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A HYBRID UNCERTAINTY QUANTIFICATION METHOD FOR ROBUST OPTIMIZATION

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Abstract. The present paper investigate the performance of a hybrid uncertainty quantification (UQ) method for robust optimization. In the beginning of the optimization this method uses a first order second moment method (FOSM) for UQ and switches during the optimization process to an adaptive stochastic collocation method (ASCM). The idea is that the disadvantages of the FOSM are a compensated by the advantages of the ASCM and vice versa. In order to assess the efficiency of this method, several configurations of an uncertain flow optimization problem are calculated. The results are examined with respect to the computational cost and reduction of the objective function. Furthermore, the results are compared to a robust optimization with a pure ASCM.

1 INTRODUCTION

Nonintrusive sampling methods for uncertainty quantification are quite popular because in this case well developed deterministic computational fluid dynamics (CFD) solvers can be used for flow simulation. The drawback of these methods such as Monte Carlo simulation or stochastic collocation is that they may become highly computationally intensive. Especially for robust optimization with many uncertain input parameters this can be a crucial issue.

In practice, this problem is often avoided by using a deterministic optimization first and afterwards examining the result with an uncertainty quantification in order to check if the result fulfills the given requirements for robustness. However, in this way not necessarily the robust optimum is found.

We propose a combination of an adaptive stochastic collocation method on sparse grids (ASCM) [1] and a sensitivity derivatives based first-order second moment method (FOSM) [2] for uncertainty quantification together with a gradient-free Nelder-Mead optimizer [3]. The idea is that the disadvantages of the FOSM are a compensated by the advantages of the ASCM and vice versa.

Section 2 presents the theoretical background of flow problems under uncertainty. Section 3 describes the key idea of robust optimization. Numerical methods for the quantification of uncertainties are presented in Section 4. Section 5 describes a gradient free optimizer. Subsequently the hybrid approach is proposed in Section 6. Several tests are computed in order to compare the performance of the hybrid scheme to a robust optimization method with a pure ASCM in Section 7. Finally, the results are summarized in section 8.

2 FLOW PROBLEMS UNDER UNCERTAINTY

In this work we focus on incompressible, steady and laminar flow problems. These flows can be modeled by the Navier-Stokes equations [4]. The corresponding equations for the mass conservation and the momentum are written as:

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial(\rho u_i u_j)}{\partial x_j} - \frac{\partial \mu \frac{\partial u_i}{\partial x_j} + \frac{\partial x_j}{\partial x_i}}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \rho f_i,$$

where u_i is the velocity vector and x_i is the position vector. The fluid density and dynamic viscosity are represented by ρ and μ. The vector f_i describes the body force. In order to get the closed equation system proper boundary conditions have to be applied. The most common conditions on the boundary Γ are:

- Dirichlet condition: $u_i = u_{bi}$
- Neumann condition: $\frac{\partial u}{\partial x_i} n_i = g_b$.

For simplicity, in the following we write only a general form of a PDE instead of the Navier-Stokes equations. A PDE can be written in the form

$$\begin{aligned} \mathcal{A}(\boldsymbol{\phi}(\mathbf{x}), \mathbf{x}) &= f(\mathbf{x}) \qquad \text{in } D \\ \mathcal{B}(\boldsymbol{\phi}(\mathbf{x}), \mathbf{x}) &= g(\mathbf{x}) \qquad \text{in } \partial D, \end{aligned} \tag{2}$$

where $\mathcal{A}$ is the differential operator which also includes all parameters such as fluid properties. $\boldsymbol{\phi}$ describes the flow field solution. The boundary conditions operator is denoted by $\mathcal{B}$. D is a spatial domain in $\mathbb{R}^d$ with its boundary ∂D. $\mathbf{x}$ refers to the elements of D. The forcing term and boundary conditions are denoted by f and g, respectively.

