On the Nature and Treatment of Uncertainties in Aerodynamic Design

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Abstract. Recently, optimization has become an integral part of the aerodynamic design process chain. Besides standard optimization routines which require some multitude of the computational effort necessary for the simulation only, also fast optimization methods based on one-shot ideas are available, which are only 4 to 10 times as costly as one forward flow simulation computation. However, the full potential of mathematical optimization can only be exploited, if optimal designs can be computed, which are robust with respect to small (or even large) perturbations of the optimization setpoint conditions. That means, the optimal designs computed should still be good designs, even if the input parameters for the optimization problem formulation are changed by a non-negligible amount. Thus even more experimental or numerical effort can be saved. In this paper, we aim at an improvement of existing simulation and optimization technology, developed in the German collaborative effort MEGADESIGN, so that numerical uncertainties are identified, quantized and included in the overall optimization procedure, thus making robust design in this sense possible. These investigations are part of the current German research program MUNA.

1 Introduction

Uncertainties pose problems for the reliability of numerical computations and their results in all technical contexts one can think of. They have the potential to render worthless even highly sophisticated numerical approaches, since their conclusions do not realize in practice due to unavoidable variations in problem data. The proper treatment of these uncertainties within a numerical context is a very important challenge. This paper is devoted to the enhancement of highly efficient optimal design techniques developed in the framework of MEGADESIGN by a robustness component, which tries to make the optimal design generated a still good design, if the setting of a specific design point is varied. The investigations presented here are part of the research effort MUNA, which has recently started.

Robust aerodynamic design is a rather recent area of research, which up to now received attention only in very few publications (cf. [10]). Most of the techniques developed so far pertain to problems with a low degree of nonlinearity [9, 11]. Here, we try to give some insight into the sources of uncertainties, their range and compare approaches for their proper treatment.

2 The nature of uncertainties in aerodynamic design

For most of what follows it will be enough to consider a rather abstract but generic form of an aerodynamic shape optimization problem

$$\min_{\mathbf{y},p} f(\mathbf{y},p) \tag{1}$$

s.t.
$$c(y, p) = 0$$
 (2)

$$h(y, p) \ge 0 \tag{3}$$

We think of the equation (2) as the discretized outer flow equation around, e.g., an airfoil described by geometry parameter $p \in \mathbb{R}^{n_p}$. The vector y is the state vector (velocities, pressure,...) of the flow model (2) and we assume that (2) can be solved uniquely for y for all reasonable geometries p. The objective in (1) $f : (y, p) \mapsto f(y, p) \in \mathbb{R}$ typically is the drag to be minimized. The restriction (3) typically denotes lift or pitching moment requirements. To make the discussion here simpler, we assume a scalar valued restriction, i.e., $h(y, p) \in \mathbb{R}$. The generalization of the discussions below to more than one restriction is straight forward.

Uncertainties arise in all aspects of aerodynamic design. However, we want to limit the discussion here to uncertainties which cannot be avoided at all before constructing a plane. We distinguish two types of uncertainties: uncertainties with respect to the flight conditions and geometry uncertainties. The main characteristics of the macroscopic flight conditions are angle of incidence and the velocity (Mach number) of the plane. One generally knows the rough values for these characteristics but nevertheless, there will be unavoidable deviations from the nominal flight condition. In the numerical discussion below, we focus on the Mach number as an uncertain parameter within limits. We assume (mainly due to lack of statistical data) a truncated normal distribution of the perturbations with the nominal Mach number as expected value. The resulting robust problem formulations discussed below require more computational effort but can be reformulated as deterministic problems similar to (1-3).

Geometry uncertainties on the other hand require to change the optimal design problem dramatically. With geometry uncertainties, we mean the case that the real geometry deviates from the planned geometry characterized typically by splines parameterized by p. The parameters p span a space of possible geometries of dimension n_p . The sources for deviations from the planned geometry may lie in manufacturing, usage and wearing of the aircraft or wheather conditions (e.g., ice crusts). The only sure information about these deviations is that they will not lie within the geometry space spanned by the spline parameters p. Here, one rather has to work in the shape space, which is in general a function space that requires at least the usage of a free node parameterization. The ultimate goal of these investigations is the robust design under moderate shape fluctuations from a function space still to be determined. We leave these discussions to subsequent publications.

