

AN ALTERNATIVE TO MONTE CARLO SIMULATION METHOD

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Abstract. The quantification and propagation of uncertainty is a growing discipline, with applications within practically all sciences. Uncertainties are present in every prediction model of each discipline (natural, structural, biological, etc), since an exact and perfect definition of geometry, boundary conditions, material properties, initial conditions and excitations (among others) is rarely possible. A common and robust approach to perform the propagation of uncertainties is the Monte Carlo method, which usually implies running a large number of simulations. Complex systems, where uncertainty propagation is particularly interesting, require time expensive computations, and large memory and storage capacities in order to process such amount of data. Even thousands of runs of a slightly non-linear model with a few degrees of freedom could take a considerable time, despite the use of state-of-the-art solvers and parallelization techniques. In this work, a methodology that could allow the reduction of the number of simulations is discussed. The idea of the method is to perform a parametric sweep for a certain parameter \mathbb{X} to be considered stochastic, then assign probabilities (according to a previously selected cumulative probability density function) to the values of \mathbb{X} , and finally map the corresponding probability values to the target variables. Hence, the probability density function of the target variables could be estimated. Within this work, the theory and implementation of the proposed method are discussed and application examples are provided.

1 INTRODUCTION

The propagation of uncertainties in physical problems can be a computer-intensive task, given the large number of simulations required to construct the statistics.

In general, the preferred method to carry out such analysis is based on Monte Carlo (MC) simulations, which rely on random sampling to reconstruct a probability density function (PDF). This approach requires a vast amount of data to attain convergence within a prescribed range. Also, there are other techniques that converge with reduced sample size, but depend on serialized calculations, such as Markov Chain Monte Carlo (MCMC). The latter, though robust and extensively used, has a drawback: the serialized nature of the method implies that calculations cannot be parallelized, therefore it becomes time consuming when complex non-linear models are considered.

In this work, the problem of uncertainty quantification and propagation in a low dimensional parameter space is analyzed, e.g. 1D or 2D. The focus will be in the modeling of stochastic variables. Particularly, keeping in mind that a parametric sweep is often carried out in an exploratory stage in an attempt to determine the qualitative behaviour of a model (e.g. to identify possible bifurcations or chaos regions), it seems interesting to re-utilise this information for stochastic analysis purposes, thus reducing the required computation time.

Throughout this text, the following nomenclature will be used: standard fonts denote deterministic variables (e.g. x, y, g), while capital blackboard bold typeface is used to represent random variables (e.g. \mathbb{X}, \mathbb{Y}).

2 IDEA OF THE METHOD

In order to gain some insight into the very basic idea of the method, a brief review of the most-common techniques is presented below.

2.1 Method I: Closed-form Solution

Let x be the value of one particular parameter used in a model, and let y be one of the output variables of interest. The model acts as a transformation that assigns values $g : x \rightarrow y$.

As discussed in many probability textbooks, eg. [Grimmet and Welsh \(2014\)](#), given a known PDF for a random variable \mathbb{X} with density function $f_{\mathbb{X}}$, the density function $f_{\mathbb{Y}}$ for a transformation $\mathbb{Y} = g(\mathbb{X})$ can be obtained analytically if the transformation is one-to-one. Therefore, if the function $g(x)$ has a known expression and is invertible, the propagation can be done by performing the calculation defined by Eq. (1).

$$f_{\mathbb{Y}}(y) = f_{\mathbb{X}}(g^{-1}(y)) \cdot \left| \frac{d}{dy} (g^{-1}(y)) \right| \quad (1)$$

Unfortunately, such calculation is not always possible. This is the case where no closed-form expression exists for the output PDF, or when the transformation is not injective.

2.2 Method II: Monte Carlo (MC)

If no analytical solution is attainable, a Monte Carlo (MC) based simulation is often employed to obtain a numerical solution. In such cases, numerous repetitions of the following procedure are involved: a set of values for the parameters are drawn, then the model is run and the output variables are stored. After a sufficiently large number of drawn results, the statistic are reconstructed e.g. by means of a kernel estimator.

