

CompuCell3D Training Workshop
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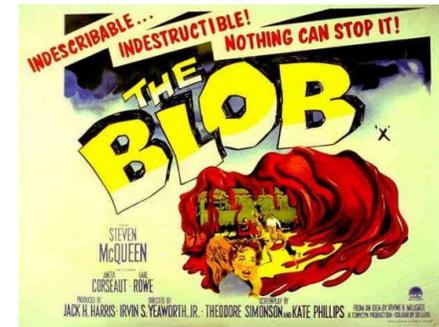
Initial Conditions in CompuCell3D: PIF files and *PIF Generator*

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Initial conditions in CompuCell3D: PIF files and PIF Generator: outline (a)

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

- Initial conditions: *Blobs, PIFs,?*



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

Initial conditions in CompuCell3D: PIF files and PIF Generator: outline (b)

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

the
simulation
context

2. What are PIF files?

the
data
context

3. How to generate PIF files?

the
application
context

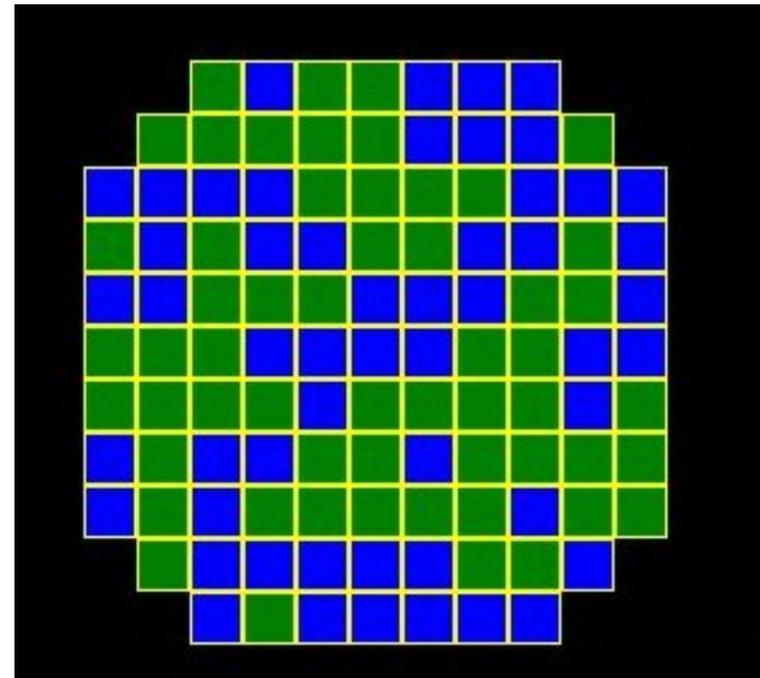
Initial conditions in CC3D XML: BlobInitializer

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>
```

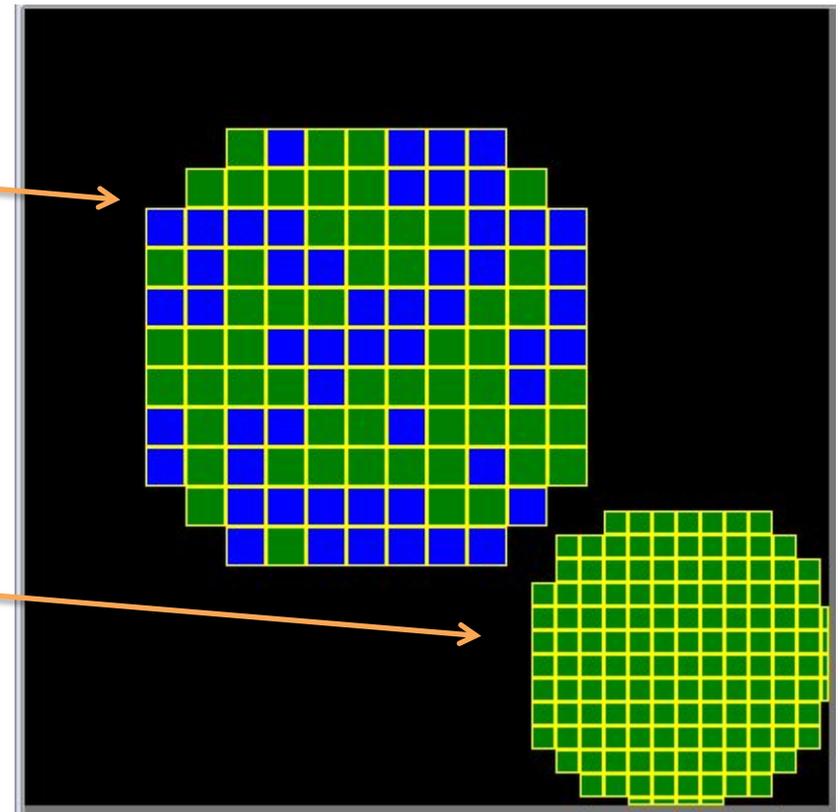
*must'nt have spaces
between cell type names*



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>
```

