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Uncertainty Propagation and Robust Design in CFD Using Sensitivity Derivatives

Michele M. Putko
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UNCERTAINTY PROPAGATION AND ROBUST
DESIGN IN CFD USING SENSITIVITY DERIVATIVES

by

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A Dissertation Submitted to the Faculty of
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ABSTRACT

UNCERTAINTY PROPAGATION AND ROBUST DESIGN IN CFD USING SENSITIVITY DERIVATIVES

Michele M. Putko
Old Dominion University, 2004
Director: Dr. Arthur C. Taylor III

This study investigates and demonstrates a methodology for uncertainty propagation and robust design in Computational Fluid Dynamics (CFD). Efficient calculation of both first- and second-order sensitivity derivatives is requisite in the proposed methodology. In this study, first- and second-order sensitivity derivatives of code output with respect to code input are obtained through an efficient incremental iterative approach.

An approximate statistical moment method for uncertainty propagation is first demonstrated on a quasi one-dimensional (1-D) Euler CFD code. This method is then extended to a two-dimensional (2-D) subsonic inviscid model airfoil problem. In each application, given statistically independent, random, normally distributed input variables, a first- and second-order statistical moment matching procedure is performed to approximate the uncertainty in the CFD output. In each model problem, a Sensitivity Derivative Enhanced Monte Carlo (SDEMC) method is also demonstrated. With this methodology, incorporation of the first-order sensitivity derivatives into the data reduction phase of a conventional Monte Carlo (MC) simulation allows for improved accuracy in determining the first moment of the CFD output. The statistical moment method and the SDEMC method are also incorporated into an investigation of output function variance. The methods that exploit the availability of sensitivity derivatives are found to be valid and computationally efficient when considering small deviations from input mean values.

In both the 1-D and 2-D problems, uncertainties in the CFD input variables are incorporated into robust optimization procedures. For each optimization, statistical moments involving first-order sensitivity derivatives appear in the objective function and system constraints. The constraints are cast in probabilistic terms; that is, the probability
that a constraint is satisfied is greater than or equal to some desired target probability. Gradient-based robust optimization of this stochastic problem is accomplished through use of both first and second-order sensitivity derivatives. For each robust optimization, the effect of increasing both input standard deviations and target probability of constraint satisfaction are demonstrated. This method provides a means for incorporating uncertainty when considering small deviations from input mean values.
This dissertation is dedicated to my children,

Chris, Bob, Marie, Joseph, Catherine, and James,

and to my wonderful husband, Chris.
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NOMENCLATURE AND ACRONYMS

A(x) area distribution in nozzle
AD automatic differentiation
AV adjoint variable
a geometric shape parameter
b geometric shape parameter
b vector of independent input variables
CFD Computational Fluid Dynamics
C_l Lift coefficient
C_m Moment coefficient
E total energy
E() expected value
e_o specific total energy
F vector of CFD output functions
FO first-order
HDII hand-differentiated, incremental–iterative
GRAPE Grids about Airfoils using Poisson's Equation
g vector of conventional optimization constraints
HOT higher order terms
k number of standard deviations
M Mach number at nozzle inlet
M Mach number distribution throughout nozzle
MC  Monte Carlo
Minf  free-stream Mach number
MPP  Most Probable Point
Mt  target inlet Mach number
n  number of input random variables
N  sample size
NDV  number of design variables
NOF  number of output functions
P  Pressure
Pb  normalized nozzle static back (outlet) pressure
PDF  Probability Density Function
Q  vector of flow-field variables (state variables)
q  mass flux through nozzle
qt  target mass flux through nozzle
R  vector of state equation residuals
S  Source
SD  sensitivity derivative
SDEMC  Sensitivity Derivative Enhanced Monte Carlo
SDES  Sensitivity Derivative Enhanced Sampling
SO  second-order
TMC  traditional Monte Carlo
u  flow velocity in x direction
V  nozzle volume
\( V() \) variance( )

\( V_t \) target nozzle volume used for optimization

\( X \) computational grid

\( x \) normalized axial position within nozzle

\( \alpha \) angle of attack

\( \gamma \) specific heat ratio

\( \sigma \) standard deviation

\( \sigma^2 \) variance

\( \rho \) density

\( \rho() \) probability density function

**super script:**
- mean value

**sub-script:**
1 based on first-order approximation
2 based on second-order approximation
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CHAPTER I
INTRODUCTION

1.1 Motivation

In Computational Fluid Dynamics (CFD), the computation of sensitivity derivatives (SD) of CFD code output, with respect to code input parameters, affords information which can be very useful in estimating uncertainty propagation; that is, the extent to which the output function is affected by uncertainties in input parameters. With such information, one may conduct a probabilistic gradient-based optimization. This optimization is in contrast to most CFD-based aerodynamic optimization and design studies where the input parameters have been assumed precisely known. Input parameters often contain uncertainties which may have a large impact upon design and therefore should be considered in design optimization. The present study demonstrates a methodology for incorporating input parameter uncertainties into CFD-based design.

Uncertainties in input parameters propagate throughout the design. An efficient and reliable quantification of this uncertainty propagation is an objective of the present study. To this end, various efficient methods which exploit the availability of the CFD SD are proposed. The methods addressed in the present study which exploit the availability of CFD SD are the approximate statistical moment method, and the Sensitivity Derivative Enhanced Monte Carlo (SDEMC) method. The methods are investigated for both accuracy and efficiency in predicting uncertainty propagation.

The journal model for this dissertation is the AIAA Journal.
The approximate statistical moment method of uncertainty quantification allows one to analytically represent uncertainties in design constraints and objectives. This analytic representation of input parameters, design constraints, and design objectives may be considered in optimization giving rise to a non-deterministic or robust optimization procedure. The successful demonstration of robust optimization on a high-fidelity CFD code is also an objective of the present work.

1.2 Literature Review

Recent advances in CFD analyses have led to much discussion of sensitivity analyses and gradient based optimization for complex aerodynamic configurations [1-4]. In most CFD-based aerodynamic optimization and design studies, the input data and parameters have been assumed precisely known giving rise to a deterministic or conventional optimization. The need to incorporate uncertainty-based design in CFD is an active area of research and currently presents an opportunity for improvement in many CFD analyses and design procedures [5].

Structural design disciplines frequently incorporate statistical uncertainties in the input data or parameters giving rise to non-deterministic design optimization studies [6-13]. Recent attention is being given to develop probabilistic design models in lieu of deterministic models throughout many engineering disciplines [14-16]. In [17], a survey of analytic probabilistic approaches used in uncertainty analysis illustrates the development of the mean value first-order second moment (MVFOSM) method. In the current study, this method is referred to as the first-order (FO) approximate statistical moment method. In [18] it is shown that this approximate statistical moment method
and Automatic Differentiation (AD) can be used to efficiently propagate input uncertainties through finite element analyses to approximate output uncertainty. Due to recent advances in AD of high-fidelity CFD codes [19], it is currently possible to employ a similar strategy to propagate uncertainties through CFD codes.

An integrated strategy for mitigating the effect of uncertainty in simulation-based design is presented in [20]. This strategy consists of uncertainty quantification, uncertainty propagation, and robust design tasks or modules. Two approaches are discussed there for propagating uncertainty through sequential analysis codes: an extreme condition approach (or worst case approach) and a statistical approach. Both approaches can be efficiently implemented using SD. For CFD code, the former approach is demonstrated in [21], whereas the latter approach is demonstrated herein.

A gradient-based robust optimization employing the approximate statistical moment method requires second-order (SO) SD from the CFD code. The efficient calculation of SO SD from CFD code is presented in [19] using a method proposed, but not demonstrated in [22]. This method first requires iterative calculation of the FO SD by both the forward-mode and by the reverse-mode differentiation methods followed by a non-iterative scheme to obtain SO SD. The procedure for obtaining SD in the current study is further described in the following section.

A demonstration of gradient-based, robust optimization involving advanced or high-fidelity (nonlinear) CFD code is presented in [23] and [24]. The analytical statistical approximation of the objective function in these robust optimizations requires SO SD. However, unlike the present endeavor, these earlier studies employed a direct numerical
random sampling technique to compute expected values at each optimization step in order to avoid the SO SD.

Two other aspects need to be noted with respect to the robust optimization demonstrations for CFD code modules presented herein and also in [23] and [24]. First, the sources of uncertainty considered were only those due to code input parameters involving geometry and/or flow conditions; i.e., due to sources external to the CFD code simulation. Other computational simulation uncertainties, such as those due to physical, mathematical and numerical modeling approximations are addressed in [25-31]. Essentially internal model error and uncertainty sources, are not considered in the present study. That is, the discrete CFD code analysis results were taken to be deterministically "certain" herein. Ultimately, all of these modeling sources of error and uncertainty must be assessed and considered as discussed. Sensitivity derivatives can also aid in this assessment as discussed in [32] since the adequacy of an internal model's (i.e., algorithm, turbulence, etc.) prediction capability generally depends, to some extent, on the modeling parameter values specified as input.

Second, as discussed in [24], uncertainty classification with respect to an event's impact (from performance loss to catastrophic) and frequency (from everyday fluctuation to extremely rare) sets the problem formulation and solution procedure. Structural reliability techniques typically deal with risk assessment of infrequent but catastrophic failure modes, identifying the most probable point (MPP) of failure and its safety index. Recent advances in probabilistic approaches for reliability-based design are discussed in [33-38]. Here, we are addressing the assessment of everyday operational fluctuations on performance loss, not catastrophe. Consequently, we are
most concerned with aero performance behavior due to probable fluctuations, i.e., near the mean of probability density functions (PDF). Structural reliability assessment is most concerned with improbable catastrophic events, i.e., probability in the tails of the PDF. Simultaneous consideration of both types of uncertainty is discussed in [39].

For a computationally expensive CFD analyses, the approximate statistical moment method for uncertainty propagation is investigated as an alternative to uncertainty propagation by an expensive direct MC simulation. The availability of the CFD SD enables calculation of the approximate statistical moments and thus analysis via an efficient probabilistic method. The availability of SD also allows for improvements in traditional MC sampling methods. In [40], it is proposed and demonstrated that SD may be incorporated into MC sampling methods for a reduction in variance. This SDEMC method is investigated herein in a high-fidelity CFD application.

The availability of CFD SD is clearly an enabling factor in the present work. There are several methods for obtaining SD as discussed in [41], however the method presented in [19] was best suited for the current study.

1.3 Sensitivity Derivatives

The current study makes extensive use of FO and SO SD of code output with respect to code input. Although the focus of this work is not on the calculation of SD, it is worth noting that this study is one of the first demonstrations of the very efficient ADIFOR (Automatic Differentiation of Fortran) assisted incremental-iterative approach for calculation of SO SD recently developed as described in [19].
In [22], the automatic differentiation software tool, ADIFOR 2.0 is demonstrated to be a viable tool for the calculation of SD for CFD codes. ADIFOR 2.0 is successfully employed in [22], [42], and [43] in forward-mode or direct differentiation procedures.

One should note that forward-mode or direct differentiation scales with the number of design variables (NDV) in contrast to reverse-mode or adjoint variable differentiation which scales with the number of output functions (NOF). An improvement in ADIFOR 3.0 enabled the execution of the reverse-mode scheme with the ADIFOR automatic differentiation software. For further information on the ADIFOR software see [44-46].

As discussed in [19], a SO SD may be constructed using both the FO forward-mode and reverse-mode SD schemes. This SO SD requires the computational effort associated with NDV+NOF, that is, the computational effort associated with a FO SD calculation in both a forward and reverse-mode.

For the current work, the FO SD are obtained by hand differentiation of the Euler codes using both a HDII (hand-differentiated, incremental–iterative) approach as well as a HDII-AV (hand-differentiated, incremental–iterative adjoint variable) approach. Following the development of the HDII and HDII-AV FO SD, a non-iterative calculation of the SO SD is obtained by using a black-box, forward-mode application of ADIFOR 3.0 to the appropriate pieces of the FO SD code, in order to construct the many SO derivative terms. The equations and theoretical development of the method are described in detail in [19].

In the present study, the non-iterative ADIFOR assisted method of calculating the SO SD is employed as a reliable scheme for the efficient and accurate calculation of SD. This method is very efficient when compared to the number of solutions required.
when computing the second derivative in a purely forward mode. That is, typically in CFD problems (NDV+NOF) is much less than the computational effort required to obtain SO SD via the traditional forward mode ((NDV^2+NDV)/2+NDV.)

The efficient calculation of sensitivity derivatives is a key enabler for the present study. Both FO and SO SD are incorporated throughout the uncertainty propagation and robust optimization procedures.

1.4 Objectives of the Present Work

The objectives of the present work are to develop and demonstrate an efficient and accurate method for estimating input parameter uncertainty propagation in CFD and to incorporate input parameter uncertainties into CFD-based robust design. In order to accomplish these objectives, the uncertainty propagation methodologies are first presented in a general context and then extended to quasi 1-D and 2-D CFD Euler flow analyses. After validation of the approximate statistical moment method of uncertainty quantification, the methodology is incorporated into the robust design procedures. Again, the development for the robust design procedures begin in a generic context, and are then extended to 1-D and 2-D Euler flow applications.
CHAPTER II

ESTIMATING UNCERTAINTY PROPAGATION IN CFD

2.1 Introduction

Two uncertainty propagation methods that exploit the availability of SD are investigated as techniques to accurately and efficiently predict uncertainty propagation through CFD code. The approximate statistical moment method and a SDEMC method are investigated with applications in quasi 1-D and 2-D Euler CFD problems. In each application, the FO and SO SD of code output with respect to code input are obtained through the method described in Sec. 1.3. For the present study, input variables are assumed to be independent, normally distributed, random variables. Although the strategy presented herein is also applicable to correlated and/or non-normally distributed variables, the analysis and resulting equations become more complex.

In the present study, the CFD output function vector, F is a function of the continuous input random variables, b, that is \( F = F(b) \). The expected value or first moment of \( F(b) \), is denoted by \( E(F) \). For a continuous input random variable, \( b \), with probability density function, \( \rho(b) \), the expected value or first moment is given as:

\[
E(F) = \overline{F} = \int F(b) \, \rho(b) \, db
\]  

(2.1)

Similarly, the variance or second moment, denoted by \( V(F) \) or \( \sigma_F^2 \) is given as:

\[
V(F) = \sigma_F^2 = \int (F(b) - E(F))^2 \, \rho(b) \, db
\]  

(2.2)

with the standard deviation of the output function vector, \( F \) represented as the square root of the variance, or \( \sigma_F \).
In the current study, the vector of input random variables is represented as a set of $n$ random variables, $b = \{b_1, \ldots, b_n\}$, with mean values, $\bar{b} = \{\bar{b}_1, \ldots, \bar{b}_n\}$, and standard deviations, $\sigma_b = \{\sigma_{b_1}, \ldots, \sigma_{b_n}\}$. For each application investigated, a single typical aerodynamic output function will represent $F$. That is $F$ will be represented by a single parameter and not the entire CFD code output. Although the CFD code produces several output parameters, only one parameter is investigated for the purpose of focusing the study.

