
HOW TO CONSTRUCT STOCHASTIC MODELS ? THEORY AND NUMERICS

by

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General background : modelling of stochastic perturbations and validation of models

The aim of this lecture is to present a set of mathematical tools and results permitting to construct a stochastic viable model from a known deterministic one and second to validate them via numerical simulations. Indeed, many dynamical systems in Biology or Physics are in a first approach modelled by a deterministic dynamical systems. We can cite for example the classical Hodgkin-Huxley model in Biology or the Landau-Lipshitz model in Physics. Then, a set of observations are made and lead to the introduction of a stochastic or random component. For the Hodgkin-Huxley model this comes from the fact that there exists an intrinsic stochastic bioelectrical activity of neurons which is observed experimentally. For the Landau-Lifshitz model this comes from the fact that the electromagnetic fields behaves very randomly. However, to take into account these stochastic effects is in general not an easy task.

The Lecture is made of two parts : the first one deals with the construction of the stochastic model. The second one is devoted to numerical methods designed in order to validate these models. All the mathematical tools and results will be illustrated by numerous examples coming from Biology, Physics, Astronomy and Celestial Mechanics.

Part I - Admissible or viable stochastic models

In a first part of this Lecture, we discuss such a modelling in the context of the theory of stochastic differential equations.

Returning to the initial deterministic model is always interesting. Indeed, it provides a set of constraints which are in general considered as fundamental by the scientists. This can be some fundamental law of Physics like conservation of energy, existence of some symmetries or invariance properties. At least these properties are in general respected by the deterministic

model and a natural way to extend such a model in the stochastic framework is to construct a suitable stochastic perturbation respecting such a constraints in an appropriate sense.

In this Lecture, we will provide many results characterizing stochastic perturbations which preserve important properties : invariance of domain (in particular positivity), first integrals, variational structures (Lagrangian or Hamiltonian), symmetries, etc. These results will then be applied in various fields : Biology (behaviour of neurons, HIV population dynamics, Virus transmission models and models for the immune system, Cellular signaling networks, Population growth models, Tumor growth), Physics (Ferromagnetism), Astronomy and Celestial Mechanics (Two-body problem, Orbits of Satellites, Earth's rotation).

Part II - Numerical methods and validation of models

In a second part of this Lecture, we discuss how to make numerical simulations in order to validate these stochastic models. The main difficulty which is not usually discussed in the literature, is to provide numerical methods respecting the constraints of the models. This problem is well known in Hamiltonian mechanics where the conservation of energy is an important feature of the models and has led to the theory of variational integrators. For invariance of domains, symmetries, etc, the state of the arts is not so clear even in the deterministic case.

In this Lecture, we will discuss the construction of variational integrators in the context of the theory of discrete embeddings and secondly we will discuss the construction of topological numerical scheme which are reminiscent of a general program initiated by R. Mickens around non-standard numerical scheme. These methods will be discussed in the deterministic and stochastic case with numerous examples.

Articles of the author on the subjects of the Lecture

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- L. Bourdin, J. Cresson, I. Greff, P. Inizan, Variational integrators for Fractional Lagrangian systems in the framework of discrete embeddings, 13.p, *Applied Numerical Mathematics*, Volume 71, September 2013, Pages 1-23.