Recall:

OpenVT – A Standardized Ecosystem for Virtual Tissue Simulation

2-year NSF grant (ends 2025-8-31)

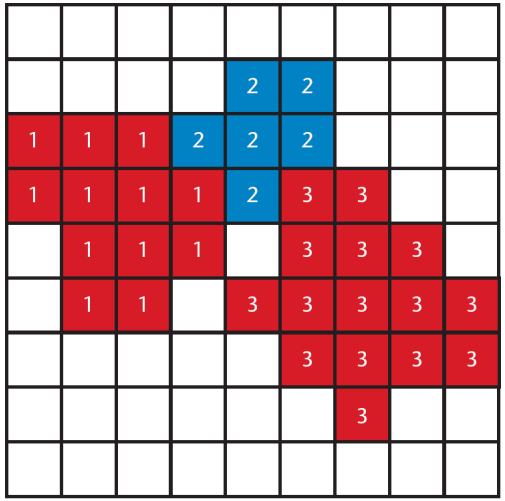
Specific aims include: development of shared standards for specification of VT models between CompuCell3D and PhysiCell, creation of cell-type description libraries, standardization of initial conditions, and description of model outputs. These standards will then be used to define the needed APIs that allow the interconnection and reuse of models.

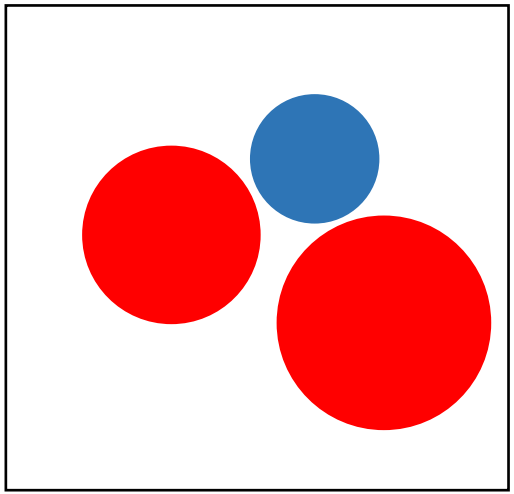
https://new.nsf.gov/funding/opportunities/pathways-enable-open-source-ecosystems-pose

PIs: Glazier, Wild, Macklin https://www.nsf.gov/awardsearch/showAward?AWD_ID=2303695

Agents: spatial definition

- CC3D: contiguous pixels on a lattice
- PhysiCell: center + volume (lattice-free)





Specifying agents initial conditions (geometry)

- CC3D: PIFF (Potts Initial File)
  https://compucell3dreferencemanual.readthedocs.io/en/latest/pif_initializer.html

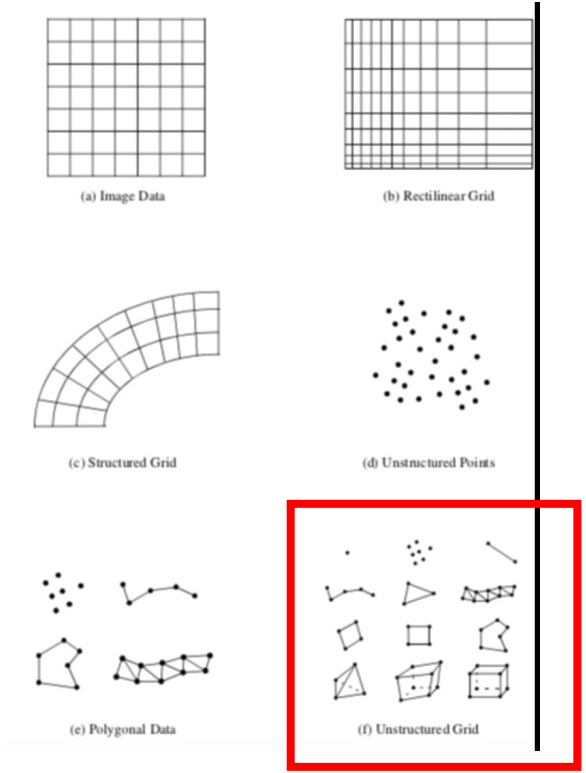
  cell# celltype x1 x2 y1 y2 z1 z2

- PhysiCell: CSV

  https://github.com/MathCancer/PhysiCell/blob/master/changes.md#1110

  x,y,z,celltype[,…]

