	Cm: STDEV	Cm: CoV
t: NORMAL	0.014574	2.668E-04	**1.83%**	0.741658	8.867E-03	**1.20%**	-0.094657	1.765E-03	**1.87%**
t: UNIFORM	0.014612	1.705E-04	**1.17%**	0.740912	2.798E-03	**0.38%**	-0.095043	4.555E-04	**0.48%**
t, M, a: NORMAL	0.014702	9.247E-04	**6.29%**	0.740377	2.764E-02	**3.73%**	-0.095525	5.204E-03	**5.45%**
deterministic	0.014600			0.740494			-0.094709		

Fig.12 PDF Coefficient of Variance in the three application cases

5. Third Application: Robust Design Optimisation of RAE 2822 airfoil, applying Bezier parameterisation in modeFRONTIER

The last application we report is an example of Robust Design Optimisation.
The baseline airfoil model is the RAE2822 (fig.9), defined as the corresponding test case of section 4. Three uncertain parameters are considered (thickness, Mach number and Angle of incidence), as follows:

- M=0.734, normal distr. σ =0.005
- Angle=2.79°, normal distr. σ =0.1°
- Relative thickness=1, normal distr. σ =0.005

The objective of the optimization is defined as the minimization of Cd coefficient and, since the optimization is stochastic, the value to be maximized is the maximum value of the distribution (truncated to 99.9 percentile); in addition to this, also two constraints are considered, the minimum Cl and the maximum Cm, to be respectively higher than a specified value (corresponding to baseline configuration values, obtained by a Polynomial Chaos sampling).

- Objective: Minimise MAX Cd
- Constraint: MIN Cl >= 0.66, MIN Cm>=-0.112

The FINE/HEXA model is the same adopted in section 4.

In addition, to perform the optimization problem, we need to parameterize the baseline geometry, and this is obtained adding to the baseline configuration ordinates the ones of a Bezier curve (fig.13).
Bezier curve is a parametric curve that remains continuous and regular at the variation of the control points position. In our case, four control points are used for both the two Bezier curves, to be added respectively on the upper profile and to the lower profile of the RAE2822 airfoil. As can be seen in the example of fig.13, the baseline profiles can be modified.

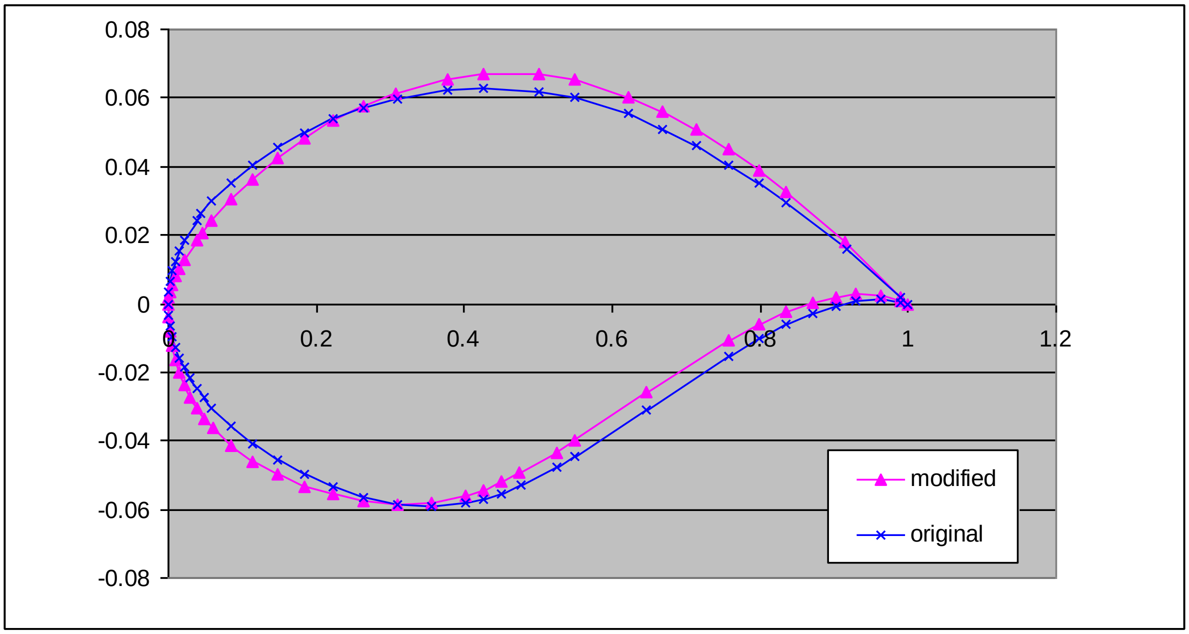

Fig.13. Baseline RAE2822 airfoil and airfoil modified adding two Bezier curves (lower and upper profile).

