Inexpensive Monte Carlo Uncertainty Analysis

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Abstract

This paper proposes a new methodology for uncertainty propagation through CFD codes using adjoint error correction[7]. The mathematical formulation is presented followed by a proof-of-concept model example. The method is further demonstrated using artificial geometric uncertainty for a 2D inviscid airfoil code. Reduced order modelling has been used to further reduce the computational costs, and results of approximate Monte Carlo(MC) simulations have been compared with full nonlinear MC simulations.

Key Words: Uncertainty Propagation, Adjoints, Manufacturing Uncertainty, Reduced Order Modelling

1 INTRODUCTION

With the availability of high performance computing and sophisticated software programs, high fidelity simulations are being increasingly used in Aerospace design. However, high fidelity computing is only used for deterministic design, which assumes a perfect knowledge of the environmental and operational parameters. In reality, there is much uncertainty in the form of manufacturing tolerances[8], uncertain modelling parameters[9] and in-service wear-and-tear.

Significant amount of work is underway to accommodate the effect of uncertainty in the design cycle using robust design and optimisation methodologies and reliability engineering. But all these methodologies are computationally expensive. Consequently, most of the reported work uses low fidelity simulation models. For example inviscid codes would be routinely used for robust design instead of the full viscous versions.

Also, it is often not very clear as to which quantities best represent uncertainty. E.g. in many cases a random variable might be represented in terms of mean and standard deviation. For quantities like total pressure loss across a compressor stage, this is an adequate representation since we are only interested in the mean. On the other hand for quantities like turbine life due to high temperature, the tail part of the distribution is the quantity of interest. Hence, complete information regarding the probability density function (PDF) is desired. PDF is also required for the calculation of the cumulative density function (CDF) which is one of the popular choices[10] for objective function in robust optimisation.

Even if we are only interested in the mean of some quantity, this might not be adequate because of the highly nonlinear nature of the flow equations. This point can be illustrated using simple functions like $y = \sin(x)$ and $y = \cos(x)$. Fig. 1 shows the output frequency distribution of these function for normally distributed x with $\mu_x = 0$ and $\sigma_x = \frac{\pi}{4}$. This comparison highlights the fact that output distributions may not have any resemblance with the input distributions for non-linear functions, and hence, mean and variance calculations might not be the best way to represent uncertainty.

Hence, there is a need for computationally inexpensive high fidelity methods for uncertainty propagation.

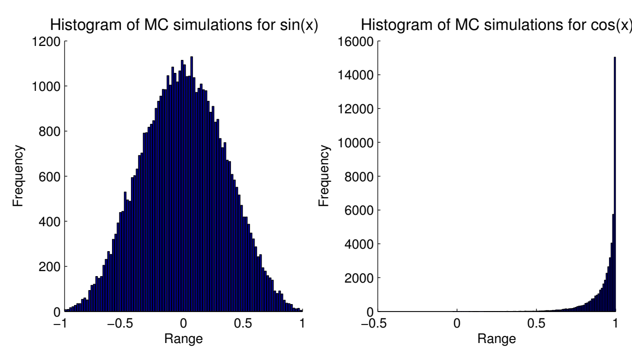

Fig.1: Resulting frequency distribution for $\sin(x)$ and $\cos(x)$ for $\sigma_x = \frac{\pi}{4}$

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Also, it might be important in many cases to obtain the full PDF for the output function instead of just the mean and standard deviation.

Reviewing the existing literature, the most straight forward and accurate method is full nonlinear MC simulations (as used by Garzon[2]). Though this method is very easy to implement, it is still prohibitively expensive for real life applications with high-fidelity models. But in many cases, if the computational tool needs to be used as a black box, this is the only alternative. Another promising method is the use of stochastic partial differential equations [14][11]. These methods can handle large uncertainties and high nonlinearities. They are also very accurate if a converged solution is obtained. But they are also relatively difficult to implement and all the effort invested may not be justified for smaller uncertainties.