2.3 Method III: Numerical Transformation Method (TM)

Alternatively, if the results from a parametric sweep are available, a re-utilization of the data can be performed and the re-calculation of the output values from the model is avoided. In this scenario two options are available.

On the one hand, if the transformation is one-to-one then the function $x = g(y)$ could be reconstructed, per example, via a spline, and the expression (1) can be numerically evaluated. This method will be referred to as the Transformation Method (TM).

On the other hand, a kernel estimator could be used in the reconstruction of the output PDF. If a numerical mapping between the original input variables and the output variables is established, then probabilities can be assigned directly, i.e. without finding an expression for $x = g(y)$. Thus the need for a one-to-one relation is eliminated. This method will be referred to as the Proposed Method (PM)

In the TM Method, the PDF is obtained via transformation of Random Variables. As already stated, given a known PDF for a random variable \mathbb{X} with density function $f_{\mathbb{X}}$, PDF $f_{\mathbb{Y}}$ for a transformation $y = g(x)$ is defined by Eq. (1), if the transformation is one-to-one. Otherwise, special care is necessary to find the distribution of \mathbb{Y} .

In this case, a parametric sweep is used to construct a discrete mapping that matches values of the input parameter x with an output y . Then, the continuous transformation is approximated via a spline method, and the derivative $\frac{d}{dy} (g^{-1}(y))$ is obtained by numerically evaluating Eq. (1). Note again that this procedure is valid only if the transformation is injective.

2.4 Method IV: Proposed Method (PM)

As stated before, a different approach to construct the PDF for the transformed random variables \mathbb{Y} is to utilize a kernel smoothing function technique, as in (Silverman, 1986). In particular, the Matlab *ksdensity* tool has been used for this purpose. This tool allows a PDF reconstruction by overlaying kernel functions according to frequencies or predefined weights. In this case, the parametric sweep and the associated probability for the response are employed in the definition of weights for the output PDF.

3 PROCEDURE

The main idea of the PM relies on finding a mapping between the input and output variables and then, assign probabilities. Therefore, distributions need be discrete.

Given a continuous input parameter and its known PDF, the distribution is discretized as follows.

Consider a regular partition of the domain. As illustrated in Fig. (1), the probability value within each interval will be concentrated and assigned to a discrete set of values x_i^* . Then, if the interval length is $\Delta = (b - a)/n$, $x \in (a, b)$, $\xi \in [0, 1]$, x_i^* is defined by Eq. (2).

$$x_i^* = a + i \cdot \xi \cdot \Delta \quad \text{with } i \in (1, 2 \dots n), \xi \in (0, 1) \quad (2)$$

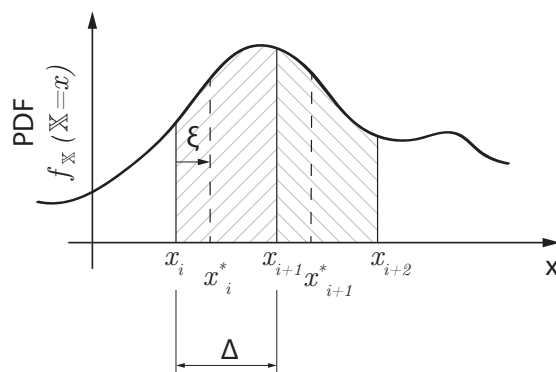


Figure 1: Discretisation of the input PDF via regular partitions

Finally, as the input variable \mathbb{X} is now discrete, it is valid to assign to each value of \mathbb{Y} the accumulated probability of all those \mathbb{X} that are mapped into \mathbb{Y} by the aforementioned transformation.

4 EXAMPLE 1: APPLICATION TO A DISCRETE DISTRIBUTION

The objective of this example is to understand the core idea of the PM with a simple discrete case.

Let the transformation $y = g(x)$ be given by Fig. (2), with an associated PDF $f_{\mathbb{X}}(\mathbb{X} = x)$.