The uncertainties associated with the output function, $F$ are investigated utilizing three methods; the traditional Monte Carlo (TMC) method, the approximate statistical moment method, and a SDEMC approach. Note that the TMC method is employed as a baseline for comparison with the other methods. With each investigation, the speed or efficiency of the method as well as the accuracy of the method is assessed.

2.2 Traditional Monte Carlo Approach

The most straightforward way of calculating approximations for the integrals in Eqs. (2.1) and (2.2) is through a traditional MC simulation. The TMC approximations for the output function mean and variance are given by

$$\bar{F}(b) \approx \frac{1}{N} \sum_{j=1}^{N} F(b_j)$$

(2.3)

$$\sigma_F^2 \approx \frac{\sum_{j=1}^{N} (F(b_j) - \bar{F}(b))^2}{N - 1}$$

(2.4)

where $N$ represents the sample size of the Monte Carlo simulation.
The difficulty with a TMC simulation is that in order to get an accurate prediction of the output mean and variance, one may have to perform thousands of runs which are often not feasible with high fidelity CFD codes. An approximation of the first moment generated via TMC contains error proportional to $\sigma_f/\sqrt{N}$. First-order and second-order approximate statistical moment methods, and the SDEMC method are investigated as more efficient alternatives to traditional MC approximations.

### 2.3 Approximate Statistical Moment Method

Approximate statistical moments are formulated for the first statistical moment (mean) and second statistical moment (variance) applying standard integration procedures to either a FO or SO Taylor series approximations of the output function of interest where derivatives are evaluated at the mean values, $\bar{b}$. The FO and SO Taylor series approximations for an output function, $F(b)$ with $n$ independent input variables are:

**FO:**
\[
F_1(b) = F(\bar{b}) + \sum_{i=1}^{n} \frac{\partial F}{\partial b_i}(b_i - \bar{b}_i)
\]  \hspace{1cm} (2.5)

**SO:**
\[
F_2(b) = F(\bar{b}) + \sum_{i=1}^{n} \frac{\partial F}{\partial b_i}(b_i - \bar{b}_i) + \frac{1}{2} \sum_{k=1}^{n} \sum_{i=1}^{n} \frac{\partial^2 F}{\partial b_i \partial b_k}(b_i - \bar{b}_i)(b_k - \bar{b}_k)
\]  \hspace{1cm} (2.6)

Utilizing these Taylor series approximations, one may obtain FO and SO approximations for the mean and variance of the output function, $F$. These approximations are derived through simplification of the following integrals:
\[
\overline{F}_1 = \int \overline{F}_1(b) \rho(b) \, db \\
\overline{F}_2 = \int \overline{F}_2(b) \rho(b) \, db \\
\sigma_{F_1}^2 = \int \left( \overline{F}_1(b) - \overline{F}_1 \right)^2 \rho(b) \, db \\
\sigma_{F_2}^2 = \int \left( \overline{F}_2(b) - \overline{F}_2 \right)^2 \rho(b) \, db
\] (2.7) (2.8)

Considering the independent, normally distributed, random input variables, \( b \) the resulting simplifications are the FO approximate statistical moments:

\[
\overline{F}_1 = F(\overline{b})
\] (2.9)

\[
\sigma_{F_1}^2 = \sum_{i=1}^{n} \left( \frac{\partial F}{\partial b_i} \sigma_{b_i} \right)^2
\] (2.10)

as well as the SO approximate statistical moments:

\[
\overline{F}_2 = F(\overline{b}) + \frac{1}{2!} \sum_{i=1}^{n} \frac{\partial^2 F}{\partial b_i^2} \sigma_{b_i}^2
\] (2.11)

\[
\sigma_{F_2}^2 = \sum_{i=1}^{n} \left( \frac{\partial F}{\partial b_i} \sigma_{b_i} \right)^2 + \frac{1}{2!} \sum_{i=1}^{n} \sum_{k=1}^{n} \left( \frac{\partial^2 F}{\partial b_i \partial b_k} \sigma_{b_i} \sigma_{b_k} \right)^2
\] (2.12)

where all derivatives are evaluated at the mean values, \( \overline{b} \). Note in Eq. (2.11) that the second-order approximate mean, \( \overline{F}_2 \), is not at the mean values of input \( \overline{b} \), i.e., \( \overline{F}_2 \neq F(\overline{b}) \). The Eqs. given in (2.9) and (2.10) represent the FO approximate statistical moment method, and Eqs. (2.11) and (2.12) represent the SO approximate statistical

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moment method for quantifying output function uncertainty. The methods are straightforward with the difficulty largely lying in computation of the SD.

2.4 Sensitivity Derivative Enhanced Monte Carlo Method

One naturally looks for ways to improve the convergence of the traditional MC method. In [40] a technique which exploits the availability of the SD to achieve variance reduction via a SDEMC method is presented. The SDEMC method also employs the calculation of a FO Taylor series approximation, \( F_i(b) \) expanded about the mean values of the input parameters, \( \bar{b} \). To illustrate the development of the SDEMC method, one may write an expression for the expected value of \( (F(b) - F_i(b)) \):

\[
\int (F(b) - F_i(b)) \rho(b) \, db = \int F(b) \rho(b) \, db - \int F_i(b) \rho(b) \, db
\]

Note that it has already been established with Eq. (2.9) that for a normal input random variable, \( b \):

\[
\int F_i(b) \rho(b) \, db = \bar{F}_i = F(\bar{b})
\]

One may accordingly rearrange Eq. (2.13) substituting as suggested by Eq. (2.14) to obtain the following expression for \( \bar{F} \):

\[
\bar{F} = F(\bar{b}) + \int (F(b) - F_i(b)) \rho(b) \, db
\]
As suggested in [40], a MC simulation may be performed to approximate the integral in Eq. (2.15). That is:

\[ \int \left( F(b) - F_i(b) \right) \rho(b) \, db \approx \frac{1}{N} \sum_{j=1}^{N} \left( F(b_j) - F_i(b_j) \right) \]  

(2.16)

Note that only one FO SD is required for the evaluation of \( F_i \), that is the FO SD at the mean values of the input parameters, \( \bar{b} \). Combining Eqs. (2.15) and (2.16) results in the SDEMC approximation for \( \bar{F} \):

\[ \bar{F}_{\text{SDEMC}} \approx F(\bar{b}) + \frac{1}{N} \sum_{j=1}^{N} \left( F(b_j) - F_i(b_j) \right) \]  

(2.17)

In [40], it is suggested that there is an order of magnitude reduction in error when a SDEMC method is compared to a TMC method. In the current work, the SDEMC prediction of the output function mean method will be investigated in both 1-D and 2-D CFD problems.

An analogous investigation into a sensitivity derivative enhanced expression for the output function variance reveals that such an expression is much more complex due to the SO order terms in Eq. (2.2). Although the SDEMC variance for the output function, \( F \) is difficult to construct, a very useful expression of variance, that of the FO Taylor series remainder is easily constructed with the availability of SD.

A Monte Carlo approximation for the variance of the FO Taylor series remainder, \( (F-F_i) \) is given by:
This statistical parameter provides considerable insight into the behavior of the output function. For a linear output function, $F$, the variance $\sigma^2_{F-F_1}$ is equal to zero, that is $F=F_1$. For a nonlinear function, the variance of the FO Taylor series remainder, $\sigma^2_{F-F_1}$ is nonzero. The value of $\sigma^2_{F-F_1}$ represents the effect of the higher order terms on the output function, $F$. The parameter, $\sigma^2_{F-F_1}$ will be calculated for both the 1-D and 2-D CFD problems as a sensitivity derivative enhanced measure of output function variation.

In order to calculate $\sigma^2_{F-F_1}$ as given by Eq. (2.18), one must perform a MC simulation of $N$ samples, as well as have the first order SD available for calculation of $F_1$. Note that in the SDEMC prediction of the output function mean, these items are also necessary. Accordingly, the additional effort to compute the variance of the Taylor series remainder as shown in Eq. (2.18) is minimal.

Note also that with knowledge of SO SD, one may predict a minimum value of $\sigma^2_{F-F_1}$ analytically without a MC simulation. For convenience, the Taylor series remainder, $F-F_1$ may be represented by:

$$F-F_1 = \text{SO terms} + \text{HOT} \quad (2.19)$$
where \[ \text{SO terms} = \frac{1}{2!} \sum_{k=1}^{n} \sum_{i=1}^{n} \frac{\partial^2 F}{\partial b_i \partial b_k} (b_i - \bar{b}_i)(b_k - \bar{b}_k) \]

\[ \text{HOT} = \text{terms of order three and higher} \]

Note that in the current study, SO SD are available and therefore the SO terms in Eq. (2.19) are known. Since the terms of order three and higher can only increase the variance of the output function, one may produce an expression for the minimum value of \[ \sigma^2_{F-F_i} \] through knowledge of SO terms. That is:

\[ \text{Minimum}(\sigma^2_{F-F_i}) = \sigma^2_{\text{SO Terms}} \]  \hspace{1cm} (2.20)

The SO SD will be employed to solve for \( \sigma^2_{\text{SO Terms}} \) and accordingly represent the lower limit on the variance of the FO Taylor series remainder.

The TMC approach, the approximate statistical moment approach, and the SDEMC approach for uncertainty propagation are now developed for 1-D and 2-D Euler CFD applications.
CHAPTER III

UNCERTAINTY PROPAGATION IN 1-D AND 2-D EULER FLOW

Estimates for uncertainty propagation are obtained through TMC techniques, the approximate statistical moment method, and the SDEMC method using both quasi 1-D and 2-D model CFD problems. In both the 1-D and 2-D applications, the aerodynamic system is represented in a conventional discretized manner, i.e. the discretized conservations laws of steady compressible fluid flow with appropriate boundary conditions are applied to a computational grid. The system may be represented with the aerodynamic output function, $F$ and the state equation residuals, $R$ in the following form:

$$F = F(Q(b),X(b),b)$$  \hspace{1cm} \text{(aerodynamic output functions)} \hspace{1cm} (3.1)$$

$$R = R(Q(b),X(b),b) = 0$$ \hspace{1cm} \text{(nonlinear state equations)} \hspace{1cm} (3.2)$$

where $Q$ is the vector of state (field) variables, $X$ is the computational grid, and $b$ is the vector of input (design) variables. The vector of state equation residuals, $R$, is driven to machine zero for a solution to the system of equations.

3.1 Uncertainty Propagation in 1-D Euler Flow

In the 1-D sample problem, two separate applications of uncertainty propagation are presented; the first involving propagation of geometric uncertainties, the second involving propagation of flow parameter uncertainties. Both uncertainty analyses are performed with quasi 1-D Euler equations and boundary conditions describing subsonic flow through a variable area nozzle depicted in Fig. 3.1. The nozzle inlet is located at $x$
= 0 with area, \( A(x = 0) = 1 \); the nozzle outlet is at \( x = 1 \). The area distribution is given by \( A(x) = 1 - ax + bx^2 \). The volume, \( V \), occupied by the nozzle, is the integration of \( A(x) \) over the length \( x = 0 \) to \( x = 1 \), that is \( V = \frac{a}{2} + \frac{b}{3} \), where \( a \) and \( b \) are the geometric design parameters. Three flow parameters are specified as input boundary conditions: the stagnation enthalpy, inlet entropy, and outlet static (back) pressure.

![Fig.3.1 Variable area nozzle.](image)

The quasi 1-D flow through this nozzle is represented by applying the discretized conservation laws of steady compressible fluid flow with boundary conditions. The steady quasi 1-D Euler equations may be represented with the addition of a flux vector and a source term:
\[
\frac{\partial E(Q)}{\partial x} + S(Q) = 0
\] 

(3.3)

where 

\[ Q = [\rho, \rho u, \rho e_0]^T \]

\[ E(Q) = [\rho u, \rho u^2 + P, (\rho e_o + P) u]^T \]

\[ S(Q) = -\frac{dA}{dx} A \left[ \rho u, \rho u^2, (\rho e_o + P) u \right]^T \]

The ideal gas law with a constant specific heat ratio at \( \gamma = 1.4 \) is used to complete (i.e. for closure of) the system of governing equations. In the 1-D Euler code, the governing equations are solved numerically with an upwind flux-vector splitting method as discussed in [47] and [48]. The computational grid, \( X \) is formed by equally dividing the nozzle with 100 grid points along the x axis.

With a quasi-1-D aerodynamic system represented in the form of Eqs. (3.1) and (3.2), two separate applications of uncertainty propagation are now presented; the first involving propagation of geometric uncertainties, the second involving propagation of flow parameter uncertainties.

### 3.2 Geometric Uncertainty Propagation in 1-D

For the discussion of geometric uncertainty propagation, geometric shape parameters, \( a \) and \( b \) will represent the statistically independent random input variables, \( b \). Recall these parameters are coefficients in the quadratic equation describing the nozzle area, \( A(x) = 1 - ax + bx^2 \). The Mach number distribution through the nozzle, \( M \), is viewed here as a component of the state variable, \( Q \); its value at the inlet, \( M \), (non
bold) is the CFD output function, $F$. Substituting these variables in Eqs. (3.1) and (3.2) yields the following aerodynamic system with geometric input variables, $a$ and $b$:

$$F = M(a,b), a,b$$  \hspace{1cm} \text{(aerodynamic output function)} \hspace{1cm} (3.4)$$

$$R = R(M(a,b), a,b) = 0 \hspace{1cm} \text{(nonlinear state equations)} \hspace{1cm} (3.5)$$

### 3.2.1 Traditional MC Simulation in 1-D

In order to establish a basis of comparison for the approximate methods being investigated, a traditional MC simulation is performed. The traditional MC approximations for the mean and variance of the output function, $M$ are given as:

$$\bar{M}(a,b) \approx \frac{1}{N} \sum_{j=1}^{N} M(a_j,b_j) \hspace{1cm} \sigma_M^2 \approx \frac{\sum_{j=1}^{N} (M(a_j,b_j) - \bar{M}(a,b))^2}{N-1} \hspace{1cm} (3.6)$$

Note the error associated with $\bar{M}(a,b)$ is $\propto \sigma_M / \sqrt{N}$. For the current study, a sample size of $N=3000$ was found to be sufficient to make conclusions regarding the behavior of the sample and the accuracy of the approximate methods.

For the investigation involving geometric uncertainties in quasi 1-D flow, five independent MC simulations (each with a sample size of $N = 3000$) were conducted. In each simulation, the mean values of the input parameters were set at, $\vec{b} = \{\vec{a}, \vec{b}\} = \{0.6, 0.3\}$. The input parameter standard deviations, $\sigma = \sigma_a = \sigma_b$, ranged from 0.01 to 0.08 as shown in Table 3.1.
Table 3.1 Input variable $\sigma$ for geometric uncertainty propagation

<table>
<thead>
<tr>
<th>Simulation</th>
<th>$\sigma = \sigma_a = \sigma_b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.01</td>
</tr>
<tr>
<td>2</td>
<td>0.02</td>
</tr>
<tr>
<td>3</td>
<td>0.04</td>
</tr>
<tr>
<td>4</td>
<td>0.06</td>
</tr>
<tr>
<td>5</td>
<td>0.08</td>
</tr>
</tbody>
</table>

The output function mean and variance, $\bar{M}(a, b)$ and $\sigma_m^2$ were calculated for each of the five simulations. These values were then incorporated as the basis for comparison when assessing approximations derived via the approximate statistical moment methods and the SDEMC method.

