GridSimM User Guide

Introduction

GridSimM is an object and agent oriented modeling framework based on an open source, multi-agent simulation software library MASON (Luke et al., 2005), which provides a general purpose, discrete event simulation engine. As a pharmacological modeling framework, GridSimM provides basic components and features for in silico experimentation and analysis, including a data processor and graphical user interface (GUI). At the core of framework is a pharmacologically responsive, virtual patient model. The current version consists of a set of interconnected two-dimensional square grids and event mechanisms that map to different physiological features and processes.

System Requirements

- 128 MB RAM
- 10 MB free had disk space
- Java Runtime Environment (https://java.com/en/download/index.jsp)

Getting Started

1. Download GridSimM.jar and the "lib" folder that contains: ecj19.jar, jcommon-1.0.16.jar, jfreechart-1.0.13.jar, mason17-with-src.jar, and opencsv-2.3.jar. Make sure that GridSimM.jar and the "lib" folder are saved in the same directory.
2. Double-click GridSimM.jar to start program (Java security prompt may ask for confirmation).

Using GridSimM

GridSimM starts in GUI mode by default. The GUI has three windows visible when initialized: Simulation Info, PlasmaChart, and the main controller. The Simulation Info window has input selectors for referent data files as well as output file selectors. Simulation outcomes are shown in the PlasmaChart as simulation unfolds. GridSimM's main controller provides an interactive interface to control and manage simulations.

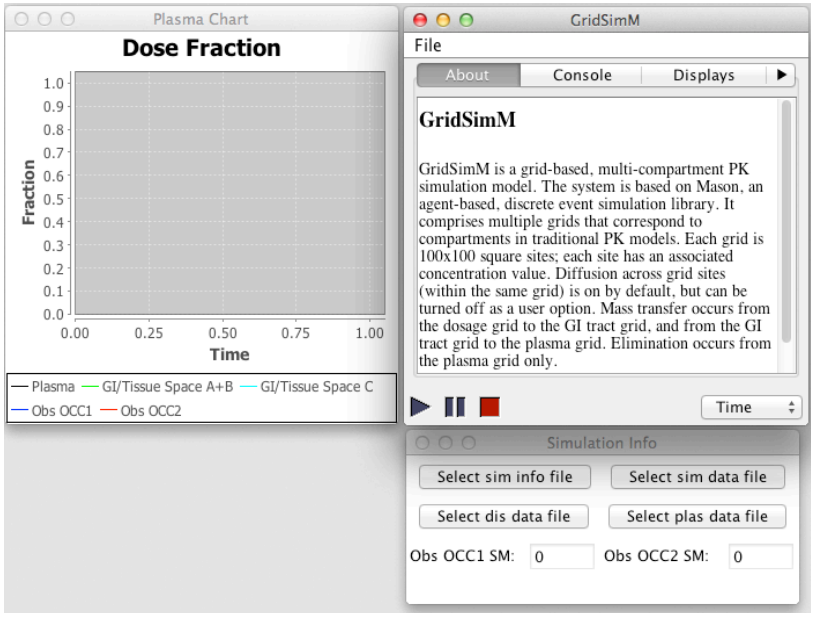

Figure 1. GridSimM Graphical User Interface

A. Simulation Info window

The Simulation Info window allows users to select referent data files and simulation output files. Two types of referent data are allowed: dose dissolution-time measurements and drug plasma concentration-time data. Both are optional and not required for running simulations. Simulation information and data are written to simulation output files if selected. If no output files are selected, simulation data are stored as a text file in the "sim_output" folder. The window also shows similarity measures (Kim et al., 2012) computed for dissolution and plasma concentrations as the simulation executes if referent data are given.

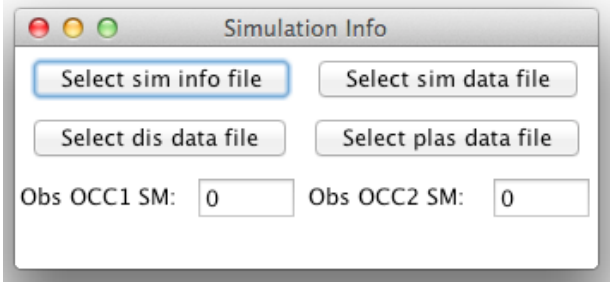

Figure 2. Simulation Info window

Click on "Select Dis Data File" button to select dissolution data (optional).
Click on "Select Plas Data File" button to select plasma concentration data (optional).
Click on "Select Sim Info File" button to select an output file (optional) to record simulation related information including parameter values and similarity values.
Click on "Select Sim Data File" button to select an output file (optional) to record simulation data including time-lapse drug amount in individual spaces.

