

CompuCell3D Training Workshop
Biocomplexity Institute
Indiana University
Bloomington
Aug 15-19 2011

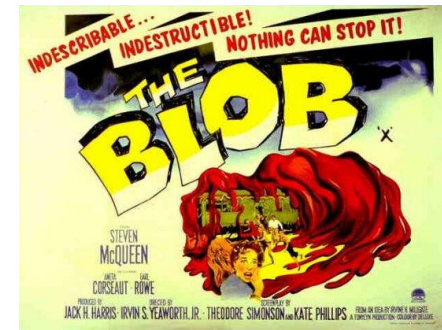
Initial Conditions in CompuCell3D: PIFF files and *CellDraw*

Maciej Swat
James Glazier
Randy Heiland
Abbas Shirinifard
Julio Belmonte
Mitja Hmeljak

Initial conditions in CompuCell3D: PIFF files and CellDraw: outline (a)

- *Initial Conditions in CompuCell3D:*
why do we care?

- Initial conditions: *Blobs, PIFFs,?*



- Drawing a scenario vs. image input
- Designing a scenario with CC3D's help

Initial conditions in CompuCell3D: PIFF files and CellDraw: outline (b)

1. Initial conditions in CompuCell3D
(and how to define them?)

the
simulation
context

2. What are PIFF files?

the
data
context

3. How to generate PIFF files?

the
application
context

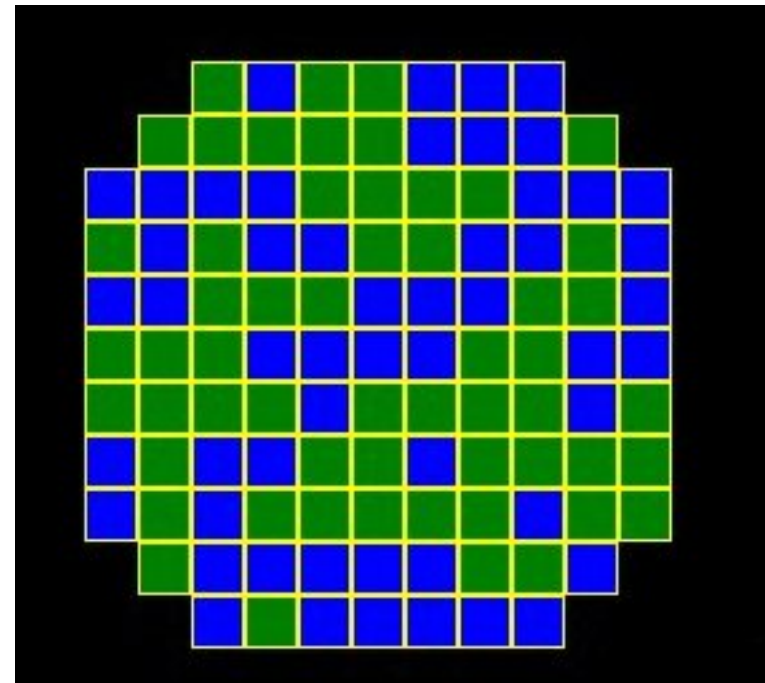
Initial conditions in CC3D XML: BlobInitializer

in CC3D XML definition files, a simple way to initialize some cells:

BlobInitializer → Fills a circle-like area with cells

```
<Steppable Type="BlobInitializer">  
  <Region>  
    <Radius>30</Radius>  
    <Center x="40" y="40" z="0"/>  
    <Gap>0</Gap>  
    <Width>5</Width>  
    <Types>Dark,Light</Types>  
  </Region>  
</Steppable>
```

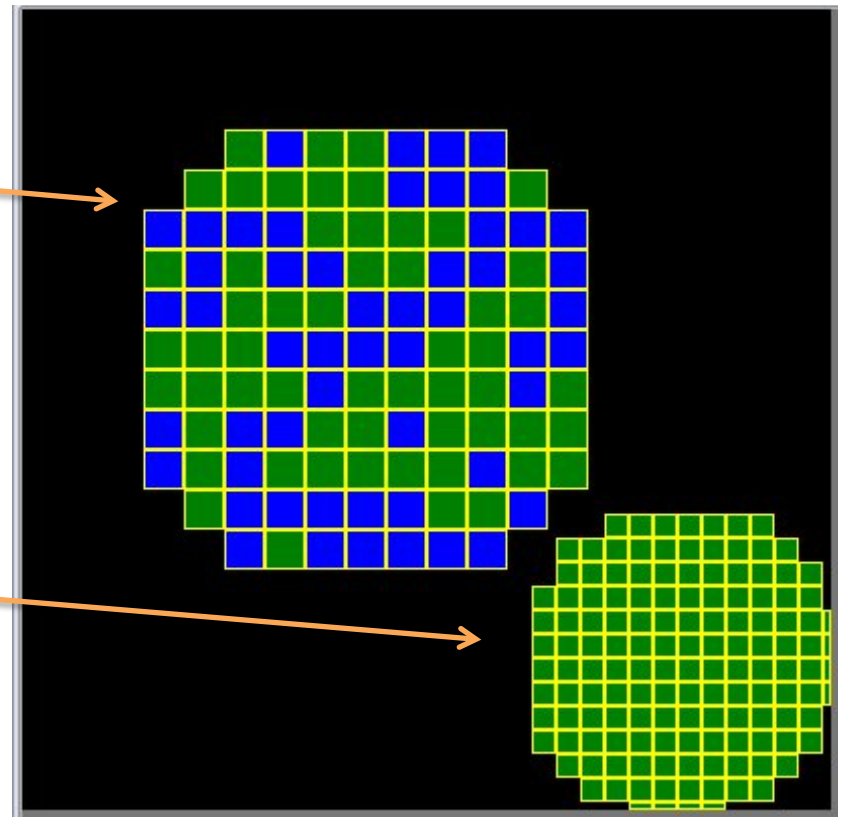
*must'nt have spaces
between cell type names*



Initial conditions in CC3D XML: BlobInitializer examples

```
<Steppable Type="BlobInitializer">  
  <Region>  
    <Radius>30</Radius>  
    <Center x="40" y="40" z="0"/>  
    <Gap>0</Gap>  
    <Width>5</Width>  
    <Types>Condensing,NonCondensing</Types>  
  </Region>
```