The workflow in modeFRONTIER is the same one illustrated in fig.1, with the addition of a calculator node to sum to the two original vector variables (the *y* ordinates of the baseline curves) the two Bezier curves defined in function of the defined control points variables (range of variation is given).
As performed in section 4 for the test case application, we adopted 12 samples using Polynomial Chaos expansion to extrapolate the performance distributions.
At this point, the optimisation can be started: the SIMPLEX algorithm (particularly rapid and efficient for single-objective problems) is selected.
In the definition of objective and constraints (from the corresponding nodes of the workflow), the MEAN value is selected for the Cd output (to be minimised as objective), while for Cl and Cm the MINIMUM value is to be constrained to be higher than the correspondent baseline limit.
Fig.14 reports the convergence of the SIMPLEX algorithm, that was stopped just after about 20 designs completed (note that, for each design, 12 samples are evaluated). The unfeasible designs, i.e. the ones that don’t respect the constraints, are visualised in red, while the best design is ID20 (the final shape of the airfoil is the one reported in purple colour in fig.13 here above, compared

to the original shape, in blue colour). Note that the ordinate of fig.14 reports the objective value, i.e. the MEAN of the Cd distribution.

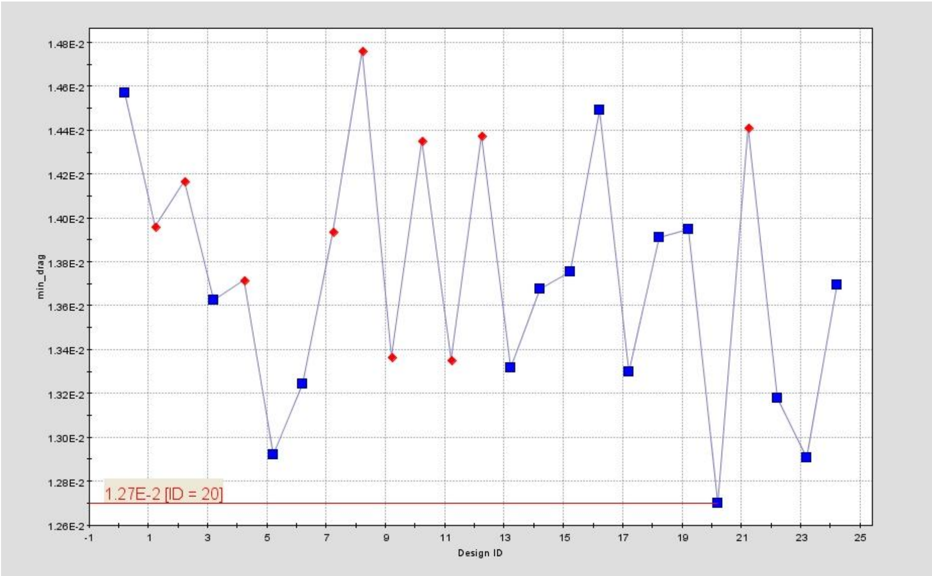

Fig.14 SIMPLEX algorithm convergence

From fig.14 we note that the mean Cd has been improved from the value 1.47E-2 of the baseline, to 1.27E-2 of the optimised shape, and this respecting the constraints.
Table.15 here below shows the comparison between the stochastic performances of the RAE2822 baseline and the optimised airfoil. Note the improvement in the mean Cd coefficient, and the small variations of other coefficients, as a consequence of the constraints satisfaction.
Finally, fig.16 shows again how the Cd mean value has been improved for the optimised design, comparing the PDF distributions, while fig.17 shows how both designs (baseline and optimised solution) respect the constraints (constraints limits are reported) on the minimum Cl and Cm.

Fig.15 Stochastic performances of the RAE2822 baseline and optimised shape

	Cd MEAN	Cd STDEV	Cl MEAN	Cl STDEV	Cm MEAN	Cm STDEV
RAE2822	0.0147	9.25E-4	0.740	2.76E-2	-0.0955	5.20E-3
Optimised	**0.0127**	6.7E-4	0.745	2.62E-2	-0.0953	4.42E-3