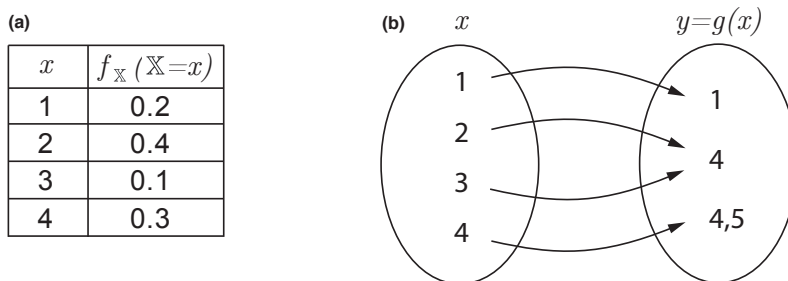


Figure 2: (a) Definition for the mapping $g(x)$ and probabilities for the input variable \mathbb{X}

Then the probabilities can be assigned in the following manner:

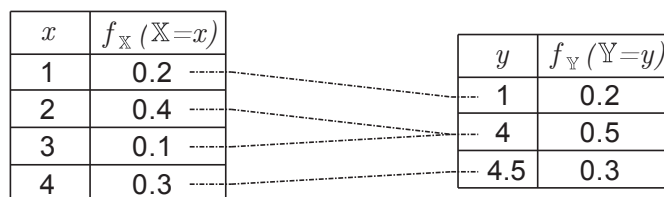


Figure 3: Output PDF $F_{\mathbb{Y}}$

Finally, the solution to this problem is a mass function $f_{\mathbb{Y}}(\mathbb{Y} = y)$, as shown in Fig. (3). Note that the mapping could have been obtained by solving a parametric sweep for any desired model.

5 EXAMPLE 2: APPLICATION TO A CONTINUOUS DISTRIBUTION

The aim of this example is to show the applicability of the PM to the continuous case, while at the same time to numerically gain some insight into the advantages of the method with regards to convergence and time consumption. To achieve this goal, PM is compared against well-known MH-MCMC simulations. The model is programmed within the MATLAB mathematical software.

Let's consider an input stochastic parameter with a normal distribution $\mathbb{X} = \mathcal{N}(\mu, \sigma) = \mathcal{N}(5, 3)$. Let \mathbb{Y} be an output random variable, after the application of a transformation $g : x \rightarrow y$ defined by Eq. (3). Note that this mapping could represent a complex model for which propagation of parameter \mathbb{X} is being performed.

$$y = g(x) = 3 \cdot (x - 1.4) \cdot (x - 3.1) \cdot (x - 4.7) \cdot (x - 7.7) \quad (3)$$

In this example, the PM utilises a regular centred partition of the form $x = a : \Delta : b$, where $\{a, b\} = \{-15, 25\}$. Different cases for the partitioning interval Δ will be considered. Then, the total number of points n can be obtained as $n = 1 + (b - a)/\Delta$. Note that the n is the total amount of executions required for the propagation analysis. In the case of MH-MCMC, n coincides with the desired number of samples.

Based on the results depicted on Fig. (5), the PM converges with a very low amount of samples when compared to MH-MCMC. Moreover, it is shown that MH-MCMC may diverge greatly depending on the initial guess for the cases with the lowest number of samples ($n = 401$), while results converge for a large amount of samples.

Finally, MH-MCMC time requirements are much higher than PM as the number of samples increases, as shown in Fig. (6).