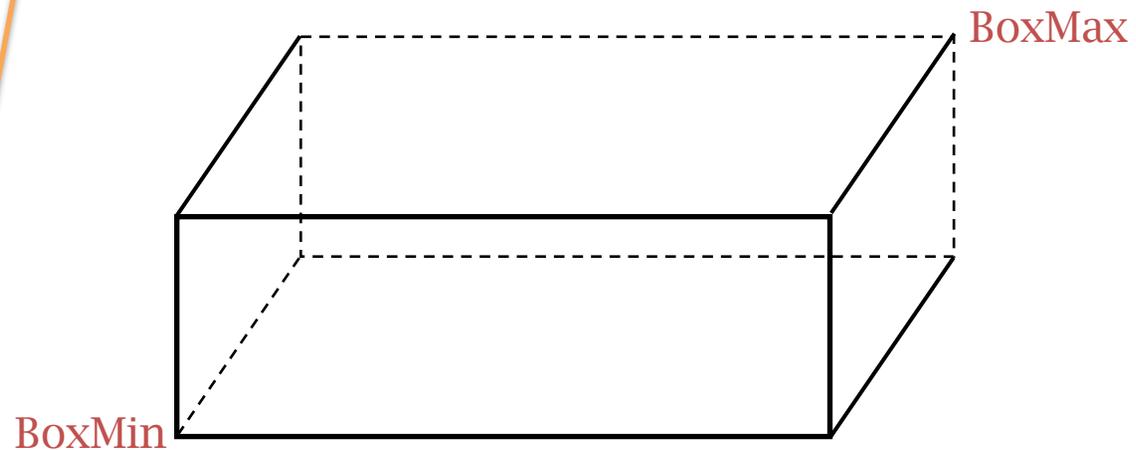
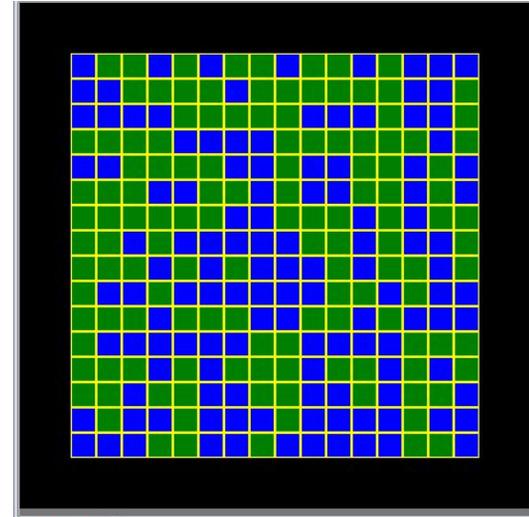
```
  <Region>  
    <Radius>20</Radius>  
    <Center x="80" y="80" z="0"/>  
    <Gap>0</Gap>  
    <Width>3</Width>  
    <Types>Condensing</Types>  
  </Region>  
</Steppable>
```



Initial conditions in CC3D XML: UniformInitializer

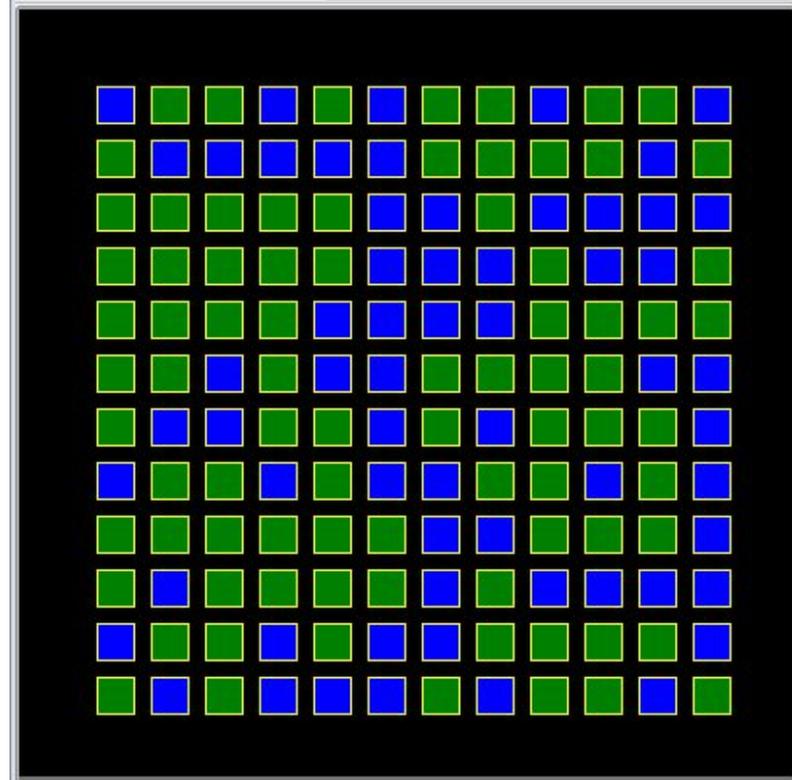
```
<Steppable Type="UniformInitializer">  
  <Region>  
    <BoxMin x="10" y="10" z="0"/>  
    <BoxMax x="90" y="90" z="1"/>  
  
    <Types>Condensing,NonCondensing</Types>  
  
    <Gap>0</Gap>  
    <Width>5</Width>  
  </Region>  
</Steppable>
```

