Laboratório Nacional de Computação Científica

Programa de Pós-Graduação em Modelagem Computacional

Uncertainty Quantification Management System

Noel Moreno Lemus

Petrópolis, RJ - Brasil

Abril de 2018

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Uncertainty Quantification Management System

Thesis submitted to the examining committee in partial fulfillment of the requirements for the degree of Doctor of Sciences in Computational Modeling.

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Abril de 2018

Dedication

To my little and special family.

Acknowledgements

O autor manifesta reconhecimentos às pessoas e instituições que colaboraram para a execução de seu trabalho.

"Essentially, all models are wrong, but some are useful."

(George Edward Pelham)

Abstract

Segundo a **??**, 3.1-3.2), o resumo deve ressaltar o objetivo, o método, os resultados e as conclusões do documento. A ordem e a extensão destes itens dependem do tipo de resumo (informativo ou indicativo) e do tratamento que cada item recebe no documento original. O resumo deve ser precedido da referência do documento, com exceção do resumo inserido no próprio documento. (...) As palavras-chave devem figurar logo abaixo do resumo, antecedidas da expressão Palavras-chave:, separadas entre si por ponto e finalizadas também por ponto.

Keywords: latex. abntex. editoração de texto.

Abstract

This is the english abstract.

Keywords: latex. abntex. text editoration.

List of Figures

List of Tables

List of abbreviations and acronyms

UQ	Uncertainty Quantification
FP	Forward Problem
QoI	Quantity of Interest

List of symbols

Γ	Letra grega Gama
Λ	Lambda
ζ	Letra grega minúscula zeta
$\in$	Pertence

Contents

1 Introduction

1.1 Research Objectives

1.2 Highlights of the Dissertation

1.3 Organization of the Dissertation

2 Related Works

2.1 Overview

HPC and computational modeling play a dominant role in shaping the methodological developments and research in uncertainty qualification. Depending on the complexity of the uncertainty qualification investigation, anywhere from 10^2 to 10^8 runs of the computational model may be required. Thus, uncertainty qualification investigations may require extreme-computing environments (e.g., exascale) to obtain results in a useful time frame, even if a single run of the computational model does not require such resources.

Advances in computing over the past few decades—both in availability and power—have led to an explosion in computational models available for simulating a wide variety of complex physical (and social) systems. These complex models—which may involve millions of lines of code, and require extreme-computing resources—have led to numerous scientific discoveries and advances. This is because these models allow simulation of physical processes in environments and conditions that are difficult or even impossible to access experimentally. However, scientists' abilities to quantify uncertainties in these model-based predictions lag well behind their abilities to produce these computational models. This is largely because such simulation-based scientific investigations present a set of challenges that is not present in traditional investigations.

Until recently, the original approach of describing model parameters using single values has been retained, and consequently the majority of mathematical models in use today provide point predictions, with no associated uncertainty. (JOHNSTONE et al., 2016)

An immediate challenge in the development of an appropriate treatment of uncertainty in an analysis of a complex system is the selection of a mathematical structure to be used in the representation of uncertainty. (HELTON et al., 2010a) Traditionally, probability theory has provided this structure [48-55]. However, in the last several decades, additional mathematical structures for the representation of uncertainty such as evidence theory [56-63], possibility theory [64- 70], fuzzy set theory [71-75], and interval analysis [76-81] have been introduced. This introduction has been accompanied by a lively discussion of the strengths and weaknesses of the various mathematical structures for the representation of uncertainty [82-90]. For perspective, several comparative discussions of these different approaches to the representation of uncertainty are available [72; 91-98]

a 'typical' UQ problem involves one or more mathematical models for a process of interest, subject to some uncertainty about the correct form of, or parameter values for, those models.

Often, though not always, these uncertainties are treated probabilistically.

but how will you actually go about evaluating that expected value when it is an integral over a million-dimensional parameter space? Practical problems from engineering and the sciences can easily have models with millions or billions of inputs (degrees of freedom).

the language of probability theory is a powerful tool in describing uncertainty

UQ cannot tell you that your model is 'right' or 'true', but only that, if you accept the validity of the model (to some quanti-fied degree), then you must logically accept the validity of certain conclusions (to some quantified degree). (SULLIVAN, 2015)

"UQ studies all sources of error and uncertainty, including the following: systematic and stochastic measurement error; ignorance; limitations of theoretical models; limitations of numerical representations of those models; limitations of the accuracy and reliability of computations, approximations, and algorithms; and human error. A more precise definition is UQ is the end-to-end study of the reliability of scientific ∞erences."