The formulation (2) assumes that all system parameters are exactly known, but actually in quantities of physical processes there is always a certain amount of fluctuation. These uncertainties can be caused by natural fluctuations like the outdoor temperature or atmospheric pressure. Another example are human-made fluctuations in manufacturing processes, so each product is slightly different due to existing tolerances. Uncertainties in simulations can also arise from lack of knowledge, if some effects are too complicated, so that values can be estimated only

approximately.
In order to account uncertainties in flow simulations the system (2) has to be extended to a stochastic system of the form

$$\begin{aligned} \mathcal{A}(\boldsymbol{\phi}(\mathbf{x},\omega),\mathbf{x},\omega) &= f(\mathbf{x},\omega) \qquad &&\text{in } D\times\Omega \\ \mathcal{B}(\boldsymbol{\phi}(\mathbf{x},\omega),\mathbf{x},\omega) &= g(\mathbf{x},\omega) \qquad &&\text{in } \partial D\times\Omega. \end{aligned} \tag{3}$$

The stochastic system (3) includes the random parameter space Ω, which contains possible realizations for the uncertain parameters. These realizations can be mapped on ω. The uncertain system parameters result in a stochastic system output which can be described with methods from the field of uncertainty quantification. An overview and description of these methods are given by [5, 6, 1].

3 ROBUST FLOW OPTIMIZATION

The aim of robust flow optimization is to obtain optimal design that are not sensitive to fluctuations of system parameters. This can be realized by minimizing the standard deviation σ_J of objective function $J(\boldsymbol{\phi}(\mathbf{a},\omega),\mathbf{a},\omega)$, where $\mathbf{a}$ is the vector of design parameters. In the following the objective function is denoted by J. To ensure that the solution of the optimization satisfies further requirements the mean value $\bar{J}$ of the objective function must be considered. An overview of several such robust optimization is provided by [7, 6]. In this work we focus on the formulation:

$$\begin{aligned} \min\ \bar{J} + \lambda\sigma_J \qquad &\text{subject to} \\ F\left(\boldsymbol{\phi}(\mathbf{a},\omega),\mathbf{a},\omega\right) = 0 & \\ \mathbf{a}_l \le \mathbf{a} \le \mathbf{a}_u, & \end{aligned} \tag{4}$$

where λ is a scalar, F is an equality constraint and $\mathbf{a}_l$ and $\mathbf{a}_u$ are the lower and upper bounds for the design parameters $\mathbf{a}$. The main equality constraints in flow optimization problems are the Navier-Stokes equations.
In order to solve the robust problem 5 conventional optimization methods can be applied. In 5 the gradient free Nelder-Mead optimization method is briefly presented. For detailed descriptions of further optimization methods we refer to [8, 6, 9].

4 NUMERICAL METHODS FOR UNCERTAINTY QUANTIFCATION

In general methods for UQ can be categorized into two classes. On the one hand there are intrusive methods, which require a reformulation of the original model to a stochastic version and on the other hand the non-intrusive methods, which only need a set of solutions of the deterministic problem. An overview of the different types of UQ is given by [5, 6].
In the following sections two methods for UQ, FOSM and ASCM, are described.

4.1 First Order Second Moment

The idea of the First Order Second Moment method is to approximate the objective function J by a Taylor series. The first order Taylor series approximation of J can be written as

$$J(\boldsymbol{\omega}) = J(\bar{\boldsymbol{\omega}}) + \sum_{i=1}^{n} \frac{\partial J}{\partial \omega_i}(\omega_i - \bar{\omega}_i), \tag{5}$$

with the uncertain input parameters $\boldsymbol{\omega} = (\omega_1, \ldots, \omega_n)$ and their means $\bar{\boldsymbol{\omega}} = (\bar{\omega}_1, \ldots, \bar{\omega}_n)$. On the basis of [5] statistical quantities of J like the mean value $\bar{J}$ and its variance σ_J^2 which depend among others on the variance σ_ω^2 of the input parameter, can be approximated by

$$\bar{J} = J(\bar{\boldsymbol{\omega}}), \qquad \sigma_J^2 = \sum_{i=1}^{n} (\frac{\partial J}{\partial \omega_i}\sigma_{\omega_i})^2. \tag{6}$$