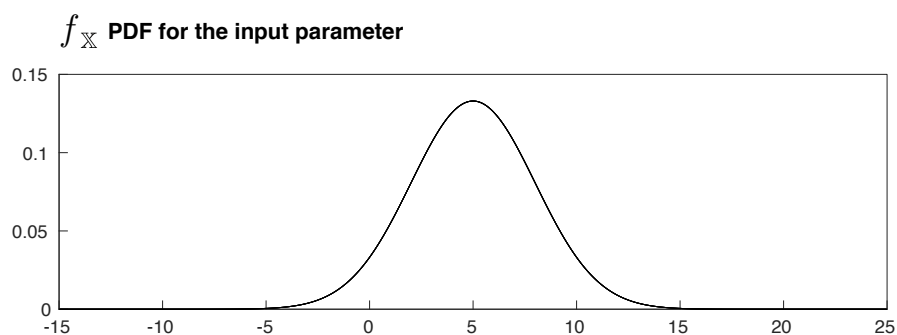


Figure 4: Input PDF $f_{\mathbb{X}}$

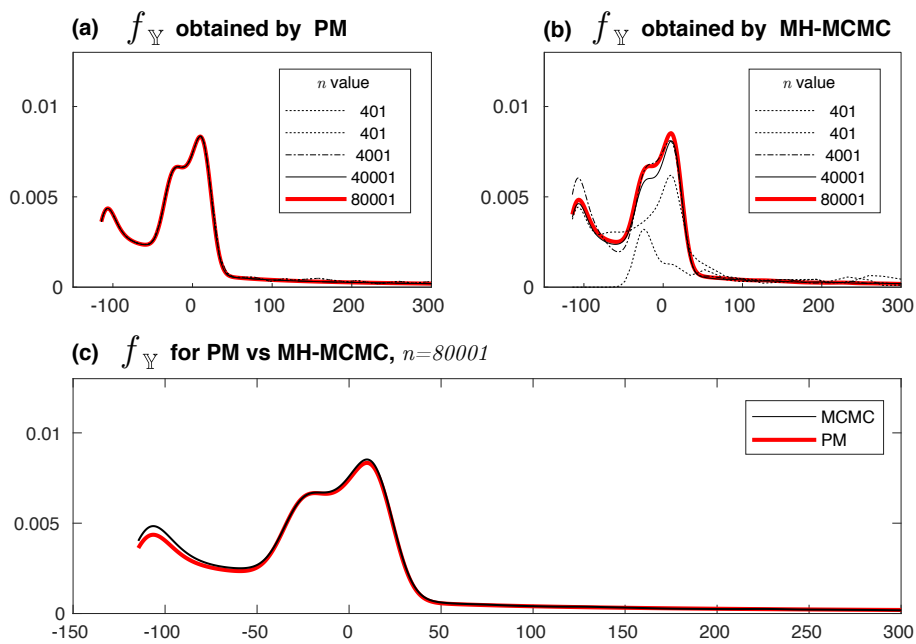


Figure 5: (a) Depicts the output f_Y PDF calculated via the proposed method (PM), for different values values of n ; (b) shows the output f_Y PDF obtained via MH-MCMC, for different values of n ; (c) A comparison between PM and MH-MCMC is established for the resulting f_Y PDFs, for $n = 80001$.

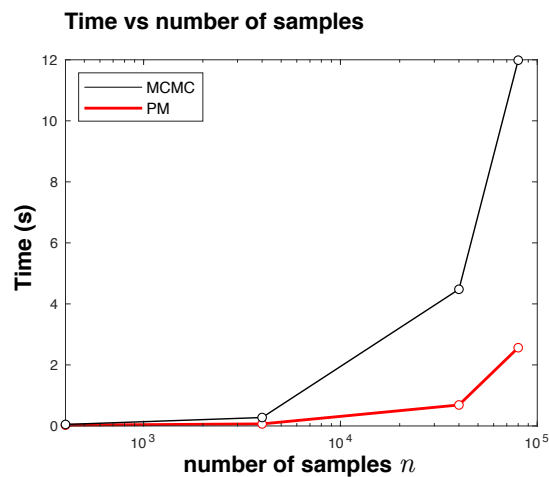


Figure 6: Time requirement for n samples

6 EXAMPLE 4: APPLICATION TO DRILL-STRING DYNAMICS

The objective of this example is to show the applicability of the PM to a non-linear problem of drill-string dynamics. Also, the PM will be compared against the transformation method (TM).

A Cosserat rod model (Antman, 2006) is considered with stochasticity on one of the parameters that define the friction model. The friction model itself is taken from the work of Tucker and Wang (2003), and it has been regularized so that the frictional torque and rate-of-penetration vanish as the drill-bit angular velocity tends to zero. The resulting model is described by Eq.

