Integrated Approaches for Stochastic Chemical Kinetics

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Introduction

In this talk I discuss how we can simulate stochastic chemical kinetics when there is a memory component. This can occur when there is spatial crowding within a cell or part of a cell, which acts to constrain the motion of the molecules which then in turn changes the dynamics of the chemistry. The counterpart of the Law of Mass Action in this setting is through replacing the first derivative in the ODE description of the Law of Mass Action by a time-fractional derivative, where the time-fractional index is between 0 and 1. There has been much discussion in the literature, some of it wrong, as to how we model and simulate stochastic chemical kinetics in the setting of a spatially-constrained domain – this is sometimes called anomalous diffusion kinetics.

In this presentation, I discuss some of these issues and then present two (equivalent) ways of simulating fractional stochastic chemical kinetics. The key here is to either replace the exponential waiting time used in Gillespie's SSA by Mittag-Leffler waiting times (MacNamara et al. [2]), which have longer tails than in the exponential case. The other approach is to use some theory developed by Jahnke and Huisinga [1] who are able to write down the underlying probability density function for any set of mono- molecular chemical reactions (under the standard Law of Mass Action) as a convolution of either binomial probability density functions or binomial and Poisson probability density functions). We can then extend the Jahnke and Huisinga formulation through the concept of iterated Brownian Motion paths to produce exact simulations of the underlying fractional stochastic chemical process. We demonstrate the equivalence of these two approaches through simulations and also by computing the probability density function of the underlying fractional stochastic process, as described by the fractional chemical master equation whose solution is the Mittag- Leffler matrix function. This is computed based on a clever algorithm for computing matrix functions by Cauchy contours (Weideman and Trefethen [3]).

References

[1] T. Jahnke and W. Huisinga, 2007, Solving the chemical master equation for monomolecular reaction systems analytically, *J. Math. Biology* **54**, 1, 1–26.

[2] S. MacNamara, B. Henry and W McLean, 2017, Fractional Euler limits and their applications, *SIAM J. Appl. Math.* **77**, 2, 447–469.

[3] J.A.C. Weideman and L.N. Trefethen, 2007, Parabolic and hyperbolic contours for computing the Bromwich integral, *Math. Comp.* **76**, 1341–1356.