UQ is not a mature field like linear algebra or single-variable complex analysis, with stately textbooks containing well-polished presentations of classical theorems bearing August names like Cauchy, Gauss and Hamilton. Both because of its youth as a field and its very close engagement with applications, UQ is much more about problems, methods and 'good enough for the job'. There are some very elegant approaches within UQ, but as yet no single, general, over-arching theory of UQ.

In

Probability theorists usually denote the sample space of a probability space by Ω; PDE theorists often use the same letter to denote a domain in $\Re^n$ on which a partial differential equation is to be solved. In UQ, where the worlds of probability and PDE theory often collide, the possibility of confusion is clear. Therefore, this book will tend to use Θ for a probability space and $\mathbf{X}$ for a more general measurable space, which may happen to be the spatial domain for some PDE.

2.2 Types of Uncertainty

It is sometimes assumed that uncertainty can be classified into two categories, (KIUREGHIAN; DITLEVSEN, 2009) although the validity of this categorization is open to debate.

Aleatory uncertainty arises from an inherent randomness in the properties or behavior of the system under study. For example, the weather conditions at the time of a reactor accident are inherently random with respect to our ability to predict the future. Other examples include the variability in the properties of a population of weapon components and the variability in the possible future environmental conditions that a weapon component could be exposed to. Alternative designa- tions for aleatory uncertainty include variability, stochastic, irreducible and type A. (HELTON, 2009)

Epistemic uncertainty derives from a lack of knowledge about the appropriate value to use for a quantity that is assumed to have a fixed value in the context of a particular analysis. For example, the pressure at which a given reactor containment would fail for a specified set of pressurization conditions is fixed but not amena- ble to being unambiguously defined. Other examples include minimum voltage required for the operation of a system and the maximum temperature that a system can withstand before failing. Alternative designations for epistemic uncertainty include state of knowledge, subjective, reducible and type B. (HELTON, 2009)

2.2.1 Aleatory uncertainty

Aleatory uncertainty arises from an inherent randomness in the properties or behavior of the system under study. For example, the weather conditions at the time of a reactor accident are inherently random with respect to our ability to predict the future. Other examples include the variability in the properties of a population of weapon components and the variability in the possible future environmental conditions that a weapon component could be exposed to. Alternative designa- tions for aleatory uncertainty include variability, stochastic, irreducible and type A. (HELTON, 2009)

2.2.2 Epistemic uncertainty

2.3 Uncertainty Representation

The question of how to represent and communicate uncertainties is a topic of research both from a practical and theoretical point of view. A fair bit of theoretical research is aimed at the mathematical calculus of uncertainty. This includes extensions and alternatives to standard probabilistic reasoning, such as Dempster-Schafer theory and imprecise probabilities. When uncertainties are needed for investigations requiring computational models, additional considerations arise. For example, if the simulation output is a daily surface-temperature field over the globe for the next 200 years, representing uncertainty and dependencies is complex. Should ensembles be used to represent plausible outcomes? How should these ensembles of simulation output be stored? How can high-consequence/low-probability outcomes be discovered in this massive output? Here some research investigations attempt to leverage theory that exploits high dimensionality to bound probabilities and system behavior. Finally, even when uncertainties are well captured,

Table 1 – The range of the GLD parameters and the minimum and maximum values corresponding to the labeling of the regions given in Figure

Region	λ_1	λ_2	λ_3	λ_4	Minimum	Maximum
1 and 5	all	< 0	< -1	> 1	$-\infty$	$\lambda_1 + \frac{1}{\lambda_2}$
2 and 6	all	< 0	> 1	< -1	$\lambda_1 - \frac{1}{\lambda_2}$	∞
3	all	> 0	> 0	> 0	$\lambda_1 - \frac{1}{\lambda_2}$	$\lambda_1 + \frac{1}{\lambda_2}$
	all	> 0	$= 0$	> 0	λ_1	$\lambda_1 + \frac{1}{\lambda_2}$
	all	> 0	> 0	$= 0$	$\lambda_1 - \frac{1}{\lambda_2}$	λ_1
4	all	< 0	< 0	< 0	$-\infty$	∞
	all	< 0	$= 0$	< 0	λ_1	∞
	all	< 0	< 0	$= 0$	$-\infty$	λ_1

how best to communicate such uncertainties to the public or to decision-makers is also a topic of ongoing research.