3 Robust formulations of aerodynamic design problems

The general deterministic problem formulation (1-3) is influenced by stochastic perturbations. We assume that there are uncertain disturbances $s \in S \subset \mathbb{R}^n$ involved in the form of random variables associated with a probability measure \mathcal{P} with Lebesgue density $\varphi : S \to \mathbb{R}_0^+$ such that the expected value of *s* can be written as

$$E(s) = \int_{S} s d\mathcal{P}(s) = \int_{S} s\varphi(s) ds$$

and the expected value of any function $g: S \to \mathbb{R}$ is written as

$$E(g) = \int_{S} g(s)d\mathcal{P}(s) = \int_{S} g(s)\varphi(s)ds$$

The dependence can arise in all aspects, i.e., a naive stochastic variant might be rewritten as

$$\min_{\mathbf{y},p} f(\mathbf{y}, p, s) \tag{4}$$

s.t.
$$c(y, p, s) = 0$$
 (5)

$$h(y, p, s) \ge 0 \tag{6}$$

This formulation still treats the uncertain parameter as an additional fixed parameter. The optimal solution should be stable with respect to stochastic variations in s. The literature can be classified in the following ideal classes: min-max formulation, semi-infinite formulation and chance constraints.

3.1 Min-max formulations

The min-max formulation aims at the worst-case scenario.

$$\min_{y_s, p} \max_{s \in S} f(y_s, p, s) \tag{7}$$

s.t.
$$c(y_s, p, s) = 0, \forall s \in S$$
 (8)

$$h(y_s, p, s) \ge 0, \ \forall s \in S \tag{9}$$

Since the state vector y depends on the uncertain parameter s, there is a different y_S for each s. The min-max formulation is obviously independent of the stochastic measure \mathcal{P} and thus needs only the perturbation set S as input. Thus, it ignores problem specific information which is usually at hand. We do not treat this formulation furthermore in this paper.

3.2 Semi-infinite formulations

The semi-infinite reformulation aims at optimizing the average objective function but maintaining the feasibility with respect to the constraints everywhere. Thus, it aims at an average optimal and always feasible robust solution. The ideal formulation is of the form

$$\min_{y_s,p} \int_{s} f(y_s, p, s) d\mathcal{P}(s)$$
(10)

s.t.
$$c(y_s, p, s) = 0, \forall s \in S$$
 (11)

$$h(y_s, p, s) \ge 0, \ \forall s \in S \tag{12}$$

Semi-infinite optimization problems have been treated directly so far only for rather small and weakly nonlinear problems, e.g. [4]. For the numerical treatment of complicated design tasks, one has to approximate the integral in the objective (10). If one assumes that the random variable confers to a multivariate truncated normal distribution, i.e. $s \sim \frac{1}{const} N(\mu, C) \cdot \mathbf{1}_S$ with expected value vector μ the integral in (10) be efficiently evaluated by a Gaussian quadrature, where the quadrature points $\{s_i\}_{i=1}^N$ are the roots of a polynomial belonging to a class of orthogonal polynomials. In the case of a lift constraint in (12) to be satisfied overall within a set of Mach numbers, we can take advantage of the fact that the lift is monotonically increasing with the Mach number. Therefore, it is enough to keep a lift constraint for the smallest Mach number under consideration. Therefore, we can reformulate problem (10-12) in an approximate fashion in the form of a multiple set-point problem for the set-points $\{s_i\}_{i=1}^N$:

$$\min_{y_i,p} \sum_{i=1}^{N} f(y_i, p, s_i) \omega_i$$
(13)

s.t.
$$c(y_i, p, s_i) = 0, \ \forall i \in \{1, \dots, N\}$$
 (14)

$$h(y_i, p, s_{\min}) \ge 0.$$
 (15)

where ω_i denote the quadrature weights. We will investigate this formulation later on. As an example, we look at the Mach number as being the uncertainty *s*, which is scalar valued, i.e. $s \sim \frac{1}{const} N(\mu, \sigma^2) \cdot \mathbf{1}_S$ and we choose just 4 Gaussian points. The following figure shows a particular choice for the density function of the Mach number with expected value $s^0 = 0.73$ and the computed Gaussian points.