(4).

$$TOB = (-a_1 + a_2 F_{bit}) a_4 \frac{\omega_L^3}{(\omega_L^2 + \epsilon^2)^2} + a_3 a_4 \frac{\omega_L^3}{(\omega_L^2 + \epsilon^2)^{3/2}} + a_5 \frac{\omega_L}{(\omega_L^2 + \epsilon^2)^{1/2}} \quad (4)$$

A more detailed description of the drill-string model can be found in (Goicoechea et al., 2018).

Variable	Symbol	Value	Units
Weight on bit	WOB	100	<i>kN</i>
Regularization parameter	ϵ	2	<i>rad s⁻¹</i>
Model parameter 1	a_1	$3.429 \cdot 10^{-3}$	<i>m s⁻¹</i>
Model parameter 1	a_2	$5.672 \cdot 10^{-8}$	<i>m N⁻¹ s⁻¹</i>
Model parameter 2	a_3	$1.374 \cdot 10^{-4}$	<i>m rad⁻¹</i>
Model parameter 4	a_4	$9.537 \cdot 10^6$	<i>N rad</i>
Model parameter 5	a_5	$1.475 \cdot 10^3$	<i>N m</i>

Table 1: Parameters for the Tucker and Wang friction model

In order to compare the two methods, consider the case where a distribution for the maximum peaks of the angular velocities is desired. In this case, each parameter maps into a different value for the peaks so the transformation is one-to-one. Moreover, $y = g(x)$ is monotonically decreasing and invertible, as shown in Fig. (7).

The random variable A_1 is considered to have a uniform PDF distribution in the interval $[0, 6.858 \cdot 10^{-3}]$, therefore its corresponding first and second moments are $\mu = 3.4290 \cdot 10^{-3}$ and $Var = 3.9193 \cdot 10^{-6}$.

The model is implemented and solved within the COMSOL (2018) FEM software.

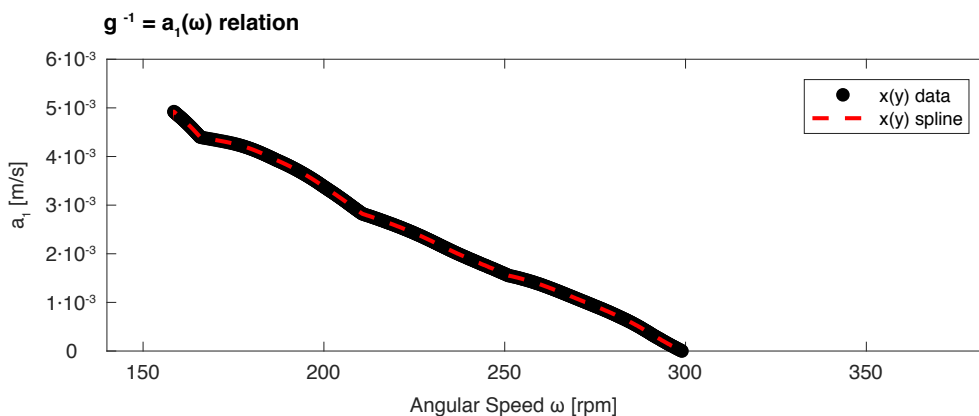


Figure 7: Inverse mapping $a_1 = g^{-1}(\omega)$ used in the TM method.

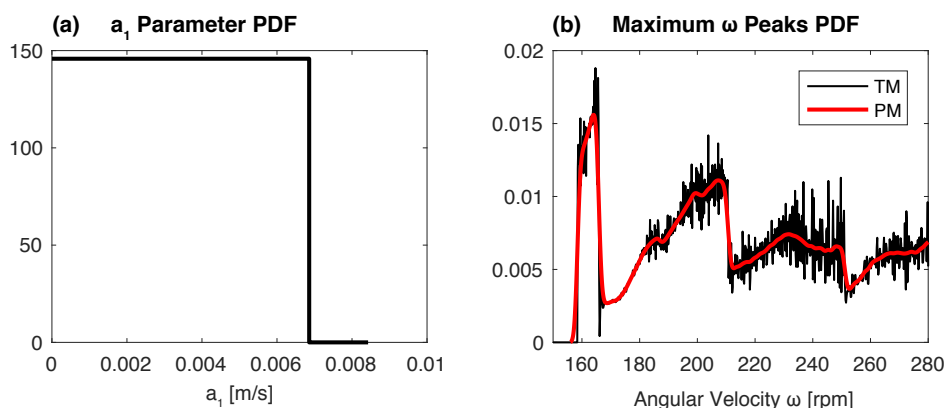


Figure 8: (a) Input a_1 PDF; (b) Construction of the output PDF for the maximum angular speed ω_z by means of PM and TM methods.