The derivatives are evaluated at the mean values of the uncertain input $\bar{\boldsymbol{\omega}}$. The relevant effort to evaluate [6] arise in the computation of the derivatives. This can be done e.g. with the finite difference method [4]. The FOSM is proposed for robust optimization in [2, 10, 11].
Compared to other methods the fast evaluation is the main advantage of the FOSM, but on the other hand there are many drawbacks. Since it is a first order approximation non-linear effects are not considered, so in practice the failure of the approximated statistical quantities increase with growing input uncertainty. Similarly, the FOSM provides poorer results, the more uncertain input parameter are taken into account.

4.2 Adaptive Stochastic collocation method

The stochastic collocation method belong to the nonintrusive methods. The idea is to decompose the stochastic problem into a finite number of deterministic problems, which can be solved with common methods. A more detailed description is given by [1, 5].
The main steps of the ASCM are the selection of a set of possible realizations of uncertain input parameters $\boldsymbol{\omega}$, the so-called collocation points. For each of this realizations the corresponding PDE 2 has to be solved. These solutions are interpolated in order to achieve a continuous representation of the random solution space. Subsequently, the interpolation error is estimated and if needed more collocation points are added. The statistical quantities $\bar{J}$ and σ_J^2 can be estimated on the basis of the interpolated random solution space. In order to ensure adequately accurate results while keeping the number of collocation points small, the collocation points can be located on a sparse grid. Despite the adaptivity and the sparse grid realization, the computational effort of the ASCM is a multiple larger than the effort of the FOSM. Nevertheless, the ASCM has the advantage that a required accuracy can be ensured. The discrepancy between the advantage of accuracy and disadvantage of computational time compared to the FOSM increases with the number of uncertain parameters.

5 NUMERICAL OPTIMIZATION METHOD

In this work we use the globalized bounded Nelder-Mead method (GBNM) for optimization. The GBNM belongs to the class of iterative, gradient free optimization methods and is based

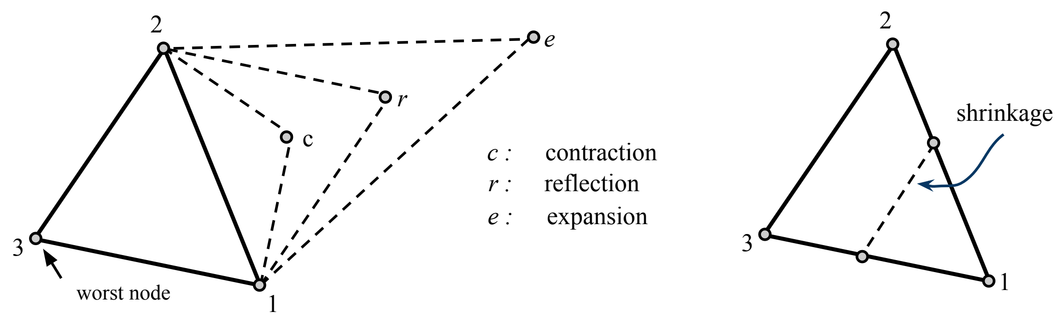


Figure 1: 2D example of the transformations of a simplex.

on the Nelder-Mead algorithm (NMA) proposed by [12].

The key idea of this method is to initialize the simplex, a polyhedron with n+1 nodes in the n-dimensional optimization space. The coordinates of each node represents a set of design parameters. In the initialization for each set, the corresponding value of the objective function is computed and assigned to the node. Subsequently, in every iteration the node with the worst value is replaced by a better one until the simplex is contracted to the optimum. The substitution is realized through reflection, contraction, expansion and shrinkage, which are illustrated in Figure 1. There is no guarantee for convergence, but in practice, the method has proven to be useful [3]. The initial radius of the simplex has a significant influence on the convergence behavior [15]. If the radius is too large, many iterations are needed to converge. On the other hand, if the radius is to small, the optimum might not be localized. The extension of NMA to GBNM by [3] allows to take into account the lower and upper bounds of the design parameters.