*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>
```

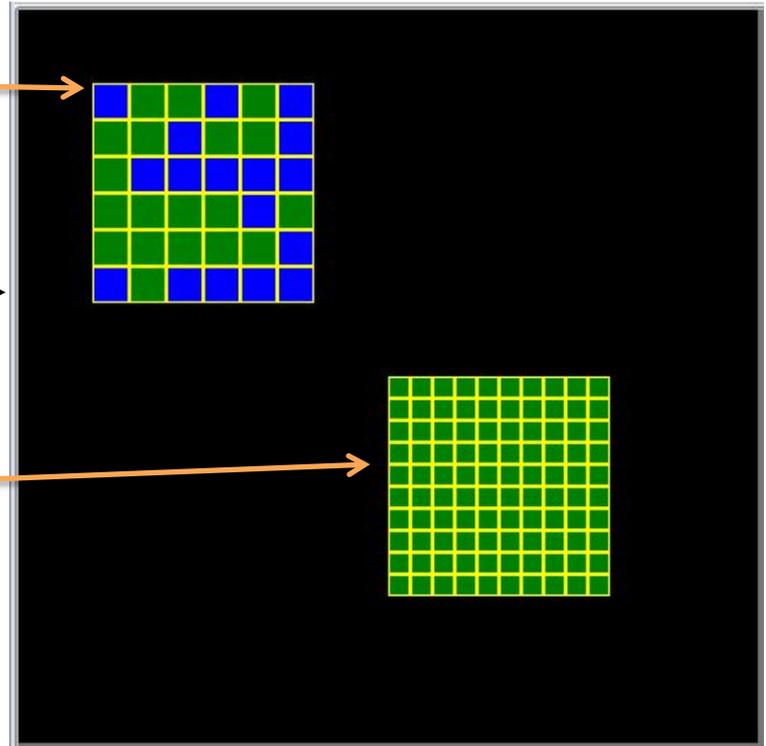


a <gap> places a gap between cells, filled with medium

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 PIF files?

PIF: “Potts Initialization File”

The PIF file format: each line contains...

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

Consecutive but otherwise arbitrary numbers. These represent the unique *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 PIF file format
more cumbersome than a PIF file, but accessible directly in XML*

</Steppable>

<Steppable Type="PIFInitializer">

tells CC3D to read a PIF file

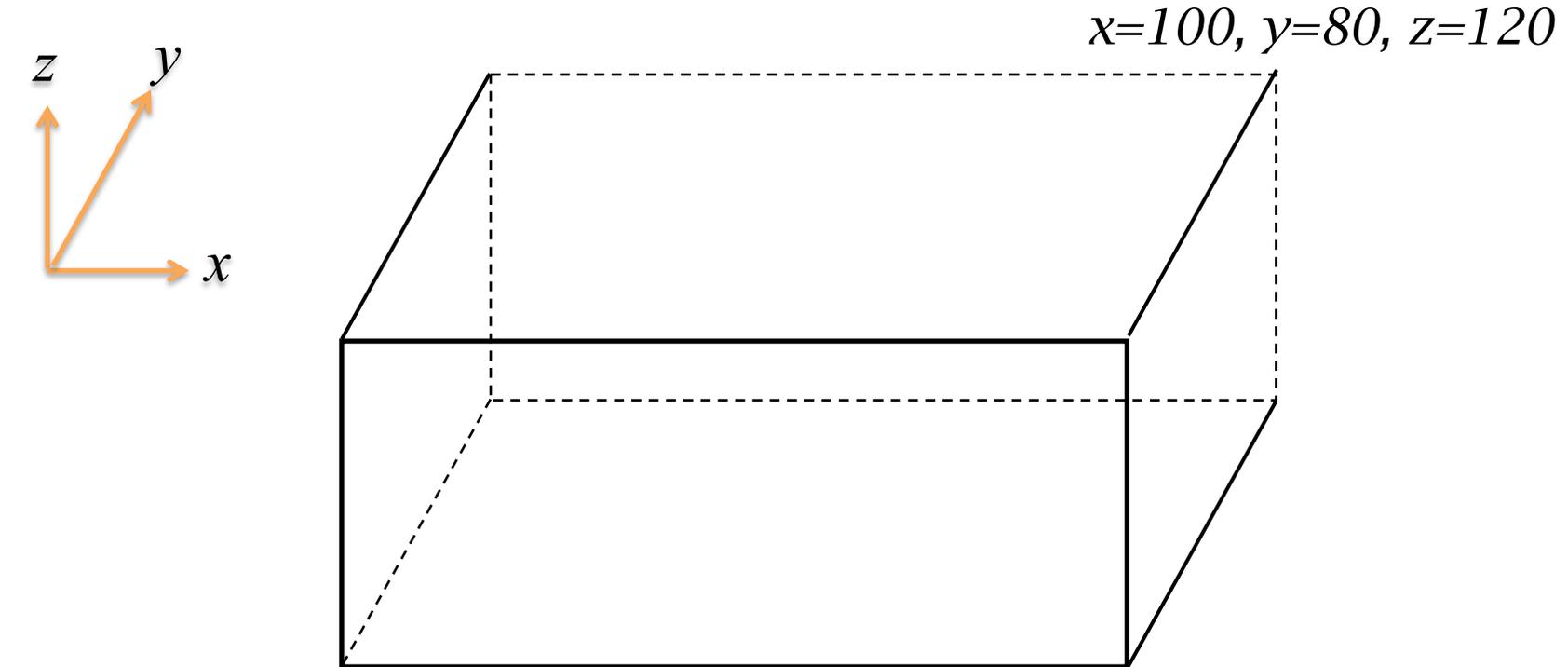
</Steppable>

<Steppable Type="PIFDumper">

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

</Steppable>

A 'box' cell as defined by a PIF line



