SimuPlant: The Virtual Root
User Documentation

The University of Nottingham

2013

Table of Contents

Overview

SimuPlant is a software suite designed to simulate vertex-based models encoded within the OpenAlea modelling framework[1]. This user documentation focuses on SimuPlant: The Virtual Root, which features multi-cellular models of auxin transport within the *Arabidopsis* root tip, as described by Band et al [2].

SimuPlant: The Virtual Root enables users with no programming experience to simulate auxin dynamics within an *Arabidopsis* root tip. Users can select from a range of model assumptions and choose model and simulation parameter values. Users can then simulate the model to investigate how their choices affect the predicted distributions of auxin and downstream network components. Simulation results are shown visually within the root geometry and can be exported and saved as PNG image files.

SimuPlant is written in Java, and is hence platform independent. It is available from **www.simuplant.org**.

Model description

The plant hormone auxin is an important regulator of plant growth and development and plays a key role in organ initiation and tropic responses. Auxin is actively transported through plant tissues via proteins on the cell membranes; the cellular and subcellular location of these membrane proteins can create auxin maxima and directed fluxes.

SimuPlant: The Virtual Root simulates auxin transport within an *Arabidopsis* root tip, using actual cell geometries. The model predicts the levels of auxin (and downstream components) within each cell and apoplast compartment. Within each compartment, both protonated and anionic auxin are present, with the proportion of each dependent on the compartmental pH.

The model incorporates

   i.   passive diffusion of protonated auxin across cell membranes,
   ii.   efflux of anionic auxin (from the cytoplasm to apoplast) mediated by members of the PIN family of membrane proteins,
   iii. efflux of anionic auxin (from the cytoplasm to apoplast) mediated by members of the PGP family of membrane proteins,
   iv.   influx of anionic auxin (from the apoplast to the cytoplasm) mediated by the AUX1 membrane proteins,
   v.   influx of anionic auxin (from the apoplast to the cytoplasm) mediated by the LAX2 membrane proteins,
   vi.   passive diffusion of auxin within the apoplast,
   vii. auxin production and degradation within each cell,
   viii. auxin-mediated degradation of the DII-VENUS fluorescent reporter (via the network of interactions shown in Fig. 1).
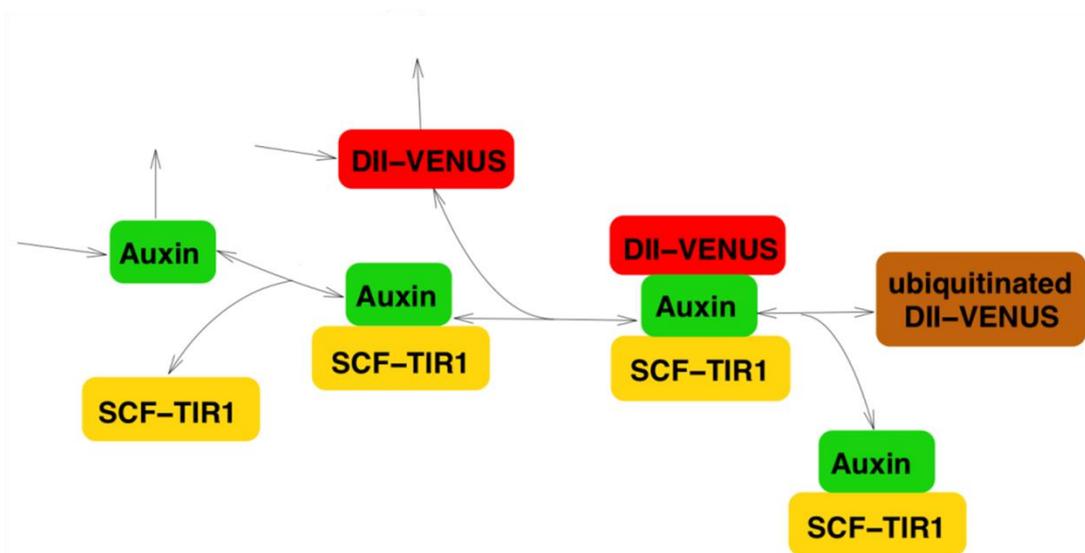

Figure 1: The network of interactions through which auxin degrades DII-VENUS.