There is an approximate alternative available in the form of moment methods first used for aerospace applications by Newman et. al.[12]. This method is explored in some detail below, but this method only gives the mean and standard deviation of the output function and complete PDF information is not available. Taylor[13] and Alekseev et. al.[1] have also reported a further speed-up of moment methods using adjoint equations.

Higher order moment methods require the computation of higher derivatives which are difficult to obtain for CFD codes. With improvements in automatic differentiation(AD) tools it might be possible in future to achieve this, as explored by Taylor et. al.[13], but at present it is very costly to calculate higher derivatives using AD for complex applications.

Though the concept of uncertainty has been discussed in the generic sense, this paper looks only at the geometric uncertainty. The two main sources of this uncertainty are manufacturing errors and in-service wear-and-tear. Because of the sophisticated manufacturing processes, this uncertainty is sufficiently small to justify the use of moment methods and the proposed methodology.

The rest of the paper discusses the moment methods and the proposed new method for Inexpensive Monte Carlo(IMC) simulations. The new method will be demonstrated using a model problem followed by a 2D inviscid code with synthetic geometric uncertainty. Results and implementation issues are discussed at the end.

2 MOMENT METHOD

Given a probability distribution for x, the aim is to determine or approximate the corresponding distribution for y, where

$$y = f(x),$$

and f can be any smooth nonlinear function.

Moment methods are based on the Taylor series expansion of the original nonlinear function about the mean of the input μ_x.

$$\begin{aligned} y =& f(\mu_x) + f'(\mu_x)(x-\mu_x) \\ &+ \tfrac{1}{2} f''(\mu_x)(x-\mu_x)^2 + O((x-\mu_x)^3) \end{aligned} \tag{1}$$

where the primes denote derivatives with respect to x. By considering various orders of the Taylor expansion and taking moments, the mean and variance of output y can be approximated in terms of its derivatives evaluated at μ_x.

After taking first and second moments of y, the various approximations to μ_y and σ_y^2 are:
First order moment method:

$$\begin{aligned} \mu_y &= f(\mu_x) + O(\sigma_x^2) \\ \sigma_y^2 &= \sigma_x^2 f'(\mu_x)^2 + O(\sigma_x^3) \end{aligned} \tag{2}$$

Second order moment method:

$$\begin{aligned} \mu_y &= f(\mu_x) + \frac{f''(\mu_x)}{2}\sigma_x^2 + O(\sigma_x^3) \\ \sigma_y^2 &= f'(\mu_x)^2\sigma_x^2 + f'(\mu_x) f''(\mu_x) S_x \sigma_x^3 \\ &\quad + \tfrac{1}{4}\left(f''(\mu_x)\right)^2 (K_x - 1)\sigma_x^4 + O(\sigma_x^4) \end{aligned} \tag{3}$$

where S_x is the skewness, and K_x is the Kurtosis. No assumptions on the input and output distributions are required here. It should also be noted that the error in the variance for second order moment is still of the order of σ_x^4. This is because the third order moment method reveals that the σ_x^4 term is incomplete in the second order expression. Hence, it is not clear *a priori* as to whether this incomplete fourth order term should be included in the expression. This depends on the magnitude of the coefficients of this term.

A set of simulations have been presented with simple functions $y = \sin(x)$ and $y = \cos(x)$ to assess the performance of moment methods with respect to MC simulations. Monte Carlo simulations have been carried out in a direct way by sampling out x according to its distribution and finding out the corresponding y. MC simulations were performed for increasing values of σ_x and the predictions from the first and second order methods are compared.

Fig. 2 and Fig. 3 show the performance of various methods as σ_x is increased progressively from 0 to $\pi/8$. x is assumed to have a normal distribution with $\mu_x = 0$. A sample size of 50,000 is used for each MC simulations.

