User guidebook for the *MorphoSim* GUI on Matlab

1. *Brief introduction*

The graphical user interface (GUI) of *MorphoSim* (Morphology Simulator) is constructed using Matlab 2018b. One can utilize this GUI to compute the morphological change of a multicellular system conveniently.

2. *Use flow*

1) Download the Folder "MorphoSim" from GitHub https://github.com/XiangyuKuang/MorphoSim.git (Fig. G1).

2) Open the MorphoSim.m in Matlab and click "Run", then an interactive interface appears (Fig. G2).

- The Matlab version should be no earlier than 2018b.
- Click "Set Path" to add the Folder "MorphoSim" with its subfolders before running the programs (Fig. G3).
- Open the MorphoSim.m in Matlab and click "Run", then an interactive interface appears (Fig. G2).

3) To compute a multicellular system with specific cell names and attraction matrix, use the upper panel:

A. Import the information of cell name and attraction matrix (Fig. G4).

- The file format is shown in "Example\Example_CellName&AttractionMatrix_*.xls", where "*" is "1" or "2".
- The number in Row j and Column i means the attraction ($\sigma_{i,j}$) from Cell j to Cell i.
- The file "Example\Example_CellName&AttractionMatrix_1.xls" contains the matrix with relatively strong attraction in ABpl-E contact (i.e., $\sigma_{\mathrm{ABpl,E}} = \sigma_{\mathrm{S}} = 0.5$) (Fig. G4(b) and (e)). The file "Example\Example_CellName&AttractionMatrix_2.xls" contains the matrix with relatively weak attraction in ABpl-E contact (i.e., $\sigma_{\mathrm{ABpl,E}} = \sigma_{\mathrm{W}} = 0$) (Fig. G4(c) and (f)).

B. Import the initial cell pattern which is kept as binary regions and can be designated arbitrarily.

- The file format is shown in "Example\Example_8Cell.mat".
- The cellular regions should be set inside the eggshell shown in "Example\Example_Eggshell.mat", in which the interior and exterior of the eggshell are labeled by 0 and 1 respectively.

C. Set the *in silico* time, step length (δt; recommended value: 2), and saving interval for computation (Fig. G4(a)).

D. Choose if the eggshell is considered.

E. Give a name like "Test" for the simulation and its output storage.

F. Click "Run", then a folder named by Step E is generated and the cell patterns at spaced time points would be saved as "Test\Test_*.mat", where "*" denotes the *in silico* time corresponding to each file (Fig. G5).

- One can know the progress through the files saved intermittently.

4) To illustrate a multicellular structure outputted by *MorphoSim*, use the lower panel (Fig. G4(b) and (c)):

A. Import the information of cell names.

- The file format is shown in "Example\Example_CellName.xls".

B. Import the selected cell pattern outputted by *MorphoSim*.

C. Click "Plot", then a figure illustrating the multicellular structure would be shown (Fig. G4(d)-(f)).

3. Contact

All the fundamental scripts of the *MorphoSim* GUI have been uploaded onto GitHub https://github.com/XiangyuKuang/MorphoSim.git. If there is any question, please contact Xiangyu Kuang (kuangxy@pku.edu.cn) or Guoye Guan (guanguoye@gmail.com) anytime.

4. Figures for the user guidebook

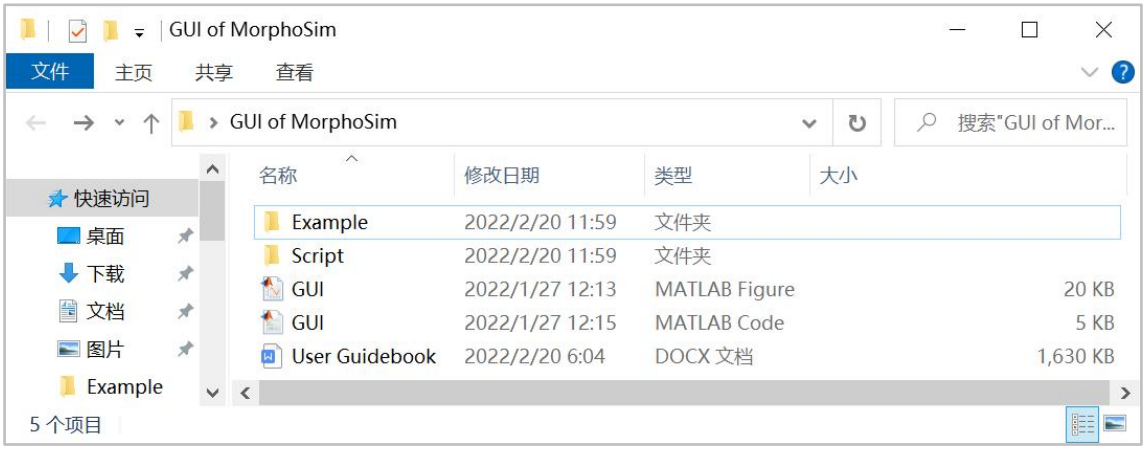

Fig. G1. The files and subfolders in the Folder "MorphoSim" downloaded from GitHub.

