UNIVERSITÀ DEGLI STUDI DI TRENTO
Dipartimento di Matematica

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Aula Seminari – Dipartimento di Matematica

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HYBRID STOCHASTIC-DETERMINISTIC MODELS FOR SIMULATION OF BIOCHEMICAL SYSTEMS

ABSTRACT:
At the molecular level, biochemical reactions are random collisions, so that the processes governing the dynamics is inherently stochastic, and would deserve a stochastic mathematical model ro obtain reliable (predictive) simulation. The chemical master equation (CME) is the fundamental evolution equation of the stochastic description of biochemical reaction kinetics. In particular, CME is especially useful when formulating mathematical models of gene regulatory networks and protein-protein interaction networks, where the numbers of molecules of most species are around tens or hundreds. However, in most applications it is impossible to solve the CME directly due to its high dimensionality. Instead, indirect approaches based on realizations of the underlying Markov jump process are used such as the stochastic simulation algorithm (SSA). In the SSA, however, every reaction event has to be resolved explicitly such that it becomes numerically inefficient when the system's dynamics include fast reaction processes or species with high population levels. Such a dynamic is termed hybrid dynamics, as requires hybrid stochastic/deterministic modelling approaches. In many hybrid approaches, fast reactions are approximated as continuous-deterministic processes or replaced by quasi-stationary distributions either in a stochastic or deterministic context, while slow reaction involving a low number of molecules are modelled with discrete-stochastic formalisms. I will present an overview of the use of hybrid models for biochemical reaction systems including also the recent results and advancements achieved in my research activity.

References:

[1] Paola Lecca, Ian Laurenzi, Ferenc Jordan, Deterministic versus stochastic modelling in biochemistry and systems biology, Woodhead Publishing Series in Biomedicine No. 21, 2012.
[2] Systemic Approaches in Bioinformatics and Computational systems Biology: Recent Advances, by Paola Lecca (Editor), Dan Tulpan (Editor), Kanagasabai Rajaraman (Editor), IGI-Global, 2012.

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