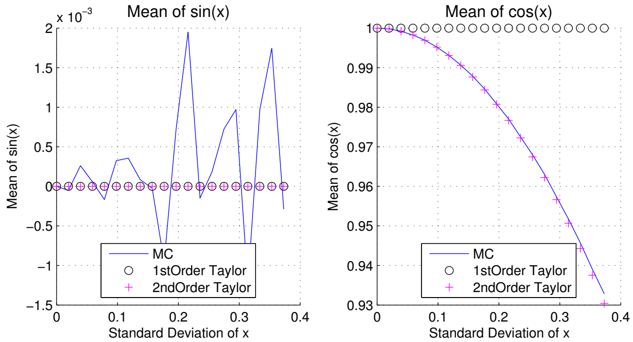

Fig.2: Prediction of μ_y with increasing σ_x

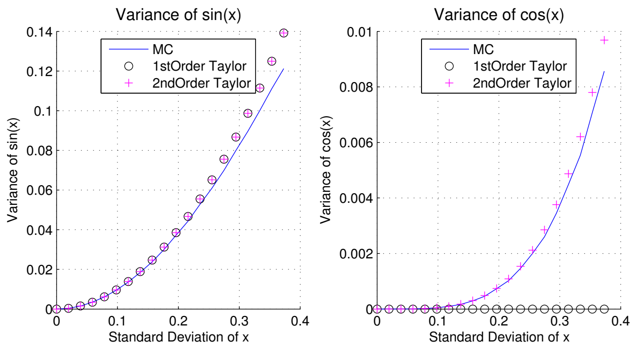

Fig.3: Prediction of σ_y^2 with increasing σ_x

It can be observed here that linear methods are only valid for small values of σ_x. The advantage obtained by moving to an higher order method solely depends on the values of higher derivatives at the mean of the input. For example, moving from first to second order moment method does not improve the variance estimate for $\sin(x)$.

Also, note that the first order method has completely missed the behaviour of the mean of the cosine function. Performance criteria like lift and efficiency are expected to behave more like the cosine function with peak values at the input mean and rapid deterioration away from the design point. This stresses the need for at least second order methods for uncertainty propagation. It should also be noted that the algebra becomes increasingly complex for higher order approximations though only univariate distributions are considered here.

3 INEXPENSIVE MONTE CARLO

In this section, a new methodology for uncertainty propagation is outlined. This is based on the idea of adjoint error correction as proposed by Giles and Pierce[7]. The formulation is first developed for simple nonlinear algebraic equations. It can then be extended to discretisations of PDEs.

Let u be the solution of a set of non-linear algebraic equations

$$N(u(x), x) = 0, \tag{4}$$

and let the functional of interest, $J(u(x), x)$, be some smooth function of u. The discrete adjoint equation corresponding to this function is

$$\left(\frac{\partial N}{\partial u}\right)^T v = \left(\frac{\partial J}{\partial u}\right)^T, \tag{5}$$

where v is the adjoint solution. Let u^* and v^* be approximations to u and v. The first order Taylor expansion of the function of interest is:

$$J(u,x) \approx J(u^*,x) - \frac{\partial J}{\partial u}(u^* - u) + O\left(\|u^* - u\|^2\right).$$

Using the adjoint equation (5), we have

$$J(u,x) \approx J(u^*,x) - v^T \frac{\partial N}{\partial u}(u^* - u) + O\left(\|u^* - u\|^2\right).$$

A first order Taylor expansion of equation (4) then gives us,

$$J(u,x) \approx J(u^*,x) - v^T N(u^*,x) + O\left(\|u^* - u\|^2\right).$$

The order of the error still remains the same. Finally if we use an approximate solution v^* instead of the exact adjoint solution v, then

$$\begin{aligned} J(u,x) \approx & J(u^*,x) - v^{*T} N(u^*,x) \\ & + O\left(\|u^* - u\|^2, \|u^* - u\|\|v^* - v\|\right) \end{aligned} \tag{6}$$

The final equation forms the basis for the new Inexpensive Monte Carlo (IMC) method. After calculating the nonlinear solution u, linear sensitivity $\frac{du}{dx}$ and adjoint solution v at the mean of x, μ_x, we consider two options:

- IMC1: Use baseline values,

$$u^* = u(\mu_x), \quad v^* = v(\mu_x) \tag{7}$$

- IMC2: Use linear extrapolation to estimate u^*, and

$$u^* = u(\mu_x) + \frac{du}{dx}(x - \mu_x), \quad v^* = v(\mu_x) \tag{8}$$

As can be clearly seen from equation (6), the first approach has an overall leading error of second order, while the second method has a leading error of third order. Just based on the leading order of error, IMC1 should perform as well as the first order moment method.