The distributions of the membrane proteins are prescribed (based on experimental images). Users can select from a range of multicellular geometries. In [2], the model is used to investigate the role of the AUX1 influx carriers and the available geometries correspond to those within this publication. We therefore have geometries obtained from wild-type plants, *aux1* null mutant plants (in which no AUX1 are present) and *aux1 J0951>> AUX1* plants (in which AUX1 is only present within the elongating epidermal and outer lateral root cap cells). Users have a range of options for adjusting the membrane protein distributions, and can change the model parameter values.

Further details of the model and associated equations can be found in [2].

Installing SimuPlant: The Virtual Root

Requirements

Java 7 is the only requirement in order to run the application.

Download

- The latest version of the SimuPlant GUI is available from **www.simuplant.org**.
- A Java 7 runtime installation is also required (available at **www.java.com** or from the system package manager on Linux).

Running the VirtualRoot Simulator

Using a command terminal, navigate to the folder where simuplant-root.jar was downloaded to and run the GUI by typing:

```
java -jar simuplant-root.jar
```

Troubleshooting

If SimuPlant doesn't run then test the Java installation by typing:

```
java -version
```

If the reported version is less than "1.7.0_xx" then Java will need to be upgraded *via* **www.java.com** or the system package manager for Linux.

On Windows, if Java7 is installed and the command prompt reports that it is unable to find java.exe:
- use Windows Explorer to browse or search for java.exe, generally located at *C:\Program Files\Java\jre7\bin or C:\Program Files(x86)\Java\jre7\bin*
- shift-right-click on the located java.exe file and select "Copy as path"
- right click on the command prompt, select paste and type " `-version`" after it and try again.
- If that succeeds and reports a version, then use that path in place of "java" at the command-prompt, ie:

```
"C:\Program Files\Java\jre7\bin\java.exe" -jar simuplant-root.org
```

If the computer is connected to a network which uses a web proxy to access the internet Java should automatically detect the settings. If this doesn't happen then the user can either:
- follow the instructions at **www.java.com/en/download/help/proxy_setup.xml**
- or modify the java command as follows:

```
java -Dhttp.proxyHost=proxy.host.name -Dhttp.proxyPort=8080 -jar simuplant-root.jar
```

Replacing 'proxy.host.name' and '8080' with the correct address and port.

The Program Interface

The SimuPlant interface consists of five major components, as seen in Fig. 2 and described below. Full details for using these components are provided in the next section.
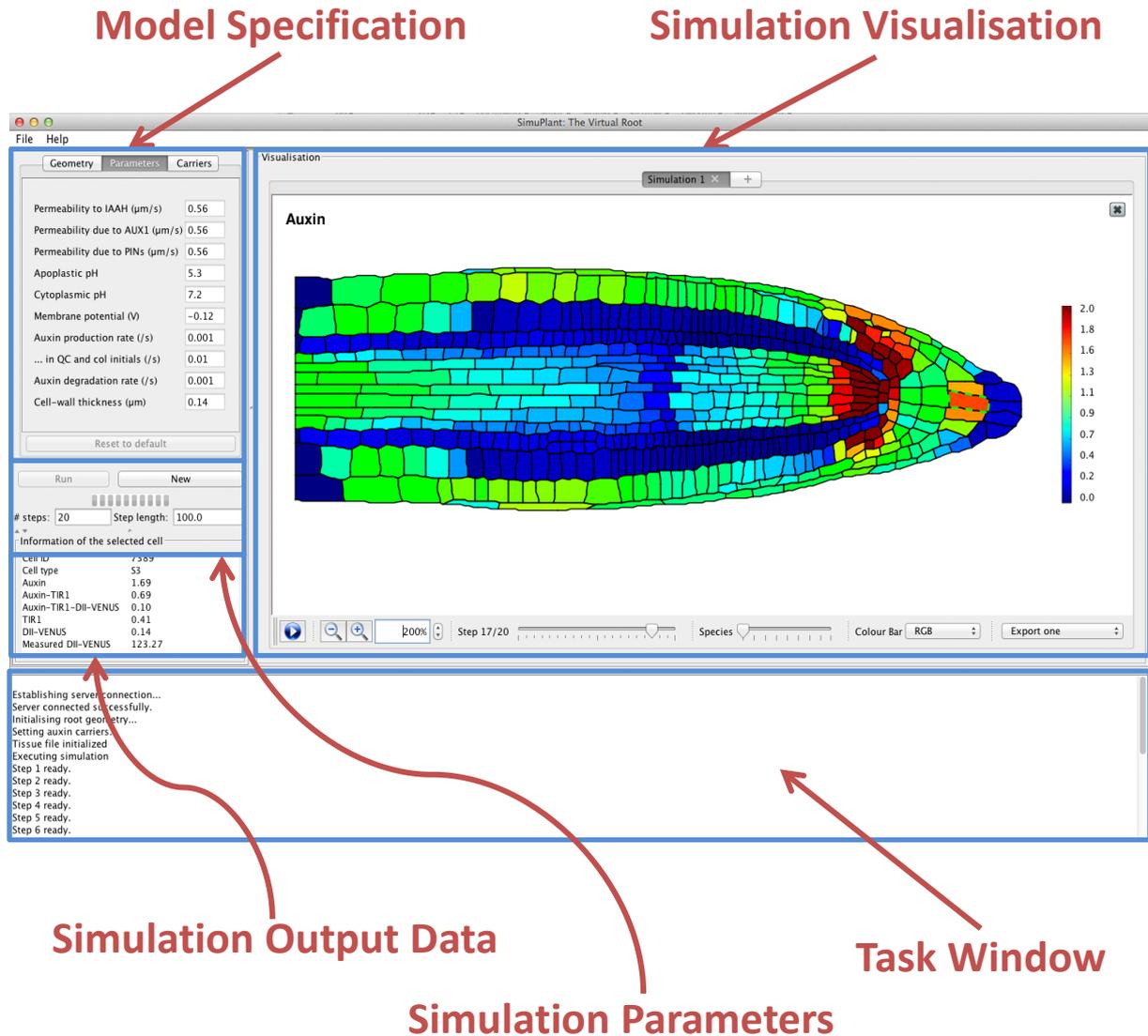
Figure 2: A standard view of the SimuPlant interface

