DIPARTIMENTO DI INGEGNERIA CIVILE E AMBIENTALE

POLITECNICO MILANO 1863

Citrini Room, Building 4, ground floor, Leonardo Campus
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Chemical Continuous Time Random Walks

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Accurately simulating reactive transport through heterogeneous media requires resolving the spatial scales at which mixing takes place. This typically requires a fine spatial discretization (Eulerian methods) or large numbers of particles (Lagrangian methods), leading to prohibitively expensive simulations for large-scale transport. We explore a different approach and consider the question: In heterogeneous chemically reactive systems, is it possible to describe the evolution of macroscopic reactant concentrations without explicitly resolving the spatial transport? Traditional Kinetic Monte Carlo methods, such as the Gillespie algorithm [1], model chemical reactions as random walks in particle number space, without the introduction of spatial coordinates. The inter-reaction times are exponentially distributed under the assumption that the system is well mixed. In real systems, transport limitations lead to incomplete mixing and decreased reaction efficiency. We introduce an arbitrary inter-reaction time distribution, which may account for the impact of incomplete mixing. The resulting process defines an inhomogeneous continuous time random walk in particle number space, from which we derive a generalized chemical Master equation and formulate a generalized Gillespie algorithm [2]. We then determine the modified chemical rate laws for different inter-reaction time distributions. We trace Michaelis–Menten-type kinetics back to finite-mean delay times, and predict time-nonlocal macroscopic reaction kinetics as a consequence of broadly distributed delays. Non-Markovian kinetics exhibit weak ergodicity breaking and show key features of reactions under local non-equilibrium.

[1] Gillespie, Daniel T. "Exact stochastic simulation of coupled chemical reactions." The journal of physical chemistry 81.25 (1977): 2340—2361.
[2] Aquino, T. and M. Dentz, Chemical continuous time random walks, Physical Review Letters, 119.23 (2017): 230601.

Reference: **Dr. Giovanni Porta** (giovanni.porta@polimi.it)

Tomás Aquino studied Theoretical Physics for his Undergraduate education at the University of Lisbon (2009), in his home country, Portugal. He obtained his Master's Degree from the same institution, specializing in Nonlinear and Statistical Physics (2011). He then completed his graduate studies in Indiana, USA, where he was awarded a PhD by the University of Notre Dame (2016).
Tomás is interested in modeling physical processes with recourse to stochastic methods, both by analytical and computational means. Currently, he is developing models of conservative and reactive transport for surface and subsurface hydrological systems that aim to capture heterogeneity through the use of stochastic descriptions. He has also worked in applying probabilistic techniques to gene expression in biological cells and to the dynamics of multi-strain diseases such as Influenza.