

# Computational Analysis and Visualization of Complex Biochemical Systems: A GUI Design Challenge

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Relating the phenotype of an organism to its genotype is one of the 'Grand Challenges' in modern biology. For example, relating a disease such as diabetes or cancer to the causative changes (mutations) in the organisms DNA or changes in the organism's environmental insults (toxins). Our lab has developed a theoretical framework that relates the genotype and environment of an organism to the behavior of its underlying biochemical systems (the phenotype).

We also have developed a computational toolbox for analysis and visualization of these important relationships. One of the current limitations has to do with 'bugs' or limitations in the GUI. Many of these issues are well documented. The following is a list of the issues to be fixed, prioritized from the simplest to the more challenging.

- Automatically change the "name" of the file for saved data to agree with the "name" of the file in which the model is saved.
- Save "Parameter constraints" and "kinetic orders" as part of the saved data
- Alphabetizing of parameters (in the parameter table, sliders, and pull-down options)
- Change index for "Add Columns" button to start with "3"
- Fix pull-down window for the 2-D stability plot option
- Create separate data files for the different saved versions of the data
- Eliminate the "-0.00" problem to specify a "true zero" in inequalities
- Eliminate the overwriting of graphics panels
- Integrate open source python ODE solver into the GUI
- Allow deletion of saved data
- Option of toggling between views of the color bar and the Design Space plots
- Coordinated coloring of phenotypes (polytopes)
- Rough- and fine-scale sliders for interactive plots
- "Graceful" halt option to avoid system crashes

We would like the assistance of computer science talent to expand the capabilities of the current toolbox, while making it more robust and user-friendly. The project involves programming in python for visualization to advance the design of the GUI. I would be happy to meet with any prospective team, to give a demonstration that would provide more detail, and to discuss the nature and relative importance of the design challenges.