1. Model Specification panel

The Model Specification panel enables the user to select from a choice of root geometries, specify model parameter values and choose different options for the distributions of the PIN, AUX1 and LAX2 membrane proteins.

2. Simulation Parameters panel

The Simulation Parameters panel enables the user to choose the time interval and number of time steps for the simulation, and to start and stop the simulation.

3. Simulation Visualisation panel

The Simulation Visualisation panel displays the root geometry, showing the distributions of the prescribed or simulated species within the model. Using the tool strip at the bottom of the panel, the user can zoom into and out of the image, choose to see different species at different time steps, select colour mappings for the model outputs and save the simulation figures.

4. Simulation Output Data

Users can click particular cells within the root geometry to see the predicted concentrations of the different species within this cell; these data are displayed in the Simulation Output Data panel.
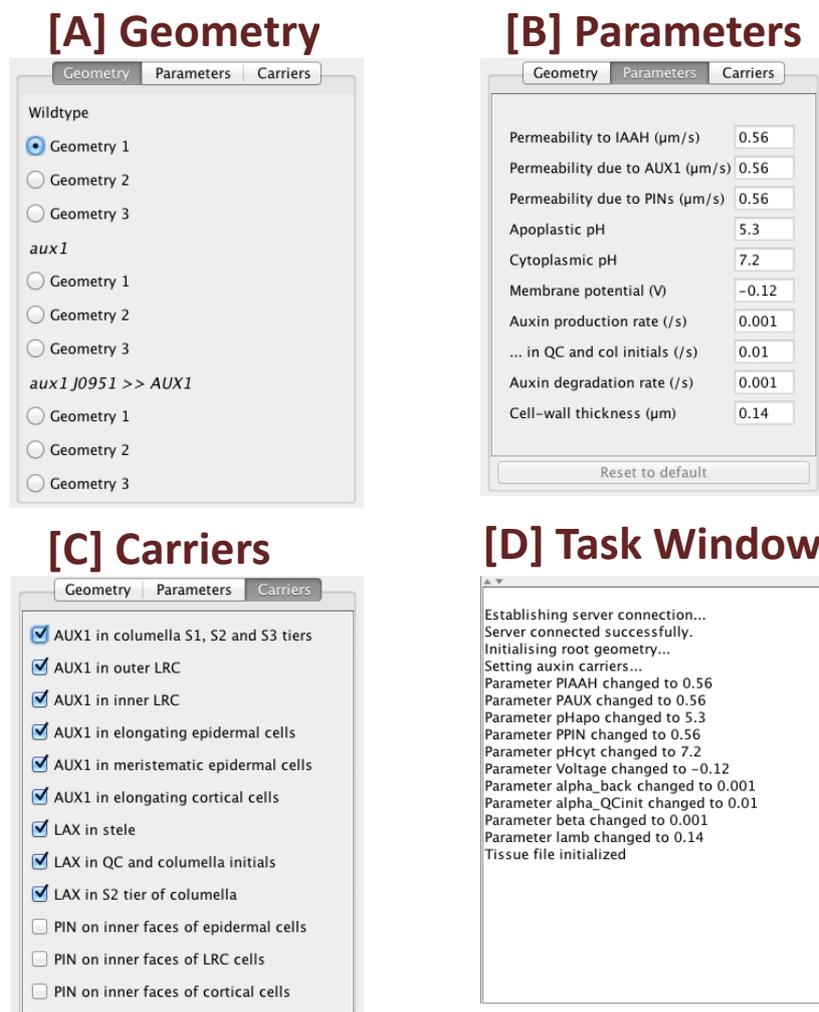
5. Task Window

