18th World IMACS / MODSIM Congress, Cairns, Australia 13-17 July 2009
http://mssanz.org.au/modsim09

Master equations in chemical kinetics: CME and beyond

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Abstract: Chemical reactions happening inside the cell are discrete, stochastic events widely modeled through the Chemical Master Equation (CME) and solved either directly, by trajectorial approaches (SSA) and their coarse-grained approximation, or by hybrid methods that bridge these two approaches. However, the CME assumes molecular well-mixedness and is prone to lack accuracy in the presence of multi-stage reactions that involve time delays and/or spatial inhomogeneities. Including these aspects requires approaches that go beyond the classical CME approach.

We will give a review of stochastic, temporal and spatio-temporal approaches within the Master Equation framework. Especially, we will focus on two generalizations of the classical CME, the CME for reaction kinetics with delays (DCME) (Barrio et al., 2006; Tian et al., 2007) and for compartment-based reaction-diffusion (RDME) (Hattne et al., 2005; Isaacson, 2009) and explain their relationship. In this context, we will also bridge from corresponding trajectorial approaches, namely delay SSAs (Bratsun et al. 2005; Barrio et al., 2006; Cai, 2007; Anderson 2007) and spatial SSAs (Hattne et al., 2005; Marquez-Lago and Burrage, 2007; Erban et al., 2007), to particle tracking models and discuss current research topics.

Keywords: *chemical master equation, reaction-diffusion master equation, delay, SSA, DSSA.*

REFERENCES

Hattne, J., Fange, D., Elf, J. (2005), Stochastic reaction-diffusion simulation with MesoRD. *Bioinformatics* **21** (12), 2923-4.
Isaacson, S.A. (2009), The reaction-diffusion master equation as an asymptotic approximation of diffusion to a small target. *SIAM J Appl Math*, **70** (1), 77-111.
Marquez-Lago, T.T., Burrage, K. (2007), Binomial tau-leap spatial stochastic simulation algorithm for applications in chemical kinetics. *J Chem Phys* **127**, 104101.
Bratsun, D., Volfson, D., Tsimring, L.S., Hasty, J. (2005), Delay-induced stochastic oscillations in gene regulation. *Proc Natl Acad Sci USA* **102**, 14593.
Barrio, M., Burrage, K., Leier, A., Tian, T. (2006), Oscillatory regulation of Hes1: discrete stochastic delay modelling and simulation. *PLoS Comp Bio* **2** (9), e117.
Tian, T., Burrage, K., Burrage, P., Carletti, M. (2007) Stochastic delay differential equations for genetic regulatory networks. *J Comp Appl Math* **205**, 696-707.
Cai, X. (2007), Exact stochastic simulation of coupled chemical reactions with delays. *J Chem Phys* **126**, 124108.
Anderson, D.F. (2007), A modified next reaction method for simulating chemical systems with time dependent propensities and delays. *J Chem Phys* **127**, 214107.
Erban, R., Chapman, S.J. and Maini, P.K. (2007), A practical guide to stochastic simulations of reaction-diffusion processes. arXiv:0704.1908v2

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