The solution of the nonlinear equations, linear equations and the adjoint equations are required at the baseline. As the function $N(u^*, x)$ only has to be evaluated at each sample point (as opposed to a complete nonlinear solution), this method is computationally much cheaper than the full nonlinear MC simulations. The use of these approaches is now demonstrate using a simple model problem.

$$
\begin{aligned}
N(u(x), x) &= u + u^3 - x \\
J(u(x), x) &= u^2
\end{aligned}
\tag{9}
$$

Input variable x is treated as a random variable with normal distribution. The standard deviation σ_x is increased from 0 to 1. The estimates for mean and standard deviation for J using first and second order moment methods and IMC methods is compared with full nonlinear MC simulations for different μ_x. Equation 9 is solved using simple Newton iterations to machine accuracy. Analytic expressions for the calculation of v and $\frac{du}{dx}$ were used at $x = \mu_x$.

Fig. 4 shows the comparison between various methods. As expected IMC1 and the first order moment method behave similarly. Also, IMC2 and the second order moment method show similar behaviour.

Fig. 5 shows a similar comparison for $\mu_x = 0$. As can be observed here the error increases rapidly in this case. Higher order effects become significant sooner in this case as opposed to the previous one. This case illustrates the problem in defining the validity range for these methods *a priori*. In other words, it is not possible in real life to define *a priori* what are "small" enough perturbations to justify these kinds of second order approximations.

4 CFD EXAMPLE

The mathematical treatment as discussed in the previous section for nonlinear set of algebraic equations is similarly valid for discretized PDEs. The discretized form of the fluid flow equations corresponds to the nonlinear algebraic equations with x as the geometry and u as the flow solution. The function of interest is typically the discretisation of an integral over the entire domain or the boundary.

An additional complexity in the CFD codes is the large number of input random variables in the form of points defining the surface geometry, which could be of the order of a thousand. If the number of input random variables is not restricted to a low number, then the computational cost would go up due to the large number of linear sensitivity calculations. To reduce this extra computational cost, a reduced order model of the geometric uncertainty is derived.

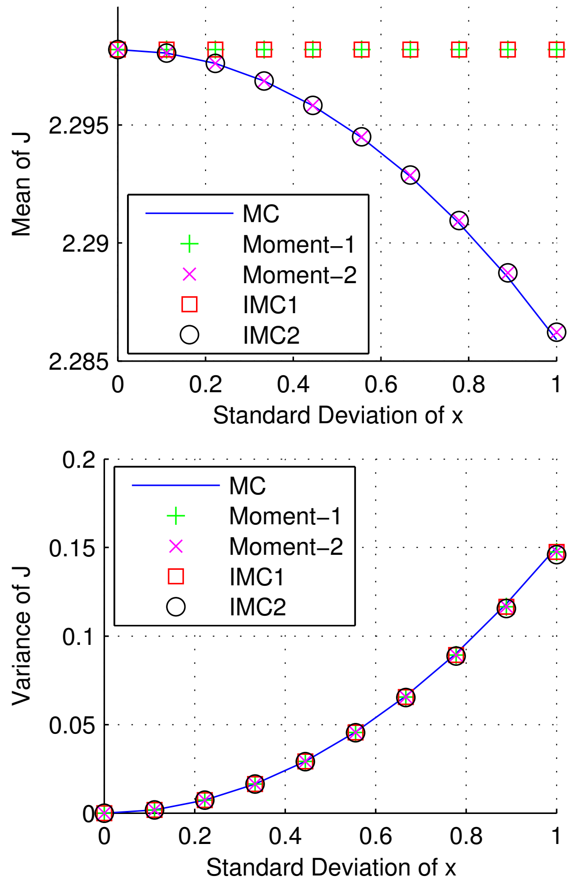

Fig.4: Comparison of different methods for model problem with $\mu_x = 5$

4.1 Reduced Order Model

Let $\widehat{x}$ denote a vector of surface perturbations. If we have p points defining the surface in m dimension then the size of $\widehat{x}$ is mp. If these perturbations are used in the original form, then we would require mp linear calculations for IMC simulations. A reduced order model for the i^{th} airfoil is defined as