The Task window displays the current task that is being undertaken by the server.

Using SimuPlant: The Virtual Root

Specifying the model

On starting SimuPlant, the Model Specification panel displays the 'Geometry' tab (Fig. 3A). Nine different root geometries are listed, which have been segmented from microscope images of wild-type, *aux1* and *aux1 J0951>>AUX1* plant root tips. On selecting a geometry, the server initialises the multicellular root geometry and auxin carrier distributions, and loads the auxin transport and DII-VENUS degradation models. As these tasks are completed, they are listed in the Task Window (Fig. 3D).

[A] Geometry

| Geometry | Parameters | Carriers |

Wildtype
- ⦿ Geometry 1
- ○ Geometry 2
- ○ Geometry 3

aux1
- ○ Geometry 1
- ○ Geometry 2
- ○ Geometry 3

aux1 J0951 >> AUX1
- ○ Geometry 1
- ○ Geometry 2
- ○ Geometry 3

[B] Parameters

| Geometry | Parameters | Carriers |

Permeability to IAAH (µm/s)	0.56
Permeability due to AUX1 (µm/s)	0.56
Permeability due to PINs (µm/s)	0.56
Apoplastic pH	5.3
Cytoplasmic pH	7.2
Membrane potential (V)	−0.12
Auxin production rate (/s)	0.001
... in QC and col initials (/s)	0.01
Auxin degradation rate (/s)	0.001
Cell–wall thickness (µm)	0.14

Reset to default

[C] Carriers

| Geometry | Parameters | Carriers |

- ☑ AUX1 in columella S1, S2 and S3 tiers
- ☑ AUX1 in outer LRC
- ☑ AUX1 in inner LRC
- ☑ AUX1 in elongating epidermal cells
- ☑ AUX1 in meristematic epidermal cells
- ☑ AUX1 in elongating cortical cells
- ☑ LAX in stele
- ☑ LAX in QC and columella initials
- ☑ LAX in S2 tier of columella
- ☐ PIN on inner faces of epidermal cells
- ☐ PIN on inner faces of LRC cells
- ☐ PIN on inner faces of cortical cells

[D] Task Window

```
Establishing server connection...
Server connected successfully.
Initialising root geometry...
Setting auxin carriers...
Parameter PIAAH changed to 0.56
Parameter PAUX changed to 0.56
Parameter pHapo changed to 5.3
Parameter PPIN changed to 0.56
Parameter pHcyt changed to 7.2
Parameter Voltage changed to −0.12
Parameter alpha_back changed to 0.001
Parameter alpha_QCinit changed to 0.01
Parameter beta changed to 0.001
Parameter lamb changed to 0.14
Tissue file initialized
```

**Figure 3: The Model Specification panel and Task Window**

Having chosen a root geometry, users can view the default model parameters or carrier distribution by selecting the relevant tabs within the Model Specification panel (Fig. 3). Model parameter choices can be changed by simply deleting and replacing the values listed, with the field turning grey when parameter changes are registered and the Task Window (Fig 3D) detailing the changes. Users can return to the default values by clicking the 'Reset to default' button within this tab (Fig. 3B).

Extreme parameter values can cause the simulation to take excessive time or lead to numerical errors. To prevent this we restrict the allowed parameters; if the parameter value entered is outside the specified range, the value is automatically reassigned to the maximum or minimum of the range.