As shown in Fig. (8), solutions for both PM and TM are consistent. The numerical transformation solution results in a noisier graph. This could either be due to the fact that a spline has been used in the obtention of derivatives, or to the usage of a high value for the kernel smoothing bandwidth.

7 EXAMPLE 5: APPLICATION TO GUYED MASTS DYNAMICS

Guyed masts are examples of structures extensively used in Civil Engineering. During the service life of the structure, the guys tension values can vary due to various circumstances. A three-dimensional guyed mast is herein represented by a 20 m beam-column and one level of three nonlinear inclined cables at the top (see Fig. 9(a)), with a prescribed dynamic lateral load acting on the mast. The top displacements of the mast exhibits a rich range of dynamic responses, within small ranges of variation of the initial pretension (see Fig. 9(b)). In this example, the initial pretension H will be considered a random variable, uniformly distributed within the interval $[2000N, 3000N]$.

Figure 10 depicts the results of the PDF of the peak displacements, for the Monte Carlo Method (10(a)) and the Proposed Method (10(b)) for different number of realizations. Note that in this problem the output (peak displacements at the top) is nonperiodic within the interval of pretension studied (see Fig. 9(b)) and then is treated as a stochastic variable. It is apparent that the Proposed Method almost reaches a very good approximation of the PDF of the peak displacements with 100 realizations, while the Monte Carlo Method needs at least 10 times more realizations to achieve similar results. In Fig. 10(c) a comparison between both methodologies is showed. The differences are insignificant and the number of realizations (and computational time invested) is, again 10 times lower for the Proposed Method than the required for the standard Monte Carlo simulations. In this case, by means of the Proposed Method, less than half of the results from the parametric sweep performed in order to study the nonlinear dynamics were necessary to obtain a good approximation to the PDF of the peak displacements.

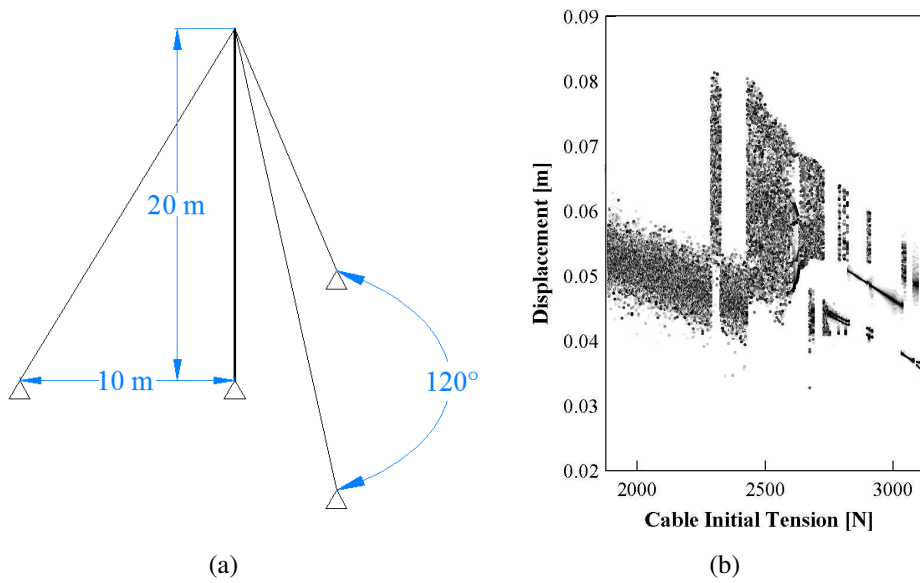


Figure 9: (a) Studied Guyed Mast. (b) Bifurcation diagram of the top displacements.