B. Plasma Chart

The PlasmaChart window shows the factional drug amount in GI/tissue spaces A+B and C and plasma. Also shown are referent plasma profiles from up to two different conditions (e.g., Obs Occ1 = fasting, Obs Occ2 = fed) if provided.

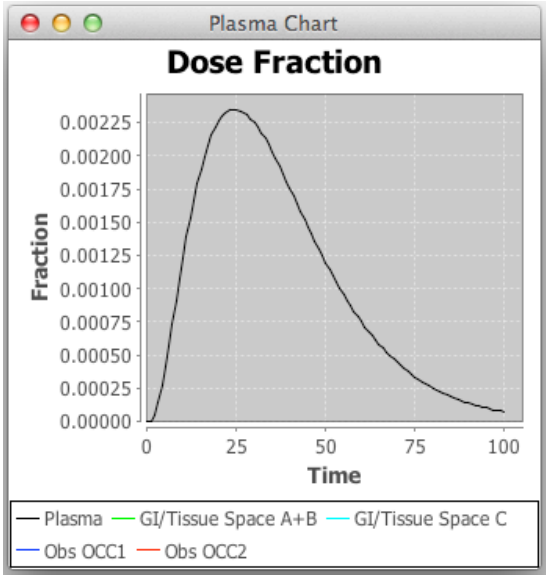

Figure 3. Plasma Chart window

C. GridSimM Controller

The main controller window provides an interactive interface through which users perform and manage simulations. It has five panels: About, Console, Displays, Inspectors, and Model. Users can access simulation related info and options via the Console, Displays, and Model panels. To start, pause or stop simulation, press the corresponding button at the bottom.

1. Console

The Console panel allows users to automatically stop or pause simulation at an arbitrary step or stop time. Users can set or alter seeds for random number generators used in simulation.

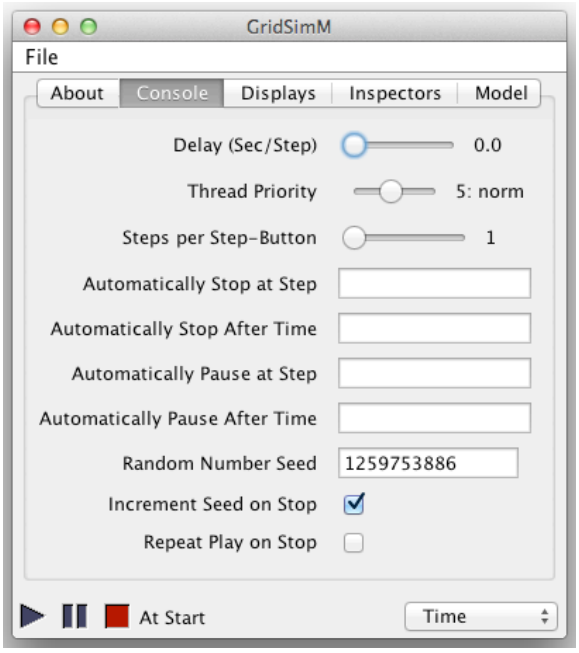

Figure 4. Console panel

2. Displays

The Display panel allows users to show or hide GUI windows. Open windows are indicated in bold. Windows not shown are greyed out. Users can show or hide individual windows listed by selecting and clicking on the "Show" or "Hide" buttons.

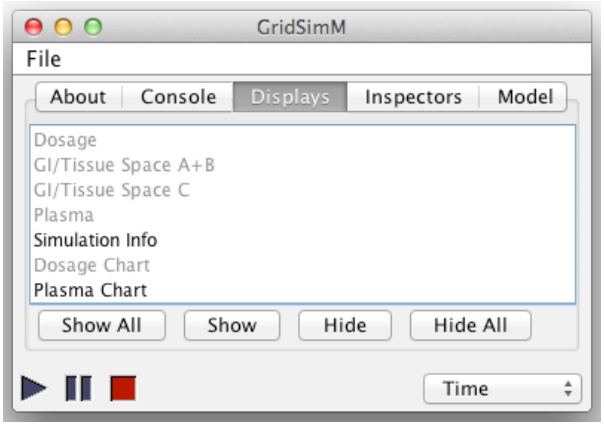

Figure 5. Displays panel

3. Model

The Model panel shows a list of model parameters that are modifiable and accessible to users. Individual parameter values can be altered by selecting each respective text field and entering a new value (must press 'return' to effect change). The panel has two pages. By clicking on the arrows on the upper-right corner, users can navigate between the two pages.