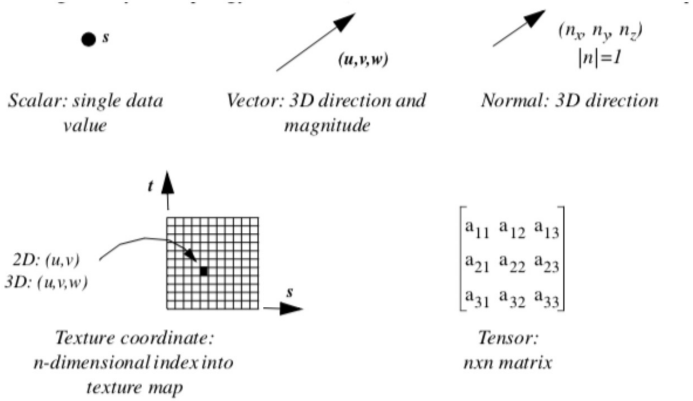
VTK data formats



Most general (.vtu)

5.5 Attribute Data

Attribute data is information associated with the structure of the dataset. This structure includes both the dataset geometry and topology. Most often, attribute data is associated with dataset points or cells, but sometimes attribute data may be assigned to cell components such as edges or faces. Attribute data may also be assigned across the entire dataset, or across a group of cells or points. We refer to this information as attribute data because it is an attribute to the structure of the dataset. Typical examples include temperature or velocity at a point, mass of a cell, or heat flux into and out of a cell face.

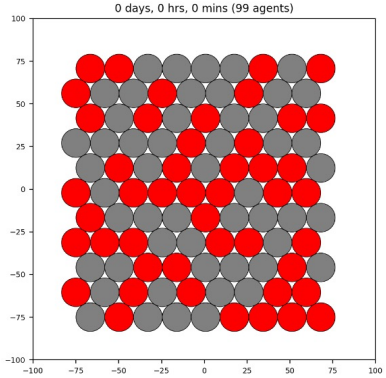


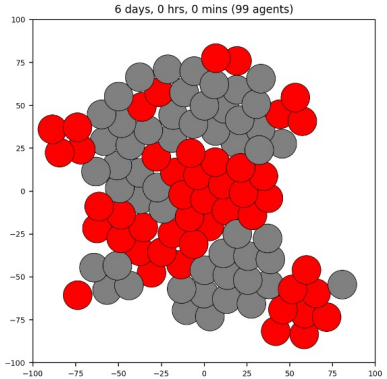
Very preliminary work

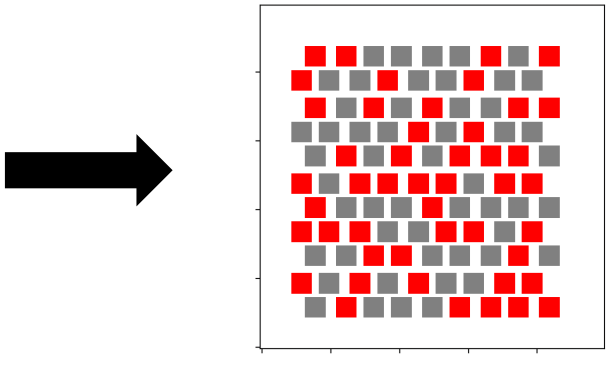
Python script to create a VTK (.vtu) file from PhysiCell cells ICs.
Python script to create native format for CC3D.

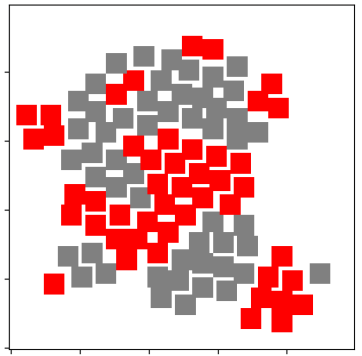
Converting a later snapshot as ICs.

