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

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MODELING and simulation of biological systems provide a framework to test and develop the understanding of experimental observations. For any given model, the output (or outputs) depends on a set of parameters (either measured or determined *ab initio*) and a topology that describes how these parameters are connected. The advent of rules-based formalisms to describe biochemical interactions has yielded a formal biochemical language that allows the generation of complex multi-parameter mathematical representations of biological systems. As large sets of experimental data become available, new tools are required to deal with the complex mathematical descriptions of biology that arise when encoding complex systems. This tutorial focuses on how multiple topologies representing a biochemical reaction network can be built and how a programming environment is used to generate varying levels of biological abstraction. We show how *PySB* can be used to build model representations whereby the model is itself a software program, which is executed to generate biochemical reaction networks and mathematical representations of biology. *PySB* allows users to use a range of existing tools to build program functions representing biological concepts, construct programs of biochemical signal transduction, carry out simulations, visualize model properties, and analyze data – all within the *Python* programming environment. We will show how models can be built to probe multiple biochemical constructs that explain the same biological observables. We will also show how a programming approach can provide a clean, clear, and concise description of a model that can be easily shareable and updated. The use of techniques such as calibration to experimental data, number theory approaches to understand model behavior, and a range of tools for model building will be discussed as tools to understand the model-to-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 will be helpful.

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