

Parrallel Exact Stochastic Simulator

Currently the applicability of Gillespie's exact stochastic simulation algorithms to large-scale genetic regulatory network models, whole-cell models, and multi-cell models is limited by simulator performance. Although improvements to these algorithms have been made by Gibson and Bruck, the simulation time required to model a single cell-cycle of E. Coli still remains on the order of years. Other more efficient techniques exist for simulating complex biochemical models such as the use of ordinary differential equations, partial differential equations, approximate stochastic simulation, and chemical langevin equations, however, these techniques can ignore or corrupt the representation of noise (stochastic fluctuation), an emerging area of study that is believed to be a critical factor in analyzing and characterizing biochemical system behavior. To improve exact stochastic simulator performance, an attempt is made to parallelize Gillespie's algorithms based on techniques that have been previously applied to parallel discrete event simulation. Modeling a large biologically-significant problem on various supercomputers at the Oak Ridge National Laboratory will be explored.

Student's Name: **Trayvon D. Leslie**
School Student Attends: Alabama A&M University
Name(s) of Mentor(s): Nagiza Samatova, Mike Leuze, Andrey Gorin
Division: Computer Science and Mathematics
Program: Research Alliance in Math and Science