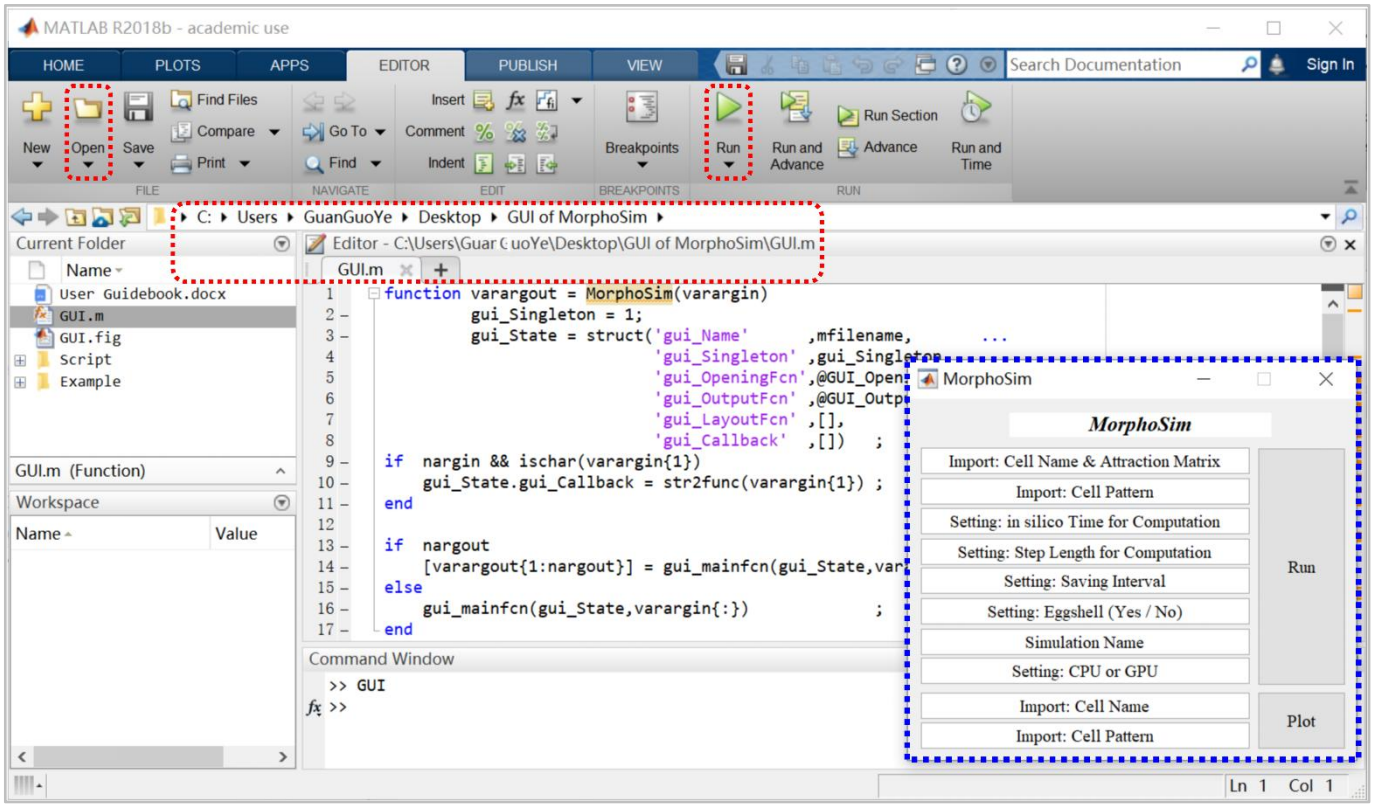

Fig. G2. Instruction to open the *MorphoSim* GUI. The script imported and the buttons for loading and running it are noted by dashed red frames; the interface of *MorphoSim* generated after clicking "Run" is noted by a dashed blue frame.

