Component Specification

Software Components

1. *Simulation Engine*

Purpose:
Handles all tasks related to model management, parameter adjustments, and running simulations

Inputs:
- Antimony model files
- Simulation settings (e.g., time range, step size, initial conditions)
- Parameter adjustments (e.g., reaction rate constants)

Outputs:
- Time-course data of molecule concentrations as a structured format (e.g., pandas dataframe)
- Updated model data after parameter changes.

2. *Visualization Manager*

Purpose:
Responsible for creating and managing visualizations, including animated bar charts and any additional plots

Inputs:
- Time-series data from the Simulation Engine
- User preferences for visualization (e.g., selected species, animation speed)

Outputs:
- Real-time animated bar charts showing molecule concentrations
- Interactive visualizations that allow users to adjust parameters and observe changes

3. *Interaction Controller*

Purpose:
Manages user interactions, bridging the gap between the user interface and backend functionality

Inputs:
User actions (e.g., uploading a model, adjusting parameters, controlling animations).

Outputs:
Triggers the Simulation Engine to update model parameters or rerun simulations
Directs the Visualization Manager to update plots or animations based on user inputs

Interactions to Accomplish Use Cases

Use Case: *Visualize a Metabolic Pathway Simulation*

Load a model:

- The Interaction Controller processes the file upload and sends it to the Simulation Engine.
- The Simulation Engine reads the file, preprocesses it, and prepares for simulation.

Run simulation:

- The Interaction Controller triggers the Simulation Manager to run the simulation using Tellurium.
- The Simulation Engine provides time-series data as output.

Visualize results:

- The Visualization Manager receives the time-series data and animates it as a bar chart.

If the user adjusts parameters:

- The Interaction Controller captures the adjustment and informs the Simulation Manager to update the parameters and rerun the simulation
- The Visualization Manager refreshes the animation to reflect the new results

Preliminary Plan

High Priority:
Develop the Simulation Engine to handle model reading, simulation execution, and parameter adjustments
Create the Visualization Manager to display animated bar charts
Implement the Interaction Controller for basic user actions like loading models, changing parameters, and running simulations

Medium Priority:
Add user controls (e.g., sliders for parameter adjustments, play/pause for animation)
Implement interactive exploratory features (e.g., selecting species to display)
Enable dynamic communication between the Interaction Controller and other modules

Low Priority:
Add export functionality for animations (e.g., save as video)
Enhance visual aesthetics (e.g., custom color schemes, labels)