MATHEMATICAL SCIENCES

DISMA - Stochastic Models of Chemical Reaction Networks and Applications

Funded By	Dipartimento DISMA
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Context of the research activity	The object of interest are stochastic chemical reaction networks and potential model extensions. Specifically, the project will deal with continuous-time Markov chains, their stationary regime (existence and description), absorption probabilities, convergence to other stochastic processes (in different topologies). Application to biology, chemistry, and industry will be of interest.
	Reaction networks are mathematical models used in biochemistry, epidemiology, ecology, and sociology with the aim to describe changes over time of the abundances of interacting particles (such as chemical species, molecules, individuals, animals, etcetera). As such, reaction networks attract the interest of both applied scientists and mathematicians: the former need the development of novel mathematical results to properly analyze specific systems, and the latter are intrigued by the non-trivial interplay between the dynamics of the system and the properties of the graph given by the finite set of allowed changes of the interacting items. On top of classical and currently active applications such as analysis and statistical inference in biomolecular, epidemiological, and ecological models, novel scientific frontiers in connection with the study of reaction networks are currently investigated: examples are the emerging field of synthetic biology aiming at controlling the cell behavior, the capability of designing and physically construct sets of chemical reactions capable to perform specific calculations, and even the possibility to build chemically implemented machine learning and neural network algorithms. Formally, stochastic models of reaction networks describe the change in the reactant molecule counts as a continuous-time Markov chain. The Ph.D. project will therefore deal with theory of continuous-time Markov chains, including connectivity properties, limit behaviour as the time goes to infinity, stopping times, and exit distributions. More specifically, during the Ph.D. the candidate is expected to learn about the following active research direction, and prove novel mathematical results related to one or more of them: a) Inferring the existence of a stationary distribution from topological

Objectives	characteristics the graph given by the finite set of allowed reaction. This is typically done via Foster-Lyapunov techniques, but alternative methods can be investigated. b) Characterizing or approximating the stationary distribution when possible. c) Studying the rate of convergence to the stationary distribution. This is typically done via Foster-Lyapunov techniques or Poincare inequalities, but alternative tools can be explored. d) Convergence of the families of stochastic reaction network models to a limit deterministic or stochastic processes, under different assumptions. The convergence of interest is typically a functional convergence over compact intervals of time. The topologies of interest can vary among uniform topology, Skorohod topology, Jakubowsky topology, etc. e) Studying the available simulation techniques and analysing their benefits and drawbacks. f) Comparing stochastic processes arising form different models, with potential use of Stochastic Ordering techniques. g) Extensions of the classical mathematical models to cases with heterogeneous space (such as in compartmental models, spatial models, diffusive models, etc). h) Application of stochastic reaction networks theory in the settings of biochemistry, epidemiology, ecology, and sociology, as described above. The Ph.D., at the end of the program, should be able to: carry out research independently, produce original and relevant results, and fit into the international scientific community. The training of the Ph.D. will be achieved via studying suggested literature, discussion with peers and senior researchers of the Politecnico di Torino, participation to international conferences and workshops to get in touch with the international scientific community, and presentations (written and oral) of the Ph.D. own work.

Skills and competencies for the development of the activity	The candidate should be familiar with mathematical techniques of proving theoretical results and possess the due rigor these require. During his or her undergraduate career he or she should have passed basic exams in probability and statistics and, possibly, have acquired an introductory knowledge of Stochastic Processes. A master's thesis in probability calculus is not required, but any additional expertise of the subject is an added value.