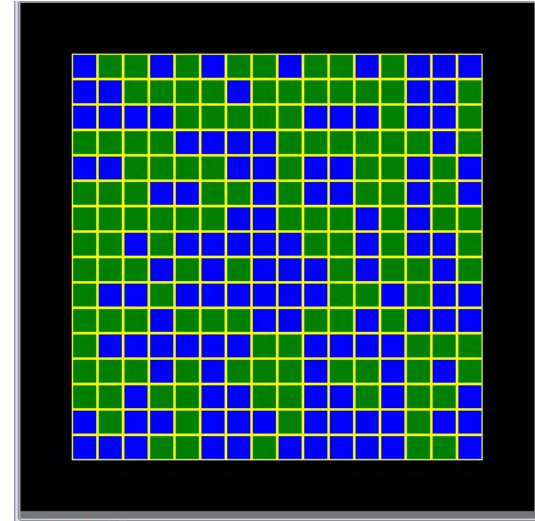
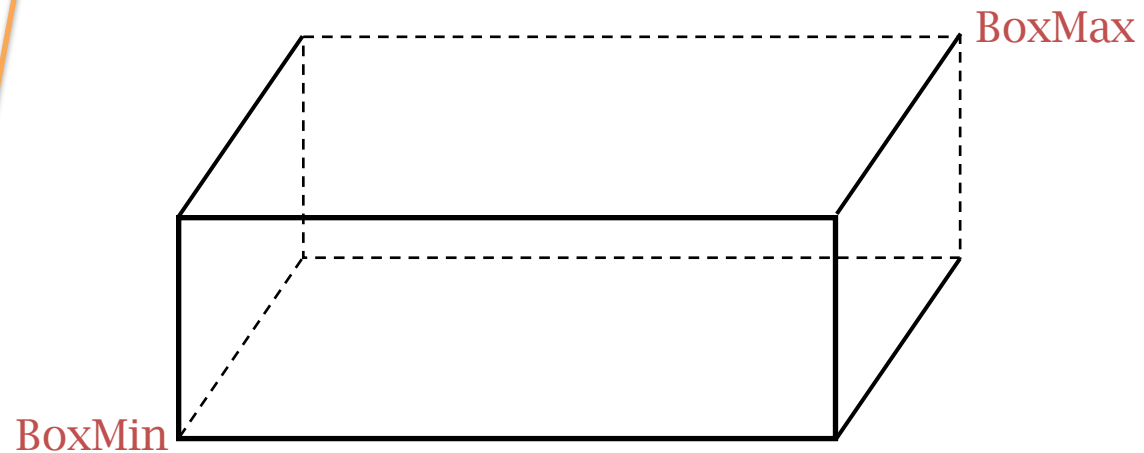
```
  <Region>  
    <Radius>20</Radius>  
    <Center x="80" y="80" z="0"/>  
    <Gap>0</Gap>  
    <Width>3</Width>  
    <Types>Condensing</Types>  
  </Region>  
</Steppable>
```



Initial conditions in CC3D XML: UniformInitializer

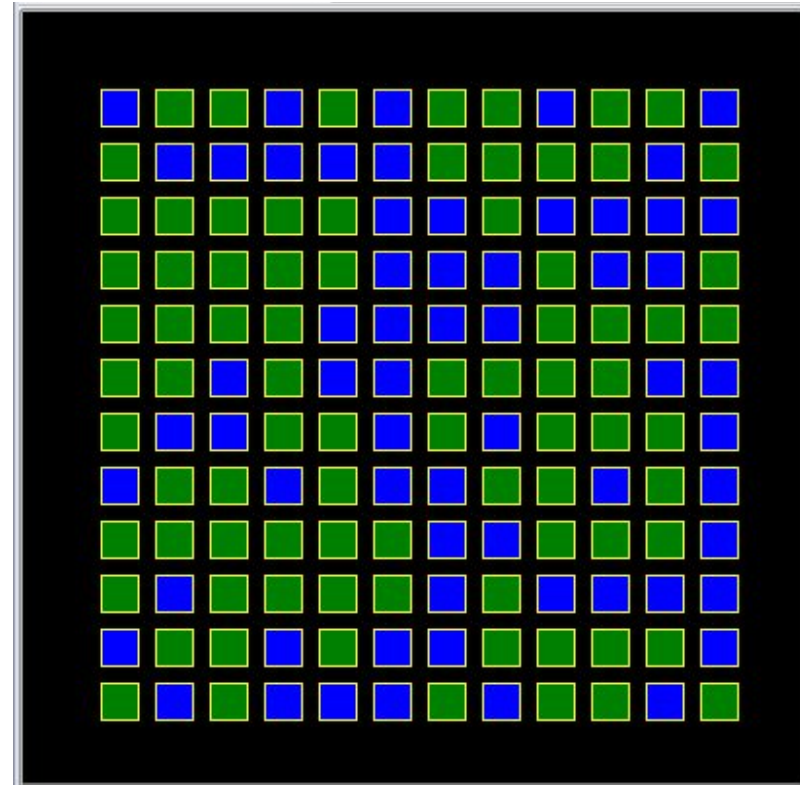
```
<Steppable Type="UniformInitializer">  
  <Region>  
    <BoxMin x="10" y="10" z="0"/>  
    <BoxMax x="90" y="90" z="1"/>  
  
    <Types>Condensing,NonCondensing</Types>  
  
    <Gap>0</Gap>  
    <Width>5</Width>  
  </Region>  
</Steppable>
```

