

Title:

Modeling Chemical Reaction Systems and Decrease Computational Time using Parallel Processing

Abstract:

In biochemistry, species/molecules undergo randomly occurring population changes due to chemical reactions. Existing stochastic simulation and tau-leaping methods are frequently used to simulate the transient solutions of biochemical reaction systems. This offers practical insight into the behavior of the system. One simulation tells us one possible randomization of the given model. We want to examine the probability distribution of large systems. By implementing parallel processes, we can spread the work among many threads simultaneously, and thereby decrease the computational time. Because Monte Carlo methods such as the SSA and Tau-Leap require many runs that are time-consuming, parallelizing them can spread their workload across multiple processors. To do so, we use the OpenMP Fortran Application Program Interface, which allows the use of directives to implement parallelism. Preliminary results show that the parallelization of complicated systems decreases the computational time significantly. Thus, allowing for larger systems with a large number of realizations to be simulated quickly. In the experiments, we use 1,2,4 and 8 processing cores. This research will provide insight into how efficient parallelization can be beneficial to many different models.