PhysiCell





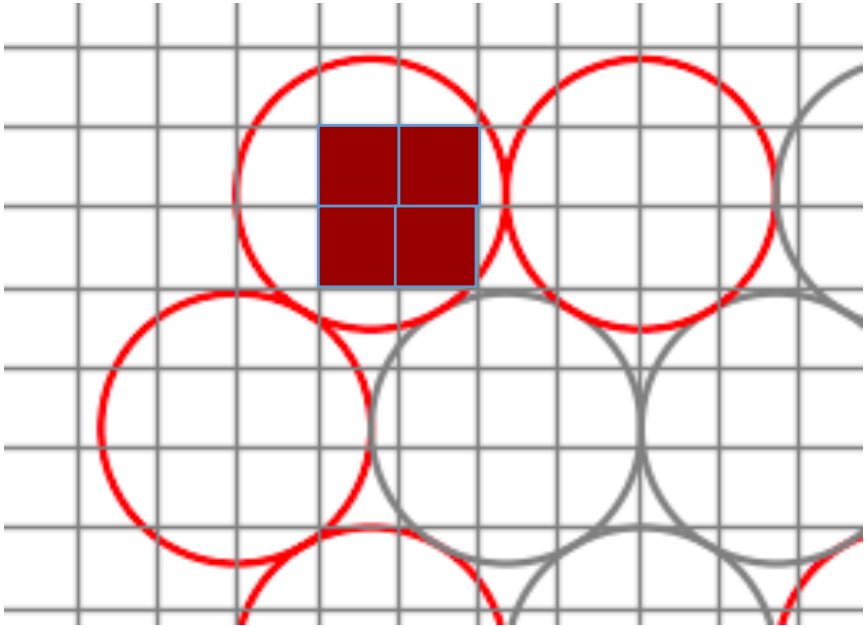




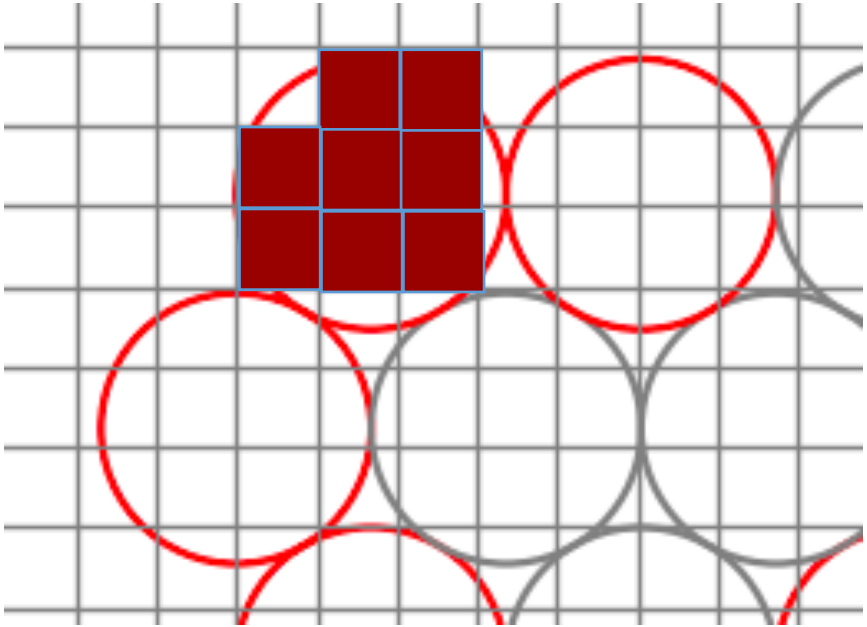
CC3D

- https://github.com/OpenVT/playground/issues/2

Converting PhysiCell ICs to CC3D: rasterizing a circle/sphere

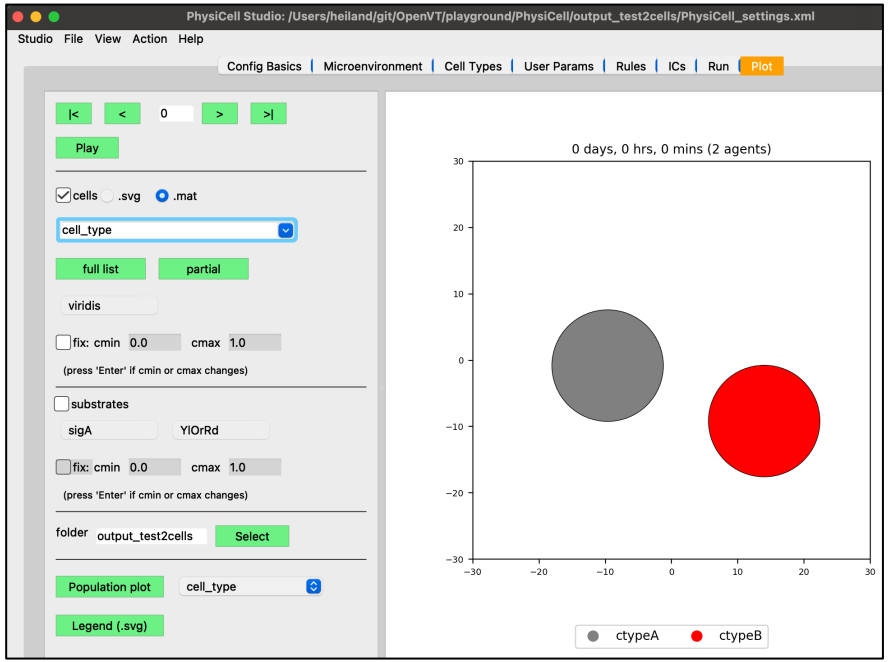


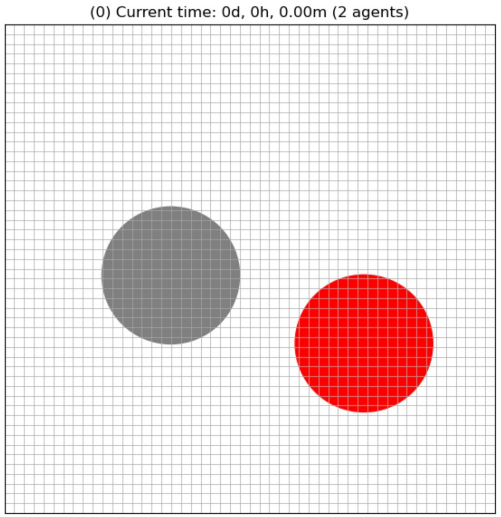
Pixel entirely inside



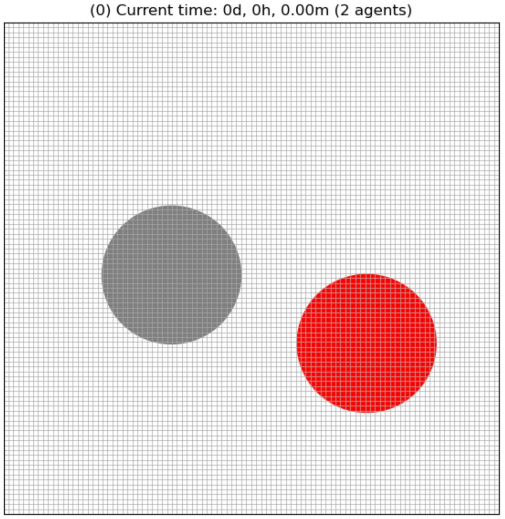
Pixel center < R

Map 2 cells into a CPM lattice





50x50



Showing original circular cells, but will just have contiguous pixels for CPM.

100x100

```
(base) M1P~/git/OpenVT/playground/PhysiCell$ python pcdl2vtu.py output_test2cells output00000000.xml
reading: output_test2cells/PhysiCell_settings.xml
Warning @ pyMCDS._read_xml : cell_definition custom_data without variable type setting detected. ['sample']
reading: output_test2cells/output00000000.xml
working on metadata ...
working on mesh data ...
reading: output_test2cells/initial_mesh0.mat
working on discrete cell data ...
reading: output_test2cells/output00000000_cells.mat
done!
bbox =  -30.000000 -30.000000 -10.000000 30.000000 30.000000 10.000000
bds= -30.0 30.0 -30.0 30.0
len(cell_type)= 2
 0) ctypeA: vol= 2494.0
 1) ctypeB: vol= 2494.0
0 ) x,y,z=  -9.649676331393135 -0.8192351629222685 0.0
1 ) x,y,z=  13.980851874014036 -9.174781047707121 0.0
-->  output00000000_pcell.vtu
```

Convert PhysiCell cells to a .vtu format, initially just:

- Centers
- Cell ID
- Volumes

```
<?xml version="1.0"?>
<VTKFile type="UnstructuredGrid" version="0.1" byte_order="LittleEndian" header_type="UInt32" compressor="vtkZLibDataCompressor">