*must'nt have
spaces between
cell type names*



Initial conditions in CC3D XML: UniformInitializer example

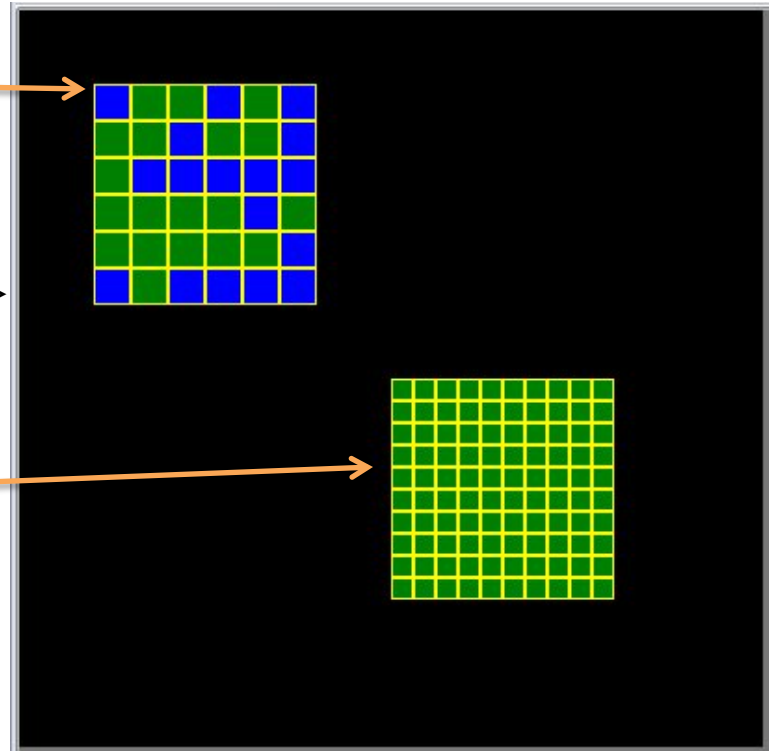
```
<Steppable Type="UniformInitializer">  
  <Region>  
    <BoxMin x="10" y="10" z="0"/>  
    <BoxMax x="90" y="90" z="1"/>  
  
    <Types>Condensing,NonCondensing</Types>  
  
    <Gap>2</Gap>  
    <Width>5</Width>  
  </Region>  
</Steppable>
```



a <gap> places a gap between cells, filled with medium

Initial conditions in CC3D XML: more UniformInitializer examples

```
<Steppable Type="UniformInitializer">  
  <Region>  
    <BoxMin x="10" y="10" z="0"/>  
    <BoxMax x="40" y="40" z="1"/>  
    <Gap>0</Gap>  
    <Width>5</Width>  
    <Types>Condensing,NonCondensing</Types>  
  </Region>  
  
  <Region>  
    <BoxMin x="50" y="50" z="0"/>  
    <BoxMax x="80" y="80" z="1"/>  
    <Gap>0</Gap>  
    <Width>3</Width>  
    <Types>Condensing</Types>  
  </Region>  
</Steppable>
```



in UniformInitializer, BoxMin,BoxMax values z=0,z=1 mean "one 2D layer at z==0"

What are PIFF files?

PIFF: "Potts Initialization File Format"

The PIFF file format: each line contains...

[cell number] [cell type name] [xLow] [xHigh] [yLow] [yHigh] [zLow] [zHigh]

Arbitrary integers.
These represent the
unique *cell ids* for
manipulating cells in
CompuCell3D.

The biological
name of a cell,
the same name as
in the XML file.

Box or individual **pixel**.

Box: [low - high] points represent
the opposite vertices of a box. In
CC3D, the box will become a single
cell of type [cell type name]. Its
unique *id* will be [cell number].

Pixel: If [low - high] values are
identical, it adds a single pixel to a
cell.

Initial conditions in XML: options

<Steppable Type="BlobInitializer">

*creates a spherical (3D) or circular (2D) cell "blob"
with one or more cell types, randomly distributed*

</Steppable>

<Steppable Type="UniformInitializer">

*creates a block-shaped cell part: it can also be used to add individual pixels
the definition is similar to the PIFF file format
more cumbersome than a PIFF file, but accessible directly in XML*

</Steppable>

<Steppable Type="PIFInitializer">

tells CC3D to read a PIFF file

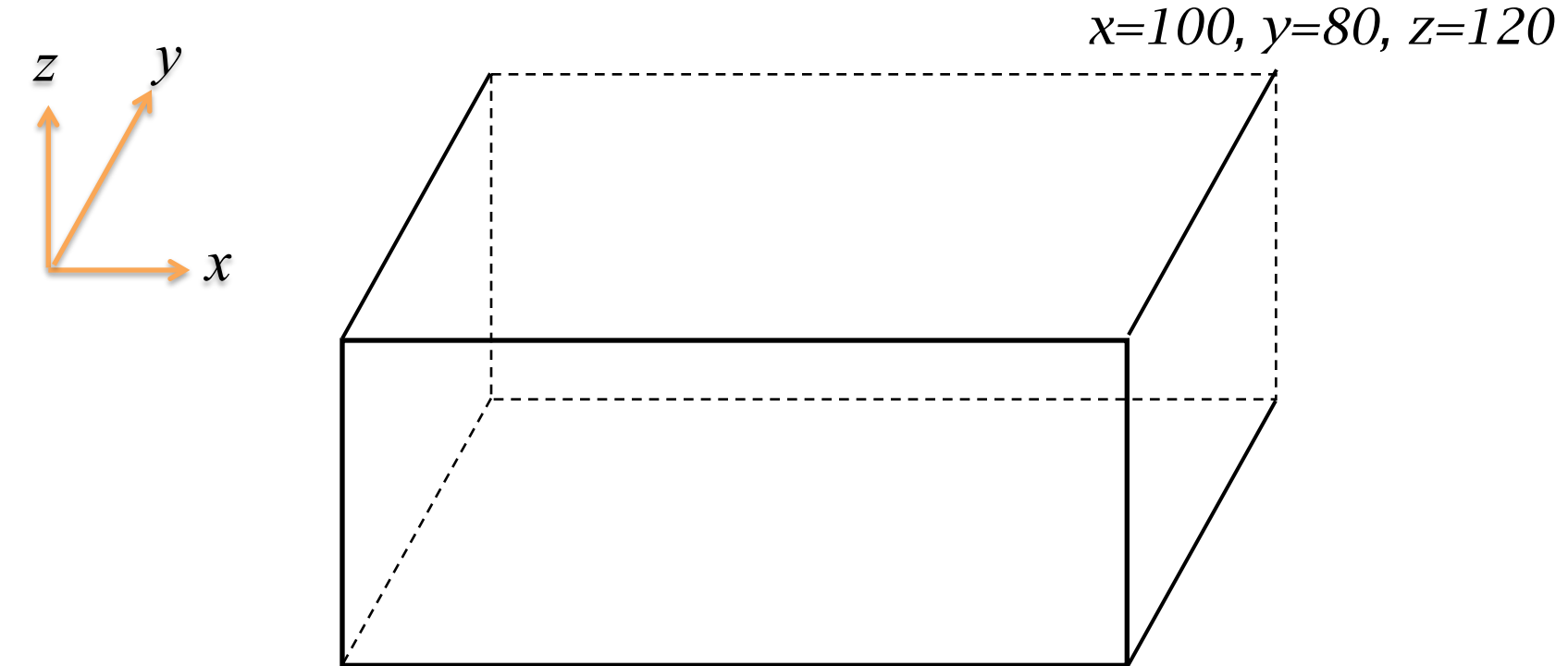
</Steppable>

<Steppable Type="PIFDumper">

*(not an initializer) tells CC3D to
dump a PIFF file from the current lattice*

</Steppable>

A 'box' cell as defined by a PIFF line



$x=20, y=40, z=100$

in the PIFF file, this cell is defined as:

...