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

in the PIF file, this cell is defined as:

...

127 Epithelium 20 100 40 80 100 120

...

...

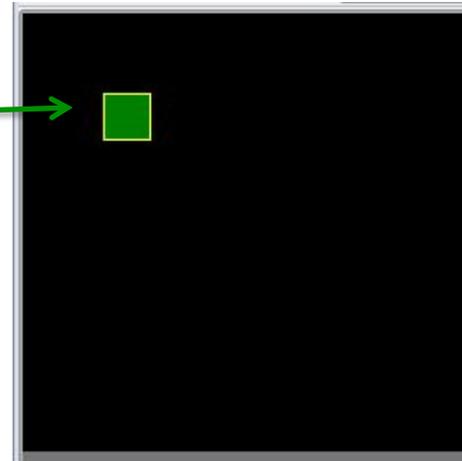
The rules of PIF (as obeyed by CC3D)

- In a PIF 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 PIF line) can be specified using multiple PIF 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 PIFs to be created in XML files
- CC3D can “dump” the current cell lattice in PIF format for restarting future simulations. Such PIF files contain one line per pixel, as from the lattice.

A little PIF example (a)

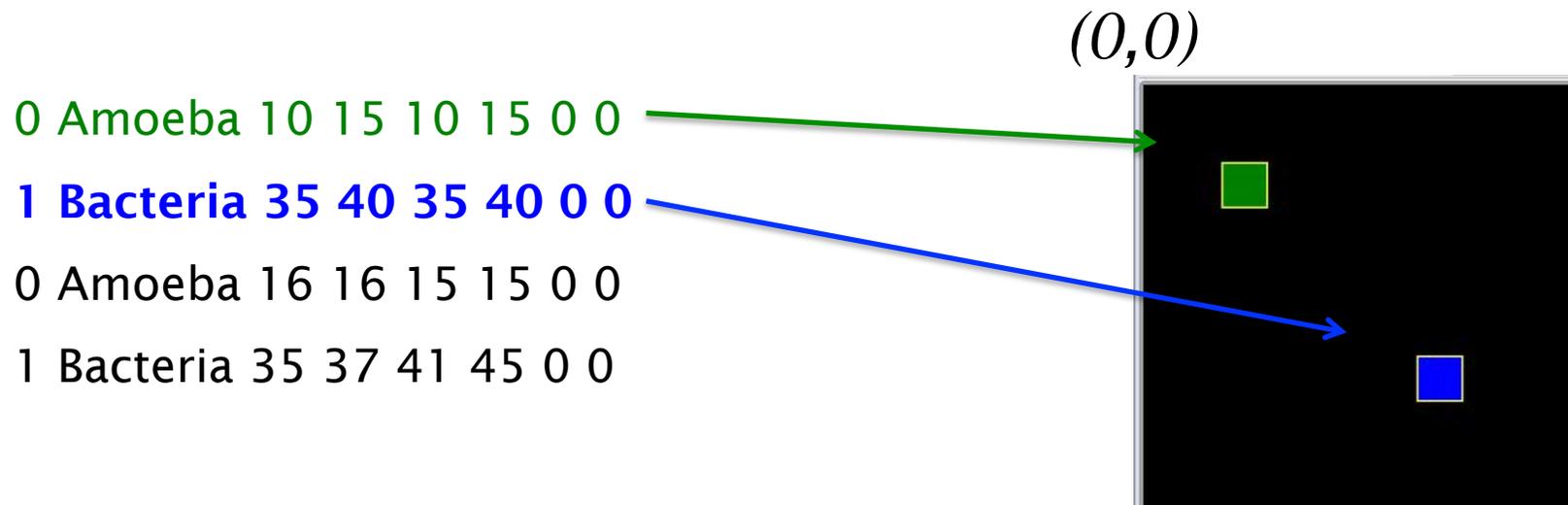
```
0 Amoeba 10 15 10 15 0 0  
1 Bacteria 35 40 35 40 0 0  
0 Amoeba 16 16 15 15 0 0  
1 Bacteria 35 37 41 45 0 0
```

$(0,0)$



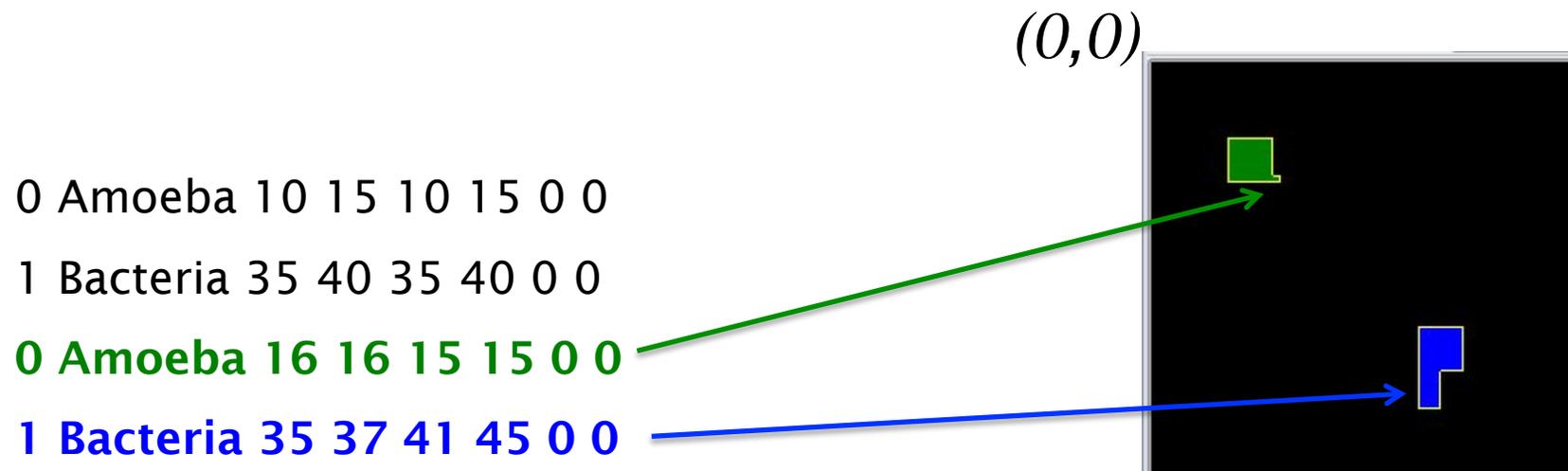
the first PIF line defines one cell

A little PIF example (b)