Additionally, each independent MC simulation of 3000 samples was subdivided into six sub-samples with $N = 500$. This division allowed for further analysis and comparison of uncertainty propagation techniques due to sample size.

### 3.2.2 Approximate Statistical Moment Method in 1-D

Applying the approach previously described in Sec. 2.3, the CFD output function, $M$, with geometric input variables, $a$ and $b$ may be represented with FO and SO Taylor series approximations:

\[
\text{FO: } M_1(a, b) = M(\bar{a}, \bar{b}) + \frac{\partial M}{\partial a}(a - \bar{a}) + \frac{\partial M}{\partial b}(b - \bar{b})
\] (3.7)
\[ M_2(a, b) = M(\overline{a}, \overline{b}) + \frac{\partial M}{\partial a}(a - \overline{a}) + \frac{\partial M}{\partial b}(b - \overline{b}) + \]
\[ \frac{\partial^2 M}{\partial a \partial b} (a - \overline{a})(b - \overline{b}) + 0.5 \left( \frac{\partial^2 M}{\partial a^2} (a - \overline{a})^2 \right) + 0.5 \left( \frac{\partial^2 M}{\partial b^2} (b - \overline{b})^2 \right) \]

(3.8)

It is important to assess the Taylor series output function approximations (see Eqs. (3.7) and (3.8)) with direct nonlinear CFD code simulations prior to assessing uncertainty propagation predictions. If the CFD output function, \( M \), is quasi-linear with respect to the input variables of interest, one can expect FO approximations to be reasonably good; that is, the FO statistical moment approximations should match well with the moments produced by an actual Monte Carlo simulation. For a more nonlinear system, one naturally expects better accuracy with SO approximations; that is, moment predictions which include SO terms should yield results which better predict the statistical moments produced by the Monte Carlo simulation.

For the 1-D geometric variable application, the FO and SO approximations for the mean, and variance of the output function, \( M \) are expressed in terms of the output function evaluated at the input parameter mean values, \( M(\overline{a}, \overline{b}) \), the FO and SO SD, and the input parameter standard deviations, \( \sigma_a \) and \( \sigma_b \):

\[ \overline{M}_1 = M(\overline{a}, \overline{b}) \]  
(3.9)

\[ \sigma_{M_1}^2 = \left( \frac{\partial M}{\partial a} \sigma_a \right)^2 + \left( \frac{\partial M}{\partial b} \sigma_b \right)^2 \]  
(3.10)
SO: \[ \overline{M}_2 = M(\overline{a}, \overline{b}) + 0.5 \left( \frac{\partial^2 M}{\partial a^2} \right) \sigma_a^2 + \frac{1}{2} \left( \frac{\partial^2 M}{\partial b^2} \right) \sigma_b^2 \] (3.11)

\[ \sigma_{M_2}^2 = \left( \frac{\partial M}{\partial a} \sigma_a \right)^2 + \left( \frac{\partial M}{\partial b} \sigma_b \right)^2 + 0.5 \left( \frac{\partial^2 M}{\partial a^2} \sigma_a^2 \right)^2 + 0.5 \left( \frac{\partial^2 M}{\partial b^2} \sigma_b^2 \right)^2 + \left( \frac{\partial^2 M}{\partial a \partial b} \sigma_a \sigma_b \right)^2 \] (3.12)

Predictions of the FO and SO statistical moments, \( \overline{M}_1, \overline{M}_2, \sigma_{M_1}, \) and \( \sigma_{M_2} \) are assessed in two fashions; they are first compared with a TMC analysis, and subsequently compared with a SDEMC analysis. The comparisons are presented and discussed in Chap. IV.

3.2.2 Sensitivity Derivative Enhanced Monte Carlo Method (SDEMC) in 1-D

The FO Taylor series approximation for \( M_1 \), that is \( M_1 \) as expressed in Eq. (3.7) is incorporated into a SDEMC scheme. The resulting first-order SDMC approximation for \( \overline{M} \) is given by:

\[ \overline{M}_{\text{SDMC}}(a, b) \approx M(\overline{a}, \overline{b}) + \frac{1}{N_{\text{SD}}} \sum_{j=1}^{N_{\text{SD}}} \left( M(a_j, b_j) - M_1(a_j, b_j) \right) \] (3.13)

where \( N_{\text{SD}} \) is the sample size for the SDEMC simulation. For the SDEMC method, the total MC sample size of \( N = 3000 \) was divided into six independent SDEMC samples with \( N_{\text{SD}} = 500 \). Thus, \( \overline{M}_{\text{SDMC}} \) was calculated six times. This repetitive analysis was advantageous in lending confidence to the statistical value, \( \overline{M}_{\text{SDMC}}(a, b) \).
For each of the six independent sub samples, the expression $\sigma^2_{M-M_1}$ was also calculated as a measure of output function variance as show in Eq. (3.14).

The variance of the Taylor series remainder, $\sigma^2_{M-M_1}$ is given as:

$$
\sigma^2_{M-M_1} = \frac{\sum_{j=1}^{N} (M(a_j, b_j) - M_1(a_j, b_j) - (\bar{M}(a, b) - \bar{M}_1(a, b)))^2}{N-1}
$$

(3.14)

with the standard deviation $\sigma_{M-M_1}$, the square root of Eq. (3.14).

The minimum value for this variance is determined with the output function, $M(a,b)$ represented in Taylor series form as:

$$
M(a, b) = M(\bar{a}, \bar{b}) + \frac{\partial M}{\partial a}(a - \bar{a}) + \frac{\partial M}{\partial b}(b - \bar{b}) + \\
+ \frac{\partial^2 M}{\partial a \partial b}(a - \bar{a})(b - \bar{b}) + \\
+ 0.5 \left( \frac{\partial^2 M}{\partial a^2}(a - \bar{a})^2 \right) + 0.5 \left( \frac{\partial^2 M}{\partial b^2}(b - \bar{b})^2 \right) + \text{HOT}
$$

(3.15)

where HOT represent the higher order terms not explicitly shown. Rearranging and substituting for $M_1$ yields:

$$
M(a,b) - M_1(a,b) = \frac{\partial^2 M}{\partial a \partial b}(a - \bar{a})(b - \bar{b}) + 0.5 \left( \frac{\partial^2 M}{\partial a^2}(a - \bar{a})^2 \right) + 0.5 \left( \frac{\partial^2 M}{\partial b^2}(b - \bar{b})^2 \right) + \text{HOT}
$$

(3.16)
The SO terms are represented by:

\[
\text{SO terms} = \frac{\partial^2 M}{\partial a \partial b} (a - \bar{a})(b - \bar{b}) + 0.5 \left( \frac{\partial^2 M}{\partial a^2} (a - \bar{a})^2 \right) + 0.5 \left( \frac{\partial^2 M}{\partial b^2} (b - \bar{b})^2 \right)
\]  

(3.17)

The variance of the SO terms may be represented by:

\[
\sigma_{\text{SO}}^2 = \int \left( \text{SO.} - \overline{\text{SO.}} \right)^2 \rho(b) \, db
\]

(3.18)

Simplifying Eq. (3.18) for the current independent, normally distributed geometric input parameters yields:

\[
\sigma_{\text{SO}}^2 = \left( \frac{\partial^2 M}{\partial a \partial b} \right)^2 \sigma_a \sigma_b
\]

(3.19)

Note that higher order terms can only increase the variance of the output function. Accordingly, Eq. (3.19) represents a lower limit on \( \sigma_{M-M_1}^2 \), i.e. \( \min(\sigma_{M-M_1}^2) \). A MC simulation will be performed to calculate the \( \sigma_{M-M_1}^2 \), and Eq. (3.19) will also be employed as an analytic expression for \( \min(\sigma_{M-M_1}^2) \). With the analytic expression and a MC simulation, one may ascertain whether this minimum value of the Taylor series remainder variance sufficiently describes the output function variation.

The results of the 1-D geometric input parameter uncertainty investigation are given in Chap. IV.
3.3 Flow Parameter Uncertainty Propagation in 1-D

A second example of uncertainty propagation in the nozzle problem involves uncertainty propagation due to fluctuations in flow parameters. For the discussion of flow parameter uncertainty propagation, the free-stream Mach number, Minf, and the nozzle static back pressure, Pb, will be taken as statistically independent random variables. Specifying the free-stream Mach number sets the stagnation enthalpy. As in the geometric uncertainty example, the Mach number distribution through the nozzle, M, is viewed as a component of the state variable, Q; its value at the inlet, M, is the CFD output, F. Applying the approach previously outlined in Eqs. (3.1) and (3.2) yields the following system of equations:

\[ F = M(\text{Minf}, \text{Pb}, \text{Minf}, \text{Pb}) = 0 \quad \text{(aerodynamic output function)} \quad (3.20) \]
\[ R = R(\text{Minf}, \text{Pb}, \text{Minf}, \text{Pb}) = 0 \quad \text{(nonlinear state equations)} \quad (3.21) \]

The input variables, Minf, and Pb were substituted for the geometric input variables, a and b, and FO and SO SD were calculated. For the investigation involving flow parameter uncertainties in quasi 1-D flow, four independent MC simulations (each with a sample size of N = 3000) were conducted. In each simulation, the mean values of the input parameters were set at, \( \overline{b} = \{\text{Minf}, \text{Pb}\} = \{0.3, 0.8\} \). The input parameter standard deviations, \( \sigma = \sigma_{\text{Minf}} = \sigma_{\text{Pb}} \), ranged from 0.01 to 0.06 as shown in Table 3.2.
Table 3.2 Input variable $\sigma$ for 1-D flow parameter uncertainty propagation

<table>
<thead>
<tr>
<th>Simulation</th>
<th>$\sigma = \sigma_{\text{Minf}} = \sigma_{\text{Pb}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.01</td>
</tr>
<tr>
<td>2</td>
<td>0.02</td>
</tr>
<tr>
<td>3</td>
<td>0.04</td>
</tr>
<tr>
<td>4</td>
<td>0.06</td>
</tr>
</tbody>
</table>

Expressions for:

- $\bar{M}(\text{Minf, Pb})$ (MC approximation for the expected value of $M$)
- $\sigma_M^2$ (MC approximation for the variance of $M$)
- $M_1(\text{Minf, Pb})$ (First-order Taylor series approximation for $M$)
- $M_2(\text{Minf, Pb})$ (Second-order Taylor series approximation for $M$)
- $\bar{M}_1$ (First-order approximate mean)
- $\bar{M}_2$ (Second-order approximate mean)
- $\sigma_{M_1}^2$ (First-order approximate variance)
- $\sigma_{M_2}^2$ (Second-order approximate variance)
- $\bar{M}_{\text{SDMC}}(\text{Minf, Pb})$ (Sensitivity derivative enhanced MC mean)
- $\sigma^2_{M-M_1}$ (Sensitivity derivative enhanced variance)
- $\sigma^2_{SO}$ (Variance of Second Order Terms)

were developed and parallel the expression given in Eqs. (3.6) through (3.19).
As in the geometric example, $\overline{M}_{SDMC}$ is calculated six times with a sample of $N_{SD} = 500$ in order to lend confidence to this statistical value. The results of the flow parameter uncertainty investigation are given in Chap. IV.

### 3.4 Flow Parameter Uncertainty Propagation in 2-D

Subsequent to the initial investigation of uncertainty propagation in CFD on a quasi 1-D Euler problem using the TMC method, the FO and SO approximate statistical moment method, and the SDEMC method, a similar investigation was extended to a 2-D Euler problem. The problem entailed 2-D inviscid steady subsonic flow over a NACA 64A410 airfoil [49], using an Euler code [19].

Here again the discretized conservation laws of steady, compressible fluid flow with appropriate boundary conditions form the aerodynamic system.

A 129 x 33 C-mesh computational grid was generated to simulate flow over the NACA 64A410 airfoil. (See Figs. 3.2 and 3.3.) The outer boundaries are located five chords upstream, ten chords downstream, five chords above and five chords below the airfoil. The radius of the arc that blends the outer boundaries together is two chords. The grid generation was performed with a FORTRAN code, GRAPE (Grids about Airfoils using Poisson's Equation.) GRAPE, an elliptic grid generator originally intended for isolated airfoils was written by Reece Sorenson at NASA Ames Research Center, and was modified by Rod Chima at NASA Glenn to allow generation of periodic C-type grids [50-41].
Fig. 3.2 Complete grid for 2-D NACA 64A410 airfoil.

Fig. 3.3 Close-up grid for 2-D NACA 64A410 airfoil.

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In the 2-D investigation only uncertainties due to flow parameters were investigated. The airfoil angle of attack, \( \alpha \) and the free-stream Mach number, \( \text{Minf} \), will be taken as statistically independent random variables, \( b \), and the lift coefficient, \( C_l \) represents the CFD output, \( F \). Substituting in Eqs. (3.1) and (3.2) yields the following aerodynamic system:

\[
F = C_l \left( \mathbf{Q} \left( \text{Minf}, \alpha \right), \mathbf{X}, \text{Minf}, \alpha \right) \quad \text{(aerodynamic output function)} \quad (3.22)
\]

\[
\mathbf{R} = \mathbf{R} \left( \mathbf{Q} \left( \text{Minf}, \alpha \right), \mathbf{X}, \text{Minf}, \alpha \right) = 0 \quad \text{(nonlinear state equations)} \quad (3.23)
\]

Note that the computational grid, \( \mathbf{X} \), is not a function of the flow input variables and remains fixed throughout the investigation.

Three independent MC simulations with a sample size of \( N = 2500 \) were conducted. In both simulations the average values of the input parameters were set at,

\[
\overline{b} = \{\alpha, \text{Minf}\} = \{4^0, 0.4\}. \quad \text{In Simulation 1, } \sigma_\alpha = \sigma_{\text{Minf}} = 0.01, \quad \text{while in Simulation 2, } \sigma_\alpha = \sigma_{\text{Minf}} = 0.02 \quad \text{and in Simulation 3, } \sigma_\alpha = \sigma_{\text{Minf}} = 0.04, \quad \text{The output function mean and variance were calculated for each simulation. Each independent MC simulation of 2500 samples was subdivided into five samples of \( N=500 \). This division allowed for further analysis and comparison of MC techniques.}

3.4.1 Traditional MC Simulation in 2-D

In order to establish an initial basis of comparison for the methods being investigated, a traditional MC simulation is performed. For the current investigation of 2-D flow parameter uncertainty propagation a sample size of \( N= 2,500 \) is used. The traditional MC approximations for the mean and variance of the output function, \( C_l \) are given as:
\[ 
\bar{C}l(\alpha, M_{\text{inf}}) \approx \frac{1}{N} \sum_{j=1}^{N} Cl(\alpha_j, M_{\text{inf}_j}) 
\]  
(3.24)

\[ 
\sigma_{\bar{C}l}^2 \approx \frac{\sum_{j=1}^{N} (Cl(\alpha_j, M_{\text{inf}_j}) - Cl(\alpha, M_{\text{inf}}))^2}{N-1} 
\]  
(3.25)

Although these expressions are approximations, a sample size of \( N=2,500 \) is found to be sufficient for making comparison with the other approximate methods.