127 Epithelium 20 100 40 80 100 120

...

...

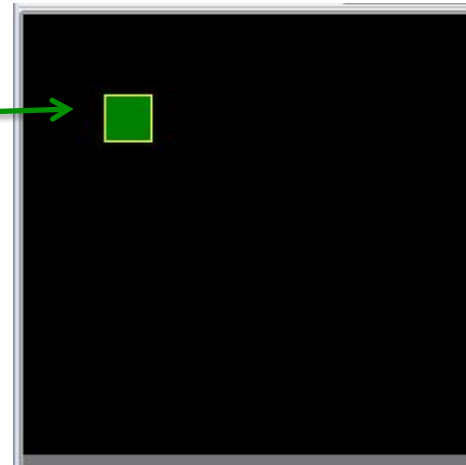
The rules of PIFF (as obeyed by CC3D)

- In a PIFF file, later data overwrites earlier data (following the "*opaque paint*" rule AKA painter's algorithm)
- A particular cell (==cell *id*, the first entry in a PIFF line) can be specified using multiple PIFF lines: useful for defining cells that are not block-shaped.
 - non-block cells are sometimes not necessary: a few "relaxation" steps can smooth the cells
- CC3D allows simple PIFFs to be created in XML
- CC3D can "dump" the current cell lattice in PIFF format for restarting future simulations. Such PIFF files contain one line per pixel, as from the lattice.

A little PIFF example (a)

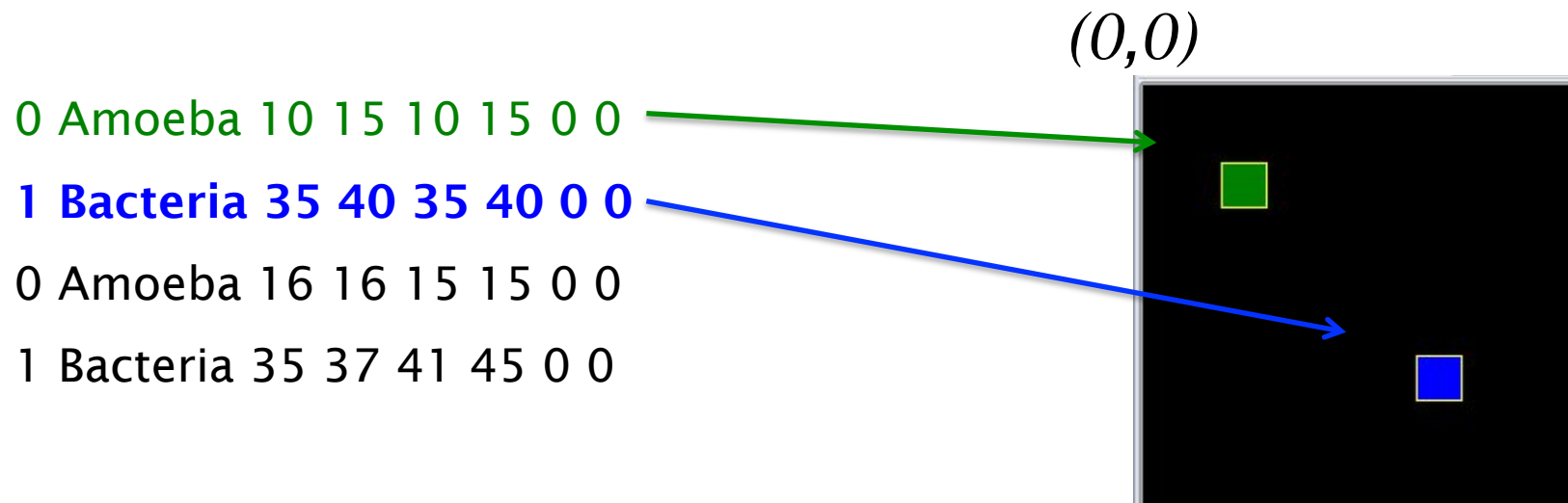
```
0 Amoeba 10 15 10 15 0 0  
1 Bacteria 35 40 35 40 0 0  
0 Amoeba 16 16 15 15 0 0  
1 Bacteria 35 37 41 45 0 0
```

$(0,0)$



the first PIFF line defines one cell

A little PIFF example (b)

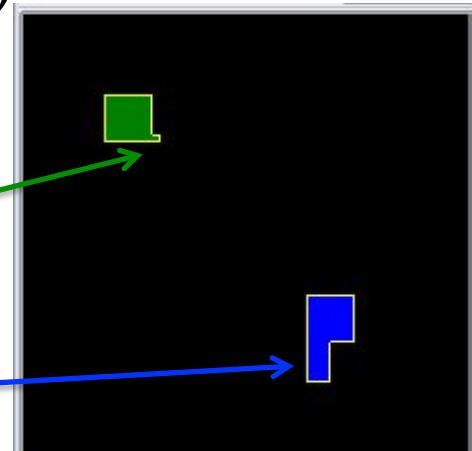


the second PIFF line defines a second cell
of a different type

A little PIFF example (c)

```
0 Amoeba 10 15 10 15 0 0  
1 Bacteria 35 40 35 40 0 0  
0 Amoeba 16 16 15 15 0 0  
1 Bacteria 35 37 41 45 0 0
```

$(0,0)$

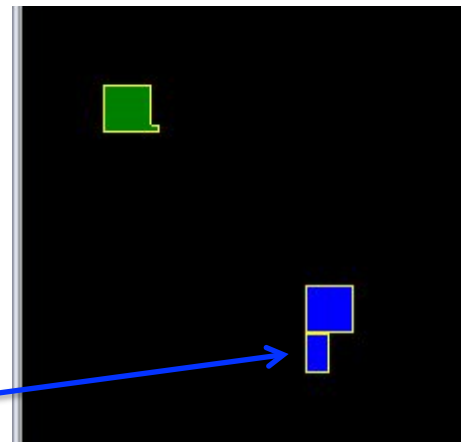


the third and fourth PIFF lines define additional pixels for the cells defined before

