Improving stochastic simulations of complex chemical systems with bitwise arithmetic

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The Gillespie algorithm is a powerful computational tool to simulate the dynamics of a system of interacting chemical species in regimes where particle numbers are small, and stochastic fluctuations are large [1]. This well-known algorithm becomes computationally demanding when one attempts to sample a large number of configurations, e.g. looking for rare samples in the dynamics, or simulating a large number of species or reactions. In this internship, we propose to develop a new method to increase the computational yield of the algorithm, by leveraging the boolean representation of numbers as they are stored in a computer [2].

This method allows for simulating *simultaneously* multiple copies of the system, which share the same random number used to draw the system samples. Because the random-number generation is the bottleneck of the simulation, this parallel algorithm yields a significant gain in performance, see Fig. 1. Most importantly, given that the copies of the system are initialized with random, independent initial conditions, their dynamics is independent, and it allows for sampling a broader part of the system's configuration space. Different applications of the algorithm will be explored in the context of simulating complex chemical systems, which are typically non-well mixed and contains a large number of species and reactions.

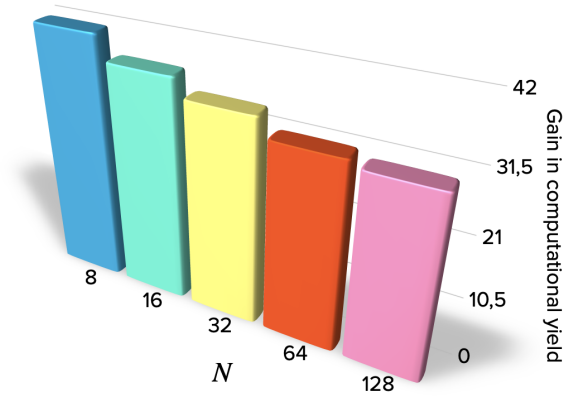

Figure 1: Gain in computational yield given by the parallel Gillespie algorithm compared to the standard algorithm, as a function of the total number of particles N in the system, for a minimal model with three chemical species. This gain has been obtained by using 64-bit registers, and is scalable to 128 and larger registers, where the gain is proportional to the register size.

The student will be tasked with the numerical implementation of this parallel Gillespie algorithm, and with its application to a few representative models of interacting chemical species. The student will acquire valuable interdisciplinary skills, such as proficiency in C++, and getting familiar with models of chemical-reaction networks.

The internship will take place at UMR 168, Institut Curie, and at Gulliver Laboratory, UMR 7083, ESPCI, Paris. For further information, please contact me at michele.castellana@curie.fr .

References

[1] D. T. Gillespie. A general method for numerically simulating the stochastic time evolution of coupled chemical reactions. *Journal of Computational Physics*, 22(4):403–434, December 1976.

[2] M. Palassini and S. Caracciolo. Universal Finite-Size Scaling Functions in the 3-d Ising Spin Glass. *Phys. Rev. Lett.*, 82(25):5128, 1999. Number: 25.