The default settings for the Geometry panel depend on the geometry chosen (reflecting whether it is from a wild-type, *aux1* or *aux1 J0951>>AUX1* plant root). Selecting different options in this panel enables the user to alter the rules specifying the carrier distributions. The distributions of the AUX1, LAX and PIN carriers can be seen on the root geometry, within the Simulation Output panel, by using the 'Species' slider to move between the different species within the model.

Specifying the simulation parameters and running the simulation

Having specified the model parameters, the user can view and alter the number and time interval of each time step (in minutes) using the Simulation Parameters panel (default parameters are provided) (Fig. 4). The simulation parameters panel also shows a progress bar whilst the server is working on completing a task.

(A)

Run	New

steps: 20   Step length: 100.0

(B)

Pause	New

steps: 20   Step length: 100.0
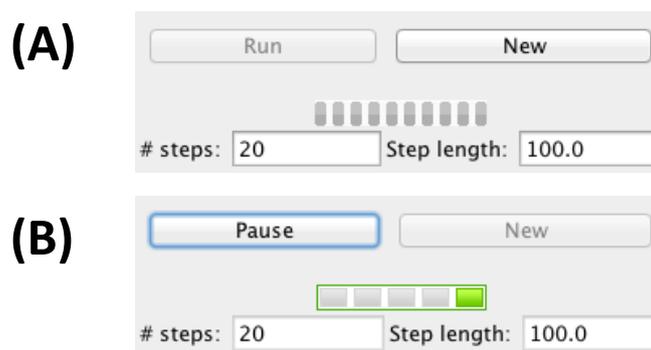
Figure 4: The Simulation Parameters panel (A) Before/after a simulation is run (B) While a simulation is running

The simulation is now ready to run by clicking the 'Run' button within the Simulation Parameters panel. The Task Window lists when each time interval has been simulated. While the simulation is running, the 'Run' button becomes a 'Pause' button (Fig. 4B) enabling the user to pause the simulation at any time. Note that on the first click of the 'Run' button, the Model Specification panel is disabled.

SimuPlant requires a continual internet connection and we do not recommend using it over unreliable wi-fi connections. If the simulator pauses for an excessive time the internet connection may have dropped briefly, in which case users should simply close the program and restart.

Viewing details of the simulation output

1. Visualising the simulation

The output of the simulation can be viewed in the Simulation Visualisation panel. The evolution of the distributions can be seen by clicking the Play button, or the distributions at particular time steps can be viewed using the Time Step slider. Users can move the root geometry within the panel by clicking and dragging, and can zoom in/out by using the mouse wheel or zoom buttons.
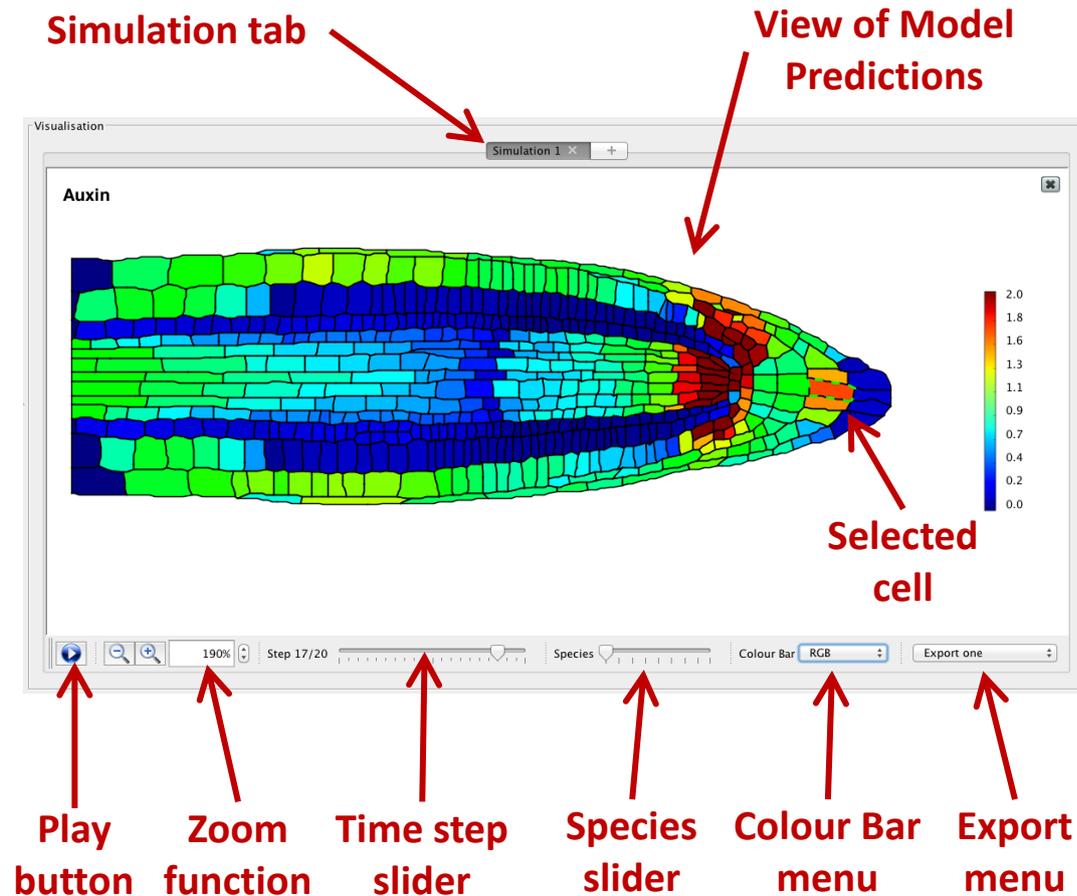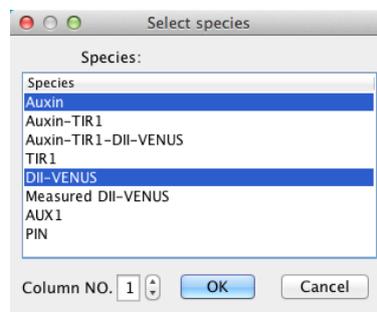