$$
\widehat{x}_i = L\alpha_i = \sum_k \alpha_{k,i} \widetilde{x}_k, \tag{10}
$$

where α is a low dimensional vector with components as random variables with zero mean and unit variance. The method of reduced order modelling derives the matrix L. The columns of L would be referred to as the leading modes. For example, Darmofal and Garzon[2][3] have used Principal Component Analysis(PCA) to achieve this. They have reported a requirement of 5 leading modes in order to capture more than 99% of geometric uncertainty for actual turbine blade measurements.

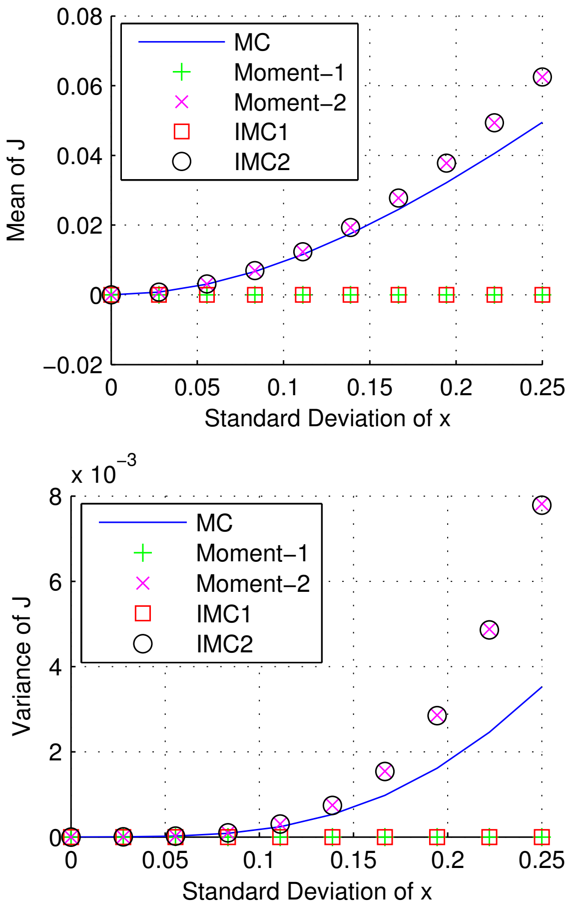

Fig.5: Comparison of different methods for model problem with $\mu_x = 0$

4.2 IMPLEMENTATION

Let x_0 be the ideal surface geometry. Then the steps for IMC2 are as follows.

- Read n sets of airfoil perturbations

$$\widehat{x}_i, \text{ where } i = 1, n$$

- Reduced order modelling for leading modes

$$\widetilde{x}_k, \text{ where } k = 1, n_r$$

- MC Sampling for M samples

$$\alpha_{k,s}, \text{ where } k = 1, n_r; \; s = 1, M$$

$$x_s = x_0 + \sum_{k=1}^{n_r} \alpha_{k,s} \widetilde{x}_k$$

Here the sampled M surface geometries could be a subset of the available n measurements. Alternatively, if n is very small, then an assumption of normal distribution could be made followed by sampling. However, it is not clear if this assumption is justified.

- Baseline nonlinear solution

$$u(x_0)$$

- n_r linear solutions at the baseline

$$\frac{du}{d\widetilde{x}_k}(u(x_0), x_0), \; k = 1, n_r$$

- One adjoint solution at the baseline

$$v(x_0)$$

- M IMC evaluations: An extra piece of code is generated for these evaluations. It is very similar to the original nonlinear code and uses the same nonlinear routines.