A little PIFF example (d)

```
0 Amoeba 10 15 10 15 0 0
1 Bacteria 35 40 35 40 0 0
0 Amoeba 16 16 15 15 0 0
2 Bacteria 35 37 41 45 0 0
```

$(0,0)$



a small change: the fourth PIFF line introduces a *new* cell ID to create a *new cell* (of the same cell type as in line two)

PIFF files without typing: CellDraw

CellDraw 1.5.0 :

editing/conversion tool for creating PIFF files

a. *drawing* the cell scenario in CellDraw:

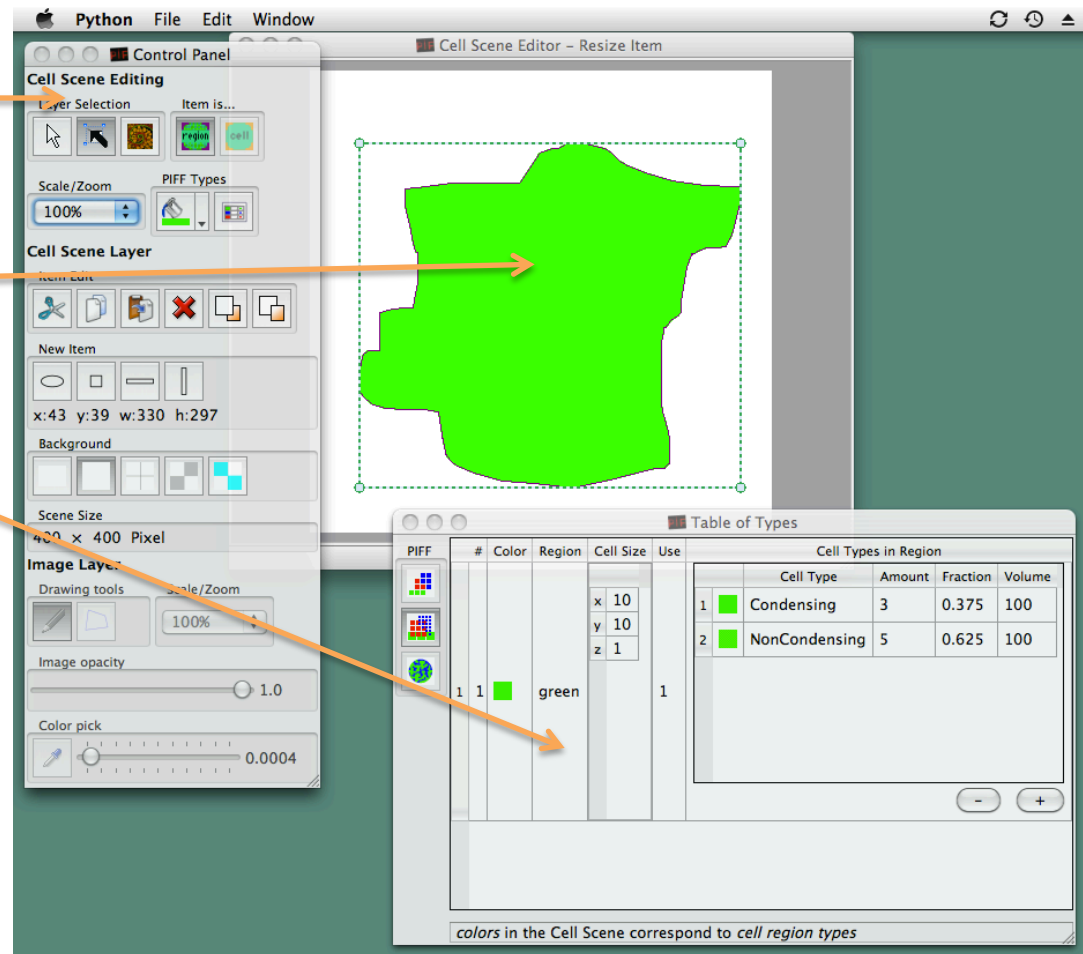
- predefined geometric shapes
- free-hand drawing of cell regions

b. *converting* images and drawings into PIFF files:

- clicking on a color in the input image creates a cell region in the PIFF Scene

CellDraw 1.5.0 : the GUI

- Control Panel
- Cell Scene Editor
- Table of Types:
 - Regions
 - Cells
 - Sizes
 - Proportions



a. drawing a cell scenario in CellDraw

scene items (regions) can be added, moved, resized

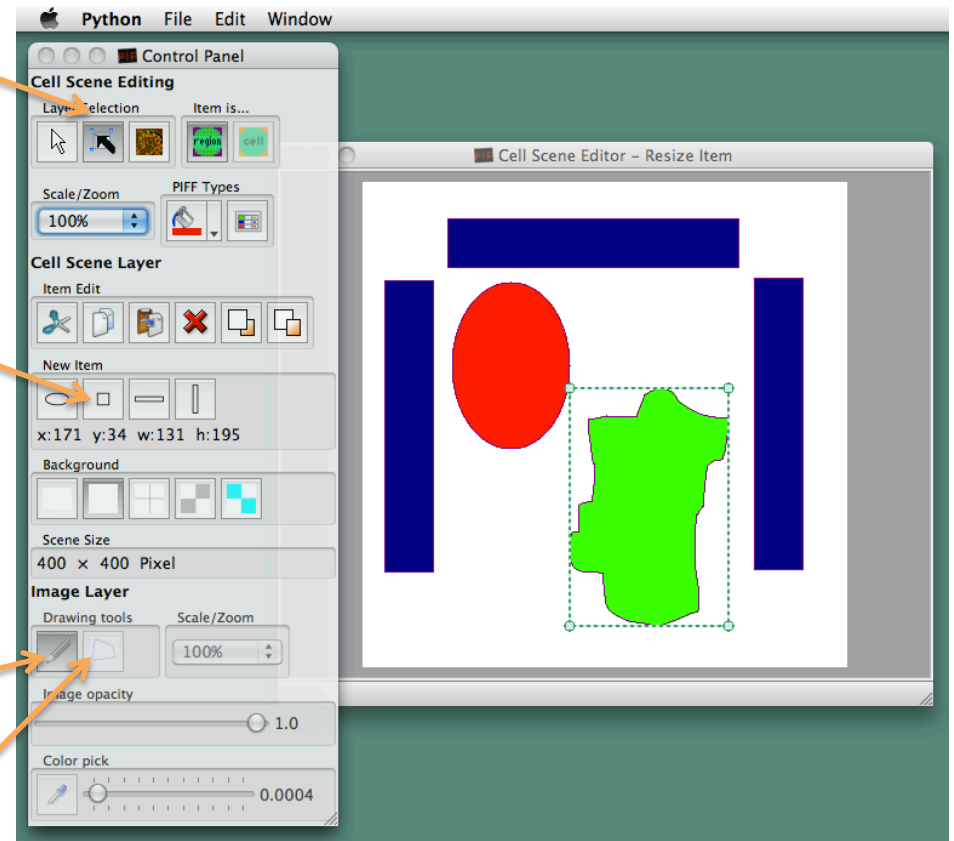
in *PIFF Scene Layer*.

