

Functional Specification

Background

Biological systems often involve complex interactions between molecules, such as enzymes, substrates, and products in a metabolic pathway. Simulating these systems is crucial for understanding their dynamics, optimizing experimental designs, and teaching concepts in systems biology. Current simulation tools lack intuitive and visually engaging methods to animate results dynamically, especially for users new to computational biology.

When visualizing biological data, there are two primary approaches: exploratory and explanatory visualizations. Explanatory visualizations aim to tell stories by surfacing key findings in a carefully constructed narrative. These are essential for communicating insights clearly and effectively, such as in scientific presentations or educational settings. Exploratory visualizations, by contrast, act as interfaces into the data or subject matter, allowing users to interact with the data and uncover their own insights. These visualizations are typically interactive, empowering users to adjust parameters, explore trends, and investigate relationships they find relevant or interesting.

This python package aims to bridge these concepts by combining explanatory elements, such as animations that clearly show changes in concentration over time, with exploratory features like adjustable parameters. This hybrid approach ensures the app can be both an effective teaching tool and a powerful resource for hypothesis-driven research.

User Profile

- Undergraduate or graduate students learning computational or systems biology.
- Researchers exploring dynamic behaviors of biological networks.

Skills and Knowledge:

- Basic understanding of systems biology and reaction networks
- Familiarity with software for simulations such as Tellurium
- General proficiency with computers and Python (browsing the web, installing software)
- Optional: Higher proficiency with Python for advanced users who want to modify or extend the app

Use Cases

Use Case 1: *Visualize a Metabolic Pathway Simulation*

Objective:

The user wants to simulate a 5-step metabolic pathway and visualize how concentrations of intermediates change over time as the simulation progresses.

Expected Interaction:

The user loads a pre-defined or custom antimony model of the metabolic pathway via a file upload.

The app runs the simulation using Tellurium and displays an animated bar chart where each bar represents a molecule's concentration.

The user observes the dynamic changes in concentrations and can pause, play, or adjust the simulation speed using controls.

The user can hover over a point to obtain more information about the species and concentration.

(Optional): The user exports the animation as a video for presentations

Use Case 2: *Interactive Parameter Exploration*

Objective: The user wants to explore how varying reaction rates affect the system dynamics in real-time.

Expected Interaction:

The user selects a reaction from the model and adjusts its parameters (e.g., rate constants) using sliders provided in the interface.

Upon making a change, the app updates the simulation results and dynamically adjusts the bar chart animation to reflect the new behavior.

The user compares outcomes of different parameter sets visually and records insights for further analysis.