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

A little PIF example (c)



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

A little PIF example (d)

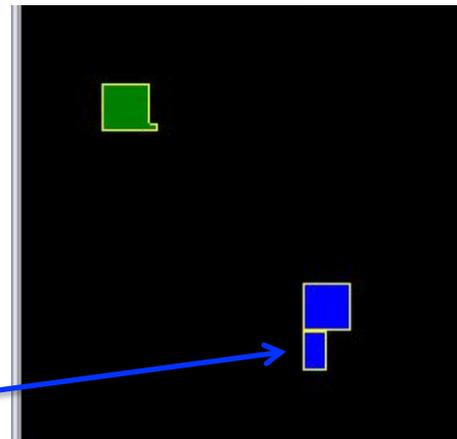
0 Amoeba 10 15 10 15 0 0

1 Bacteria 35 40 35 40 0 0

0 Amoeba 16 16 15 15 0 0

2 Bacteria 35 37 41 45 0 0

$(0,0)$



in this case, the fourth PIF line introduces a new cell ID to create a new cell (of the same cell type as in line two)

PIF files without typing: PIF Generator

PIF Generator 1.4.0 :

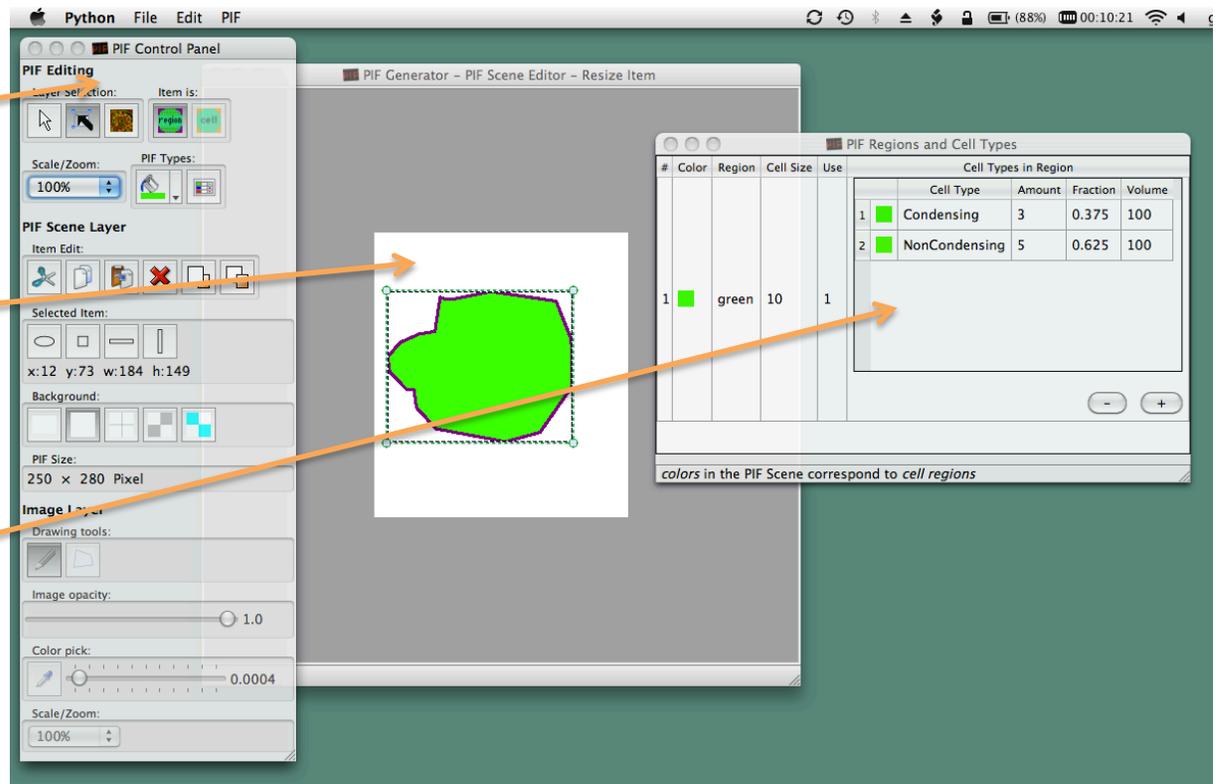
editing/conversion tool for creating PIF files

- a. *drawing* the cell scenario in PIF Generator:
 - predefined geometric shapes
 - free-hand drawing of cell regions

- b. *converting* images and drawings into PIF files:
 - clicking on a color in the input image creates a cell region in the PIF Scene

PIF Generator 1.4.0 : the GUI