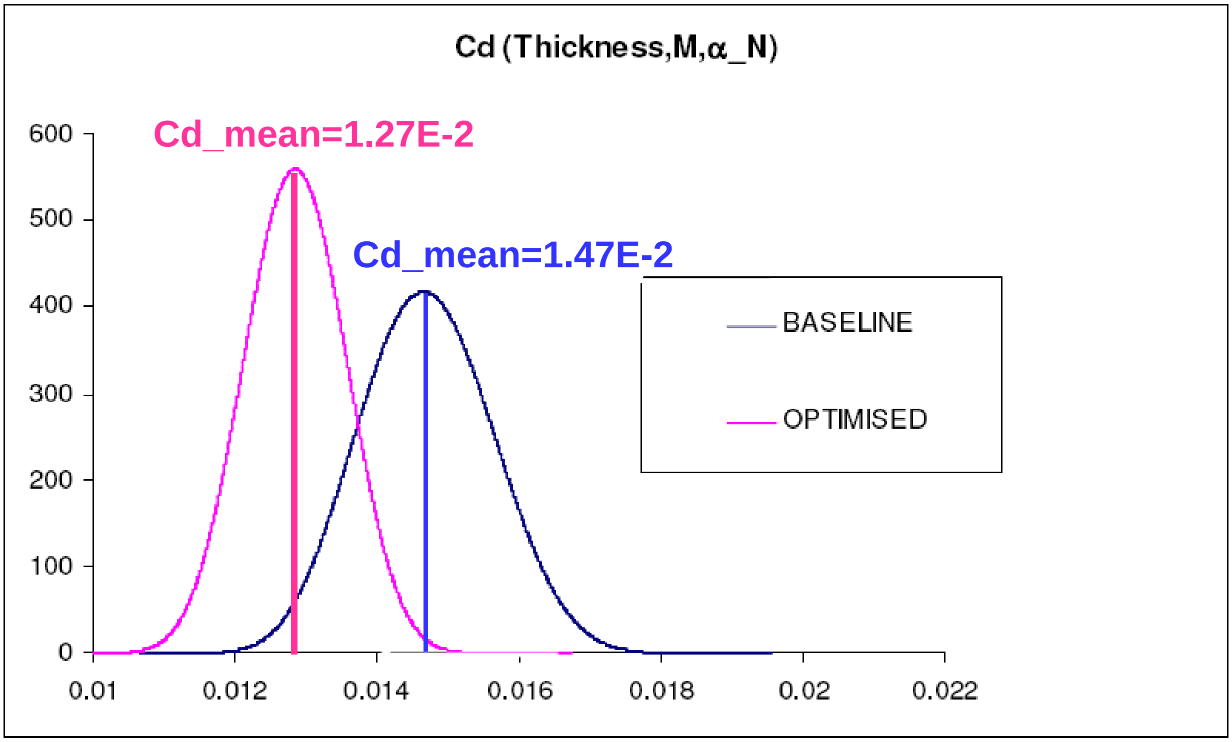

Fig.16 Probability distribution function of the RAE2822 baseline and optimised shape (Cd)

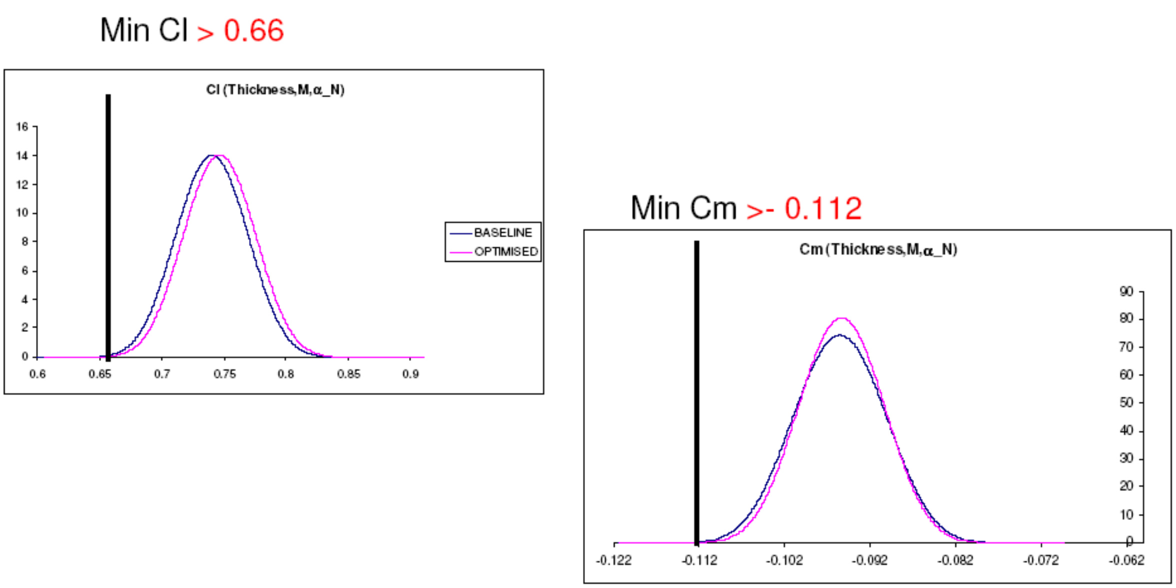

Fig.17 Probability distribution function of the RAE2822 baseline and optimised shape (Cl and Cm)

Acknowledgments

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