

Decreasing the Computational Time of Biochemical Systems via Parallelism

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Short Abstract — Existing stochastic simulation and tau-leaping methods are frequently used to simulate the transient solutions of biochemical reaction systems. These Monte Carlo type methods require averaging their results over many time-consuming runs to obtain a probability distribution. Therefore, we want to speed up the computational time without compromising the accuracy of the transient solutions. By implementing parallel processes, we can spread the work among many threads simultaneously, and thereby decrease the computational time. Here we describe some strategies used for that purpose.

Keywords — Stochastic Simulation Algorithm, SSA, Parallel, OpenMP, Tau-Leap, First Reaction Method

I. INTRODUCTION

IN biochemistry, species/molecules undergo randomly occurring population changes due to chemical reactions. We want to examine the probability distribution of a system. We explore the behavior and performance of simulation methods on a number of biological models. The following models/systems will be used in this study: Gene Toggle Model, Michaelis-Menten System, Schlogl Reactions, p53 and Map-K. Examining the transient solutions of each method offers practical insight into the behavior of the system, i.e. what happens to the population of molecules in a given system over a period of time. One simulation tells us one possible randomization of the given model. For this study, we run simulations many times in order to examine the probability distribution of the final population of each element. We seek to expand upon the well-known stochastic simulation and tau-leaping methods [1,2]. The goal is to extend to large or stiff models; models that take a long time to compute. In order to decrease the computational time, we implement parallel processes. This will significantly decrease the computational time.

II. BIOCHEMICAL SYSTEMS

We consider a chemical reaction system of N molecular species $\{S_1, \dots, S_N\}$ and N reaction channels $\{R_1, \dots, R_M\}$. The state vector of the system is defined as $\mathbf{X}(t) = \{X_1(t), \dots, X_N(t)\}$ where $X_i(t)$ is the number of molecules of species S_i at time t . The propensity functions $a_j(\mathbf{x})\tau$ tells us the probability that reaction R_j will occur in $[t, t+\tau)$ and v_{ij} gives the change in the population after each reaction. The system is updated by $\mathbf{X}(t+\tau) = \mathbf{x} + \mathbf{v}_j$.

A. SSA

The Stochastic Simulation Algorithm (SSA) is used to simulate the random behavior of the species and reactions using one reaction at a time [1]. Multiple runs can be performed in parallel.

B. Tau-Leap

The Tau-Leap method speeds up the SSA by simulating multiple reactions in each time interval. This method starts by determining how many times a reaction will fire in a subinterval. The system is then updated after simulating the group of reactions [1]. Multiple runs can also be performed in parallel.

C. First Reaction Method

The classic SSA and Tau-Leap methods assume that the reaction rates are constant. When reaction rates are time varying, other methods such as the First Reaction Method that take into account variable rates are more appropriate [3].

D. Parallel Computing

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.

III. CONCLUSION

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 work provides insight into how efficient parallelization can be beneficial to many different models.

REFERENCES

- [1] Cao Y, Gillespie DT, Petzold LR (2006) Efficient step size selection for the tau-leaping simulation method. *Journal of Chemical Physics* **124**, 224101-1 – 224101-11
- [2] Cao Y, Gillespie DT, Petzold LR (2007) Adaptive explicit-implicit tau-leaping method with automatic tau selection. *Journal of Chemical Physics* **126**, 224101-1 – 224101-9
- [3] Tian T, Burrage K. (2005) Parallel implementation of stochastic simulation for large-scale cellular processes. *8th International Conference on High-Performance Computing in Asia-Pacific Region*. 621-626.

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