- PIF Control Panel
- PIF Scene Editor
- Table of Regions and Cell Types



a. drawing a cell scenario in PIF Generator

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

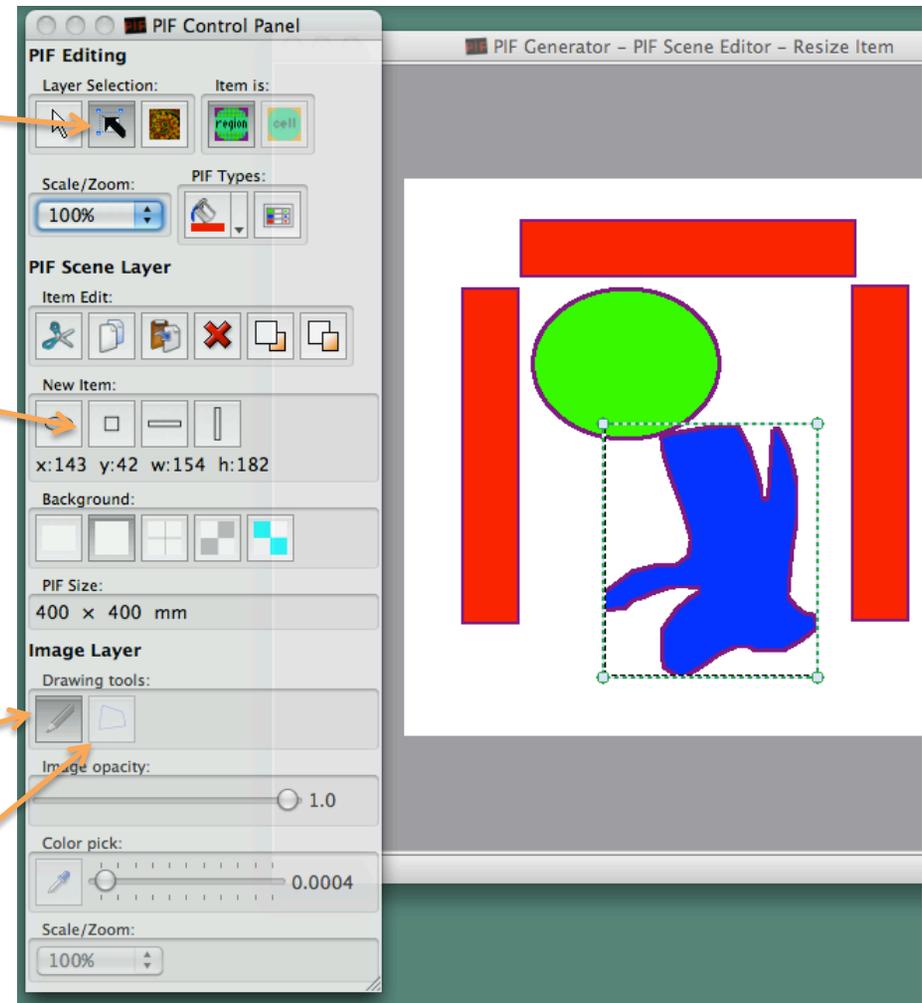
in *PIF Scene Layer*.

use predefined geometric shapes to add cell regions

in *Image Layer*.

free-hand drawing of cell regions

polygonal drawing of cell regions

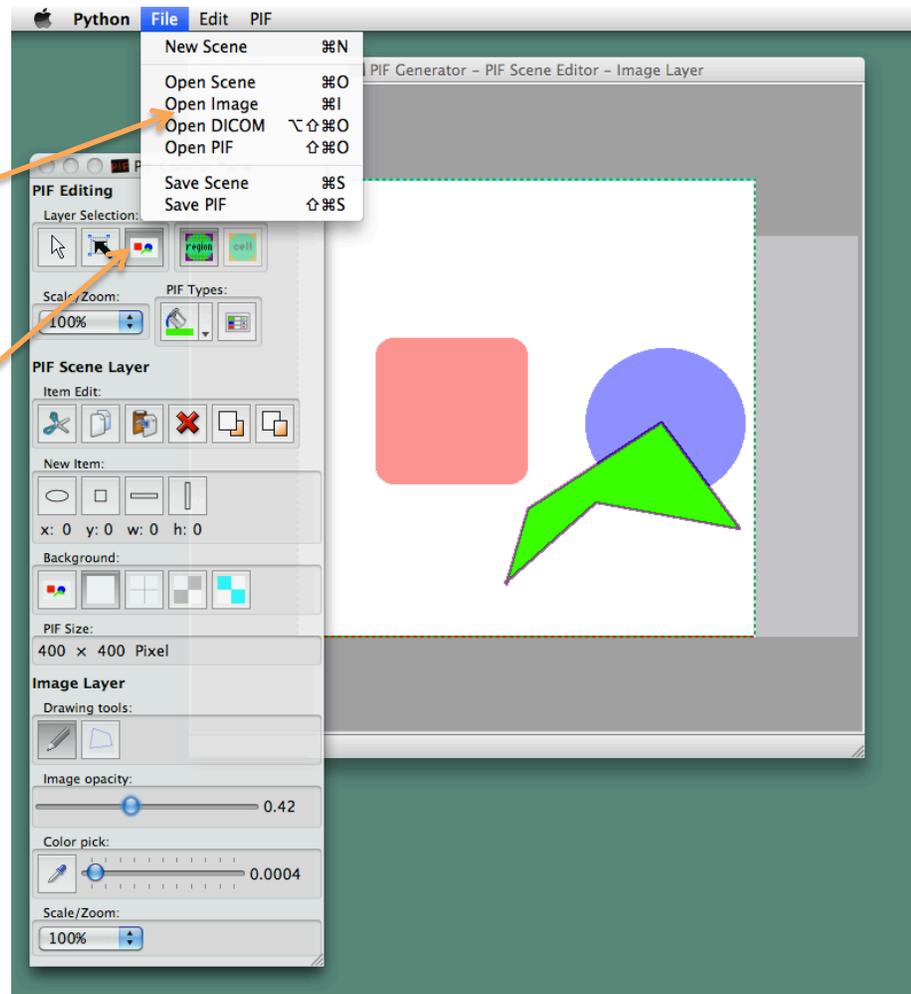


b. converting drawings and images to PIF files

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

use File → Open Image

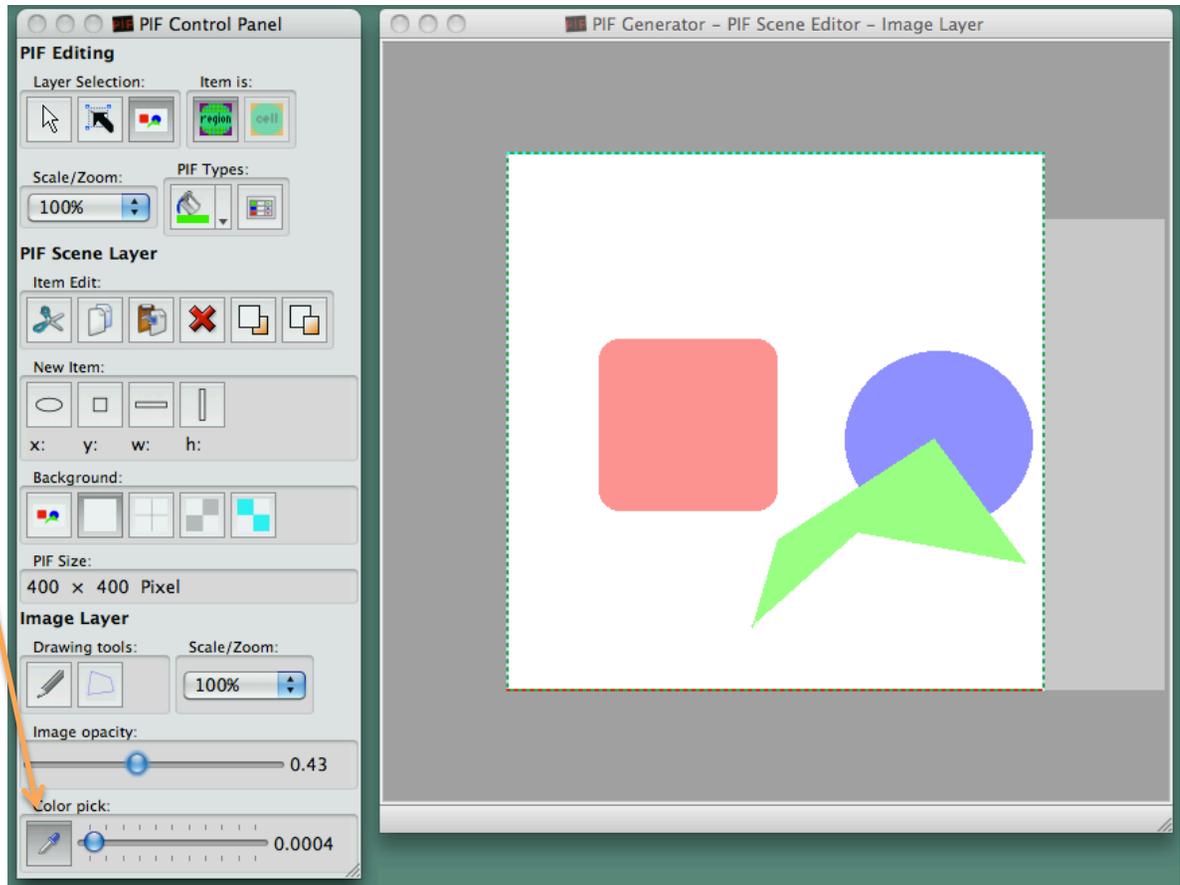
1. select the Image Layer to work with the imported image



b. converting drawings and images to PIF 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 PIF Scene

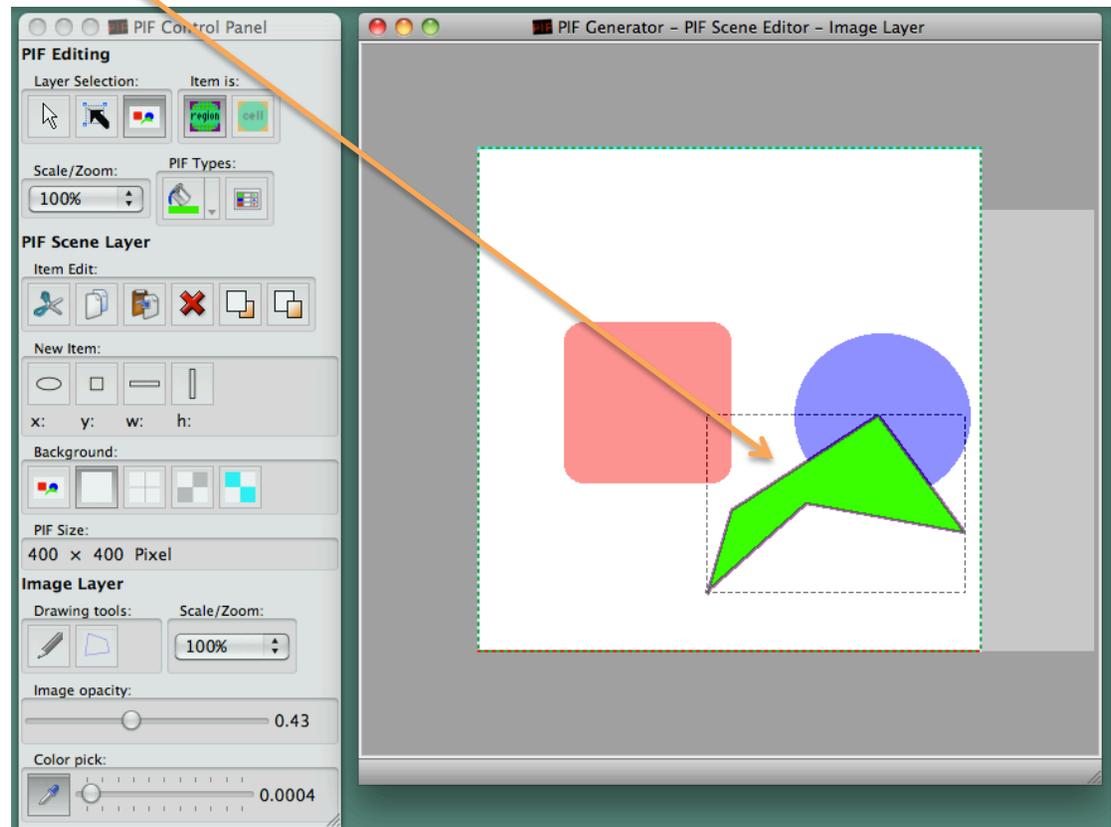


b. converting drawings and images to PIF files