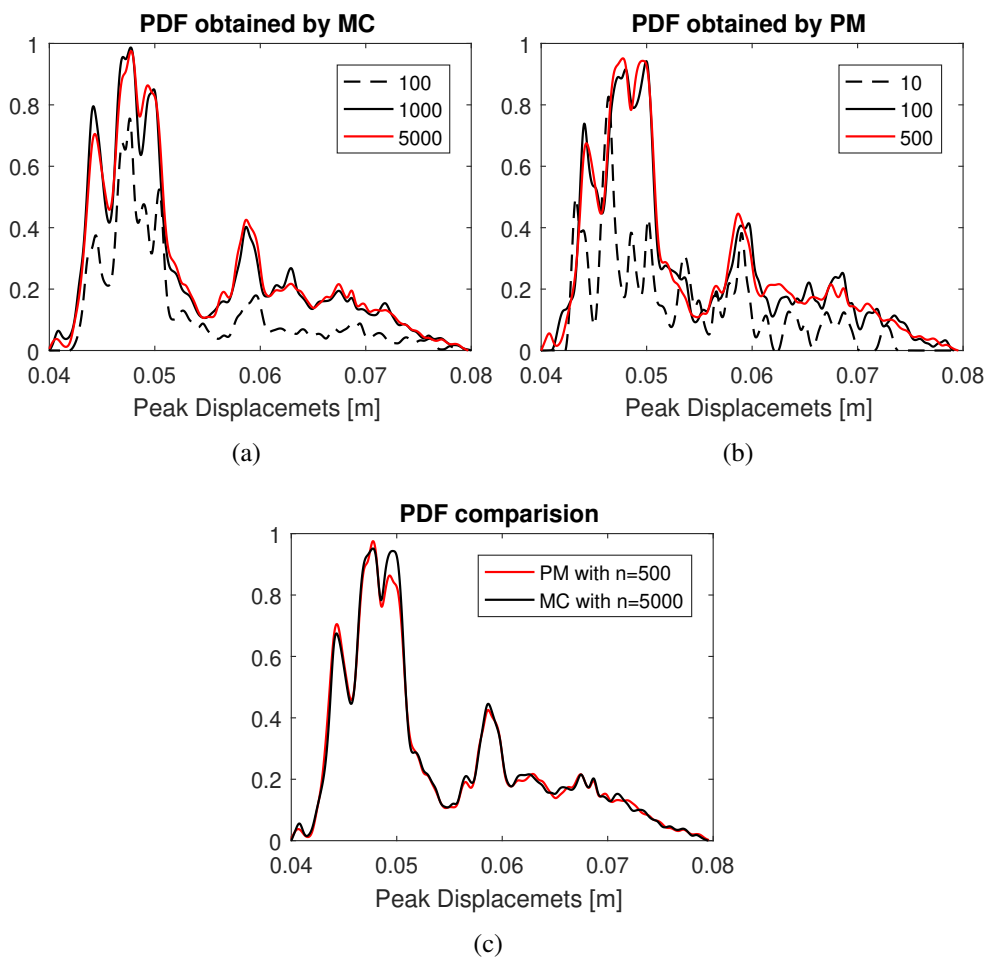


Figure 10: PDF convergence with the number of realizations. (a) Monte Carlo Method. (b) Proposed Method. (c) Comparison between Monte Carlo and the Proposed Method Results.

8 FINAL COMMENTS

In this work a method to obtain the uncertainty propagation avoiding a large number of simulations is presented. The supporting theory and application examples are discussed.

The method presented proves to be an interesting approach when performing uncertainty propagation, in the sense that convergence can be attained with a coarser partition, that is, less numerical calculations and computational time is required. This is particularly interesting in order to spread the use of uncertainty quantification to professional applications, where no powerful servers nor time are available.

Despite in this work the application to random variables is addressed, the extension to stochastic processes is direct, if deterministic models with random parameters are considered.

The most important application is thought to be low dimensional parameter spaces, especially if a parametric sweep has been previously performed.

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