  Linear extrapolation of the flow variables

$$u_s^* = u(x_0) + \sum_{k=1}^{n_r} \alpha_{k,s} \frac{du}{d\widetilde{x}_k},$$

  and adjoint correction for approximate functional

$$J(u_s, x_s) \approx J(u_s^*, x_s) - v^T N(u_s^*, x_s).$$

Note that the calculation of $J(u^*, x_s)$ only involves values of u^* at the airfoil surface, but $v^T N(u_s^*, x_s)$ involves a computation over the entire grid. However, both of these are simple evaluations which are much cheaper than the iterative nonlinear solutions. For IMC1, we leave out the linear extrapolation step while for linear extrapolation, we leave out the adjoint correction. Further implementation details can be found in reference[4].

Assuming there are n_r leading modes and one functional of interest, the cost of IMC2 is:

- One nonlinear solution on baseline geometry,
- One adjoint solution at baseline,
- n_r linear solutions for $\frac{du}{d\widetilde{x}_k}$
- M approximate MC simulations (which are equivalent to M residual evaluations)

This is much cheaper than the full nonlinear MC simulations involving M nonlinear solutions.

A 2D unstructured inviscid airfoil code[5] was developed to test these ideas on a CFD code. This is a cell centred explicit local time marching solver with smoothing. The linear and adjoint versions of the code are developed using AD. More on the development of this code can be found in reference[6]. The effect of synthetically generated geometric uncertainty is assessed on the lift calculation.

4.3 RESULTS

An O-grid was generated for a NACA-0012 airfoil using conformal mapping. The grid is coarse with 99×100 vertices. The grid was rotated through angles of -0.5^o to 0.5^o with the step size of 0.1^o in order to generate artificial grid perturbations, mimicking the angle of attack uncertainty for an airfoil. The non-dimensional farfield conditions are:

- Pressure = 1,
- Density = 1,
- Mach = 0.4, and
- Flow Angle = 3^o.

The lift was calculated using full nonlinear calculations at each point. Adjoint and linear solutions were also obtained at the baseline solution. Lift predictions are also obtained using simple linear extrapolation as well as IMC1 and IMC2. All the calculations are converged to machine precision. Fig. 6 shows the error in the predictions and the actual nonlinear solutions with respect to the angle of perturbation. As expected, the error in linear extrapolation and IMC1 shows quadratic behaviour while IMC2 is cubic.

After this validation, a set of airfoils are generated introducing artificial uncertainty. Three principal modes of perturbation are introduced:

- thickness,
- angle of attack, and
- leading edge shape.

The thickness perturbation is introduced using

$$\delta y = 0.04\ t\ x^b (1-x)^c$$

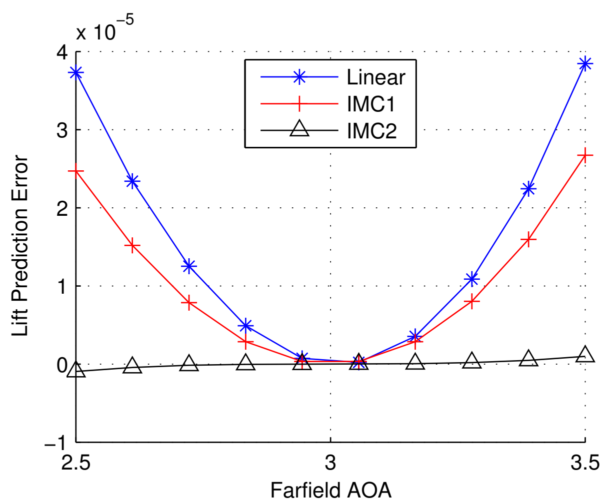

Fig.6: Error plot for linear extrapolation, IMC1 and IMC2

where $b = 3$, $c = 3$ and t is a normal random variable with zero mean and unit variance. This ensures thickness perturbation at one standard deviation equal to 4% of the chord length. The coefficient b and c control the variation of the thickness perturbation along the chord.

