

How does reactant size affect the propensity functions of the SSA?

Sotiria Lampoudi^{1,*}, Dan T. Gillespie², Linda R. Petzold¹

1. Dept. of Computer Science, University of California, Santa Barbara, USA

2. Dan T. Gillespie Consulting, Castaic, California, USA

*email: slampoud@cs.ucsb.edu

The Stochastic Simulation Algorithm (SSA) is the computational method of choice for simulating the time evolution of systems of coupled chemical reactions in which some molecules are present in low copy number. The propensity functions of the SSA, which give the stochastic “rates” of the participating reactions, were originally derived in the dilute gas limit. However, the SSA is widely used to simulate biological systems, in which some of the dilute gas assumptions are typically violated. For instance, biological systems are frequently crowded, either due to the presence of many inert molecules (which we will not address), or due to the large size of molecules of interest. Dilute gas conditions, on the other hand, require that the molecules be well-approximated by *points*, i.e. that they have negligible size.

We have studied the effect of reactant-excluded volume analytically and computationally for the $A+A \rightarrow \text{products}$ reaction in a ballistic setting, and found that the mass action form of the propensity function does not correctly capture the probability of a reaction in a reactant-crowded environment. We showed that in one dimension the correct propensity function can be determined theoretically: it is simply the original mass action propensity, with the system volume reduced by the volume of the reactants¹. In two dimensions we have no equivalent analytical formula, but simulation results suggest that it is necessary to modify the original mass action formula by subtracting a volume that is *larger* than the volume of the reactants². We expect that the impact of reactant-excluded volume is also significant in three dimensions.

References

1. D.T. Gillespie, S. Lampoudi, L.R. Petzold, *Effect of reactant size on discrete stochastic chemical kinetics*, J Chem Phys 126(3):034302, 2007.
2. S. Lampoudi, D.T. Gillespie, L.R. Petzold, *Effect of reactant size on 2D discrete stochastic chemical kinetics*, submitted to J Chem Phys, August 2007.