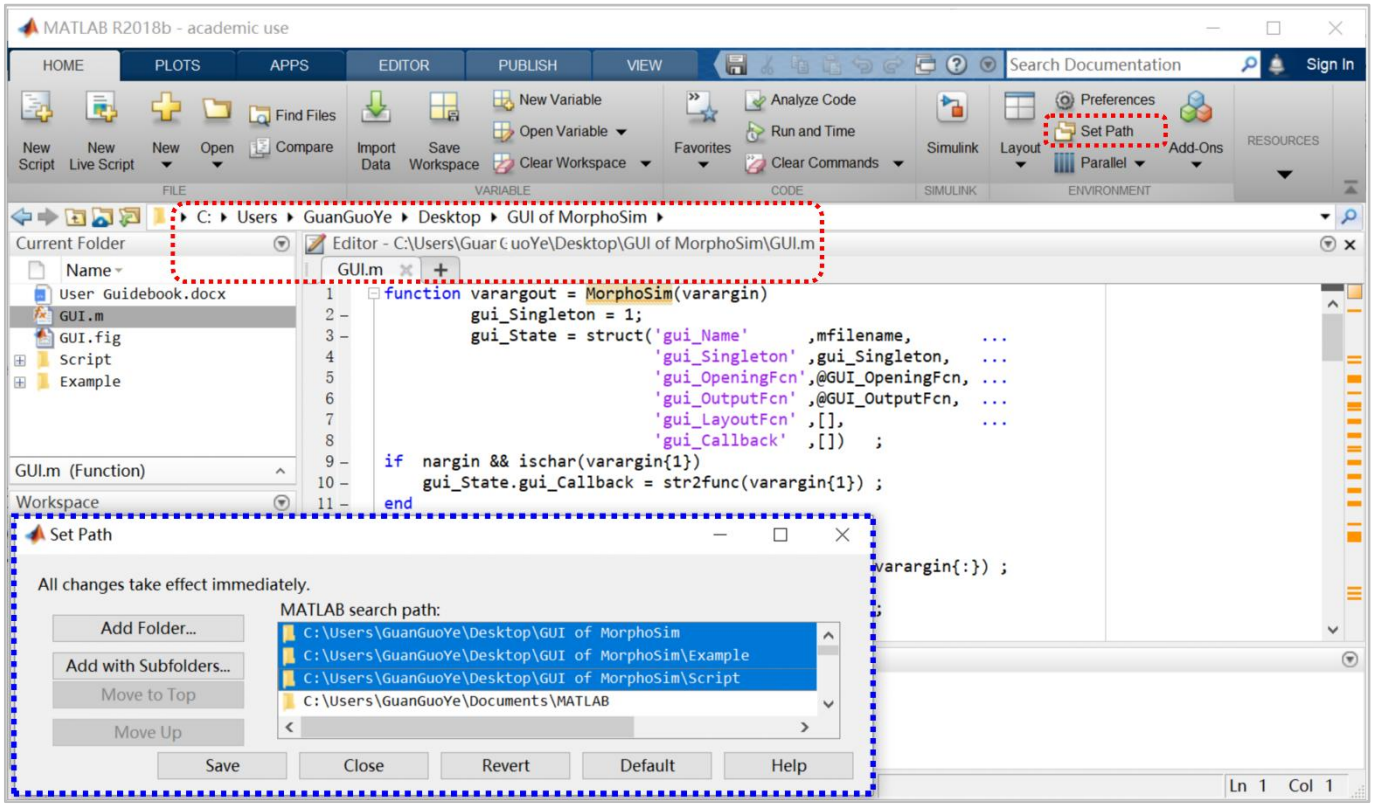

Fig. G3. Instruction to set the path for the *MorphoSim* GUI. The script imported and the button for setting path are noted by dashed red frames; the interface for setting path generated after clicking "Set Path" is noted by a dashed blue frame.