use predefined geometric shapes to add cell regions

in *Image Layer*.

free-hand drawing of cell regions

polygonal drawing of cell regions

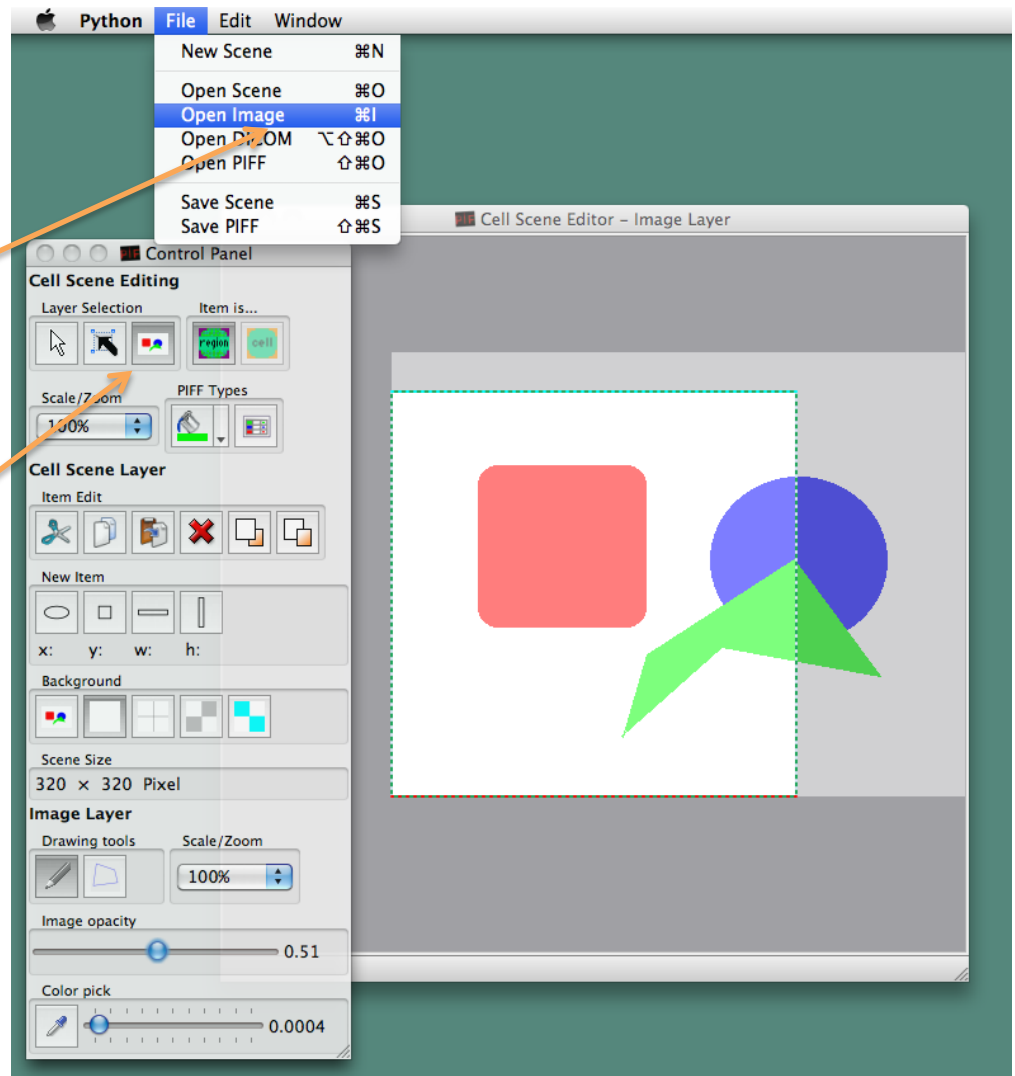


b. converting drawings / images to PIFF files

images, pictures, etc. can be imported into the Image Layer:

use File → Open Image

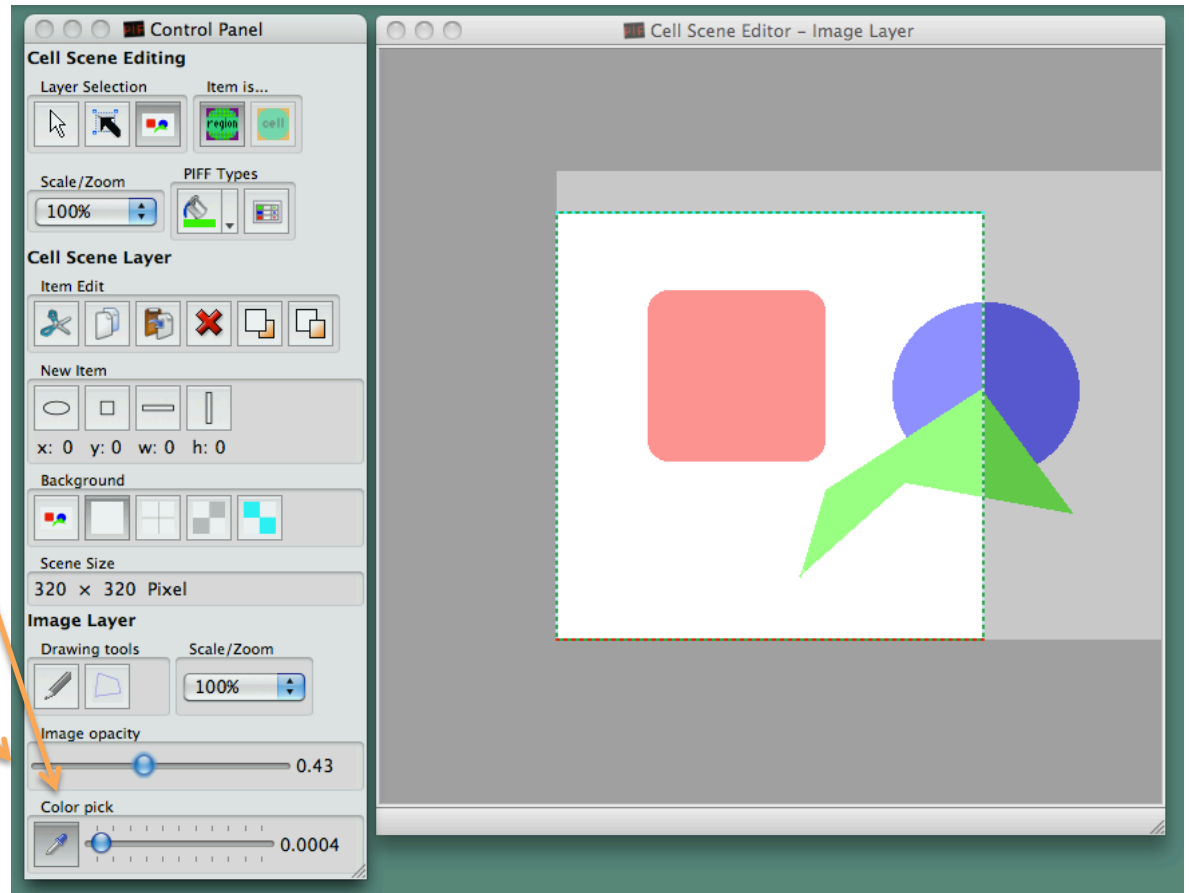
1. select the Image Layer to work with the imported image



