Using Probabilistic Methods and Ordinary/Stochastic Differential Equations to Simulate Biological Processes

Achim, Tudor; Dr. Ta'asan, Shlomo; Rand, Alex Department of Mathematics Carnegie Mellon University

Abstract: Agent-based models are used for simulating cellular and subcellular processes because they are straightforward to visualize and use and easily extensible. BioLogic is an agent-based simulator of cells, which adapts to the high variability of experimental data by simple logical variables such as high, low, or none. Extensions were added to the simulator to be able to simulate reactions using 1) probabilistic models, when the number of agents is small 2) stochastic differental equations, when the number of agents is moderate and 3) ordinary differential equations when the number of agents is large. Ideally, the algorithm shold use a combination of the three methods for maximal efficiency. In the probabilistic model we calculate probabilities for reactions based on rate constants and the law of mass action. Both the stochastic differential equations as well as the ordinary differential equations models use Euler's method to approximate the solution. The software uses as input descriptive XML files to represent the hierarchy of structures within the simulation environment and regular text files to define the reaction rates.