3.4.2 Approximate Statistical Moment Method in 2-D

Applying the approach previously described, the CFD output function, \( Cl \) is represented with FO and SO Taylor series approximations:

FO:  
\[ Cl_1(\alpha, M_{\text{inf}}) = Cl(\bar{\alpha}, \bar{M}_{\text{inf}}) + \frac{\partial Cl}{\partial \alpha} (\alpha - \bar{\alpha}) + \frac{\partial Cl}{\partial M_{\text{inf}}} (M_{\text{inf}} - \bar{M}_{\text{inf}}) \]  
(3.26)

SO:  
\[ Cl_2(\alpha, M_{\text{inf}}) = Cl(\bar{\alpha}, \bar{M}_{\text{inf}}) + \frac{\partial Cl}{\partial \alpha} (\alpha - \bar{\alpha}) + \frac{\partial Cl}{\partial M_{\text{inf}}} (M_{\text{inf}} - \bar{M}_{\text{inf}}) + \]  
\[ + \frac{\partial^2 Cl}{\partial \alpha \partial M_{\text{inf}}} (\alpha - \bar{\alpha})(M_{\text{inf}} - \bar{M}_{\text{inf}}) + \]  
\[ + 0.5 \left( \frac{\partial^2 Cl}{\partial \alpha^2} (\alpha - \bar{\alpha})^2 \right) + 0.5 \left( \frac{\partial^2 Cl}{\partial M_{\text{inf}}^2} (M_{\text{inf}} - \bar{M}_{\text{inf}})^2 \right) \]  
(3.27)

The FO and SO approximations for the mean, \( \bar{Cl} \), and variance \( \sigma_{\bar{Cl}}^2 \) of the output function are expressed as:
\[
\text{FO: } \bar{C}_1 = C_l(\alpha, Minf) \tag{3.28}
\]

\[
\sigma_{C_{l1}}^2 = \left( \frac{\partial C_l}{\partial \alpha} \right)^2 \sigma_\alpha^2 + \left( \frac{\partial C_l}{\partial Minf} \right)^2 \sigma_{\text{Minf}}^2 \tag{3.29}
\]

\[
\text{SO: } \bar{C}_2 = C_l(\alpha, Minf) + 0.5 \left( \frac{\partial^2 C_l}{\partial \alpha^2} \right) \sigma_\alpha^2 + 0.5 \left( \frac{\partial^2 C_l}{\partial \text{Minf}^2} \right) \sigma_{\text{Minf}}^2 \tag{3.30}
\]

\[
\sigma_{C_{l2}}^2 = \left( \frac{\partial C_l}{\partial \alpha} \sigma_\alpha^2 + \left( \frac{\partial C_l}{\partial \text{Minf}} \right) \sigma_{\text{Minf}}^2 \right)^2 + 0.5 \left( \frac{\partial^2 C_l}{\partial \alpha \partial \text{Minf}} \sigma_\alpha \sigma_{\text{Minf}} \right)^2 \tag{3.31}
\]

Calculations of $C_l(\alpha, \text{Minf})$, $C_l(\alpha, \text{Minf})$, $\bar{C}_1$, $\bar{C}_2$, $\sigma_{C_{l1}}^2$ and $\sigma_{C_{l2}}^2$ are compared with CFD solutions and Monte Carlo analyses based on CFD solutions. The comparisons are presented and discussed in Chap. IV.

### 3.4.2 Sensitivity Derivative Enhanced Monte Carlo Method in 2-D

The FO Taylor series approximation for $C_l$, that is $C_l$ as expressed in Eq. (3.26) is also incorporated into a SDEMC method. The SDMC approximation for $\bar{C}_l$ is given by:

\[
\bar{C}_{l_{\text{SDMC}}} (\alpha, \text{Minf}) \approx C_l(\alpha, \text{Minf}) + \frac{1}{N} \sum_{j=1}^{N} \left( C_l(\alpha_j, \text{Minf}_j) - C_l(\alpha_j, \text{Minf}_j) \right) \tag{3.32}
\]
For the SDEMC method, the total MC sample size of $N = 2500$ was divided into five independent MC samples with $N=500$. Thus, $\overline{Cl}_{SDMC}$ was calculated five times in order to lend confidence to this statistical value.

For each of the five independent sub samples, the expression $\sigma^2_{C_l-C_{li}}$ was also calculated as a measure of output function variance. The development of an expression for the variance of the second-order terms, parallels the development shown in Eqs. (3.14) through (3.19) with the result for $\sigma^2_{so}$ expressed in terms of the 2-D parameters as:

$$
\sigma^2_{so} = \left( \frac{\partial^2 C_l}{\partial a \partial M_{inf}} \right)^2 \sigma_a \sigma_{M_{inf}}
$$

(3.33)

Here again note that $\sigma^2_{so}$ is calculated as a lower limit for $\sigma^2_{C_l-C_{li}}$. The actual value of $\sigma^2_{C_l-C_{li}}$ is approximated through successive MC simulations.

The results of the flow parameter uncertainty investigation in 2-D Euler flow are presented in Chap. IV.
CHAPTER IV
UNCERTAINTY PROPAGATION RESULTS AND DISCUSSION

Presentation and discussion of results for the quasi 1-D Euler CFD and the 2-D Euler CFD uncertainty propagation are divided into four sections: function approximations, statistical first moment approximations, statistical second moment approximations, and probability density function approximations.

4.1 Function Approximations

In this section the FO and SO Taylor series output function approximations (Eqs. (3.7) and (3.8)) are compared with direct nonlinear CFD code simulations. All comparisons have been normalized, with respect the output function (M in the case of the 1-D applications, and Cl in the case of the 2-D applications.) In each application, two traces are made through the design space. Trace 1 varied the first input variable, while the second remained fixed at its mean value, and vice versa for trace 2. The required FO and SO SD needed for construction of the FO and SO Taylor series approximations were obtained as described in Sec. 1.3.

In each plot, the degree of nonlinearity associated with each individual input parameter is evident. In some applications, the CFD output function is quasi-linear with respect to the input variable of interest and therefore the FO approximations are expected to produce reasonably good results, that is, the FO statistical moment approximations and the SDEMC approximation should match well with the moments produced by an actual MC simulation.
4.1.1 Geometric Input Variable Function Approximations (1-D)

For the investigation of quasi 1-D Euler flow with geometric uncertainty, Figs. 4.1 and 4.2 illustrate that for $F = M(a,b)$, $M$ behaves as a quasi-linear function in the neighborhood of $(\bar{a}, \bar{b})$. The SO terms only contribute a discernable difference in the SO Taylor series approximations at distances further away from $(\bar{a}, \bar{b})$.

![Graph showing comparison of Taylor series function approximations vs. CFD solution, geometric input variable, b Fixed at $\bar{b}$.

Fig. 4.1 Comparison of Taylor series function approximations vs. CFD solution, geometric input variable, b Fixed at $\bar{b}$.](image)
4.1.2 Flow Input Variable Function Approximations (1-D)

For the investigation of quasi-1-D Euler CFD with flow input parameter uncertainty, Figs. 4.3 and 4.4 illustrate that for $F = M(M_{\infty}, P_b)$, the behavior of $M$ is well approximated in the neighborhood of $(\overline{M}_{\infty}, \overline{P}_b)$. In contrast to the geometric variable traces (Figs. 4.1 and 4.2), in the flow parameter traces there is noticeable nonlinear...
behavior close to the mean values of the input parameters. In general, the SO terms greatly improve the Taylor series approximations, however, Fig. 4.3 illustrates that there appears to be an inflection point in the behavior of the CFD output function when $\text{Minf} > \overline{\text{Minf}}$, that is, the FO result is better than the SO result.

Given the relatively large degree of nonlinear behavior in the flow parameter example, one would expect the SO uncertainty approximations to better predict the MC simulation output, however, one should expect even the second order approximations to loose accuracy as one encounters fluctuations further from $\text{Minf} = \overline{\text{Minf}}$ and $P_b = \overline{P_b}$.

Fig. 4.3 Comparison of Taylor series function approximations vs. CFD solution, flow input variable, $P_b$ fixed at $\overline{P_b}$.
4.1.3 Flow Input Variable Function Approximations (2-D)

For the investigation of 2-D Euler CFD with flow input parameter uncertainty, Figs. 4.5 and 4.6 illustrate that for $F = Cl(Minf, \alpha)$, the behavior of $Cl$ is well approximated in the neighborhood of $(\overline{Minf}, \overline{\alpha})$. The CFD output parameter, $Cl$, is noticeably nonlinear with respect to the free stream Mach number, Minf as shown in Fig. 4.5, whereas the first order approximation remains accurate throughout the trace in Fig. 4.6. That is, $Cl$
is quasi-linear with respect to angle of attack and nonlinear with respect to free stream Mach number. Since the function is investigated as both input parameters fluctuate, the function $C_l(M_{\infty}, \alpha)$ will exhibit nonlinear behavior largely due to fluctuations in $M_{\infty}$. As such, one would expect the SO statistical moment approximations to generate more accurate predictions of the statistical moments.

**Fig. 4.5** Comparison of Taylor series function approximations vs. CFD solution, flow input parameter, $\alpha$ fixed at $\bar{\alpha}$.
Fig. 4.6 Comparison of Taylor series function approximations vs. CFD solution, flow input parameter, Minf fixed at \( \overline{\text{Minf}} \).
4.2 First Moment Approximations

Approximations of the output function mean values are calculated for the 1-D and 2-D applications as described in Secs. 3.2-3.4. Results for all three applications, (1-D with geometric uncertainties, 1-D with flow parameter uncertainties, and 2-D with flow parameter uncertainties) are presented in this section. Recall that a range of input variance was investigated for each application. A summary of input parameter standard deviations is given in Table 4.1 below:

<table>
<thead>
<tr>
<th></th>
<th>1-D Geometric Uncertainties</th>
<th>1-D Flow Parameter Uncertainties</th>
<th>2-D Flow Parameter Uncertainties</th>
</tr>
</thead>
<tbody>
<tr>
<td>.01</td>
<td>.01</td>
<td>.01</td>
<td></td>
</tr>
<tr>
<td>.02</td>
<td>.02</td>
<td>.02</td>
<td></td>
</tr>
<tr>
<td>.04</td>
<td>.04</td>
<td>.04</td>
<td></td>
</tr>
<tr>
<td>.06</td>
<td>.06</td>
<td></td>
<td></td>
</tr>
<tr>
<td>.08</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

For each investigation, the physical nature of the problem limited the extent to which the input parameters could vary. That is, a solvable subsonic flow regime was maintained throughout each analysis.
4.2.1 First Moment Approximations with TMC Baseline

In order to assess the output function mean value approximations, a baseline for comparison must be established. The difficulty with establishing a baseline for the current investigation is that the “true” output function mean value is not known, that is the full MC simulation predicted mean contains error $\sigma_F / \sqrt{N}$. Although the sample size selected for each comparison is sufficiently large such that trends and patterns can be seen, it must be noted that even the full MC simulation is only an approximation.

For the initial assessment of the output function mean value accuracy, the mean value for each full TMC simulation serves as the baseline for comparison. That is, for the 1-D applications, the output function mean for the total sample size of $N=3000$ is the basis and for the 2-D application, the mean for the total sample of $N=2,500$ is the basis.

For the comparison of approximate methods, each total sample was divided into sub-samples with $N=500$. For each sub-sample, a mean was calculated via the traditional approach as well as the SDEMC approach. Thus we have several (six for 1-D, five for 2-D) traditional MC mean values and SDEMC mean values as well as the FO and SO first moment approximations. All values are compared to the mean values generated from the full TMC simulation. The following twelve charts depict the percent difference of each approximation from the full TMC approximation where the percent is given by:

$$\text{% Difference} = \left| \frac{\text{TMC Mean} - \text{Approximation}}{\text{TMC Mean}} \right|$$  \hspace{1cm} (4.1)

Note the “Avg MC” and the “Avg SDEMC” shown in each figure are simply an average percent difference in the given category.
Fig. 4.7 Percent difference in prediction of output mean, $\bar{M}(a, b)$ for $\sigma_a = \sigma_b = 0.01$.

(Input $\sigma = 0.02$, TMC Basis)

Fig. 4.8 Percent difference in prediction of output mean. $\bar{M}(a, b)$ for $\sigma_a = \sigma_b = 0.02$. 

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Fig. 4.9 Percent difference in prediction of output mean, $\bar{M}(a, b)$ for $\sigma_a = \sigma_b = 0.04$.

$(\text{Input } \sigma = 0.04, \text{TMC Basis})$

Fig. 4.10 Percent difference in prediction of output mean, $\bar{M}(a, b)$ for $\sigma_a = \sigma_b = 0.06$.

$(\text{Input } \sigma = 0.06, \text{TMC Basis})$
Fig. 4.11 Percent difference in prediction of output mean, $\bar{M}(a,b)$ for $\sigma_a = \sigma_b = 0.08$.

Fig. 4.12 Percent difference in prediction of output mean, $\bar{M}(\text{Minf,Pb})$ for $\sigma_{\text{Minf}} = \sigma_{\text{Pb}} = 0.01$. 

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Fig. 4.13 Percent difference in prediction of output mean, $\bar{M}(\text{Minf}, \text{Pb})$ for $\sigma_{\text{Minf}} = \sigma_{\text{Pb}} = 0.02$.

Fig. 4.14 Percent difference in prediction of output mean, $\bar{M}(\text{Minf}, \text{Pb})$ for $\sigma_{\text{Minf}} = \sigma_{\text{Pb}} = 0.04$. 

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Fig. 4.15 Percent difference in prediction of output mean, $\bar{M}(\text{Minf,Pb})$
for $\sigma_{\text{Minf}} = \sigma_{\text{Pb}} = 0.06$.

Fig. 4.16 Percent difference in prediction of output mean, $\bar{C}(\alpha,\text{Minf})$
for $\sigma_{\alpha} = \sigma_{\text{Minf}} = 0.01$. 

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Fig. 4.17 Percent difference in prediction of output mean, $\overline{Cl}(\alpha, M_{\text{inf}})$ for $\sigma_\alpha = \sigma_{M_{\text{inf}}} = 0.02$.

Fig. 4.18 Percent difference in prediction of output mean, $\overline{Cl}(\alpha, M_{\text{inf}})$ for $\sigma_\alpha = \sigma_{M_{\text{inf}}} = 0.04$.
The two most remarkable trends in each of the twelve previous figures are 1) the SDEMC approximations are much more consistent, i.e., they do not fluctuate as much as the conventional MC predictions and 2) the "Avg SDEMC" percent difference is most often smaller than the "Avg MC" percent difference. That is, the SDEMC method appears to be a better approximation for the output function mean when compared with a conventional MC simulation of similar size. With the indication that the SDEMC mean is a better approximation, one may make the conclusion that a full SDEMC baseline would be better than a full TMC baseline. Thus, another series of charts may be generated with an "Improved Baseline."