The angle of attack perturbation is introduced in the form of plain rotation of the airfoil about the trailing edge. A variation of $\pm 0.1^o$ is introduced with normal distribution.

The leading edge shape perturbation is introduced using

$$\delta y = 0.02\ l\ x^d (1-x)^e$$

where $d = 0.5$, $e = 6$ and l is a random variable with beta distribution. Coefficients for the distribution were selected in such a way as to introduce a bias towards leading edge bluntness. Though all the errors introduced here are artificial, we believe that they represent the actual geometric errors for engine blades[2].

Stratified sampling is used to generate the sample set for nonlinear MC simulations. A sample size of 1000 is used. Each nonlinear calculation took around 17 minutes so the full set took eighteen hours on a Linux cluster of 16 nodes. All the solutions are converged to machine accuracy. IMC simulations along with linear extrapolation are also carried out using the procedure explained above. Table 4.3 shows the mean and variance predictions for lift using the above methods. As can be seen IMC2 performs better than linear extrapolation and IMC1. However, in this case, linear and IMC1 methods are certainly good enough for engineering purposes.

Fig. 7 shows the histograms for the four methods discussed above. As can be seen, the IMC methods closely capture the actual histograms (and consequently PDF) of the distribution.

5 CONCLUSION

A new method for uncertainty propagation through CFD codes is presented here. Together with the use of AD tools and reduced order modelling this becomes an efficient and easy to implement method. Use of IMC

	Mean	Variance
Nonlinear	3.720894e-02	1.513875e-06
Linear Extrap.	3.721927e-02	1.500570e-06
IMC1	3.721417e-02	1.509853e-06
IMC2	3.720903e-02	1.512292e-06

Table 1: Comparison of Mean and Variance predictions for non-dimensionalised lift parameter

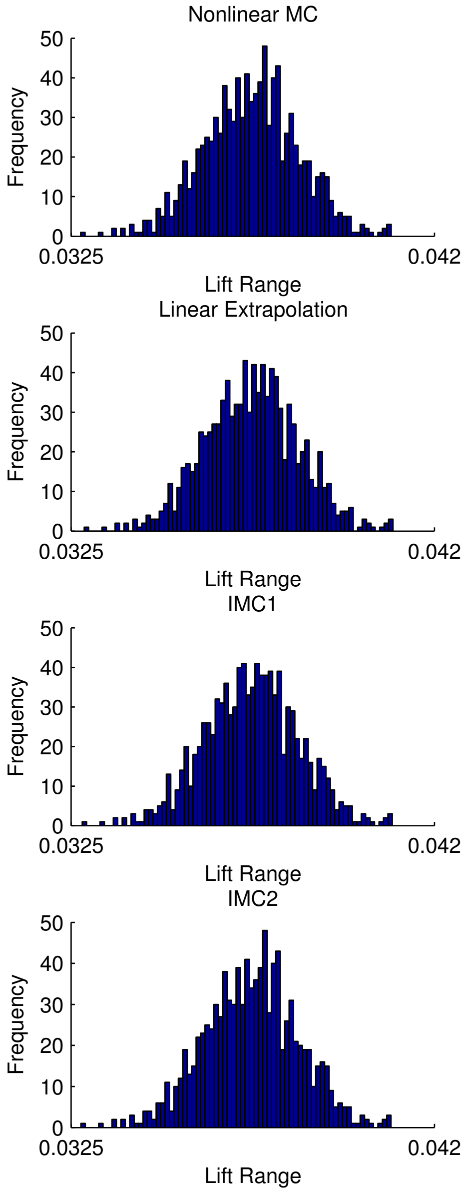

Fig.7: Histograms for Lift perturbations using various methods

method has been demonstrated using a simple 2D inviscid code which has many features of more complex 3D applications.

In future, this work will be extended to full 3D Navier-Stokes solver with blade measurements for manufacturing uncertainty. Also, further investigation into the PCA methodology is required.

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