6 HYBRID APPROACH

The idea of the proposed hybrid method is that the less computationally intensive but less accurate FOSM is used in the beginning of the optimization for uncertainty quantification in order to get a first rough estimation of the optimum. As soon as the optimizer begins to converge the method for the uncertainty quantification is switched to ASCM and the optimizer starts from this point with adapted parameters to determine a more precise (local) robust optimum. This is a common procedure for hybrid optimizers [16, 15].

The aim of this approach is that fewer iterations of the expensive ASCM are needed to find the robust optimum. This requires that an optimum which is localized by the FOSM is closer to a real optimum than a randomly chosen start point.

A characteristic of GBNM is that the simplex determine the rough location of the optimum quickly but needs many iterations and function evaluations in order to find an accurate one. Therefore, in the first phase of the optimization, when the FOSM is used, the convergence criterion is set relatively high. Thus, the computational costs of the expensive contraction of

Figure 2: Shape of a NACA5320 airfoil.

the simplex are reduced. In the second part, the convergence criterion is set to the desired value in order to determine the optimum sufficiently accurately. In addition, a small radius for the initialization of the simplex is chosen. This can reduce the number of iterations until the simplex converges, but only if the simplex is already close to an (local) optimum. Otherwise, the movement through the search space towards a minimum becomes very slow.

7 TEST CASE

7.1 Numerical framework

As flow solver we utilize our in-house flow solver FASTEST [13]. The software uses a fully conservative finite-volume method in order to discretize the incompressible Navier-Stokes equations [4]. The discretized system is solved by an iterative pressure-correction procedure with a SIP solver for inner iterations. The implementation of the ASCM is based on the work of Bettina Schieche [1] and written in MATLAB. For the generation of sample points on the sparse grid the Smolyak algorithm is used and combined with Gauss-Patterson-Legendre nodes. The interpolation of the random parameter space is done with Lagrange interpolation. The derivatives of the objective function in FOSM are calculated with a finite difference method.

7.2 Problem description

In order to analyze the performance of the presented hybrid robust optimization approach, we investigate a 2-d flow around an airfoil at low Reynolds numbers. The basis of this test case is an airfoil of the NACA 4-digit series as shown in Figure 2. This type of airfoil is described by three shape parameters. These are the maximum camber position c_{pos}, the maximum camber c_{max} and the thickness t of the airfoil. The parameter values are specified in percents of the chord, as defined in [14]. The modeled flow region and the detail of an airfoil is shown in Figure 3. At the curved inlet and on the airfoil surface Dirichlet boundary conditions are applied. Neumann boundary conditions are used at the outlet. For this purpose, it was ensured that the distance between the outlet and the airfoil is sufficiently large. A mirror boundary condition is set to the upper and lower boundaries. For this it is guaranteed that near to these areas the fluid flows only in x-direction. The domain has a total length of 32m and a height of 24m. The distance between the leading and trailing edge of the airfoil is 1m. The fluid is imaginary with a density $\rho = 1$kg/m^3, a dynamic viscosity $\eta = 1$kg/(ms) and a Reynolds number $Re = 100$. The flow field is divided into 10 structured blocks and is discretized with 30,720 control volumes. The objective function J of the optimization problem (4) is defined as

