

PySB, a programming environment to generate algorithmic representations of biological systems

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COMPUTATIONAL modeling and simulation of biological systems facilitate understanding of experimental observations and testing of novel hypotheses. A model is defined by its output(s), its parameters (initial concentrations, reaction rates) and its topology, which describes how outputs and parameters are connected. As large experimental datasets become available, new tools are required to describe the complex mathematical relationships that arise when encoding complex biological systems. This is made possible by the advent of rules-based formalisms to precisely describe biochemical interactions. This tutorial introduces PySB, a Python-based software framework used to build biological models which are themselves computer programs—an approach which facilitates the development of models which are clear, concise, shareable and modular. PySB allows access to a range of existing tools to build program functions representing biological concepts, construct programs of biochemical signal transduction, run simulations, visualize model properties and analyze data. We will demonstrate how multiple topologies representing a set of biochemical reactions can be built to explain the same set of observed data, and how a programming environment can be used to examine the resulting models at varying levels of abstraction. We will introduce techniques such as calibration to experimental data, number theory approaches to understand model behavior, and tools for elucidating the model–experimental-data relationship. Although the tutorial will be presented for a general audience, familiarity with the Python programming language and the BioNetGen or Kappa languages would be helpful.

Please visit the PySB site (PySB.org) to download and install a copy of PySB on your laptop to follow the tutorial.