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

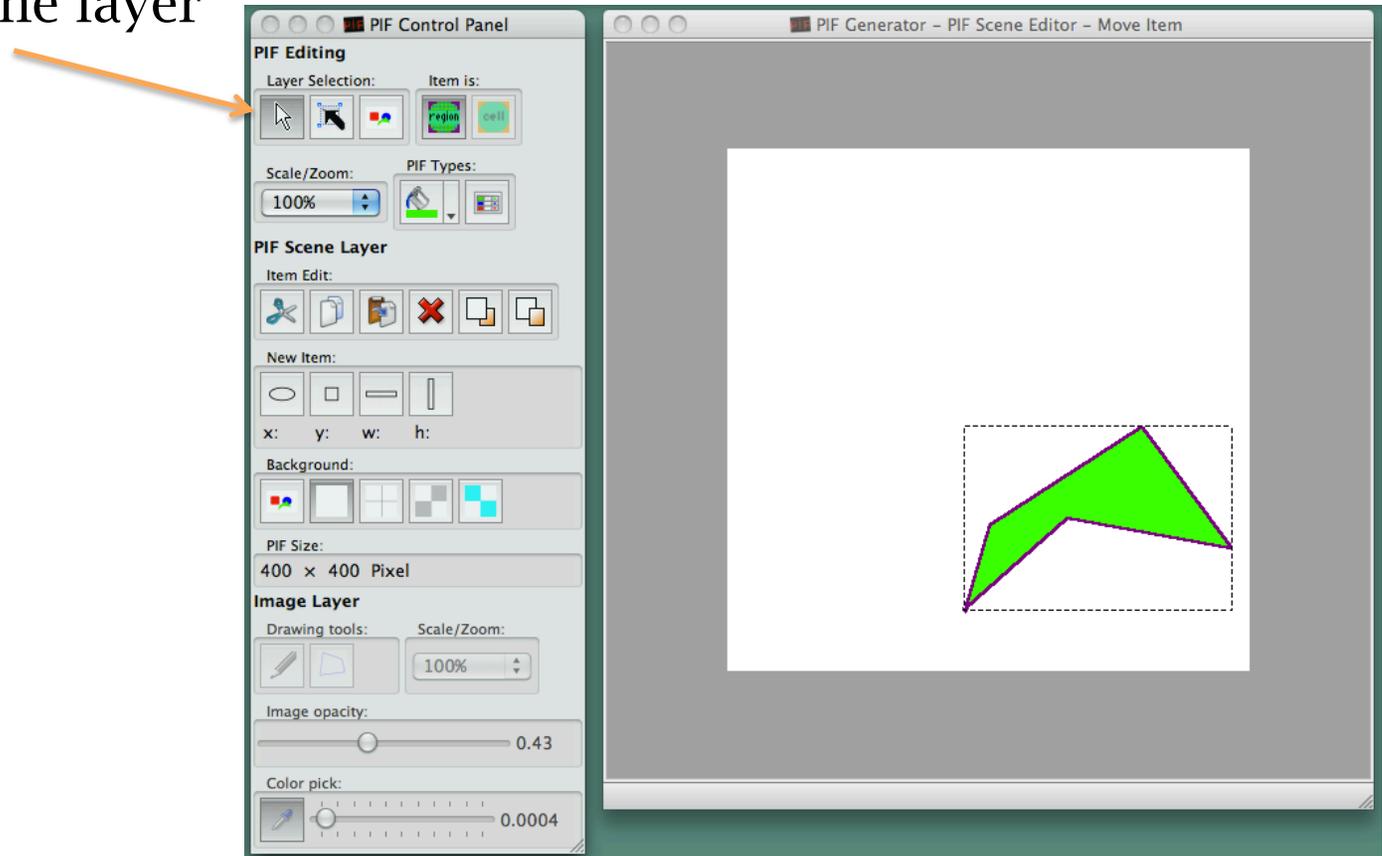
...creates a new cell region in the PIF Scene layer

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



b. converting drawings and images to PIF files

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



PIF 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 PIF file are generated as *squares* of the *chosen cell size* for each region color.

The screenshot shows the 'PIF Regions and Cell Types' window. It features a main table for regions and two sub-tables for cell types within those regions. Orange arrows point from the text on the left to specific elements in the interface: one to the 'green' region, one to the 'blue' region, and one to the 'Condensing' cell type.

#	Color	Region	Cell Size	Use
1	green	7	1	1
2	blue	10	1	1

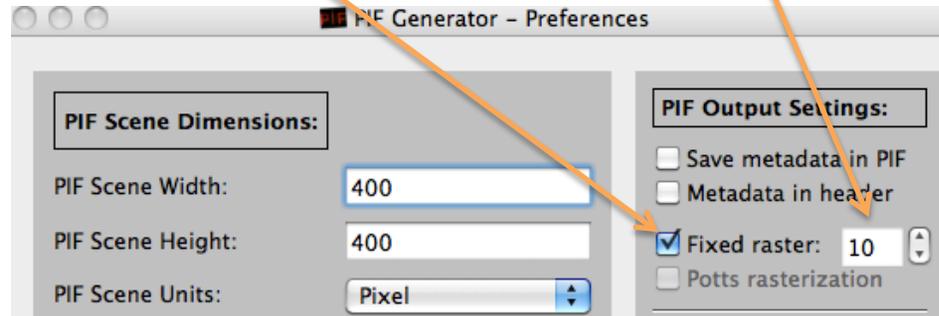