Figure 1: Gaussian points and the density function

3.3 Chance constraint formulations

Chance constraints leave some flexibility with respect to the inequality restrictions. The inequality restrictions are only required to hold with a certain probability \mathcal{P}_0

$$\min_{y_s,p} \int_{S} f(y_s, p, s) d\mathcal{P}(s)$$
(16)

s.t.
$$c(y_s, p, s) = 0, \forall s \in S$$
 (17)

$$\mathcal{P}(\{s \mid h(y_s, p, s) \ge 0\}) \ge \mathcal{P}_0 \tag{18}$$

So far, chance constraints are used mainly for weakly nonlinear optimization problems [9, 8]. In the context of structural optimization (which is typically a bilinar problem), this formulation is also called reliability-based design optimization. For more complex problems, we need again some simplification. In [10] this is performed by applying a Taylor series expansion about a nominal set-point $s^0 := \mu$, which is at the same time the expected value of the random variable *s*. Suppressing further arguments (y, p) for the moment, the Taylor approximation of 2nd order of *f* in (16) gives

$$\hat{f}(s) := f(s^0) + \frac{\partial f(s^0)}{\partial s}(s - s^0) + \frac{1}{2}(s - s^0)^\top \frac{\partial^2 f(s^0)}{\partial s^2}(s - s^0)$$

Integrating this, we observe

$$\int_{S} \hat{f}(s)ds = f(s^{0}) + \frac{1}{2} \sum_{i=1}^{k} \frac{\partial^2 f(s^{0})}{\partial s_i^2} Var(s_i)$$

where $Var(s_i)$ is the variance of the *i*-th component of *s*. Obviously, a first order Taylor series approximation would not give any influence of the stochastic information, which is the reason, why we use an approximation of second order for the objective. In order to deal with the probabilistic chance constraint (18), we have to approximate its probability distribution by something simple, e.g., again a truncated normal distribution. Therefore, we use a first order Taylor approximation there, since we know that this is again a truncated Normal distribution (unlike the second oder approximation).

$$\hat{h}(s) := h(s^0) + \frac{\partial h(s^0)}{\partial s}(s - s^0) \quad \sim \quad \frac{1}{const} N\left(h(s^0), \sigma_h^2\right) \cdot \mathbf{1}_{S_h}$$

where we assume for simplicity that h is scalar valued.

Now we can put the Taylor approximations together and achieve a deterministic single set-point optimization problem. Since the flow model (17) depends also on the uncertainties s, we should be aware that the derivaties with respect to s mean total derivaties. We express this by reducing the problem in writing y = y(p, s) via (17).

$$\min_{p} f(y(p, s^{0}), s^{0}) + \frac{1}{2} \sum_{i=1}^{k} \frac{\partial^{2} f(y(p, s^{0}), s^{0})}{\partial s_{i}^{2}} Var(s_{i})$$
(19)

s.t.
$$\mathcal{P}(\{s \mid \hat{h}(y(p,s),s) \ge 0\}) \ge \mathcal{P}_0$$
 (20)

For the computation of the total derivatives we can introduce a sensitivity equations as in [12].