$$J = (c_d - c_d^*)^2 + (c_l - c_l^*)^2, \tag{7}$$

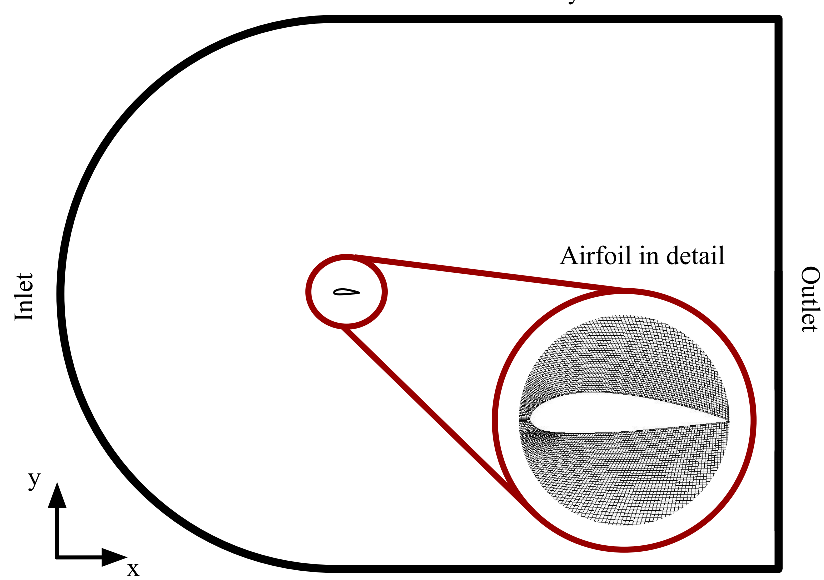


Figure 3: Flow region and detail view of the NACA5320 test case.

where c_d and c_l are the drag and lift coefficients of the airfoil. c_l^* and c_d^* are predefined values and both are set to 0.5. The vector of design parameter is $\mathbf{a} = c_{pos}, c_{max}, t$ with the lower and upper bounds $\mathbf{a}_l = 0.1, 0.1, 0.1$ and $\mathbf{a}_u = 0.8, 0.8, 0.4$. The test case has up to five uncertain parameters, the three shape parameters of the NACA airfoil and the inlet velocity v_{in} and the angle of attack α. These parameters are assumed to be normally distributed. The coefficient of the variation is set to 0.1. For the performance analysis of the hybrid method the optimization is done several times with different uncertain parameters that are taken into account. For each combination of uncertain parameters, multiple starting points for the optimization are used. The combinations of uncertain parameters that are used are given in Table 1. In order to compare

Name	Uncertain parameters
TS1	v_{in}
TS2	α
TS3	v_{in}, α
TS4	c_{max}, c_{pos}, t
TS5	$v_{in}, \alpha, c_{max}, c_{min}, t$

Table 1: Overview of the test case configurations and which parameters are treated as uncertain.

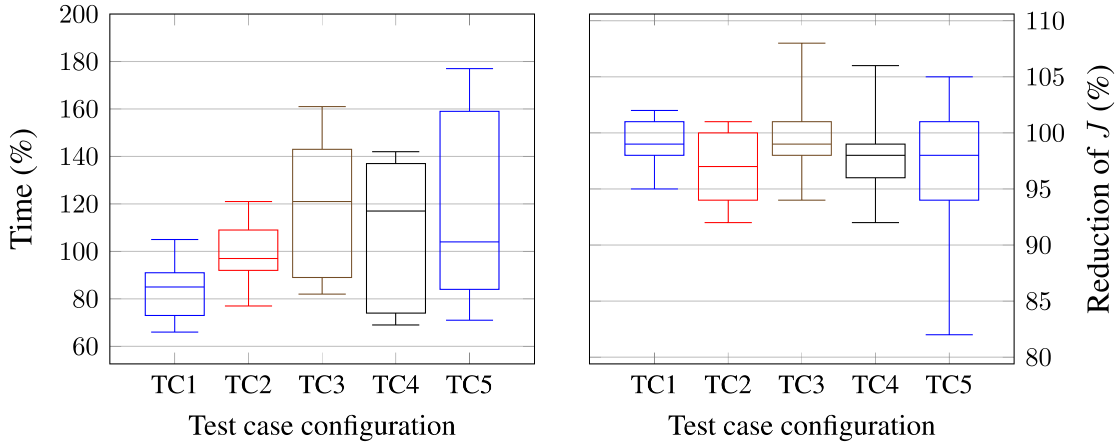
the results each problem is additionally calculated with a pure ASCM. The comparison is made with respect to the computational time as well as the reduction of the objective function.