b. converting drawings / images to PIFF files

2. select the Color Pick tool

it can be helpful to reduce the imported image's *opacity*, to discern newly added cell regions in the PIFF Scene

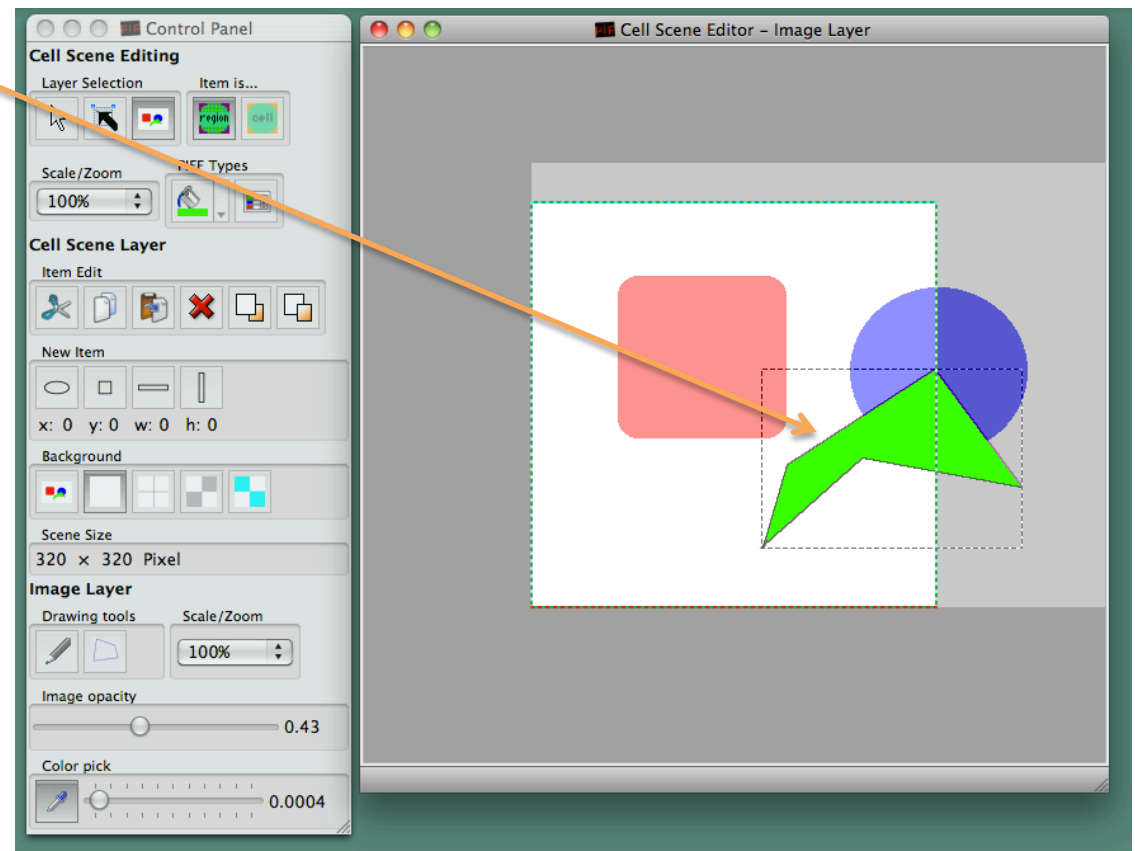


b. converting drawings / images to PIFF files

3. clicking on a color in the Image Layer...

