

Version 3.2.0 changes.

This is a major release featuring greatly improved Python scripting numerous bug fixes, simplified syntax for neighbor pixel management and hexagonal lattice.

- 1) Users can describe entire simulation (i.e. plugins, steppables and Potts Section) using Python only XML is still supported. As a matter of fact part of the simulation can be described in Python and part in the XML. However, unless users know exactly what they are doing we recommend to either use XML or Python.
- 2) We have separated XML parsing from object initialization therefore currently users can mix the order of Potts section , plugins and steppables in the XML file. However, we recommend that you stick to the old “ordered” format for clarity purposes.
- 3) Using <NeighborOrder> tag instead of <Depth> or <FlipNeighborMaxDistance> users can more easily include higher order neighbors in appropriate modules. Note, this eliminate the need of knowing the actual distance for ppixel neighbors.
- 4) We support hexagonal lattice. For 2D simulations using hex lattice you have to use xy plane for the lattice to be correctly displayed in the Player. If you use other planes the calculations will be done correctly but the Player will display other planes as if they were based on square lattice. also in 3D Orthnogonal projections for hex do not make much sense so you may slice the lattice with a plane parallel to xy plane or look at the 3D view. We will support lattice projections appropriate for hex lattices in the future.
- 5) We have fixed numerous small but annoying bugs present in the previous release

Known issues

Player limitations in displaying hexagonal lattice. For 2D simulations using hex lattice you have to use xy plane for the lattice to be correctly displayed in the Player. If you use other planes the calculations will be done correctly but the Player will display other planes as if they were based on square lattice. also in 3D Orthnogonal projections for hex do not make much sense so you may slice the lattice with a plane parallel to xy plane or look at the 3D view. We will support lattice projections appropriate for hex lattices in the future.

Version 3.1.17 changes

- 1) Added options to the Player to specify output directory or disable output completely
- 2) Greatly simplified syntax of simulation main Python script
- 3) Fixed problem with screenshot frequency and screen update frequency setting through xml file

Known issues

Player compiled with VTK support will not run properly through VNC session but will run fine using ssh. This appears to be VTK issue. We will try finding the solution and will post it on the web.

Version 3.1.16 changes

- 1) Did major refactoring to the Player so that now CompuCell3D can be run in a silent mode without connecting to the X-server. this is important if people run CompuCell3D on clusters where there is no X-server installed. Screenshots are still taken despite the fact that there is no X-server connection.

- 2) Improved Vector plot visualization in the Player – there are more options available
- 3) Improved PlayerSettings plugin so that essentially all Player options can be now configured from xml level. This may be useful when people want to run multiple different simulation at the same time and yet want to use different cell colors, concentration ranges etc... for each of the simulation.
- 4) Changed the name of run script to computecell3d.sh

Known issues

When running simulation in silent mode without X-server connection and plotting 2D screenshots of concentration or vector field with legend, the legend will not contain any text. This is due to limitation of Qt4. We hope to solve it soon. For now we store text file with min and max values of concentration and vector magnitude and having that users can deduce color assignments in color map and vector plots.

If you are using 3D visualization in silent mode with no X-server connection you need to have VTK compiled with OffScreenRendering ON and OSMesa support ON (this is how it is done on clusters with no X-server). This will however prevent QVTK widget from functioning correctly (it will crash). This means that if you are using VTK compiled with offscreen rendering you will not be able to see 3D visualization in through GUI -with connection to X-server (but you will get screenshots in the silent mode with no connection to X-server!). And vice versa, if you are using default compiled version of VTK library – the one that connects to X-Server and want to run simulation in the silent mode but without connecting to X-server the simulation will crash with an error “no connection to X-server”.

Version 3.1.15 changes

- 1) Implemented cell velocity plugin that calculates instantaneous velocity of the cell as a difference between center of mass of cells. It also precalculates after-spin-flip Center of Masses so this information is available before the actual spin flip has occurred. This plugin **has not been tested** yet.
- 2) Improved Cell Orientation plugin.
- 3) Fixed Connectivity plugin using Tinri Aegerter algorithm
- 4) Improved Energy Statistics output module so that now users can output energies for every spin flip and spin flip attempt. See cellsort_2D_statistics_spin_flip.xml example
- 5) Fixed non-vtk version of the Player. This player does not have 3D visualization capabilities
- 6) Improved installation manuals. Included step-by-step installation directions using ccmake interface. Check docs directory
- 7) Wrote short manual explaining how to run CompuCell3D from command line. See docs/Running_CompuCell3D.pdf