Supplement A: GUI Application

We developed a graphical user interface (GUI) application associated with the proposed data assimilation method to provide an enabling tool for biomedical scientists without full expertise in computational modeling and programming. This document is a comprehensive guide to the software for installation and core functions. The software package can be downloaded at: `https://github.com/haedong31/Kv_data_assim`.

1 Installation

Although the application is developed in MATLAB, it does not require the programming language installed on a computer. Instead, `MyAppInstaller_web` installs the application and MATLAB Runtime, which allows running the application without the language installed. Note that an Internet connection is required. `KvApp` is the execution file that runs the application once the installation is completed. Fig. 1 shows the main page of the application.

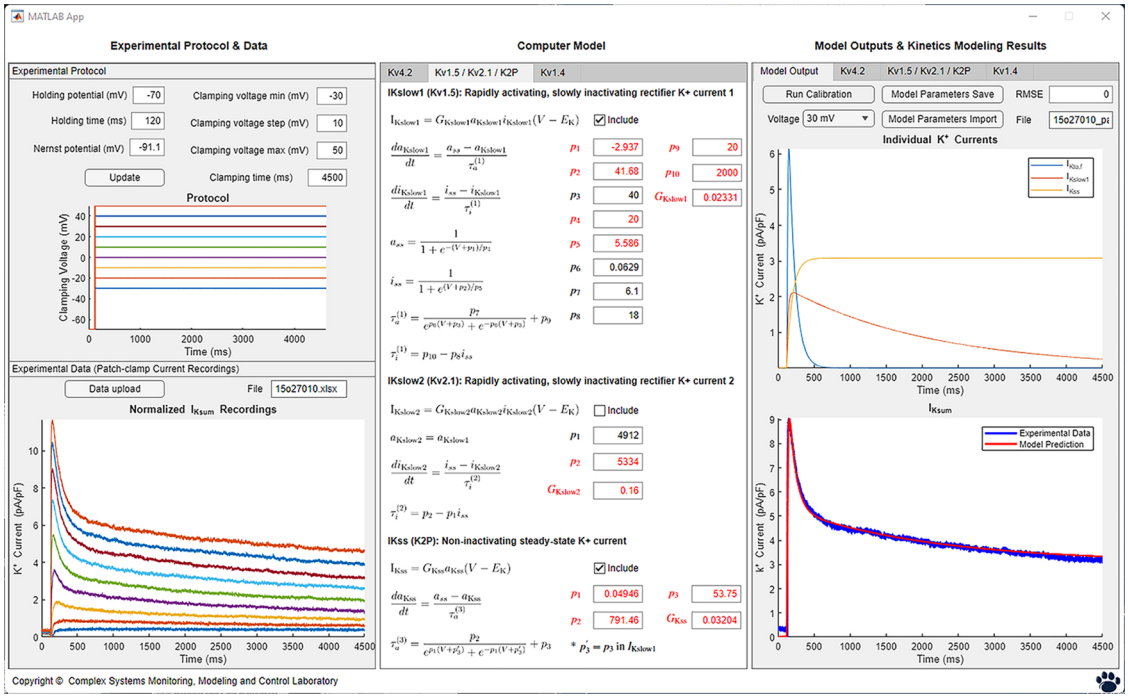

Figure 1: Main page of the application.

2 Data Import

Among three modules in the main page, Experimental Protocol & Data is designed to specify voltage-clamp protocol and corresponding *in-silico* I_{Ksum} recordings to be analyzed. Data should be stored in an Excel file, with the first column corresponding to time and the other columns normalized currents for voltage steps in increasing order. This is a default format when I_{Ksum} traces are transferred to a tabular format in ClampFit.

3 Model Calibration

The Computer Model module shows equations and kinetics parameters of computers models of K_v isoforms separated by tabs. The Computer Model module shows equations and kinetics parameters of computers models of potassium isoforms, separated and grouped by tabs. The $K_v4.2$ model in the first tab is the only stand-alone model in which every kinetic variables and parameter are independent of other models. The second tab contains three closely connected models. Each model can be chosen to be or not be included in calculating the total potassium current by checking or unchecking the Include boxes. The kinetic parameters can be adjusted manually by entering the number in the corresponding box and pressing the enter/return key. Parameters in red are identified as having significant impacts on the model behavior.

These parameters in red can be calibrated automatically using the Turn Calibration button in the Model Output tab of the third module. This function calibrates the models by minimizing discrepancies between model prediction and experimental I_{Ksum} traces. The fitness of calibration results is visualized, and the drop-down button allows to select different voltage steps. The calibrated parameter values can be saved using the Model Parameters Save button in an Excel file. It is desirable to perform model calibration separately, utilizing more computing power and time for better results. Other tabs named after the K_v isoforms show kinetic variables such as steady states, time constants, and transition rates as shown in Fig. 2.

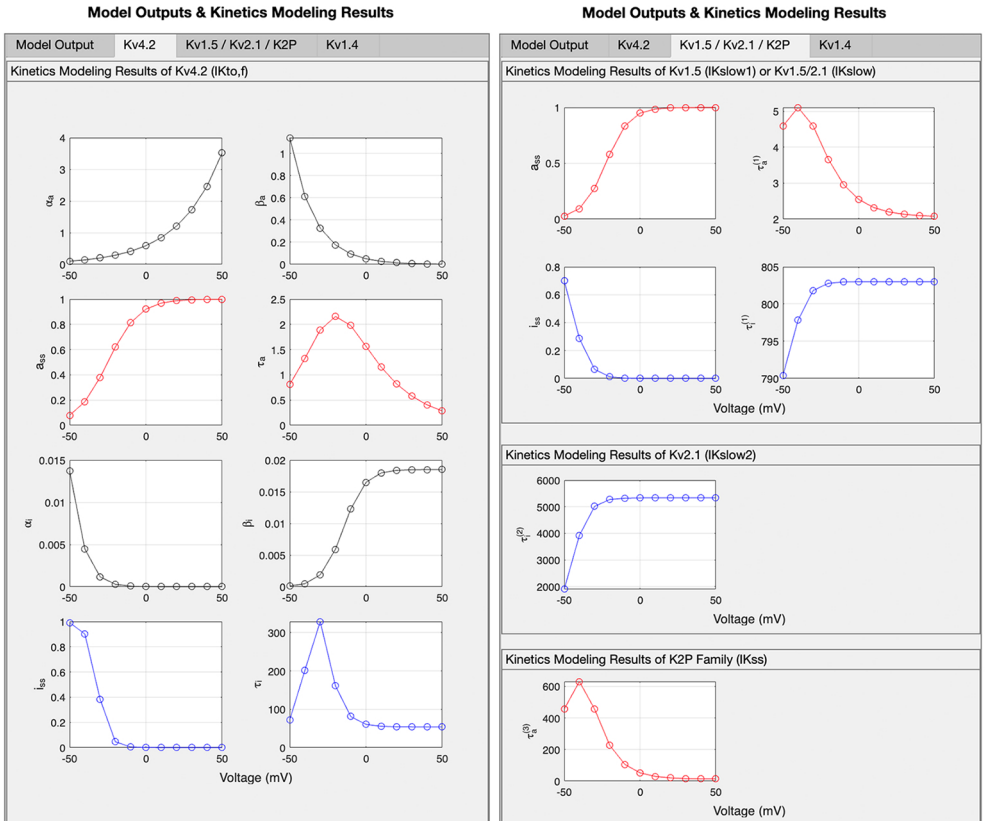

Figure 2: Data assimilation outputs. Kinetics modeling of K_v isoforms.