Computational Systems Biology: Chapter 13. Stochastic Simulations of Cellular Processes: From Single Cells to Colonies

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All chemical reactions are inherently random discrete events; while large numbers of reacting species in well-stirred vessels my appear to be governed by deterministic expressions, the biochemistry at the heart of the living cell—which may involve only a single copy of a gene or only a handfull of proteins—can exhibit significant fluctuations from mean behavior. Here we describe the Lattice Microbes software for the stochastic simulation of biochemical reaction networks within realistic models of cells, and explore its application to two model systems. The first is the lac genetic switch, which illustrates how stochastic gene expression can drive identical cells in macroscopically identical environments toward very different cell fates, and the second is the MinDE system, whose oscillatory behavior along the length of the E. coli cell illustrates the necessity of detailed spatial resolution in accurately modeling cellular biochemistry. We conclude by describing the use of a hybrid methodology that couples the Lattice Microbes' reaction-diffusion modeling capability with a genome-scale flux-balance model of metabolism in order to describe the collective metabolism of a dense colony of cells.

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