As an example, again we look at the case that s is scalar valued, i.e.

$$s \sim \frac{1}{const_s} N(\mu, \sigma^2) \cdot \mathbf{1}_{[l,u]}$$
, where $const_s = \int_{l}^{u} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx$ is the scaling factor to normalize the density function. Hence, we obtain the distribution of the

factor to normalize the density function. Hence, we obtain the distribution of the probabilistic constraint

$$\hat{h}(s) \sim \frac{1}{const_{\hat{h}}} N\left(h(s^0), \left(\frac{\partial h(s^0)}{\partial s}\right)^2 \sigma^2\right) \cdot \mathbf{1}_{\left[\frac{\partial h(s^0)}{\partial s}l + h(s^0), \frac{\partial h(s^0)}{\partial s}u + h(s^0)\right]}$$

where $const_{\hat{h}} = \frac{1}{\sqrt{2\pi (\frac{\partial h(s^0)}{\partial s})^2 \sigma^2}} \int_{\frac{\partial h(s^0)}{\partial s} l + h(s^0)}^{\frac{\partial h(s^0)}{\partial s} u + h(s^0)} \exp\left(-\frac{(x - h(s^0))^2}{2(\frac{\partial h(s^0)}{\partial s})^2 \sigma^2}\right) dx.$

Finally, the following equivalent representations of the chance constraint

$$\mathcal{P}(\{s \mid \hat{h}(y(p,s),s) \ge 0\}) \ge \mathcal{P}_0 \iff \mathcal{P}(\{s \mid \hat{h}(y(p,s),s) \le 0\}) \le 1 - \mathcal{P}_0$$

lead to the deterministic optimization problem

$$\min_{p} f(y(p, s^{0}), s^{0}) + \frac{1}{2} \sum_{i=1}^{k} \frac{\partial^{2} f(y(p, s^{0}), s^{0})}{\partial s_{i}^{2}} Var(s_{i}) \quad (21)$$

s.t.
$$\frac{1}{const_{\hat{h}}\sqrt{2\pi (\frac{\partial h(s^{0})}{\partial s})^{2} \sigma^{2}}} \int_{\frac{\partial h(s^{0})}{\partial s} l+h(s^{0})}^{0} \exp\left(-\frac{(x-h(s^{0}))^{2}}{2(\frac{\partial h(s^{0})}{\partial s})^{2} \sigma^{2}}\right) dx \leq 1 - \mathcal{P}_{0} \quad (22)$$

The propagation of the input data uncertainties is estimated by the combination of a First Order Second Moment (FOSM) method and a Second Order Second Moment (SOSM) method, presented for example in [10].

Since there is no closed form solution for the integral, the chance constraint is evaluated by a numerical quadrature formula. Below, we will compare this formulation with one, where the objective in (21) omits a Taylor expansion.

4 One-shot aerodynamic shape optimization and its coupling to robust design

Novel one-shot aerodynamic shape optimization in the form (1-3) have been introduced in [7, 6]. They have the potential of fast convergence in only a small multiple of cpu-time compared to on flow simulation. These methods are based on approximate reduced SQP iterations in order to generate a stationary point satisfying the first oder KKT optimality conditions.

In this context, a full SQP-approach reads as

$$\begin{bmatrix} \mathcal{L}_{yy} \ \mathcal{L}_{yp} \ h_x^{\top} \ c_x^{\top} \\ \mathcal{L}_{py} \ \mathcal{L}_{pp} \ h_p^{\top} \ c_p^{\top} \\ h_x \ h_p \ 0 \ 0 \\ c_x \ c_p \ 0 \ 0 \end{bmatrix} \begin{pmatrix} \Delta y \\ \Delta p \\ \Delta \lambda \end{pmatrix} = \begin{pmatrix} -\mathcal{L}_y^{\top} \\ -\mathcal{L}_p^{\top} \\ -h \\ -c \end{pmatrix}, \quad \begin{pmatrix} y^{k+1} \\ p^{k+1} \\ \mu^{k+1} \\ \lambda^{k+1} \end{pmatrix} = \begin{pmatrix} y^k \\ p^k \\ \mu^k \\ \lambda^k \end{pmatrix} + \tau \cdot \begin{pmatrix} \Delta y \\ \Delta p \\ \Delta \mu \\ \Delta \lambda \end{pmatrix}$$
(23)

