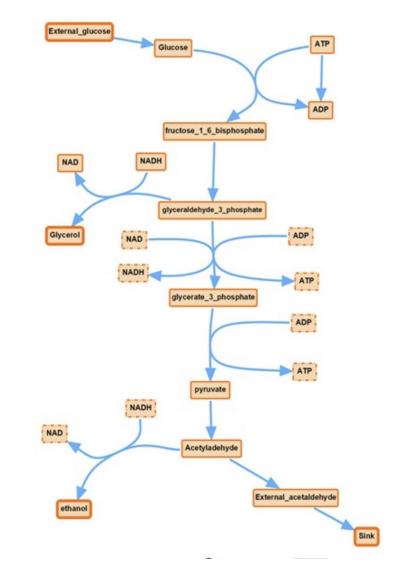


BACKGROUND

- Systems Biology Markup Language (SBML) [1]
- Used to visualize chemical reaction networks
- Works in conjugation with Tellurium (modeling software)



Α

https://doi.org/10.1093/bioinformatics/btac730.

PROBLEM STATEMENT

- The model doesn't show the difference between fluxes
- My project aims to visualize more of that

```
# Define and load a model
    r = te.loada('''
    A -> B; V
    B -> C; v
    C -> D; v
    111)
    # Load the model into SBMLDiagrams
    df = SBMLDiagrams.load(r.getSBML())
    # Apply autolayout to arrange species and reactions
    df.autolayout()
    # Set line thickness for specific reactions
    # Draw the model with specified line widths
    df.draw()
```

https://doi.org/10.1093/bioinformatics/btac730.

PROJECT: SB VISUALIZER

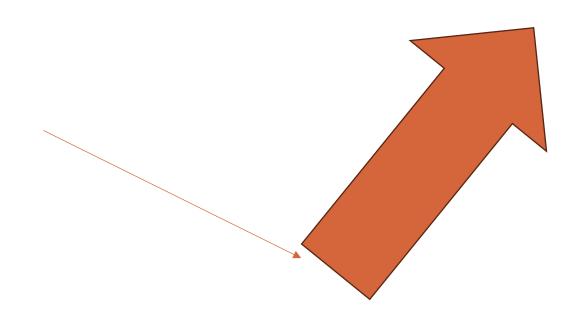
- My project aims to illustrate the flux of a species
- This is something that is not a feature of SBML
- SBML shows arrows from one species to another
- My project aims to change the thickness of the arrow to show flux
- And a color gradient representing fluxes

USERS AND COMPONENTS

- The main users of my project will be existing Python programmers
- Tellurium users
- SBML users (can use features of SBML)

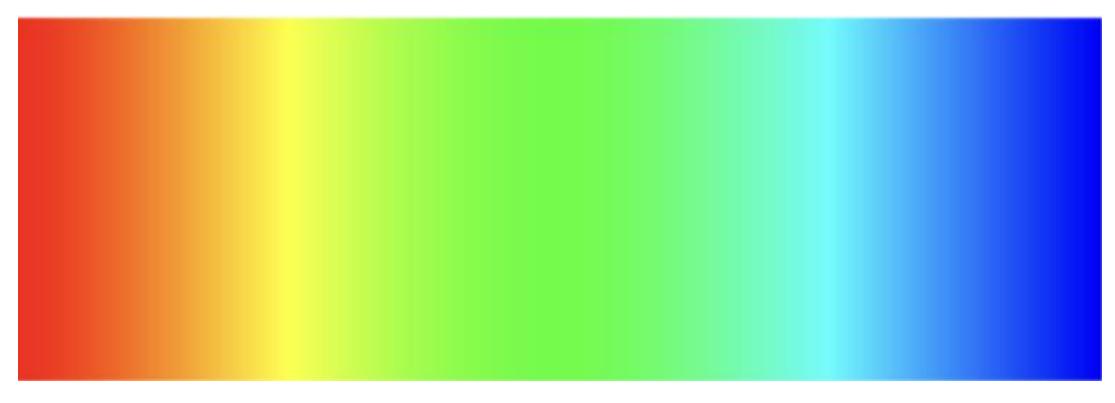
THICKNESS

- After flux calculated
- Calculate the max flux
- Scale all the fluxes



COLOR GRADIENT

- Color scheme to represent positive and negative fluxes
- Based on RGB (255, 255, 255)



https://behreajj.medium.com/color-gradients-in-processing-v-2-0-e5c0b87cdfd2

CALCULATE GRADIENT

- Obtain the maximum flux out of all the reactions
- Divide the rest of the fluxes by that maximum flux
- Multiplied this by 255 for red/blue and 1-this by 255 for green (depending on positive/negative)

DEMO AND GITHUB

- The colors still don't show up in main
- Need to figure out how to make the colors show up
- https://github.com/ptalur559/SBVisualizer

FINISHED PRODUCT

```
r = te.loada("""

J1: S1 -> S2; k1*S1;

J2: S2 -> S3; k2*S2;

S1 = 10; S2 = 0; S3 = 0; k1 = 0.1; k2 = 0.05;
""")
```

S2

S1

LESSONS LEARNED

- I learned a lot more about how to use GitHub and VSCode
- I learned more about SBML and what it's used for
- I need to figure out how to see the color changes in VSCode if I try it out in main

CITATIONS

[1] J. Xu, J. Jiang, and H. M. Sauro, "SBMLDiagrams: a python package to process and visualize SBML layout and render," *Bioinformatics*, vol. 39, no. 1, Nov. 2022, doi: https://doi.org/10.1093/bioinformatics/btac730.