

**Institute for Universal Biology (IUB)**  
**NASA Astrobiology Institute Seminar Lecture Series**  
Monday, April 27, 2015  
11:00 – Noon  
Lecture Hall 612

Institute for Genomic Biology  
Directions: <http://www.igb.illinois.edu/about/directions>

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## Simulations of cellular processes in *E.coli*, *M. acetivorans*, and *S. cerevisiae*

High-performance computing now allows integration of data from structural, biochemical, genetic and single-molecule studies into computational models of cellular processes functioning in live cells. Using our GPU based Lattice Microbe software, we analyze the stochastic reaction-diffusion dynamics of ribosome assembly and responses of a genetic switch in *Escherichia coli* cells on time scales of a cell cycle. Protein/mRNA distributions observed in single molecule and RNA seq experiments are integrated in the steady-state treatment of metabolic networks for both bacteria and yeast. The corresponding distribution of growth rates can be correlated to changes in fluxes through the metabolic network arising from various subpopulations. Reaction-diffusion kinetics of metabolites in the surrounding medium are coupled with the cellular metabolic networks to demonstrate how dense colonies of interacting bacterial cells differentially respond to the competition for resources according to their position in the colony. Finally, we report on the progress to develop similar computational models for a methane producing archaeum.

### References:

- J. Cole, et al. (2014). Stochastic Simulations of Cellular Processes: From Single Cells to Colonies. (Chapter 13) In *Computational Systems Biology: From Molecular Mechanisms to Disease, 2<sup>nd</sup> Ed.* (Eds Kriete, A, Eils, R), Elsevier, San Diego **2014**, pp. 278-292
- P. Labhsetwar et al. (2013): Heterogeneity in protein expression induces metabolic variability in a modeled *Escherichia coli* population, *Proc. Natl. Acad. Sci. USA* 110(34):14006-11
- H. Kim, S. Abeyvirigunawardena, Ke Chen, M. Mayerle, Z. Luthey-Schulten, TJ Ha, and S. Woodson. (2014) "Protein-guided RNA dynamics during early ribosome assembly" *Nature* 50:334-8.