The symbol \mathcal{L} denotes the Lagrangian function. We assume that the lift constraint *h* is active at the solution, which is the reason that we formulate is rather as an equality condition in the single setpoint case. The approach (23) is not implementable in general, because one usually starts out with a flow solver for c(y, p) = 0 and seeks a modular coupling with an optimization approach, which does not necessitate to change the whole code structure, as would be the case with formulation (23). A modular but nevertheless efficient alternative is an approximate reduced SQP approach as justified in [5].

$$\begin{bmatrix} 0 & 0 & 0 & A^{\mathsf{T}} \\ 0 & B & \gamma & c_p^{\mathsf{T}} \\ 0 & \gamma^{\mathsf{T}} & 0 & 0 \\ A & c_p & 0 & 0 \end{bmatrix} \begin{pmatrix} \Delta y \\ \Delta p \\ \Delta \lambda \end{pmatrix} = \begin{pmatrix} -\mathcal{L}_y^{\mathsf{T}} \\ -\mathcal{L}_p^{\mathsf{T}} \\ -h \\ -c \end{pmatrix}, \quad \begin{pmatrix} y^{k+1} \\ p^{k+1} \\ \lambda^{k+1} \end{pmatrix} = \begin{pmatrix} y^k \\ p^k \\ \mu^k \\ \lambda^k \end{pmatrix} + \tau \cdot \begin{pmatrix} \Delta y \\ \Delta p \\ \Delta \mu \\ \Delta \lambda \end{pmatrix}$$
(24)

where

$$\gamma = h_p^{\top} + c_p^{\top} \alpha$$
, such that $A^{\top} \alpha = -h_x^{\top}$

The matrix A denotes an appropriate approximation of the system matrix c_x , which is used in the iterative forward solver. An algorithmic version of this modular formulation is given by the following steps

- (1) generate λ^k by performing *N* iterations of an adjoint solver with right hand side $f_{\nu}^{\top}(y^k, p^k)$ starting in λ^k
- (2) generate α^k by performing *N* iterations of an adjoint solver with right hand side $h_{\nu}^{\top}(y^k, p^k)$ starting in α^k
- (3) compute approximate reduced gradients

$$g = f_p^\top + c_p^\top \lambda^{k+1}, \quad \gamma = h_p^\top + c_p^\top \alpha^{k+1}$$

- (4) generate B_{k+1} as an approximation of the (consistent) reduced Hessian
- (5) solve the QP

$$\begin{bmatrix} B & \gamma \\ \gamma^{\top} & 0 \end{bmatrix} \begin{pmatrix} \Delta p \\ \mu^{k+1} \end{pmatrix} = \begin{pmatrix} -g \\ -h \end{pmatrix}$$

- (6) update $p^{k+1} = p^k + \Delta p$
- (7) compute the corresponding shep geometry and adjust the computational mesh
- (8) generate y^{k+1} by performing *N* iterations of the forward state solver starting from an interpolation of y^k at the new mesh.

This highly modular algorithmic approach is not an exact transcription of equation (24), but is shown in [5] to be asymptotically equivalent and to converge to the same solution. The overall algorithmic effort for this algorithm is typically in the range of factor 7 to 10 compared to a forward stationary simulation.

Now we generalize this algorithmic framework to the semi-infinite problem formulation (10-12). Numerical approaches to this problem class have been proposed already in [3, 2])..

For the sake of simplicity, we restricted the formulation to a problem with two set-points coupled via the objective, which is a weighted sum of all set-point objectives (weights: ω_1, ω_2), and via the free optimization variables p, which are the same for all set-points. The generalization to more setpoints (i.e., 4 below) is then obvious. Furthermore, in the case of the restriction h being the lift, we know that it is monotonic in the Mach number. Therefore, it is enough to formulate the constraint for the smallest value s_{\min} . The corresponding Lagrangian in our example is

$$\mathcal{L}(y_1, y_2, p, \lambda_1, \lambda_2) = \sum_{i=1}^{2} \omega_i f_i(y_i, p, s_i) + \sum_{i=1}^{2} \lambda_i^{\top} c_i(y_i, p, s_i) + \mu h(y_{\min}, p, s_{\min})$$
(25)