7.3 RESULTS

All combinations of uncertain parameters that are provided in Table 1 are examined. For each combination several robust optimizations runs with different starting points are executed in order to consider the influence of the (random) choice of the starting points. The ranges of the results are illustrated in Figure 4, represented as box plots with whiskers from minimum to maximum. Figure 4a shows the results with respect to the computational time relative to the time of an optimization using a pure ASCM. This means the values below 100% indicates that the hybrid approach needs less time. Figure 4a illustrates the resulting reduction of the robust objective function. The reduction is defined as

$$r = \frac{(J_0 - J^*)}{J_0}, \tag{8}$$

where J_0 is the value of the robust objective function at the starting point and J^* is the value at the optimum. Both values are calculated with the ASCM. Again the results of the hybrid approach are relative to the results of an optimization with pure ASCM. For the test TC1, where only the inlet velocity v_{in} is treated as uncertain, the results show that the hybrid approach needs in average less time for the optimization. The median is 81%. Only the upper whisker exceeds the 100% mark to 105%. In addition to the optimization time, the reduction of the objective function is for all start points near to 100%, since the lower and upper quartils are 98% and 101%. For TC2 the median of the computational time is 97% and therefore slightly faster than a pure ASCM, but the upper quartil is 109%. This means that for this configuration more than 25% of the optimization runs with the hybrid approach require more than 9% more time. The targeted reduction of the objective function to 100% is only achieved with 25% of the chosen starting points. The consideration of more than one uncertain parameter is realized in TC3-5. In all three configurations the difference to the computational time of the pure ASCM optimization cover a large range of more than 50%. No median reaches a desired value lower than 100%. The worst result is provided by TC5, where 25% of the optimization runs requires more than 1.5 times the time of the pure ASCM. Examining the results of TC3-5 in Figure 4b, it is noticable that each lower quartil is below the 100% mark and therefore worse than the non-hybrid solution. Based on these results it can be asserted that the hybrid approach is not advantageous for non-trivial flow problems. The reason for this is that approximations of statistical quantities through FOSM are too inaccurate. The consequence is that a robust optimization using this method converges to a random point, which is not necessarily close to a (local) optimum. Thus, in the second part of the optimization the simplex radius is adjusted based on false assumptions. Due to this unfavorable choice of the parameters the convergence behavior is negatively effected ([15]).



(a) Resulting optimization times of TC1-5.

(b) Resulting reduction of the robust objective function J.

Figure 4: Results of optimization with the hybrid approach in relation to an optimization with pure ASCM. The results for all used start points of the different configurations (TC1-5) are grouped in box plots with minimum and maximum values as whiskers. (a) show the resulting relative optimization times and (b) the relative amount of the reduction of the robust objective function J.

8 CONCLUSIONS

A hybrid robust optimization method has been presented. We introduced the basics for flow problems under uncertainty. Furthermore, we described the general idea of robust optimization. Two methods for uncertainty quantification were presented, the First Order Second Moment method as well as the adaptive stochastic collocation method. Furthermore, the gradient free optimization method GBNM was introduced. Subsequently, the idea of the combination of FOSM, ASCM and GBNM to a hybrid optimization scheme was presented. This scheme was applied to a 2-dimensional flow test case of a NACA airfoil. In several tests different combinations of uncertain parameters were considered during the robust optimization. The results showed that the hybrid approach is not suitable. Only for one simple configuration the approach achieved satisfactory results. In all other tests the hybrid optimization is even worse than a pure ASCM with random starting points. Due to the linear properties of the FOSM this approach is limited to very smooth problems. Otherwise in the first part of the optimization the FOSM propose a random point as a starting point for the second part. If this point is not close to an optimum, the adaption of the simplex radius has a negative effect on the convergence.

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