Cell Types in Region				
	Cell Type	Amount	Fraction	Volume
1	type1	4	0.5	100
2	type2	2	0.25	100
3	type3	1	0.125	100
4	type4	1	0.125	100

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

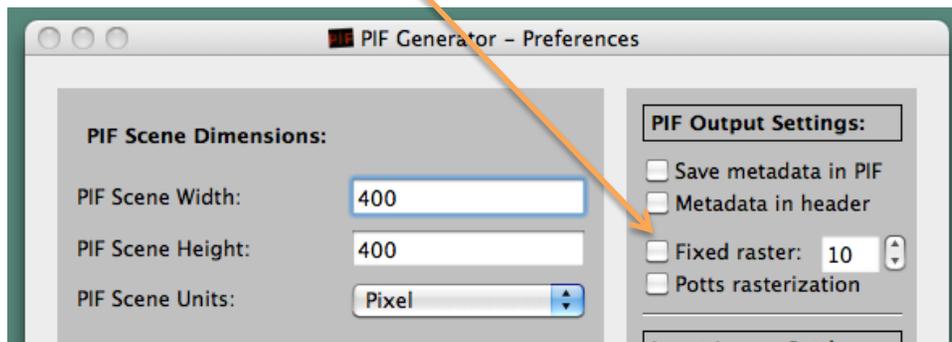
colors in the PIF Scene correspond to cell regions

generating PIF files: options (Preferences window)

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



- b. if *Fixed raster* is *not* selected, each region's cells will be saved as square blocks with *cell sizes* as set in the Table of Regions



#	Color	Region	Cell Size	Use
1	green	7	1	
2	blue	8	1	

advanced features (still in beta functionality in PIF Generator 1.4.0) : Potts-generated regions of cells

PIF Generator can invoke
CompuCell3D...

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

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