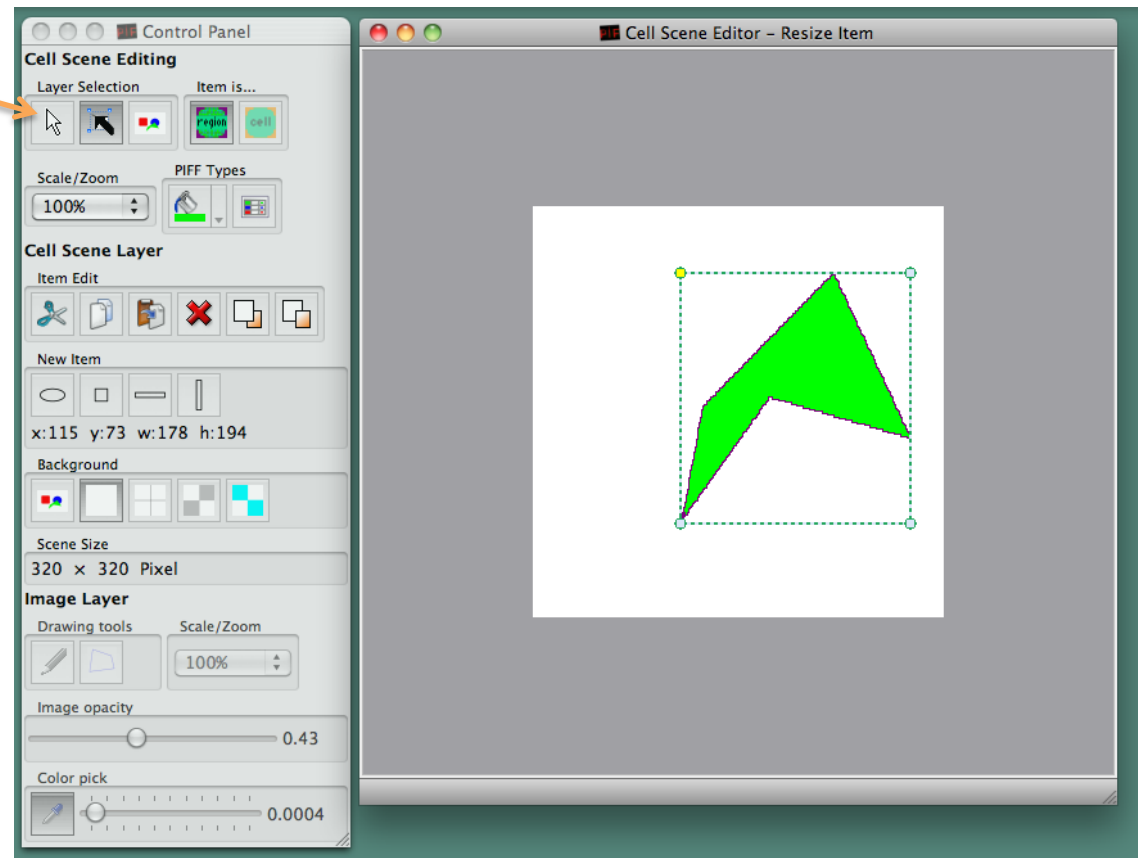
...creates a new cell region in the PIFF Scene layer

4. additional clicks on colors in the Image Layer create new cell regions in the PIFF Scene layer, one new cell region per click



b. converting drawings / images to PIFF files

5. the newly created cell region(s) can be now edited by returning to the PIFF Scene layer



PIFF Regions, Cell Types, Sizes and Amounts

Assigning cell types to cell regions:

Each *cell region* is identified by a *color*, and may contain one or more cell types.

Cell types are randomly placed within *cell regions* of the same *color*, in relative proportions as per chosen amount / fraction values.

Cells in the PIFF file are generated as *rectangular blocks* of the *chosen cell size* for each region color.

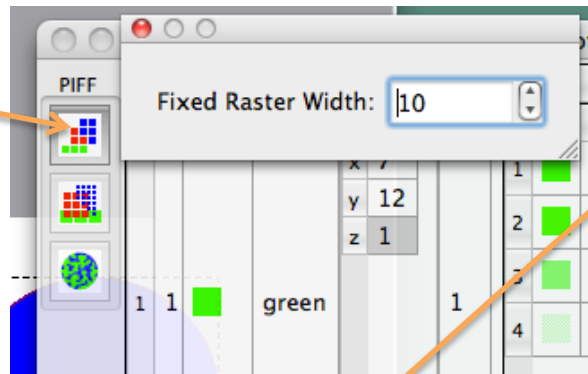
The screenshot shows the 'Table of Types' window in the Cell Scene Editor. It contains two tables, one for a green region and one for a blue region. The green region table lists four cell types (type1, type2, type3, type4) with their respective amounts, fractions, and volumes. The blue region table lists two cell types (Condensing and NonCondensing) with their respective amounts, fractions, and volumes. Arrows from the text on the left point to the 'Color' column in the first table, the 'Cell Type' column in the second table, and the 'Cell Size' column in the first table.

Cell Types in Region				
	Cell Type	Amount	Fraction	Volume
1	type1	4	0.5	100
2	type2	2	0.25	100
3	type3	1	0.125	100
4	type4	1	0.125	100

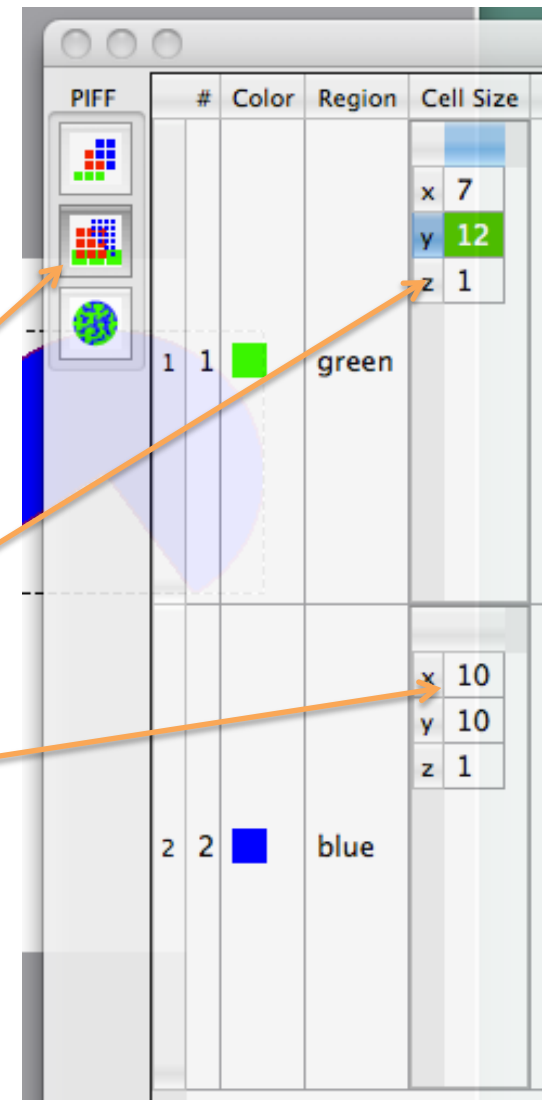
Cell Types in Region				
	Cell Type	Amount	Fraction	Volume
1	Condensing	1	0.33...	100
2	NonCondensing	2	0.66...	100

generating PIFF files: options

- a. if *Fixed Raster* is selected, all cells in *all* regions will be saved as square blocks in a fixed-size raster



- b. if *Region Rasters* is selected (the default) each region's cells will be saved as rectangular blocks with *cell sizes* as set in the Table of Types



advanced features (still ~beta in CellDraw 1.5.0) : Potts-generated regions of cells

CellDraw can invoke
CompuCell3D...

...to run a Potts model simulation...

...to prepare a PIFF scenario with
different-sized cells within each
region