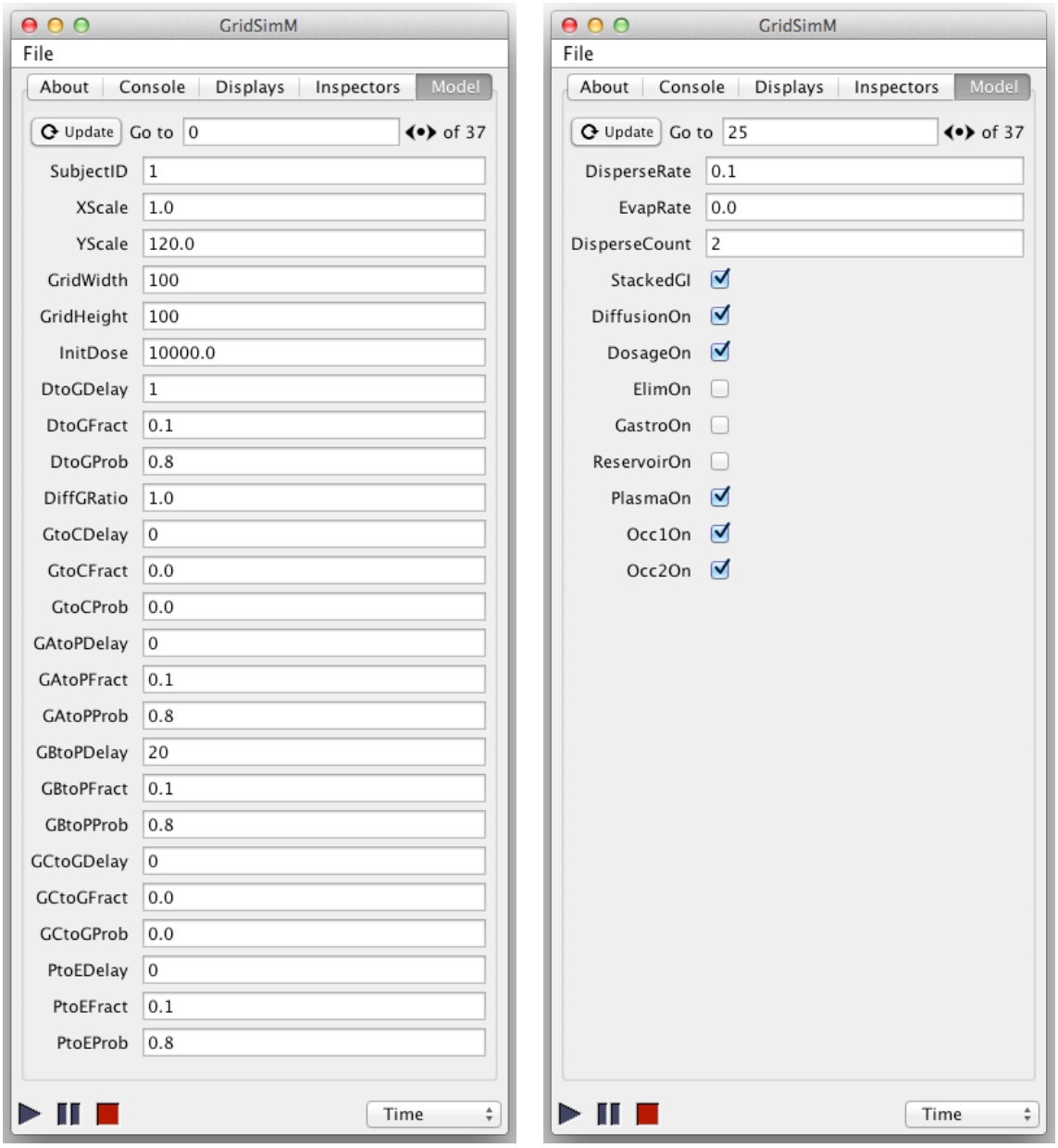

Figure 6. Model panel

References

[1] Luke S, Cioffi-Revilla C, Panait L, Sullivan K, Balan G (2005) MASON: a multi-agent simulation environment. Simulation 82: 517-527.

[2] Kim SH, Jackson AJ, Hur R, Hunt CA (2012) Individualized, discrete event, simulations provide insight into inter- and intra-subject variability of extended-release, drug products. Theor Biol Med Model 9: 39.