

Tutorial on StochSS: An Integrated Development Environment for Simulation and Analysis of Discrete Stochastic Biochemical Models

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We present StochSS: Stochastic Simulation as-a-Service, an integrated development environment for modeling and simulation of deterministic and discrete stochastic biochemical systems. An easy to use WebUI enables researchers to quickly develop and simulate biological models on a desktop or laptop, which can then be expanded or combined to incorporate increasing levels of complexity. As the demand for computational power increases, StochSS is able to seamlessly scale by deploying cloud computing resources. The cloud computing facilities also make it possible to deploy StochSS as a multi-user software as-a-service (SaaS) environment with the capability to share and exchange models via a public model repository. StochSS currently supports simulation of ordinary differential equations and well-mixed discrete stochastic models, as well as parameter estimation of discrete stochastic models and efficient mesoscale simulation of spatial stochastic models. StochSS is available for download at www.StochSS.org.

Keywords — Biochemical Modeling, Stochastic Simulation, Spatial Stochastic Simulation, Cloud Computing, Parameter Sensitivity, Parameter Estimation.

I. INTRODUCTION

A striking outcome of the past decade of Systems Biology research is the insight that stochasticity plays an important role in many biological processes. As a result, discrete stochastic simulation is now an important and widely-used tool for modeling of biological systems. To facilitate this type of research, StochSS provides a powerful platform for the development of biochemical models, as well as a complete suite of tools for simulation and analysis, 2D and 3D visualization, and the ability to scale up computational resources using the Amazon EC2 cloud [1].

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StochSS employs a hierarchy of models the associated simulation software. StochSS uses CVODES for deterministic simulation and sensitivity. On the stochastic well-mixed level, the SSA and adaptive tau-leaping are provided via integration of StochKit2[2], and parameter estimation is available via StochOptim[3]. For spatial stochastic simulation, StochSS offers the NSM and ADFSP algorithms via PyURDME[4].

II. OUTLINE OF TOPICS

This tutorial will take approximately 2 hours and will provide an introduction to systems biology modeling of biochemical systems with StochSS.

- Fundamentals of computational modeling
- Developing a well-mixed biochemical model
- Stochastic simulation of biochemical systems
- Transition from deterministic to stochastic models
- Modeling of spatially inhomogenous systems
- Developing spatial stochastic models
- Model analysis: parameter estimation / sensitivity

The tutorial will be interactive, with demonstration and examples. Attendees are encouraged to bring their own computer, and models from their own research to discuss.

III. CONCLUSION

StochSS offers users a unique modeling experience by providing an integrated solution that addresses model specification on multiple levels, features state-of-the-art simulation algorithms for efficient simulation, and removes the barrier of scaling computational resources when needed.

REFERENCES

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