Component specification

Brizzia Munoz Robles

Software components. High level description of the software components such as: *data manager*, which provides a simplified interface to your data and provides application specific features (e.g., querying data subsets); and *visualization manager*, which displays data frames as a plot. Describe at least 3 components specifying: what it does, inputs it requires, and outputs it provides.

1. theoretical photokinetics()

a. **Purpose:** Calculates theoretical photouncaging values using the following first order kinetic equation for photouncaging:

$$Y = Y_o + (plateau - Y_o)(1 - \exp(-k * x))$$

- b. Input:
 - i. Array of x values separated by commas.
 - ii. Photokinetic constant, k
- c. Output:
 - i. Table of x and corresponding y values (normalized to 1)
 - ii. Scatter plot of theoretical data

2. exp association()

- **a. Purpose:** Calculates the photouncaging constant k using the first order equation from above using raw data inputted from user as an excel file. It uses scipy.optimize.curve fit to calculate the k value.
- b. Input:
 - i. Excel file uploaded into Colaboratory folder, titled example_2 formatted such that the first column is labelled time and has all the time values and the corresponding y values titles labelled value
- c. Output:
 - i. Table of x and y values
 - ii. Kinetic constant
 - iii. Data normalized and plotted in a scatter plot

3. cell migration()

- **a. Purpose:** Simulates cell migration using a stochastic agent based model designed by Fadai et al. 2019.
 - i. Input: V,rm,rp,rd,tf,C_start,C_end,rhox
 - ii. **Output:** Matrix consisting of cell location using a heat map, where white equates to occupancy by a cell and black equates to an empty compartment
- **4. Interactions to accomplish use cases**. Describe how the above software components interact to accomplish at least one of your use cases.
 - **a.** Use case: For calculating theoretical photokinetics, after the user has entered the desired x values and photokinetic constant, the user should select "run" on the cell and the values will be outputted.
 - b. Use case: For calculating a kinetic constant from raw data, after uploading the excel file, the user should run the cell, k value will be calculated. It will call a check_excel() function to verify that the excel file is in the correct format. If it is

- not, then it will return an error to the user and description of proper excel file format. Display() will call exp_association() which returns the equation used to calculate the kinetic constant.
- **c.** Use case: For modeling cell migration, the user will input the various parameter values from a slider tool using Colab Forms. Cell_migration() will call on check_param() function to verify that all values are within a given range. If they are not, an error will be returned to the user.

5. Preliminary plan.

- a. Run check functions for inputs from users to verify inputs are correct format
 - Fix errors
- b. Update output from cell_migration() to make it more user friendly/understandable