4.2.2 First Moment Approximations with Improved (SDEMC) Baseline

In both the 1-D and 2-D examples, the SDEMC predictions of the output mean are more accurate and more consistent when compared to the conventional MC predictions of equal sample size. As such, an improved baseline may be generated and used for comparison of approximate techniques. The improved baseline is taken as the average SDEMC mean value. The following figures compare the various mean values with a SDEMC baseline where the percent difference given by:

\[
\% \text{ Difference } = \frac{|\text{Avg SDEMC Mean} - \text{Approximation}|}{\text{Avg SDEMC Mean}} \quad (4.2)
\]
Fig. 4.19 Percent difference in prediction of output mean value, $\bar{M}$ for geometric input parameters, $\sigma = 0.01$ with a SDEMC baseline.

Fig. 4.20 Percent difference in prediction of output mean value, $\bar{M}$ for geometric input parameters, $\sigma = 0.02$ with a SDEMC baseline.
Fig. 4.21 Percent difference in prediction of output mean value, $\overline{M}$ for geometric input parameters, $\sigma = \sigma = 0.04$ with a SDEMC baseline.

Fig. 4.22 Percent difference in prediction of output mean value, $\overline{M}$ for geometric input parameters, $\sigma = \sigma = 0.06$ with a SDEMC baseline.
(input $\sigma = 0.08$, SDEMC Basis)

Fig. 4.23 Percent difference in prediction of output mean value, $\bar{M}$ for geometric input parameters, $\sigma = \sigma = 0.08$ with a SDEMC baseline.

(input $\sigma = 0.01$, SDEMC basis)

Fig. 4.24 Percent difference in prediction of output mean value, $\bar{M}$ for flow input parameters, $\sigma = \sigma = 0.01$ with a SDEMC baseline.
(input $\sigma = 0.02$, SDEMC Basis)

Fig. 4.25 Percent difference in prediction of output mean value, $\bar{M}$ for flow input parameters, $\sigma = \sigma = 0.02$ with a SDEMC baseline.

Fig. 4.26 Percent difference in prediction of output mean value, $\bar{M}$ for flow input parameters, $\sigma = \sigma = 0.04$ with a SDEMC baseline.
Fig. 4.27 Percent difference in prediction of output mean value, $\bar{M}$ for flow input parameters, $\sigma = \sigma = 0.06$ with a SDEMC baseline.

Fig. 4.28 Percent difference in prediction of output mean value, $\bar{C}_1$ for flow input parameters, $\sigma = \sigma = 0.01$ with a SDEMC baseline.
Fig. 4.29 Percent difference in prediction of output mean value, $\bar{C}_l$ for flow input parameters, $\sigma = \sigma = 0.02$ with a SDEMC baseline.

Fig. 4.30 Percent difference in prediction of output mean value, $\bar{C}_l$ for flow input parameters, $\sigma = \sigma = 0.04$ with a SDEMC baseline.
The most remarkable trends in each of the twelve charts comparing predictions of mean value to the improved baseline are that 1) the SDEMC approximations present an order of magnitude improvement in accuracy when compared to a traditional MC simulation of equivalent sample size (as suggested in [40]), and that 2) the SO approximate statistical first moment approximation provides a very accurate prediction of the output mean, far better than the FO in all cases. This conclusion was not apparent without the improved baseline. (Compare for example, Fig. 4.13 with 4.25 both of which pertain to prediction of output mean, $\bar{M}(M_{inf}, P_{b})$ for $M_{inf} = \sigma_{P_{b}} = 0.02$.)

In Table 4.2, each prediction of the output function mean is assessed for computational requirements. For the given investigation, clearly the FO and SO approximate statistical moment prediction of mean are most efficient, that is the computational cost of obtaining SD is minimal when compared to the large number (500) of samples required in the MC and SDEMC approaches. Note that when obtaining SD via the approach demonstrated in [19], the calculation of SO SD is direct once the forward and reverse FO SD are obtained. In the present study where NDV = 2 and NOF = 1, the calculation of the forward and reverse FO SD were approximately equal in computational requirements to the calculation of one CFD analysis.

<table>
<thead>
<tr>
<th></th>
<th>MC</th>
<th>SDEMC</th>
<th>FO</th>
<th>SO</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFD Analyses</td>
<td>500</td>
<td>500</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>FO SD Analyses</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2a</td>
</tr>
<tr>
<td>SO SD Analyses</td>
<td>0</td>
<td>0</td>
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<td>1</td>
</tr>
</tbody>
</table>

$^a$ One forward and one adjoint variable calculation of FO SD required for SO SD

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Although both the FO and SO approximate statistical first moments are computationally efficient, the increase in accuracy afforded by the SO analysis makes this method a much better prediction at higher input parameter variance. Figs. 4.31 through 4.33 illustrate how the accuracy of the FO, SO and MC predictions is effected with increases in input parameter standard deviation. Although the FO prediction loses accuracy, the SO prediction continues to consistently approximate the output function well even at increased input variance. Also note the lack of consistency in the full MC predictions. The SO prediction of output function mean appears to a consistent, accurate and efficient method for prediction of the first statistical moment.

Fig. 4.31 Trends in accuracy for FO, SO and MC mean value approximations, with geometric uncertainties in 1-D flow.
Fig. 4.32 Trends in accuracy for FO, SO and MC mean value approximations, with flow parameter uncertainties in 1-D flow.

Fig. 4.33 Trends in accuracy for FO, SO and MC mean value approximations, with flow parameter uncertainties in 2-D flow.
The current investigation has demonstrated that 1) the SDEMC prediction of the first moment affords an order of magnitude increase in accuracy when compared to traditional MC methods, 2) the FO and SO approximate statistical moments are accurate and very efficient methods for approximating the output function mean, and 3) the SO approximate statistical moment is a very accurate prediction even at increased input parameter standard deviations. Results for the prediction of the second moment are now presented.

4.3 Second Moment Approximations

Approximations of the output function variance are calculated for the 1-D and 2-D applications. Results for all three applications, (1-D flow with geometric uncertainties, 1-D flow with flow parameter uncertainties, and 2-D flow with flow parameter uncertainties) are presented in this section. The same twelve sets of input parameters (see Table 4.1) are presented.

4.3.1 Second Moment Approximations with TMC Baseline

In order to assess the output function variance approximations, a baseline for comparison must be established. Similar to the first statistical moment analysis, the difficulty with establishing a baseline is that the "true" output function variance is not known. Note that the error associated with a MC predicted variance is greater than that associated with predicting the mean. The sample size selected for this investigation may not be sufficiently large in order to determine an accurate baseline for comparison. That is, the error associated with the baseline may make it difficult to determine trends.
or patterns associated with the FO and SO variance approximations. Note that there is not a SDEMC prediction of variance or standard deviation for the output function. A percent difference is calculated with respect to the full TMC standard deviation:

\[
\text{\% Difference} = \frac{|\text{TMC STDEV} - \text{Approximation}|}{\text{TMC STDEV}}
\]  

(4.3)

The standard deviation is presented in lieu of the variance for the sake of better resolution with values in the "\% Difference" calculations.

For each input parameter investigation, the full MC sample was again divided into sub-samples. For the 1-D applications, the total sample size of $N=3000$ was divided into six sub-samples of $N=500$ and for the 2-D applications, the total sample size of $N=2,500$ was divided into five sub-samples of $N=500$. For each sub-sample, a variance was calculated using Microsoft Excel software. The square root of the variance, the standard deviation was then calculated. These MC standard deviation values as well as the FO and SO approximations are compared to the standard deviation generated from the complete TMC simulation. The following twelve charts depict the percent difference of each approximation from the TMC standard deviation.
Fig. 4.34 Percent difference in prediction of output standard deviation, $\sigma_M$
for $\sigma_a = \sigma_b = 0.01$.

Fig. 4.35 Percent difference in prediction of output standard deviation, $\sigma_M$
for $\sigma_a = \sigma_b = 0.02$. 

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Fig. 4.36 Percent difference in prediction of output standard deviation, $\sigma_M$
for $\sigma_a = \sigma_b = 0.04$.

Fig. 4.37 Percent difference in prediction of output standard deviation, $\sigma_M$
for $\sigma_a = \sigma_b = 0.06$. 

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Fig. 4.38 Percent difference in prediction of output standard deviation, $\sigma_M$
for $\sigma_a = \sigma_b = 0.08$.

Fig. 4.39 Percent difference in prediction of output standard deviation, $\sigma_M$
for $\sigma_{Minf} = \sigma_{Pb} = 0.01$. 

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Fig. 4.40 Percent difference in prediction of output standard deviation, $\sigma_M$ for $\sigma_{Minf} = \sigma_{Pb} = 0.02$.

Fig. 4.41 Percent difference in prediction of output standard deviation, $\sigma_M$ for $\sigma_{Minf} = \sigma_{Pb} = 0.04$.

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4.42 Percent difference in prediction of output standard deviation, $\sigma_M$ for $\sigma_{\text{Minf}} = \sigma_{\text{Pb}} = 0.06$.

Fig. 4.42

4.43 Percent difference in prediction of output standard deviation, $\sigma_C$ for $\sigma_{\text{Minf}} = \sigma_{\text{a}} = 0.01$.

Fig. 4.43
Fig. 4.44 Percent difference in prediction of output standard deviation, $\sigma_{C1}$ for $\sigma_{Minf} = \sigma_\alpha = 0.02$.

Fig. 4.45 Percent difference in prediction of output standard deviation, $\sigma_{C1}$ for $\sigma_{Minf} = \sigma_\alpha = 0.04$.
The most remarkable trends in each of the twelve charts are 1) the accuracy of the MC standard deviation predictions tends to fluctuate a large amount, 2) the FO and SO predictions are occasionally a better prediction than the average MC (Avg MC) prediction, and 3) the SO prediction does not offer much improvement in accuracy over the FO prediction. Clearly the lack of significant trends is in part attributed to the error contained in the basis for comparison.

Although such results may not seem significant it is worthy to note that the FO and SO predictions are obtained without great computational expense. Table 4.2, “Computational Requirements for Prediction of Output Function Mean” also applies to the prediction of output function variance or standard deviation. Thus the FO and SO predictions of variance are efficient, but the level of accuracy in such predictions is still questionable.

4.3.2 Variance of the FO Taylor Series Remainder

In order to more fully investigate the variation in the output function of interest, the variance of the FO Taylor series remainder, $\sigma^2_{M-M_1}$ for the 1-D flow regime, and $\sigma^2_{CI-Cl_1}$ for the 2-D flow regime are considered. In the following figures the standard deviation of the actual CFD function minus the FO approximation are presented. i.e. $\sigma_{M-M_1}$ and $\sigma_{CI-Cl_1}$ for each sub-sample where N=500 samples. Here again the standard deviation is presented in lieu of the variance for the purpose of bringing better resolution to the values. For each input parameter $\sigma$, the resulting $\sigma_{M-M_1}$ for 1-D flow, or $\sigma_{CI-Cl_1}$ for 2-D flow is plotted.
Fig. 4.46 Standard deviations of Taylor series remainder for 1-D flow with uncertainties in geometric parameters.

Fig. 4.47 Standard deviations of Taylor series remainder for 1-D flow with uncertainties in flow parameters.
Fig. 4.48 Standard deviations of Taylor series remainder for 2-D flow with uncertainties in flow parameters.

As expected, the results indicate that for small input standard deviations, the standard deviation of the FO Taylor series remainder is small. As the standard deviations of the input parameters increase, so does the standard deviations of the FO Taylor series remainder. That is, with increases in input parameter \( \sigma \), the higher order terms have a greater impact on the output function and the CFD function is no longer well represented by a FO Taylor series approximation. This result is clearly seen in the preceding three figures, however, great computational expense was dedicated to creating such results. The figures were created through analysis of the 3,000 sample 1-D MC simulation and the 2,500 sample 2-D simulation. As suggested in Chap. II, knowledge of the SO SD may be employed to predict the minimum value of the FO Taylor series variance.
In the following five figures, the straight dashed line below each solid line represents the Minimum($\sigma_{F_i-F_i}$) or $\sigma_{\text{SOTerms}}$. The calculation of the $\sigma^2_{\text{SOTerms}}$ as well as the standard deviation, $\sigma_{\text{SOTerms}}$, is performed with knowledge of the SO SD, that is without any MC simulation. One can see that $\sigma_{\text{SOTerms}}$ (represented as “SO Pred”) is indeed a true minimum for the standard deviation of the FO Taylor series remainder. The ability to calculate this value without computationally expensive MC simulations is very useful for the value provides insight into how spread out the Taylor series remainder is. It can be deduced that if the Taylor series remainder has a large spread or variance, then so does the function itself for the Taylor series remainder is a component of the actual function.

Although the standard deviation, $\sigma_{\text{SOTerms}}$ is only a minimum standard deviation for the FO Taylor series reminder, one should notice the scaling of figures, is intended to illustrate the distance between $\sigma_{F_i-F_i}$ and the “SO Pred”. The order of magnitude for this difference is in the thousandths (i.e. relatively small) in Figs. 4.49 and 4.51.
Fig. 4.49 SO predictions of $\sigma$ for Taylor series remainder, small uncertainties ($\sigma = 0.01, 0.02$) in geometric parameters.

Fig. 4.50 SO predictions of $\sigma$ for Taylor series remainder, larger uncertainties ($\sigma = 0.04, 0.06, 0.08$) in geometric parameters.
Fig. 4.51 SO predictions of $\sigma$ for Taylor series remainder, 1-D Flow with small uncertainties ($\sigma = 0.01, 0.02$) in flow parameters.

Fig. 4.52 SO predictions of $\sigma$ for Taylor series remainder, 1-D flow with larger uncertainties ($\sigma = 0.04, 0.06$) in flow parameters.
Fig. 4.53 SO predictions of $\sigma$ for Taylor series remainder, 2-D flow with uncertainties in flow parameters.

With limited knowledge of the output function mean, the output function variance, and the variance of the Taylor series remainder, one may draw conclusions about the propagation of input parameter uncertainty through CFD. Employing FO and SO CFD SD, these conclusions can be made with much less computational expense. None of these parameters however, fully describe the probability distribution of the CFD output function. The following section presents an in-depth look at the actual probability distribution for the CFD output.

### 4.4 Probability Density Function Approximations

Given the mean and standard deviation of the CFD output function (from either a Monte Carlo simulation or a FO or SO prediction) and assuming a normal distribution,
one may then construct a probability density function to approximate the behavior of the non-deterministic output function. This normal curve approximation is compared to the PDF histogram generated from the full Monte Carlo simulation. In Figs. 4.54-4.63, the bars depict the Monte Carlo simulation histograms representing 3000 samples for the 1-D investigations, or the 2500 samples for the 2-D investigations. The solid curves are the normal distributions at the Monte Carlo mean value and Monte Carlo standard deviation. The Monte Carlo simulation size of either 3000 or 2500 is certainly not sufficient to obtain a smooth PDF but the degree to which the output function produces a normal distribution may be ascertained.

It is apparent that in most cases the normal approximations are good for a significant region about the mean but tend to break down in predicting the tails of the distribution. This is significant, for if one is primarily interested in reliable failure predictions, as for structural design, this prediction may not be good enough. It is felt, however that in aerodynamic performance optimization using CFD, where robustness about the mean is desired, these approximations may be good enough.