The approximate reduced SQP method above applied to this case can be written in the following form

$$\begin{bmatrix} 0 & 0 & 0 & 0 & A_1^{\top} & 0 \\ 0 & 0 & 0 & 0 & 0 & A_2^{\top} \\ 0 & 0 & B & \gamma_1 & c_{1,p}^{\top} & c_{2,p}^{\top} \\ 0 & 0 & \gamma_1 & 0 & 0 & 0 \\ A_1 & 0 & c_{1,p} & 0 & 0 & 0 \\ 0 & A_2 & c_{2,p} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta y_1 \\ \Delta y_2 \\ \Delta p \\ \Delta \mu \\ \Delta \lambda_1 \\ \Delta \lambda_2 \end{bmatrix} = \begin{pmatrix} -\mathcal{L}_{y_1}^{\vee} \\ -\mathcal{L}_{p}^{\vee} \\ -\mathcal{L}_{p}^{\vee} \\ -h \\ -c_1 \\ -c_2 \end{pmatrix}$$
(26)

We notice that the linear sub-problems involving matrices A_i^{\top} are to be solved independently, and therefore trivially in parallel. The information from all these parallel adjoint problems is collected in the reduced gradient

$$g = \sum_{i=1}^{2} \omega_i f_p^{\top} + \sum_{i=1}^{2} c_p^{\top} \lambda_i$$

Next, the solution of optimization step

$$\begin{bmatrix} B & \gamma_1 \\ \gamma_1^\top & 0 \end{bmatrix} \begin{pmatrix} \Delta p \\ \mu^{k+1} \end{pmatrix} = \begin{pmatrix} -g \\ -h \end{pmatrix}$$

is distributed to all approximate linearized forward problems

$$A_i \Delta y_i + c_{i,p} \Delta p = -c_i ,$$

which can then again be performed in parallel.

5 Numerical results

We investigate the problem discussed in [7], i.e. the shape optimization of a transonic RAE2822 profile, by the use of the code Flower within a one-shot framwork. In this section, we perform numerical comparisons between a single set-point problem formulation at the setpoint $s^0 = 0.73Mach$ with the robust formulations in sections 3.2 and 3.3. In particular, we compare four formulations: (1) non-robust optimization at the Mach number 0.73 (fixed Mach number 0.73), (2) semi-infinite formulation of equations (13-15), (3) chance constraint formulation of equations (21, 22) without higher order terms in the objective and (4) with higher order terms in the objective.

The following figures show evaluations of the objective (drag) in these cases as well as the constraint (lift).

We state the following observations: first, the higher oder terms in the objective of the chance constraint formulation (21, 22) seem to make no difference, which means that they can be safely omitted. Second, the semi-infinite robust formulation



Figure 3: Comparison of lift constraint

has a better lift to drag ratio than the chance constraint formulation, in particular in the region above the set-point 0.73.

Furthermore, we consider the angle of attack as an additional uncertain parameter. The following figure shows the drag performance of the solution of the

semi-infinite optimization problem.



Figure 4: Drag performance of optimized airfoil

As required, the solution of the semi-infinite formulation is always feasible.



Figure 5: Lift performace of optimized airfoil

The different optimized shapes are shown in Fig.6. The semi-infinite formu-

lation differs the most from the single set point case due to the requirement of feasibility over the whole range of uncertainties.



Figure 6: Comparison of optimized shapes

6 Conclusions

Robust design is an important task to make aerodynamic shape optimization relevant for practical use. It is also highly challenging because the resulting optimization tasks become much more complex than in the usual single set-point case. Essentially two robust optimization formulations are compared in this paper. The discretized semi-infinite formulation seems to be of advantage in a numerical test case close to a real configuration.

Acknowledgements. This research has been supported by BMWA within the collaborative effort MUNA.

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