(HELTON et al., 2010b)

2.3.1 Representation of Uncertainty with Probability

2.3.2 Dempster-Shafer theory

2.3.3 The Bayesian Methodology

2.4 Methods for Uncertainty Propagation

2.5 Probabilistic Background

2.5.1 The Generalized Lambda Distribution

The Generalized Lambda Distribution (GLD) was defined by Ramberg and Schmeiser in 1974 by the quantil function:

$$F^{-1}(p|\lambda) = F^{-1}(p|\lambda_1, \lambda_2, \lambda_3, \lambda_4) = \lambda_1 + \frac{p^{\lambda_3} - (1-p)^{\lambda_4}}{\lambda_2} \tag{2.1}$$

where p are the probabilities, $p \in [0, 1]$, λ_1 and λ_2 are the location and scale parameteres, and λ_3 and λ_4 determine the skewness and kurtosis of the $GLD(\lambda_1, \lambda_2, \lambda_3, \lambda_4)$.

Some restrictions in the values of $\lambda_1, \lambda_2, \lambda_3$ and λ_4 define if the GLD is valid. Those restrictions define 6 regions as is shown in table

The probability density function of the GLD at the point $x = F^{-1}(p)$ is given by:

$$f(x) = f(F^{-1}(p)) = \frac{\lambda_2}{\lambda_3 p^{\lambda_3 - 1} + \lambda_4 (1-p)^{\lambda_4 - 1}} \tag{2.2}$$

Note that the valid parameteres of λ guaranty that:

$$f(x) \geqslant 0 \tag{2.3}$$

$$\int f(x)dx = 1 \tag{2.4}$$

2.5.2 Fitting Mixture Distributions Using a Mixture of Generalized Lambda Distributions

Esto esta en (TOBERGTE; CURTIS, 2013)

2.5.3 Sampling Methods

2.5.3.1 Monte Carlo

2.6 Summary

2.7 Concepts

high-dimensional parameter spaces computationally demanding forward models nonlinearity and/or complexity in the forward model

2.8 Software and Tools for UQ

These include both free software, like OpenTURNS (Andrianov et al., 2007), DACOTA (Adams et al., 2009) and DUE (Brown and Heuvelink, 2007), commercial, like COSSAN (Schuëller and Pradlwarter, 2006), or free, but written for a licenced software, e.g. SAFE (Pianosi et al., 2015) or UQLab (Marelli and Sudret, 2014) toolboxes for MATLAB. A broad review of existing software packages is available in Bastin et al. (2013). To the best of our knowledge, however, none of the existent software is specifically designed to be extended by the environmental science community. The use of powerful but complex languages like C++ (e.g. Dakota), Python (e.g. OpenTURNS) or Java (e.g. DUE) often discourages relevant portions of the non-highly-IT trained scientific community from the adoption of otherwise powerful tools. spup-R package (**??**). De aqui saque lo de arriba tambien, aunque lo de arriba lo puedo buscar en sus respectivos papers y hablar un poco de cada uno de ellos.

Currently, advances in uncertainty propagation and assessment have been paralleled by a growing number of software tools for uncertainty analysis, but none has gained recognition for a universal applicability, including case studies with spatial models and spatial model inputs. (**??**)

3 Uncertainty Quantification Process

3.1 Measures of Information and Uncertainty

3.1.1 Variance, Information and Entropy

Variance.

Information and Entropy.

3.1.2 Information Gain, Distances and Divergences

3.2 Sensitivity Analysis

Sensitivity analysis is the systematic study of how model inputs—parameters, initial and boundary conditions—affect key model outputs. Depending on the application, one might use local derivatives or global descriptors such as Sobol's functional decomposition or variance decomposition. Also, the needs of the application may range from simple ranking of the importance of inputs to a response surface model that predicts the output given the input settings. Such sensitivity studies are complicated by a number of factors, including the dimensionality of the input space, the complexity of the computational model, limited forward model runs due to the computational demands of the model, the availability of adjoint solvers or derivative information, stochastic simulation output, and high-dimensional output. Challenges in sensitivity analysis include dealing with these factors while addressing the needs of the application. (**??**)

$$E = mc^2 \tag{3.1}$$

4 The Generalized Lambda Distribution

4.1 From Emperimental Data to GLD Paremeters

(??)

5 Our Approach

5.1 Fit the spatio-temporal dataset to the GLD

Aqui tengo que poner:

- Fit each spatio-temporal point to a corresponding GLD.
- Evaluate if the resulting GLD is valid on each spatio-temporal location.
- Perform a ks-test to evaluate if the quality of the fit on each spatio-temporal location.

