## MS11 - Stochastic Modeling and Uncertainty Quantification

## Apresentador: Pablo Martin Rodriguez, UFPE

Título: Modelos estocásticos para a propagação de informação

Resumo: A disseminação de informação em uma população tem um impacto crescente em nossa vida cotidiana devido ao acesso cada vez mais rápido à informação, confiável ou não. Apresentaremos alguns modelos estocásticos que servem para representar de formas simples o fenômeno de propagação de informação. Para isto, realizaremos um breve resumo e comparação das técnicas usadas para o estudo rigoroso de ditos modelos e discutiremos resultados da literatura.

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### Apresentador: Haroldo F. de Campos Velho, INPE

Autores: Vinicius S. Monego, Juliana A. Anochi, Haroldo F. de Campos Velho

Título: Optimal Decision Tree for Uncertainty Quantification to the Climate Precipitation Prediction

Resumo: Numerical weather and climate predictions are important advance for the society, with very good impact to several sectors: natural disasters, agriculture, energy production, industry for tourism and entertainment, pollutant contaminant, for citing few of them. The codes for atmospheric dynamics are very sophisticated, modeling the geophysical fluid dynamics, as well as other physical processes involved (complex topography, ground covering, exchange fluxes between atmosphere and the surface, radiation, turbulence, cloud formation, and precipitation). The numerical processing has a high computational effort. The standard formulation for the forecasting uncertainty quantification (pedictability) is to apply a type of Monte Carlo method (ensemble prediction), enhancing the computer power. We apply a decision tree approach for addressing two fold: climate precipitation prediction, and forecasting UQ. Experiments over South America will be shown during our presentation, with significant reduction of the computer effort, without lost of quality to the forecasting and the predictability estimation. A comparison with global model differential equation and ensemble prediction are also shown.

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#### Apresentador: Carlile Campos Lavor, Unicamp

Título: Incertezas em Geometria de Distâncias

Resumo: O principal problema da Geometria de Distâncias pode ser definido como um problema inverso: dadas algumas distâncias entre pares de objetos, determinar suas posições em algum espaço geométrico. Dentre inúmeras aplicações, passando por astronomia, estatística, nanotecnologia, robótica e telecomunicações, destaca-se o cálculo da estrutura 3D de proteínas (as "moléculas da vida"), conhecido na literatura por Molecular Distance Geometry Problem (MDGP). Por conta de propriedades químicas e geométricas das proteínas, o MDGP pode ser representado por um grafo e "resolvido" por um método tipo Branch and Prune (BP). Considerando distâncias "precisas", o algoritmo BP é muito eficiente e robusto, mas há grandes desafios quando temos que lidar com incertezas nos valores das distâncias. Apresentaremos alguns deles e estamos na expectativa de que o minissimpósio possa contribuir com novas ideias para a modelagem e "solução" do MDGP com incertezas.

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## Apresentador: Héctor E. Goicoechea, PUC-Rio

Autores: Héctor E. Goicoechea, Roberta Lima e Rubens Sampaio

Título: Analysing the variability in the computational burden of a Monte-Carlo simulation

Resumo: To present ideas, a model problem consisting of a moving mass-belt system with random friction showing the stick-slip phenomenon is treated. The dynamics is simulated. The objective is to assess the behavior of the computation cost in terms of the run-time, which is random, and its relationship with some of the output variables that define the dynamical behavior of the mechanical system. The variables that will be studied are the duration of the phases present in the simulation, sticks and slips, and the number of phases that occur in each realization. All this is analysed from a stochastic perspective. However, the probabilistic model to analyse the distribution of a threedimensional random vector, formed by the run-time, duration and number, belongs to R4, thus it is difficult to characterize and visualize. Hence, in this study, random variable transformations are used to produce new variables in an attempt to reduce the number of dimensions that need to be considered. In this exploration, the sliced Wasserstein distance is used as a measure to evaluate the independence of the variables in the new distributions. Also, the change of variables is used to assess the link between the behaviour of the results and the chosen integration method. The results show that the predictions obtained with the Monte Carlo method combined with a Multiple Scales analytical approximation are influenced by the number of transition phases rather than their durations.

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# Apresentador: João Pedro Freitas, PUC-Rio

Autores: Ioão Pedro Freitas, Roberta Lima e Rubens Sampaio

Título: Comparison among techniques to get mass functions in a branching process

Resumo: In this work, the spread of an epidemiological disease over time is modeled as a Bienaymé-Galton-Watson process. Therefore, a discrete random variable models the number of infections per infector and rules the branching process. Given this probabilistic model, the aim is to compare theoretically and computationally methodologies to get mass functions of further generations' size: probability generating functions, polynomial identities, Markov chain and Monte Carlo simulation. Comparisons are done in two distinct levels. The first is a local one, in which for the same generation, the analysis are done state by state. The other is a global, which focus on the whole support of each generation. Results show that the first two methodologies are not able to cover the entire support, due runtime issues in the probability generating functions approach and lack of RAM in the polynomial one. On the other hand, they give likelihood functions for bayesian inference, because their algorithm works with symbolic computation. Moreover, they are the only ones to also perform a local analysis. Despite of the limitation of the random variable modeling the contagion in Markov chain's technique, it has more advantages in terms of runtime and storage than the previous methods and still provides analytical relations, since it also works with symbolic computation. The further the generation is, Monte Carlo seems to be the only feasible approach, but as a consequence all the features evaluated are then random objects that need a more careful analysis and the requirement to perform bayesian inference is lost.

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Autores: Roberta Lima e Rubens Sampaio

Título: How to deal with uncertainty quantification and propagation

Resumo: Over the last years, stochastic models have called the attention of researchers. The number of publications in the subject has grown and the topic is being analyzed in different applications. Observing the new literature produced in the field, it is possible to verify that new expressions, as uncertainty quantification and uncertainty propagation, have emerged. These expressions become largely used and fashionable, however there is no consensus of their meanings. Each author arbitrates a meaning according to its own convenience. Sometimes the disarray is such that different meanings, some of them contradictory, can be found throughout the same work. The objective of this work is to clarify the concepts. We define what is and what is not uncertainty quantification and propagation. We also show, with simple examples, that several strategies found in literature called strategies to compute uncertainty quantification and propagation are not. They can lead to errors and misleadingness. The examples were chosen to be as simple as possible in order to highlight different problems that can arise when one uses these strategies.

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Título: Revolução, entropia, informação, aleatório: uma visão histórica

Resumo: A Revolução Industrial, com o desenvolvimento das máquinas térmicas levou acarretou o conceito de Entropia, mesmo antes do estabelecimento do conceito de conservação de energia. Paralelamente, as idéias Newtonianas, e o seu sucesso na descrição da Mecânica Celeste, levou a uma nova Física, a Mecânica Estatística. Essa nova visão levou ao desenvolvimento de um novo conceito de Entropia, baseado na Mecanica Estatística e em Informação, uma idéia criado por Shannon. Como essas entropias estão associadas? Uma, determínista, originada das máquinas térmicas, e a outra, aleatória, associada à informação? O trabalho mostrará, com uma ótica histórica, a relação entre essas idéias. A ênfase será na introdução do conceito de aleatório em Física.