The following figures illustrate that for small input standard deviations, the output function distributions are well approximated by normal distribution curves. As the input standard deviations increase, the normal curves tend to loose accuracy in the tails of the distribution and in some cases also near the mean of the distribution.

In the investigation of quasi 1-D flow with geometric uncertainties, recall that M(a,b) exhibits quasi-linear behavior in regions near the input parameter mean values as shown in Figs. 4.1 and 4.2. As one moves further away from the input mean values, the nonlinearities in the function become more pronounced. Accordingly, with a small
input standard deviation \((\sigma_a = \sigma_b = 0.01)\), the output function histogram is somewhat well approximated by a normal curve as shown in Fig. 4.54. (Note that the jaggedness in the PDF may be attributed to the fine bin spacing which is necessary to give resolution to the tails of the PDF.) As the input standard deviations increase, one begins to loose accuracy in predicting the distribution, especially the tails of the distribution as shown in Figs. 4.55 and 4.56.

Fig. 4.54 Probability density function for \(M(a,b)\) for \(\sigma_a = \sigma_b = 0.01\).
Fig. 4.55 Probability density function for $M(a,b)$ for $\sigma_a=\sigma_b=0.04$. 

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Fig. 4.56 Probability density function for $M(a,b)$ for $\sigma_a = \sigma_b = 0.08$. 

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Recall that in the quasi-1-D investigation, the flow parameter uncertainty study illustrated a much more nonlinear system (see Figs. 4.3 and 4.4.) Accordingly, the PDFs deviate more from the normal distribution curves as the system fluctuations grow. In Figs. 4.57 and 4.58 where the input standard deviations are relatively small, the normal PDF approximates the MC histogram reasonably well near the mean value and at the tails of the distribution. (Here again note that the bin size must be small to provide adequate visibility into behavior at the tails of the distribution.) As the input standard deviations increase, the normal behavior of the output function deteriorates to the point where the normal PDF is not a good representation of the output function distribution both at the tails and at the means values of the PDF as shown in Figs. 4.59 and 4.60. In summary, one can only expect a normal PDF to replicate the CFD histogram for a quasi-linear function.
Fig. 4.57 Probability density function for $M(M_{\text{inf}},P_b)$ for $\sigma_{M_{\text{inf}}} = \sigma_{P_b} = 0.01$. 

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Fig. 4.58 Probability density function for $M(M_{\text{in}}, P_b)$ for $\sigma_{M_{\text{in}}} - \sigma_{P_b} = 0.02$. 

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Fig. 4.59 Probability density function for $M(M_{\text{inf}}, P_b)$ for $\sigma_{M_{\text{inf}}} = \sigma_{P_b} = 0.04$. 

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Fig. 4.60 Probability density function for $M(M_{\text{inf}}, P_b)$ for $\sigma_{M_{\text{inf}}}=\sigma_{P_b}=0.06$. 

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In the 2-D investigations, Figs. 4.61-63 illustrate the effect of increasing the input flow parameter standard deviation on the shape of the PDF. All three figures depict slight skewness, that is the normal curve and the actual MC histograms are slightly offset. Note that the extent of this offset or disagreement increases as the input standard deviation increases. As seen in the 1-D examples, behavior of the non-deterministic output functions is not well approximated by the normal curves when one is concerned with the tails of the distributions.

Fig. 4.61 Probability density function for Cl ($\alpha, M_{inf}$) for $\sigma_\alpha = \sigma_{M_{inf}} = 0.01$. Reproduced with permission of the copyright owner. Further reproduction prohibited without permission.
Fig. 4.62 Probability density function for $C_l (\alpha, M_{\infty})$ for $\sigma_{\alpha} = \sigma_{M_{\infty}} = 0.02$. 

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Fig. 4.63 Probability density function for $\text{Cl} (\alpha, \text{Minf})$ for $\sigma = \sigma_{\text{Minf}} = 0.04$. 

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This section illustrates that no matter how accurate the prediction of the first and second statistical moments, a normal curve approximation may not adequately represent the CFD output function PDF. It is apparent that in most cases the normal approximations are good for a significant region about the mean but tend to break down in predicting the tails of the distribution. This is significant, for in applications where robustness about the mean is desired, the normal curve approximations may suffice.
CHAPTER V
ROBUST OPTIMIZATION IN CFD

5.1 Introduction

In gradient-based optimization, input data and parameters are often assumed precisely known leading to deterministic or conventional optimization. When statistical uncertainties exist in the input data or parameters, however, these uncertainties affect the design and therefore should be accounted for in the optimization. In the present work, robust optimization procedures are applied to the 1-D and 2-D model problems with input parameter uncertainties as presented in Chap. III.

Note again the importance of the SD. Not only does the SD contain information which is valuable in the prediction of output parameter uncertainties, the SD are also employed to direct the optimization search; that is, the objective and constraint gradients are functions of the CFD SD. The gradient-based robust optimization demonstrated herein for both the 1-D and 2-D model problems requires both FO and SO SD from the CFD code.

5.2 Conventional Optimization

Conventional optimization for an objective function, Obj, that is a function of the CFD output, F, state variables, Q, and input variables, b, is routinely expressed as shown in Eq. (5.1). Herein, the CFD state equation residuals, R, are represented as an equality constraint, and other system constraints, g, are represented as inequality constraints.
constraints. The input variables, \( b \), are precisely known, and all functions of \( b \) are therefore deterministic.

\[
\min \text{ Obj}, \quad \text{Obj} = \text{Obj}(F,Q,b) \\
\text{subject to} \quad R(Q,b) = 0 \\
\quad g(F,Q,b) \leq 0 \tag{5.1}
\]

5.3 Robust Optimization

For robust design, the conventional optimization shown in Eq. (5.1) must be treated in a probabilistic manner. Given uncertainty in the input variables, \( b \), all functions in Eq. (5.1) are no longer deterministic. The design variables are now the mean values, \( \bar{b} = \{ \bar{b}_1, ..., \bar{b}_n \} \), where all elements of \( \bar{b} \) are assumed statistically independent and normally distributed with standard deviations \( \sigma_b \). The state equation residual equality constraint, \( R \), is deemed to be satisfied at the expected values of \( Q \) and \( b \), that is the mean values \( \bar{Q} \) and \( \bar{b} \). The objective function is cast in terms of expected values and becomes a function of \( \bar{F} \) and \( \sigma_F \). The other constraints are cast into a probabilistic statement: the probability that the constraints are satisfied is greater than or equal to a desired or specified probability, \( P_k \). This probability statement is transformed into a constraint involving mean values and standard deviations under the assumption that variables involved are normally distributed as suggested in [20]. The robust optimization can be expressed as
\[
\begin{align*}
\text{min} & \quad \text{Obj} = \text{Obj}(\overline{F}, \sigma_F, \overline{Q}, \overline{b}) \\
\text{subject to} & \quad \mathbf{R}(\overline{Q}, \overline{b}) = 0 \\
& \quad g(\overline{F}, \overline{Q}, \overline{b}) + k\sigma_g \leq 0,
\end{align*}
\]

where \( k \) is the number of standard deviations, \( \sigma_g \), that the constraint \( g \) must be displaced in order to achieve the desired or specified probability, \( P_k \). First-order approximations of the mean values, and the standard deviations may be employed as shown in Eqs. (2.9) and (2.10) to generate a FO robust optimization scheme. Note the square root of the variance must be taken to generate the FO standard deviations terms: An example of this FO standard deviation approximation is given in Eq. (5.3).

\[
\sigma_{F_1} = \sqrt{\frac{\sigma_{F_1}^2}{\sum_{i=1}^{n} \left( \frac{\partial F}{\partial b_i} \sigma_{b_i} \right)^2}}
\]

Accordingly, a FO robust optimization applied to CFD code can be expressed as:

\[
\begin{align*}
\text{min} & \quad \text{Obj} = \text{Obj}(\overline{F}_1, \sigma_{F_1}, \overline{Q}, \overline{b}) \\
\text{subject to} & \quad \mathbf{R}(\overline{Q}, \overline{b}) = 0 \\
& \quad g(\overline{F}_1, \overline{Q}, \overline{b}) + k\sigma_{g_1} \leq 0,
\end{align*}
\]

Note that the standard deviation terms, \( \sigma_{F_1} \) and \( \sigma_{g_1} \) contain FO SD and therefore, a gradient-based optimization will then require SO SD to compute both the objective and constraint gradients. Note that for a SO approximation of the standard deviations, a third-order SD would be required for these gradients.
The conventional and robust optimizations as represented with Eqs. (5.1) and (5.4) were performed for the 1-D and 2-D model CFD problems incorporating the input variables and output functions described in Chap. III. Both conventional and robust optimizations are performed using the Sequential Quadratic Programming (SQP) method option in the Design Optimization Tools, DOT [52]. The SD required for the optimization are obtained as described in Sec. 1.3 or by hand.

### 5.4 Robust Optimization in Euler CFD

Applying the methodology described in Sec. 5.1 allows for demonstration of three robust optimization examples. In each of the three examples, (1-D with geometric variables, 1-D with flow variables, and 2-D with flow variables), the robust optimization results will be compared to conventional optimization results.

#### 5.4.1 Robust Shape Optimization in 1-D Euler CFD

For the 1-D shape optimization, the objective function will be a function of the aerodynamic output function as described in Sec. 3.2, i.e. \( F = M(M(a,b),a,b) \). Applying the conventional optimization previously described yields

\[
\begin{align*}
\min & \quad \text{Obj}, \\
\text{subject to} & \quad R(M,a,b) = 0 \\
& \quad V(a,b) \leq 0,
\end{align*}
\]

(5.5)

where the system constraint, \( V \), is a constraint on the nozzle volume and depends only on \( a \) and \( b \); and the objective does not explicitly depend on the state variable, \( M \).
Formulating the robust optimization problem as described by Eq. set (5.4) yields:

\[
\min \text{Obj,} \quad \text{Obj} = \text{Obj}(\bar{M}_1, \sigma_{M_1}, \bar{a}, \bar{b})
\]

subject to

\[
\begin{align*}
\mathbf{R}(\bar{M}_1, \bar{a}, \bar{b}) &= 0 \\
V(\bar{a}, \bar{b}) + k\sigma_V &\leq 0,
\end{align*}
\]

where

\[
\sigma_V = \sqrt{\left(\frac{\partial V}{\partial a} \sigma_a\right)^2 + \left(\frac{\partial V}{\partial b} \sigma_b\right)^2}.
\] (5.7)

With \(a\) and \(b\) subject to statistical uncertainties, the nozzle volume, \(V\) becomes uncertain. Recall the nozzle volume is linearly dependent on \(a\) and \(b\) and therefore is also normally distributed. Therefore, its standard deviation, \(\sigma_V\), is given exactly by Eq. (5.7).

To demonstrate the optimizations, a simple target-matching problem is selected; a unique answer is obtained when an equality volume constraint is enforced. The CFD code is run for a given \(a\) and \(b\); the resulting \(M(a,b)\) and corresponding \(V(a,b)\) are taken as the target values \(M_t\) and \(V_t\), respectively. For this conventional optimization, the objective function and constraint functions are represented as:

\[
\begin{align*}
\min \text{Obj} \quad \text{Obj}(M,a,b) &= [M(a,b) - M_t]^2 \\
\text{Subject to} \quad \mathbf{R}(M,a,b) &= 0 \\
&\quad V(a,b) - V_t = 0 \quad \text{(5.8)}
\end{align*}
\]

enforced as

\[
\begin{align*}
V(a,b) - V_t &\leq 0 \quad \text{and} \quad V_t - V(a,b) \leq 0
\end{align*}
\]

For robust optimization, the corresponding objective and constraints become:
min \text{Obj} \quad \text{Obj} (\bar{M}_t, \sigma_{M_t}, \bar{a}, \bar{b}) = [\bar{M}(\bar{a}, \bar{b}) - M_t]^2 + \sigma_{M_t}^2

Subject to \quad R(\bar{M}_t, \bar{a}, \bar{b}) = 0
\quad V(\bar{a}, \bar{b}) - V_t + k \sigma_V = 0
enforced as
\quad V(\bar{a}, \bar{b}) - V_t + k \sigma_V \leq 0
and
\quad V_t - V(\bar{a}, \bar{b}) - k \sigma_V \leq 0 \tag{5.9}

Note that for \sigma_a = \sigma_b = 0 in Eq. (5.9), the conventional optimization is obtained.

Also, in the probabilistic statement of the constraint on \( V \), it is assumed that the desired volume is less than or equal to the target volume, \( V_t \).

The 1-D geometric robust optimization scheme represented by Eq. set (5.9) is investigated for various input parameter standard deviations and for various probabilities of constraint satisfaction.

5.4.2 Robust Design For Flow Control in 1-D Euler CFD

For the 1-D flow control optimization, the objective function will be a function of the aerodynamic output function as described in Sec. 3.3; \( F=M(M(\text{Minf, Pb}), \text{Minf, Pb}) \).

The conventional optimization is expressed as

\[ \text{min Obj} \quad \text{Obj} = \text{Obj}(\text{M, Minf, Pb}) \]
\[ \text{subject to} \quad \text{R}(\text{M, Minf, Pb}) = 0 \]
\[ q(\text{Minf, Pb}) \leq 0 \tag{5.10} \]

where \( q \) is a constraint on the mass flux through the nozzle.
The robust optimization is expressed as

\[
\min \text{Obj}, \quad \text{Obj} = \text{Obj}(\bar{M}_1, \sigma_{M_1}, \bar{M}_{\text{inf}}, \bar{P}_b)
\]

subject to

\[
\begin{align*}
\mathbf{R}(\bar{M}, \bar{M}_{\text{inf}}, \bar{P}_b) &= 0 \\
\mathbf{q}(\bar{M}_{\text{inf}}, \bar{P}_b) + k \sigma_{q_1} &\leq 0
\end{align*}
\]

(5.11)

For the free stream Mach number, \(M_{\text{inf}}\), and the nozzle back pressure, \(P_b\), subject to statistical uncertainties, the mass flux, \(q\), becomes uncertain. Since \(q\) is dependent on \(M_{\text{inf}}\) and \(P_b\), its FO standard deviation, may be approximated by

\[
\sigma_{q_1} = \sqrt{\left(\frac{\partial q}{\partial M_{\text{inf}}} \sigma_{M_{\text{inf}}}\right)^2 + \left(\frac{\partial q}{\partial P_b} \sigma_{P_b}\right)^2}
\]

(5.12)

Since \(q\) is not a linear function of \(M_{\text{inf}}\) and \(P_b\), the equation for \(\sigma_q\) is not exact (unlike the previous example where \(\sigma_V\) was exactly known).