Figure 5: The Simulation Visualisation Panel.

Within the Simulation Visualisation Panel, users can:

i.   Use the zoom function to see more details of a particular area of the root geometry.
ii.   View the predicted distribution of the different species within the model (auxin, TIR1 and DII-VENUS) and the prescribed distributions of the membrane proteins using the 'Species' slider.
iii. Use the Colour bar menu to view the simulations using different colour heat mappings.

2. Viewing multiple panels

Users can create and view multiple Simulation Visualisation Panels. Right clicking the Simulation tab at the top of the Simulation Visualisation Panel (see Fig 5), the user can choose to 'Select species' which brings up the box seen in Fig 6.

Figure 6: The Select species box.

From here, users can select multiple species (using shift-left-click or ctrl-left-click [cmd-left-click on a Mac]) and specify the number of columns of Visualisation panels required. For example, selecting 'Auxin' and 'DII-VENUS' and setting the column number to be 1, the user can generate the two panels shown in Fig 7. Users can change the species and heat map options for each panel, and can remove a particular panel by clicking the close button at the top right-hand corner of the panel (see Fig 7).
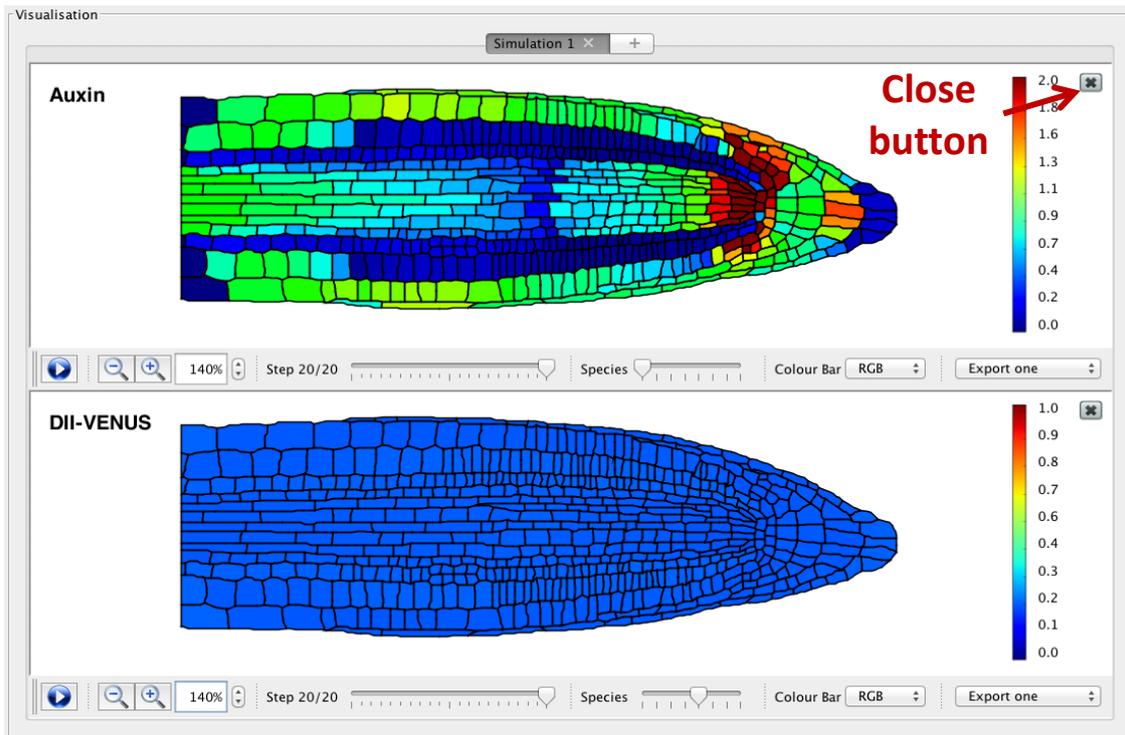
Figure 7: View with multiple Visualisation panels.