5.2 Clusterizing the GLD based in its lambda values

5.3 Use of GLD mixture to characterize the uncertainty in an spatio-temporal region

5.4 Information entropy as a measure of the uncertainty in an spatio-temporal region

5.5 Information entropy and model selection

5.6 Conclusions

6 Applicability

In the present chapter we are going to test the UQMS in three different scenarios, spatial only domain, section 6.1 , spatio-temporal domain, section 6.2, and finally a multidisciplinary system, section 6.3.

6.1 Case Study: Wave Propagation Problem

The first one is a geophysical tests for wave propagation problems

As a first case study we use the “HPC4E Seismic Test Suite”, a collection of four 3D models and sixteen associated tests that can be downloaded freely at the project’s website (https://hpc4e.eu/downloads/datasets-and-software). The models include simple cases that can be used in the development stage of any geophysical imaging practitioner (developer, tester ...) as well as extremely large cases that can only be solved in a reasonable time using ExaFLOPS supercomputers. The models are generated to the required size by means of a Matlab/Octave script and hence can be used by users of any OS or computing platform. The tests can be used to benchmark and compare the capabilities of different and innovative seismic modelling approaches, hence simplifying the task of assessing the algorithmic and computational advantages that they pose.

In our case, we are going to use the “HPC4E Seismic Test Suite” as a case study of the porposed UQMS. As we mention in the introduction of this chapter this model is a spatial only domain problem, because we are going to consider a multidimentional array as an Input and a multidimentional array as an output, but of them time independet.

6.1.1 Mathematical Formulation

6.1.2 Model and Dataset Description

The models have been designed as a set of 16 layers with constant physical properties. The top layer delineates the topography and the other 15 different layer interface surfaces or horizons. In the following, an interface horizon is associated with properties that apply to the layer that exists between itself and the immediately next layer horizon. The model covers an area of 10 x 10 x 5 km, with maximum topography at about 500 m and maximum depth at about 4500 m. The layer horizons have been sampled very finely with 1.6667 m spacing so that a highly accurate representation can be honored at high frequencies. For simulation schemes based on unstructured grids, the layer horizons can be used easily to constrain model blocks. For simulation schemes based upon Cartesian grids, a simple

Table 2 – Layer constant properties and their depth range. “Star” layers are only used in the flat case, in substitution of their non-star equivalents

Layer Id	**Vp (m/s)**	**Vs (m/s)**	**Density (Kg/m3)**	**Max. depth (m)**	**Min. depth (m)**
1	1618.92	500.00	1966.38	-135.55	-476.35
2	1684.08	765.49	1985.88	41.50	-394.90
3					
4					
5					
6					
7					
8					
9					
10					
11					
12					
13					
14					
15					
16					
2*					
3*					

script is provided that can generate 3D grids for any desired spatial sampling. Table 2 shows the properties of each of the layers included in the models.

6.1.3 Adding uncertainty into the model

The “HPC4E Seismic Test Suite” does not provide uncertainty sources, because all the input parameters of the model have fixed values. Then, to the purpose of our work we need to add some uncertainties into the inputs. Let’s suppose the variable V_p is uncertain. As this variable have 16 different values, one for each layer, we can consider it as a random vector, equation 6.1. We associate to each of the V_{p_i} a Normal distribution with μ_i equal to the value reported in Table 2 and $\sigma = 2$.

$$V_p = < V_{p_i}, \mathcal{N}(\mu_i, \sigma_i) > \tag{6.1}$$

6.2 Case Study: Austin, queso library

6.3 Case Study: Multidisciplinary System (NASA)

6.4 Case Study: Spatio-temporal Nicholson-Bailey model

Este esta en el software uqlab, en la carpeta Doc Manuals

7 Conclusions and Future Works

7.1 Revisiting the Research Questions

7.2 Significance and Limitations

7.3 Open Problems and Future Work

7.4 Final Considerations

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Appendix

APPENDIX A – uqms R package

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A.1 Título da seção

Aqui temos uma seção dentro do Apêndice.

Figure 1 – Legenda para a figura.

APPENDIX B – Título do apêndice B

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APPENDIX C – Título do apêndice C

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Annex

ANNEX A – Título do anexo A

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A.1 Título da seção

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ANNEX B – Título do anexo B

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ANNEX C – Título do anexo C

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