To demonstrate the optimizations, a simple target-matching problem is again chosen. The CFD code is run for given \(M_{\text{inf}}\) and \(P_b\); the resulting \(M\) and corresponding \(q\) are taken as the target values \(M_t\) and \(q_t\), respectively. For this conventional optimization, the objective function and constraint functions are:

\[
\begin{align*}
\min \text{Obj} &\quad \text{Obj}(M, M_{\text{inf}}, P_b) = [M(M_{\text{inf}}, P_b) - M_t]^2 \\
\text{Subject to} &\quad \mathbf{R}(M, M_{\text{inf}}, P_b) = 0 \\
&\quad q(M_{\text{inf}}, P_b) - q_t = 0 \\
enforced as &\quad q(M_{\text{inf}}, P_b) - q_t \leq 0 \\
&\quad q_t - q(M_{\text{inf}}, P_b) \leq 0
\end{align*}
\]

(5.13)
For robust optimization, the corresponding objective and constraints become:

\[
\begin{align*}
\min \text{Obj} & \quad \text{Obj}(\overline{M}_1, \sigma_{M_1}, \overline{M}_{\text{inf}}, \overline{P}_b) = [\overline{M}(\overline{M}_{\text{inf}}, \overline{P}_b) - M_t]^2 + \sigma_{M_t}^2 \\
\text{Subject to} & \quad R(\overline{M}, \overline{M}_{\text{inf}}, \overline{P}_b) = 0 \\
& \quad q(\overline{M}_{\text{inf}}, \overline{P}_b) - q_t + k \sigma_{q_t} = 0 \\
\text{enforced as} & \quad q(\overline{M}_{\text{inf}}, \overline{P}_b) - q_t + k \sigma_{q_t} \leq 0 \\
& \quad \text{and } q_t - q(\overline{M}_{\text{inf}}, \overline{P}_b) - k \sigma_{q_t} \leq 0
\end{align*}
\]

Again note that for \( \sigma_{M_{\text{inf}}} = \sigma_{P_b} = 0 \) in Eq. (5.14), the conventional optimization is obtained. Also, in the probabilistic statement of the constraint on \( q \), it is assumed that the desired mass flux is less than or equal to the target mass flux, \( q_t \).

As in the geometric robust optimization scheme, the robust optimization for flow control represented by Eq. set (5.14) is investigated for various input parameter standard deviations and for various probabilities of constraint satisfaction.

### 5.4.3 Robust Design For Flow Control in 2-D Euler CFD

For the 2-D flow control optimization, the objective function will be a function of the aerodynamic output function as described in Sec. 3.4; \( F = \text{Cl}(Q(\overline{M}_{\text{inf}}, \alpha), X, \overline{M}_{\text{inf}}, \alpha) \)

Note that the computational grid remains fixed throughout the optimization, and that the state variables, \( Q \) are not explicitly found in the input or output terms. Accordingly, one can simplify the output function notation as \( F = \text{Cl}(\overline{M}_{\text{inf}}, \alpha) \).
The conventional optimization may be expressed as

\[
\begin{align*}
\min \text{Obj} & \quad \text{Obj} = \text{Obj}(C_l, M_{\text{inf}}, \alpha) \\
\text{subject to} & \quad R(M_{\text{inf}}, \alpha) = 0 \\
& \quad C_m(M_{\text{inf}}, \alpha) \leq 0
\end{align*}
\]

(5.15)

where \( C_m \) is the pitching moment coefficient for the airfoil.

The robust optimization may be expressed as

\[
\begin{align*}
\min \text{Obj}, & \quad \text{Obj} = \text{Obj}(\overline{C_l}, \sigma_{C_l}, M_{\text{inf}}, \overline{\alpha}) \\
\text{subject to} & \quad R(M_{\text{inf}}, \overline{\alpha}) = 0 \\
& \quad C_m(M_{\text{inf}}, \overline{\alpha}) + k \sigma_{C_m} \leq 0
\end{align*}
\]

(5.16)

For the free stream Mach number, \( M_{\text{inf}} \), and the angle of attack, \( \alpha \), subject to statistical uncertainties, the pitching moment coefficient, \( C_m \), becomes uncertain. Since \( C_m \) is dependent on \( M_{\text{inf}} \) and \( \alpha \), its FO standard deviation, \( \sigma_{C_m} \), may be approximated by

\[
\sigma_{C_m} = \sqrt{\left( \frac{\partial C_m}{\partial M_{\text{inf}}} \sigma_{M_{\text{inf}}} \right)^2 + \left( \frac{\partial C_m}{\partial \alpha} \sigma_{\alpha} \right)^2}
\]

(5.17)

To demonstrate the optimizations, a simple target-matching problem is again selected; a unique answer is obtained when an equality constraint is enforced. The CFD code is run for given \( \alpha \) and \( M_{\text{inf}} \); the resulting \( C_l(\alpha,M_{\text{inf}}) \) and corresponding \( C_m(\alpha,M_{\text{inf}}) \) are taken as the target values \( C_{lt} \) and \( C_{mt} \), respectively. For this conventional optimization, the objective function and constraint are cast as
\[
\begin{align*}
\min \text{Obj} \quad & \text{Obj} = \text{Obj}(C_l, \alpha, M_{\text{inf}}) = [C_l(\alpha, M_{\text{inf}}) - C_{lt}]^2 \\
\text{Subject to} \quad & R(\alpha, M_{\text{inf}}) = 0 \\
& C_m(\alpha, M_{\text{inf}}) - C_{mt} = 0 \\
\text{enforced as} \quad & C_m(\alpha, M_{\text{inf}}) - C_{mt} \leq 0 \\
& \text{and } C_{mt} - C_m(\alpha, M_{\text{inf}}) \leq 0.
\end{align*}
\] (5.18)

For robust optimization, the corresponding objective and constraints become:

\[
\begin{align*}
\min \text{Obj} \quad & \text{Obj}(\bar{C}_l, \sigma_{C_l}, M_{\text{inf}}, \bar{\alpha}) = [\bar{C}_l(M_{\text{inf}}, \bar{\alpha}) - C_{lt}]^2 + \sigma_{C_l}^2 \\
\text{Subject to} \quad & R(M_{\text{inf}}, \bar{\alpha}) = 0 \\
& C_m(M_{\text{inf}}, \bar{\alpha}) - C_m + k \sigma_{C_m} = 0 \\
\text{enforced as} \quad & C_m(M_{\text{inf}}, \bar{\alpha}) - C_{mt} + k \sigma_{C_m} \leq 0 \\
& \text{and } C_{mt} - C_m(M_{\text{inf}}, \bar{\alpha}) - k \sigma_{C_m} \leq 0.
\end{align*}
\] (5.19)

Again note that for $\sigma_{M_{\text{inf}}} = \sigma_\alpha = 0$ in Eq. (5.19), the conventional optimization is obtained. Also, in the probabilistic statement of the constraint on $C_m$, it is assumed that the desired moment coefficient is less than or equal to the target coefficient, $C_{mt}$. Eq. set (5.19) is investigated for various input parameter standard deviations and for various probabilities of constraint satisfaction. The results for the robust optimization investigations are presented in Chap. VI.
CHAPTER VI

ROBUST OPTIMIZATION RESULTS AND DISCUSSION

Optimization results were generated using the methodology described in Chap. V for each model problem. For each set of objective functions and system constraints, two probabilistic cases are presented. For case 1, the probability of constraint satisfaction $P_k$ is fixed at $k=1$, i.e., $P_1=84.13\%$, and the effect of increasing the input variable standard deviations is addressed. For case 2, the standard deviations of the input variables are fixed at 0.01 and $P_k$ increases from 50\% (conventional optimization), to 99.99\%.

6.1 Robust Shape Optimization Results

Robust shape optimization results were generated using the quasi 1-D Euler CFD code and the procedure described in Sec. 5.4.1. As noted earlier, conventional optimization is obtained for $\sigma_a = \sigma_b = 0$. Note that FO SD are required to obtain $\sigma_{M_1}$; and therefore, SO SD will be required for the derivative of, $\sigma_{M_1}$ which is necessary in the gradient-based optimization. The SO SD required for the robust optimization were obtained by the manner presented in Sec. 1.3 with the exception of derivatives involving the nozzle volume. Since the nozzle volume is a linear function with respect to the geometric shape parameters, all SD were obtained by hand differentiation.
It is seen from Eq. (5.9) that the robust optimization results depend on the probabilistic parameters \((\sigma_a, \sigma_b)\) and \(k\). The desired probability, \(P_k\), is that from the normal cumulative distribution function since \(\sigma_Y\) here is also normally distributed.

In Fig. 6.1 and Table 6.1, results for case 1 of the robust shape optimization are displayed. For \(\sigma_a=\sigma_b\) ranging from 0 to 0.08, optimal values for the input variables \((a, b)\) are listed. As \(\sigma_a=\sigma_b\) increases, so does \(\sigma_V\). Accordingly, the mean values, \((\bar{a}, \bar{b})\), which minimize the objective function and satisfy the probabilistic constraint, become increasingly displaced from the values which yield the target volume, \(V_t\) as shown. Mean values \((\bar{a}, \bar{b})\) change, keeping the mean value, \(\overline{M(a, b)}\), of the probabilistic output near the target value, \(M_t\). The robust design points track the dashed curve for \(\overline{M} = M_t\) with some displacement due to the \(\sigma_{M_t}^2\) term of the objective function as given in Eq. (5.9). Also notice that \(V(\bar{a}, \bar{b})\) is displaced from the solid curve \(V = V_t\) by \(k\sigma_V\), as required by the probabilistic constraint. This displacement can be viewed as the solution dependent or "effective" safety margin.
Fig. 6.1 Optimization results in design space (a,b) for case 1, P_k fixed at P_1.
In Fig. 6.2 the changing area distribution of the robust optimization presented in case 1 is illustrated. As the standard deviations of design variables increase, the optimal design point, $(\overline{a}, \overline{b})$, changes resulting in a non-deterministic area distribution. With increasing input parameter $\sigma$, it is evident that the shape parameter optimization significantly alters the nozzle shape.

![Graph showing changing area distribution for robust shape optimization as input $\sigma$ increases.](image)

**Fig. 6.2** Changing area distribution for robust shape optimization as input $\sigma$ increases.

The results for case 2 of the robust shape optimization, where $\sigma_a = \sigma_b$ is fixed at 0.01, and $P_k$ increases from 50 percent to 99.99 percent ($k=0$ to 4) are given in Table 6.2.
Again mean values \((\bar{a}, \bar{b})\) change, keeping the mean value, \(\bar{M}(\bar{a}, \bar{b})\), of the probabilistic output near the target value, \(M_t\). Since \(\sigma_t = \sigma_b\) remains small, the \(\sigma_{M_1}^2\) term of the objective remains small, and the displacement of \(\bar{M}\) from the dashed line depicting \(M_t\) due to the \(\sigma_{M_1}^2\) term remains small as shown in Fig. 6.3. With an increase in \(P_k\), \(V(\bar{a}, \bar{b})\) is displaced from the solid curve \(V = V_t\) by \(k\sigma_V\), as required by the probabilistic constraint. Accordingly, the mean values, \((\bar{a}, \bar{b})\), which minimize the objective function and satisfy the constraint, again become increasingly displaced from those at the target volume, \(V_t\). Note the significant displacement of the solution from the target volume when \(P_k\) is large, i.e., when one is attempting to incorporate the tails of the pdf. In order to increase the probability of constraint satisfaction from 97.77 percent to 99.99 percent, one sees a significant change in \((\bar{a}, \bar{b})\) for a mere gain of 2 percent in constraint satisfaction.
Table 6.2 Robust shape optimization results for case 2

<table>
<thead>
<tr>
<th>K</th>
<th>P_k</th>
<th>(\bar{a})</th>
<th>(\bar{b})</th>
<th>Obj</th>
<th>(\sigma_{M_t})</th>
<th>(\sigma_V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.5000</td>
<td>0.5996</td>
<td>0.2995</td>
<td>0.000104</td>
<td>0.0101</td>
<td>0.006</td>
</tr>
<tr>
<td>1</td>
<td>0.8413</td>
<td>0.6246</td>
<td>0.3189</td>
<td>0.000118</td>
<td>0.0101</td>
<td>0.006</td>
</tr>
<tr>
<td>2</td>
<td>0.9772</td>
<td>0.6698</td>
<td>0.3687</td>
<td>0.000104</td>
<td>0.0101</td>
<td>0.006</td>
</tr>
<tr>
<td>3</td>
<td>0.9986</td>
<td>0.7052</td>
<td>0.4037</td>
<td>0.000104</td>
<td>0.0102</td>
<td>0.006</td>
</tr>
<tr>
<td>4</td>
<td>0.9999</td>
<td>0.7406</td>
<td>0.4388</td>
<td>0.000104</td>
<td>0.0102</td>
<td>0.006</td>
</tr>
</tbody>
</table>

Fig. 6.3 Optimization results in design space (a,b) for case 2, \(a\) fixed at 0.01.

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6.2 Results for Robust Design For Flow Control in 1-D

Similar results are seen in the flow parameter example. In Table 6.3, the results for case 1 are displayed. For $\sigma_{Minf} = \sigma_{Pb}$ ranging from 0 to 0.06, optimal values for the input variables ($\bar{M}inf, \bar{P}b$) are listed. As $\sigma_{Minf} = \sigma_{Pb}$ increases, so does $\sigma_{q_1}$. Accordingly, the mean values, $(\bar{M}inf, \bar{P}b)$, which minimize the objective function and satisfy the constraint, become increasingly displaced from the target mass flux, $q_t$. This is shown in Fig. 6.4. Mean values $(\bar{M}inf, \bar{P}b)$ change, keeping the mean value, $\bar{M}(\bar{M}inf, \bar{P}b)$, of the probabilistic output near the target value, $M_t$. The robust design points again track the dashed curve for $\bar{M} = M_t$ with displacement due to the $\sigma_{M_t}^2$ term of the objective, Eq. (5.14). The optimized mass flux, $q(\bar{M}inf, \bar{P}b)$, is displaced from the solid curve $q = q_t$ by $k\sigma_{q_1}$ as required by the probabilistic constraint.
Table 6.3 Robust 1-D flow parameter optimization results for case 1

<table>
<thead>
<tr>
<th>σ_{\text{Min}}</th>
<th>\bar{M}_{\text{inf}}</th>
<th>\bar{P}_b</th>
<th>\text{Obj}</th>
<th>\bar{M}</th>
<th>\sigma_{M_1}</th>
<th>\sigma_{q_1}</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>0.3000</td>
<td>0.8000</td>
<td>0.0000</td>
<td>0.3933</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.02</td>
<td>0.2861</td>
<td>0.7883</td>
<td>0.0001</td>
<td>0.3974</td>
<td>0.0116</td>
<td>0.0058</td>
</tr>
<tr>
<td>0.04</td>
<td>0.2655</td>
<td>0.7801</td>
<td>0.0005</td>
<td>0.3985</td>
<td>0.0231</td>
<td>0.0112</td>
</tr>
<tr>
<td>0.06</td>
<td>0.2555</td>
<td>0.7653</td>
<td>0.0012</td>
<td>0.4050</td>
<td>0.0327</td>
<td>0.0163</td>
</tr>
<tr>
<td>0.08</td>
<td>0.2468</td>
<td>0.7498</td>
<td>0.0020</td>
<td>0.4118</td>
<td>0.0407</td>
<td>0.0209</td>
</tr>
</tbody>
</table>