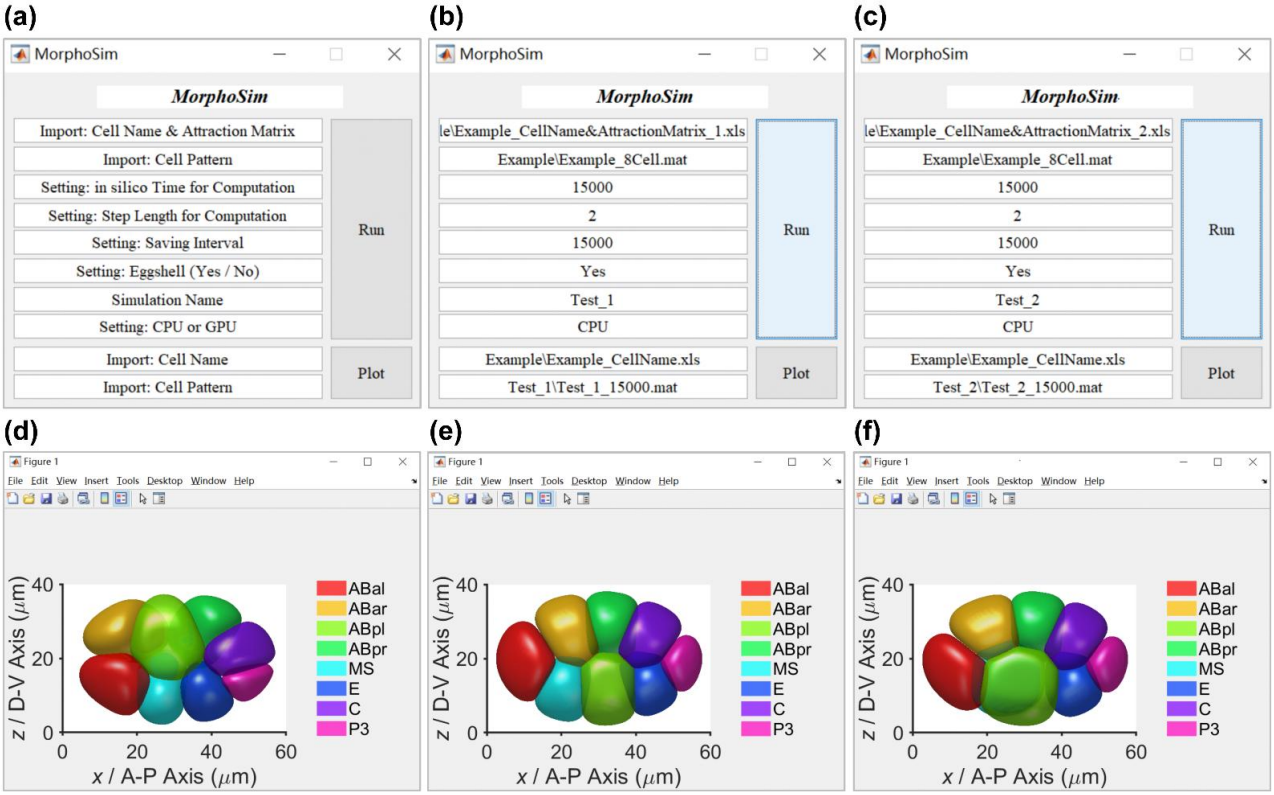

Fig. G4. The graphical user interface of *MorphoSim*. (a) The interface and instruction of inputs required. (b)(c) The simulation inputs for 8-cell *C. elegans* embryogenesis with relatively strong (i.e., $\sigma_{\mathrm{ABpl,E}} = \sigma_{\mathrm{S}} = 0.5$) and weak (i.e., $\sigma_{\mathrm{ABpl,E}} = \sigma_{\mathrm{W}} = 0.5$) adhesion in ABpl-E contact respectively. (d) The initial state (*in silico* time = 0) of the 8-cell embryo. (e)(f) The final state (*in silico* time = 15000) of the 8-cell embryo with relatively strong (i.e., $\sigma_{\mathrm{ABpl,E}} = \sigma_{\mathrm{S}} = 0.5$) and weak (i.e., $\sigma_{\mathrm{ABpl,E}} = \sigma_{\mathrm{W}} = 0.5$) adhesion in ABpl-E contact respectively. Note that this whole figure is the same as Fig. 4 in the main text of the paper.

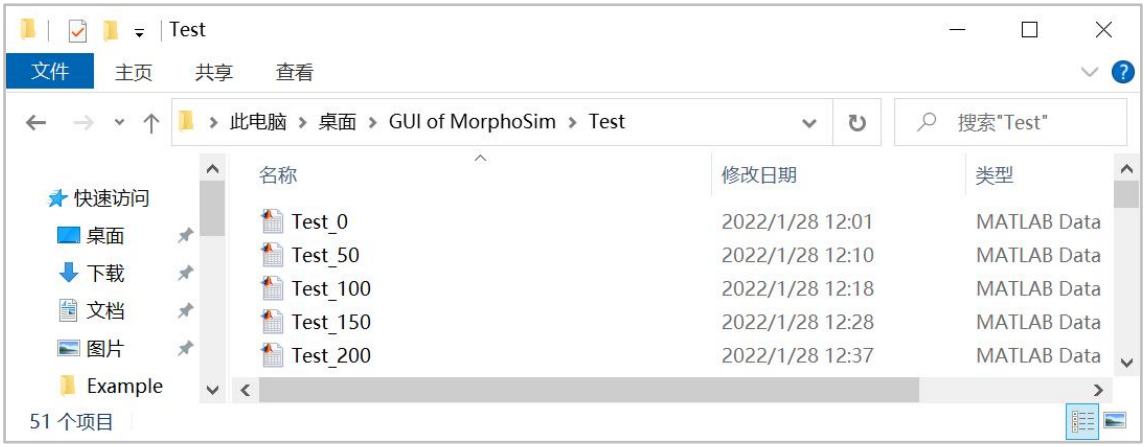

Fig. G5. The files outputted and saved intermittently.