  <UnstructuredGrid>
    <Piece NumberOfPoints="2" NumberOfCells="0">
      <PointData>
        <DataArray type="Float32" Name="volume" format="ascii" RangeMin="2494" RangeMax="2494">
          2494 2494
        </DataArray>
        <DataArray type="Int32" Name="cell_id" format="ascii" RangeMin="0" RangeMax="1">
          0 1
        </DataArray>
      </PointData>
      <CellData>
      </CellData>
      <Points>
        <DataArray type="Float32" Name="Points" NumberOfComponents="3" format="ascii" RangeMin="9.684389467693235" RangeMax="16.722464823246124">
          -9.649676322937012 -0.8192351460456848 0 13.980852127075195 -9.17478084564209 0
          <InformationKey name="L2_NORM_RANGE" location="vtkDataArray" length="2">
            <Value index="0">
              9.6843894677
            </Value>
            <Value index="1">
              16.722464823
            </Value>
          </InformationKey>
        </DataArray>
      </Points>
      <Cells>
        <DataArray type="Int64" Name="connectivity" format="ascii" RangeMin="1e+299" RangeMax="-1e+299">
        </DataArray>
        <DataArray type="Int64" Name="offsets" format="ascii" RangeMin="1e+299" RangeMax="-1e+299">
        </DataArray>
        <DataArray type="UInt8" Name="types" format="ascii" RangeMin="1e+299" RangeMax="-1e+299">
        </DataArray>
      </Cells>
    </Piece>
  </UnstructuredGrid>
</VTKFile>
```

output00000000_pcell.vtu

Disregard (range of data)

No (VTK) “cells” for PhysiCell .vtu