Fig. 6.4 Optimization results in design space (P_b, Minf) for case 1, P_k fixed at P_1.
The results for case 2 of the robust design for flow control, where $\sigma_{\text{Min}} = \sigma_{\text{Pb}}$ is fixed at 0.01, and $P_k$ increases from 50 percent to 99.99 percent, $(k=0$ to $4)$ are given in Table 6.4. Again, mean values $(\text{Minf, Pb})$ change, keeping the mean value, $\overline{M}(\text{Minf, Pb})$, of the probabilistic output near the target value, $M_t$. As in the preceding example, since $\sigma_{\text{Minf}} = \sigma_{\text{Pb}}$ remains small, the $\sigma_{M_1}^2$ term of the objective remains small and the displacement due to the $\sigma_{M_1}^2$ term remains small, as shown in Fig. 6.5. With an increase in $P_k$, $q(\text{Minf, Pb})$ is displaced from the solid curve $q = q_t$ by $k \sigma_{q_1}$, as required by the probabilistic constraint. Accordingly, the mean values, $(\text{Minf, Pb})$, which minimize the objective function and satisfy the constraint again become increasingly displaced from the target mass flux, $q_t$. Again, note the significant displacement from the target mass flux incurred in the higher probability optimizations, i.e., when one is attempting to incorporate the tails of the PDF.
Table 6.4 Robust 1-D flow parameter optimization results for case 2

<table>
<thead>
<tr>
<th>k</th>
<th>$P_k$</th>
<th>$\bar{M}_{\text{inf}}$</th>
<th>$\bar{P}_b$</th>
<th>Obj</th>
<th>$\bar{M}$</th>
<th>$\sigma_M$</th>
<th>$\sigma_q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.5000</td>
<td>0.3000</td>
<td>0.8000</td>
<td>0.00003</td>
<td>0.3933</td>
<td>0.0060</td>
<td>0.0030</td>
</tr>
<tr>
<td>1</td>
<td>0.8413</td>
<td>0.2919</td>
<td>0.7953</td>
<td>0.00003</td>
<td>0.3945</td>
<td>0.0059</td>
<td>0.0029</td>
</tr>
<tr>
<td>2</td>
<td>0.9772</td>
<td>0.2825</td>
<td>0.7916</td>
<td>0.00003</td>
<td>0.3949</td>
<td>0.0059</td>
<td>0.0029</td>
</tr>
<tr>
<td>3</td>
<td>0.9986</td>
<td>0.2688</td>
<td>0.7896</td>
<td>0.00003</td>
<td>0.3936</td>
<td>0.0060</td>
<td>0.0028</td>
</tr>
<tr>
<td>4</td>
<td>0.9999</td>
<td>0.2598</td>
<td>0.7867</td>
<td>0.00003</td>
<td>0.3938</td>
<td>0.0060</td>
<td>0.0028</td>
</tr>
</tbody>
</table>

Fig. 6.5 Optimization results in design space ($P_b$, $M_{\text{inf}}$) for case 2, $\sigma$ fixed at 0.01.
6.3 Results for Robust Design For Flow Control in 2-D

In Table 6.5, results for case 1 of the robust flow parameter optimization in 2-D are displayed. For $\sigma_\alpha = \sigma_{\text{Minf}} = \sigma$ ranging from 0 to 0.08, optimal values for the input variables $(\bar{\alpha}, \bar{\text{Minf}})$ are listed. As $\sigma$ increases, so does $\sigma_{\text{Cm}}$. Accordingly, the mean values, $(\bar{\alpha}, \bar{\text{Minf}})$ which minimize the objective function and satisfy the probabilistic constraint, become increasingly displaced from the target moment coefficient, $\text{Cmt}$. This is shown in Fig. 6.6. The robust design points track the dashed curve for $\bar{\text{Cl}} = \text{Cl}_t$ with some displacement due to the $\sigma_{\text{Cl}_t}^2$ term of the objective, Eq. (5.19). Again note that $\text{Cm}(\bar{\alpha}, \bar{\text{Minf}})$ is displaced from the solid curve $\text{Cm} = \text{Cmt}$ by $k \sigma_{\text{Cm}}$, as required by the probabilistic constraint. Here again, this displacement can be viewed as the probabilistic solution dependent or "effective" safety margin.
Table 6.5 Robust 2-D flow parameter optimization results for case 1

<table>
<thead>
<tr>
<th>$\sigma_{\text{min}}=\sigma_{\alpha}=\sigma$</th>
<th>$\bar{\alpha}$</th>
<th>$\bar{\text{M}_{\infty}}$</th>
<th>Obj</th>
<th>$\sigma_{C_{l}}$</th>
<th>$\sigma_{C_{m}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>4.00</td>
<td>0.400</td>
<td>0.0000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>0.01</td>
<td>3.95</td>
<td>0.411</td>
<td>0.0000</td>
<td>0.006</td>
<td>0.0005</td>
</tr>
<tr>
<td>0.02</td>
<td>3.86</td>
<td>0.428</td>
<td>0.0001</td>
<td>0.012</td>
<td>0.0010</td>
</tr>
<tr>
<td>0.03</td>
<td>3.81</td>
<td>0.437</td>
<td>0.0004</td>
<td>0.019</td>
<td>0.0016</td>
</tr>
<tr>
<td>0.04</td>
<td>3.79</td>
<td>0.443</td>
<td>0.0007</td>
<td>0.026</td>
<td>0.0022</td>
</tr>
<tr>
<td>0.05</td>
<td>3.72</td>
<td>0.455</td>
<td>0.0011</td>
<td>0.034</td>
<td>0.0029</td>
</tr>
<tr>
<td>0.06</td>
<td>3.66</td>
<td>0.465</td>
<td>0.0018</td>
<td>0.042</td>
<td>0.0037</td>
</tr>
<tr>
<td>0.07</td>
<td>3.52</td>
<td>0.484</td>
<td>0.0029</td>
<td>0.053</td>
<td>0.0047</td>
</tr>
<tr>
<td>0.08</td>
<td>3.42</td>
<td>0.498</td>
<td>0.0042</td>
<td>0.064</td>
<td>0.0058</td>
</tr>
</tbody>
</table>

Fig. 6.6 Optimization results in design space ($\alpha$, $\text{M}_{\infty}$) for case 1, $P_k$ fixed at $P_1$. 

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The results for case 2 of the robust optimization, where \( \sigma_a = \sigma_{\text{Minf}} \) is fixed at 0.01, and \( P_k \) increases from 50 percent to 99.99 percent (\( k = 0 \) to 4) are given in Table 6.6. With an increase in \( P_k \), \( C_m(\overline{\alpha}, \overline{\text{Minf}}) \) is displaced from the solid curve \( C_m = C_{\text{mt}} \) by \( k\sigma_{C_m} \), as required by the probabilistic constraint. Accordingly, the mean values, \( (\overline{\alpha}, \overline{\text{Minf}}) \), which minimize the objective function and satisfy the constraint, again become increasingly displaced from those at the target value, \( C_{\text{mt}} \). Note the significant displacement of the solution from the target when \( P_k \) is large, i.e., when one is attempting to incorporate the tails of the pdf. In order to increase the probability of constraint satisfaction from 97.77 percent to 99.99 percent, one sees a significant change in \( (\overline{\alpha}, \overline{\text{Minf}}) \) for a mere gain of 2 percent in constraint satisfaction.
Table 6.6 Robust 2-D flow parameter optimization results for case 2

<table>
<thead>
<tr>
<th>K</th>
<th>( P_k )</th>
<th>( \alpha )</th>
<th>( \overline{\text{Minf}} )</th>
<th>Obj</th>
<th>( \sigma_{\text{Cl}} )</th>
<th>( \sigma_{\text{Cmt}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.500</td>
<td>4.00</td>
<td>0.400</td>
<td>0.000000</td>
<td>0.000</td>
<td>0.0000</td>
</tr>
<tr>
<td>1</td>
<td>0.841</td>
<td>3.95</td>
<td>0.411</td>
<td>0.000033</td>
<td>0.0057</td>
<td>0.00047</td>
</tr>
<tr>
<td>2</td>
<td>0.977</td>
<td>3.86</td>
<td>0.428</td>
<td>0.000037</td>
<td>0.0061</td>
<td>0.00051</td>
</tr>
<tr>
<td>3</td>
<td>0.998</td>
<td>3.85</td>
<td>0.433</td>
<td>0.000039</td>
<td>0.0063</td>
<td>0.00052</td>
</tr>
<tr>
<td>4</td>
<td>0.999</td>
<td>3.83</td>
<td>0.439</td>
<td>0.000043</td>
<td>0.0064</td>
<td>0.00054</td>
</tr>
</tbody>
</table>

Fig. 6.7 Optimization results in design space \((\alpha, \text{Minf})\) for case 2, \(\sigma\) fixed at 0.01.
The present results represent an implementation of the approximate statistical moment method for robust optimization in 1-D and 2-D inviscid subsonic CFD codes. Assuming statistically independent, random, normally distributed input variables, the uncertainties in the input variables were incorporated into a robust optimization procedure where statistical moments involving FO SD appeared in the objective function and system constraints. Second-order SD were used in a gradient-based robust optimization. The approximate methods used throughout the analyses are valid when considering robustness about input parameter mean values.

Collectively, these results demonstrate the possibility for an approach to treat input parameter uncertainty and its propagation in gradient-based design optimization that is governed by complex CFD analysis solutions. It has been demonstrated on relatively simple CFD problems.
CHAPTER VII.

SENSITIVITY DERIVATIVES IN TRANSONIC FLOW

The uncertainty propagation and robust design procedures presented in Chaps. III through VI were applied to subsonic 1-D and 2-D flow regimes. The demonstrated procedures should be easily extended to transonic flow regimes, for there is nothing unique to the procedures which would limit the applications to subsonic flow. A prerequisite however, for successful implementation of the uncertainty propagation and robust design is knowledge of the CFD SD.

Although calculations of the SD for transonic flow follow the same procedures as outlined in Sec. 1.3 and in [19], in the transonic flow regime, the SD may develop a noisy or nonsmooth appearance as shown in Figs. 7.1 and 7.2. In these figures, the FO SD for the 2-D airfoil problem described in Chap. III are plotted for $\alpha = 1^\circ$, and a range of free stream Mach numbers ($\text{M}_{\infty} = 0.6$ to 0.78) where the flow transitions from subsonic to transonic. One can see the smooth behavior of the output function FO SD until approximately $\text{M}_{\infty} = 0.68$, at which time the FO SD begin to sharply fluctuate.
Fig. 7.1 Fluctuations in FO SD, $\frac{\partial C_l}{\partial \alpha}$ in transonic flow.

Fig. 7.2 Fluctuations in FO SD, $\frac{\partial C_l}{\partial \text{Minf}}$ in transonic flow.

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Such fluctuations obviously have a tremendous effect on the SO SD. With this jaggedness in the FO curve, the SO SD only describe the local behavior at the given design point. That is, the SO SD do not effectively represent the behavior of the output function. One can see in Fig. 7.3 (an example of output function behavior expanded about \( \text{Minf}=0.7 \), while \( \alpha \) remained fixed at 1°), that the SO Taylor series approximation using SO SD as calculated, does not represent the global behavior of the output function in the transonic region. Accordingly, all procedures which utilize the SO SD to include SO statistical approximations and robust optimization, do not produce meaningful results.

Fig. 7.3 Example Taylor series approximations for \( C_l(\text{Minf}, \alpha) \) in a transonic flow regime expanded at \( \text{Minf} = 0.7, \alpha = 1^\circ \).

It is interesting to note that the sharp fluctuations in the FO SD are somewhat masked when looking at the behavior of the output function. In Fig. 7.4, the CFD output function is plotted for the same range of input variables as show in Figs. 7.1 and
7.2, (for $\alpha = 1^\circ$, $\text{Minf} = 0.6$ to 0.78). Note that although a wobble is seen as the shock wave intensifies at approximately $\text{Minf} = 0.73$, the behavior of the output function appears smooth at first look. For example in Fig. 7.4 the output function appears to be smooth until $\text{Minf} = 0.73$, however looking more closely at the function behavior at $\text{Minf}=0.7$, one can see fluctuations as evident in the CFD solutions alternating on either side of the FO approximation in Fig. 7.5.

![Graph showing CFD solutions for $\text{Cl}(\text{Minf}, \alpha)$ as flow transitions to supersonic.](image-url)

Fig. 7.4 Example CFD solutions for $\text{Cl}(\text{Minf}, \alpha)$ as flow transitions to supersonic.
In [53], the problem of non-smooth SD in flows with discontinuities such as shock waves is addressed. A methodology for smoothing the SD while preserving the accuracy of the analysis is presented. In order to successfully implement the uncertainty propagation and robust optimization procedures as presented in the current study, such a procedure must be implemented. The non-smooth behavior of the SD is not however the focus of the current work. CFD SD in flows with discontinuities remains an area for further investigation.

Fig. 7.5 Example CFD solutions for $Cl(\text{Minf}, \alpha)$ compared to FO Taylor series approximation.
CHAPTER VIII

CONCLUSION

The present study demonstrates that SD may enable efficient and accurate prediction of uncertainty propagation, and robust design in CFD. With 1-D and 2-D Euler CFD codes, it has been established that the approximate statistical first moment method for prediction of output function mean is a feasible and accurate prediction. Both the FO and SO approximations are accurate at small input variable standard deviations, and the SO approximation retains accuracy as input deviations grow. It is also demonstrated that SD can be incorporated into a MC scheme to create a SDEMC method for improved prediction of the output function mean. Although the SDEMC method offers improvement over a traditional MC method, the SDEMC method is not as computationally efficient as a FO or SO direct calculation of the first moment via the approximate statistical moment method.

The utility of the SD is again seen in quantifying the output function variance through calculation of the FO and SO approximate statistical second moments, as well as the variance of the FO Taylor series remainder. The prediction of the output function variance is found to be more accurate at small input standard deviations. The ability to calculate a lower limit or minimum value for the variance of the FO Taylor Series remainder is demonstrated to be feasible at all input standard deviations, lending much insight into the stochastic behavior of the output function.

The FO second statistical moments obtained though direct calculation were successfully incorporated into a robust optimization procedure. The approximate second moments were incorporated in both objective function safety margins and probabilistic constraints. A gradient-based design optimization was accomplished with knowledge of the SO SD. Collectively, these results demonstrate the possibility for an approach to treat input parameter uncertainty and its propagation in gradient-based design optimization that is governed by complex CFD analysis solutions.
The uncertainty propagation and robust design methods presented have been demonstrated on relatively simple 1-D and 2-D Euler CFD codes in a subsonic flow regime with small numbers of CFD input variables and output functions. The results were first published in [54] for the quasi 1-D applications and in [55-56] for the 2-D applications. Issues with the SD in transonic flow have precluded the successful implementation of SD based uncertainty propagation and robust design in a transonic flow regime.

It is suggested that future studies investigate improvements in the ability to accurately predict the output function variance as this value is an important parameter in uncertainty quantification as well as the proposed robust design task. Also, the inclusion of a SO term in the SDEMC prediction of mean is an area where one might further improve the efficiency in MC prediction of the mean. One may also attempt to extend the approaches to larger systems which contain a higher number of output functions and design variables, as well as to CFD codes which include viscous effects. The feasibility of the extending the presented methodology to transonic flow should also be addressed through increased study of the behavior of CFD SD in transonic flow.
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