3. Viewing the simulation output data

The Simulation Output Data panel (Fig 8) enables users to view the data corresponding to any particular cell. Clicking on a cell within the Simulation Visualisation panel (within any of the species views) highlights the cell with a dashed green outline (see Fig 5). Information about the selected cell is displayed in the Simulation Output Data panel.

Figure 8: The Simulation Output Data panel.

Saving the simulation

Users can save both the visual predictions of the simulation as images, by using the Export menu in the toolbar within each Simulation Visualisation panel, or the simulation data which can be uploaded and viewed using SimuPlant.

Saving images of the simulation predictions

Users have the option of exporting one or all of the predicted distributions as PNG image files.

Selecting 'Export one' saves the image currently shown within the Simulation Visualisation panel (which corresponds to a particular species at a particular time step). Users select a folder and specify the name of the resulting file in the dialog box.

Selecting 'Export all' saves the predicted distributions of the currently selected species (as shown in the Simulation Visualisation panel) for each time step, in the selected folder. If the user specifies a name in the 'Save as' field a new sub-folder will be created to hold the images.

Saving the simulation data

Users can save the simulation data using the File -> Save Simulation option in the menubar. These saved simulations can be reopened for viewing in SimuPlant using the File -> Load Simulation option within the menubar.

Creating a new simulation

Users can create a new simulation in three ways:

i)   Clicking the 'New' button within the Simulation Parameters panel. This deletes the current simulation and returns the program interface to its initial configuration (with no geometry selected and the parameter values and carrier distributions returned to their default settings).

ii)   In the File menu, the user can select 'New Simulation'. This also deletes the current simulation and returns the program interface to its initial configuration.

iii)   Clicking the '+' tab at the top of the Simulation Visualisation panel. This creates a new tab, containing 'Simulation 2', leaving 'Simulation 1' within the first tab. The Simulation tabs can be deleted, either by clicking the 'x' within the Simulation tab (see Fig 6) or right clicking the Simulation tab and selecting 'close'.

In all of these cases, users should then use the geometry tab within the Model Specification panel to select a new root geometry for their new simulation.

References

[1] Pradal C, Dufour-Kowalski S, Boudon F, Fournier C & Godin C (2008) OpenAlea: a visual programming and component-based software platform for plant modelling. Functional Plant Biology *35*, 751–760. doi:10.1071/FP08084

[2] Leah R. Band, Darren M. Wells, John A. Fozard, Teodor Ghetiu, Andrew P. French, Michael P. Pound, Michael H. Wilson, Lei Yu, Wenda Li , Hussein I. Hijazi, Jaesung Oh, Simon P. Pearce, Miguel A. Perez-Amador, Jeonga Yun, Eric Kramer, Jose Alonso, Christophe Godin, Teva Vernoux, T. Charlie Hodgman, Tony P. Pridmore, Ranjan Swarup, John R. King & Malcolm J. Bennett. PIN efflux carriers direct auxin flux but the AUX1 influx carrier controls auxin level in root cells. *Submitted to Molecular Systems Biology*