Workflows for Parameter Studies of Multi-Cell Modeling

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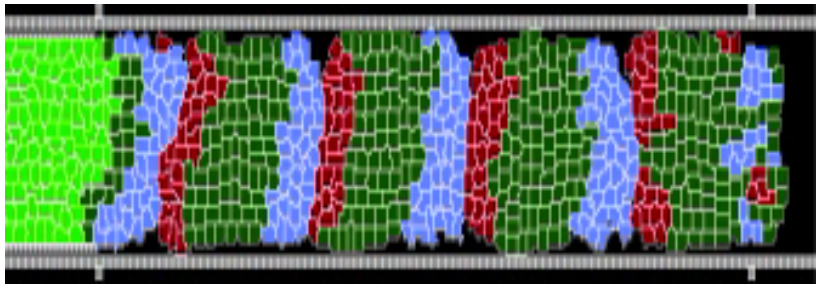
Outline

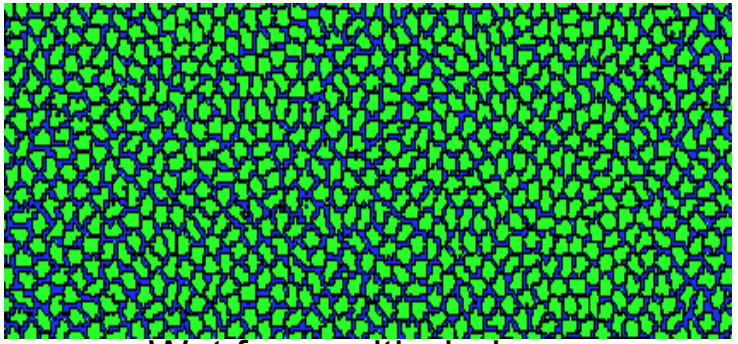
- Overview of CompuCell3D (for multi-cell modeling)
- Overview of VisTrails (for workflows)
- Overview of TeraGrid (for HPC; parameter study)
- Implicitly promote Python and FOSS
- Use case of parameter study for biological cell sorting

Multi-Cell Modeling: CompuCell3D

- Indiana University (started at Notre Dame)
- Software framework/application
  - Framework: general-purpose cell-based modeling
  - Application: standalone app w/ GUI; run batch (no GUI)
- Cells: biological or other (e.g. foams, grains)



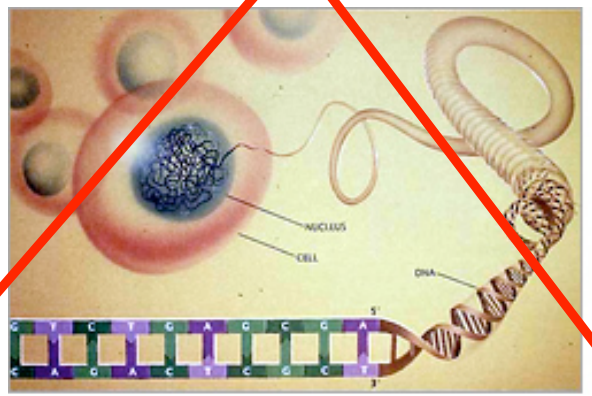
Somite sim (Julio Belmonte, IU)



Wet foam with drainage

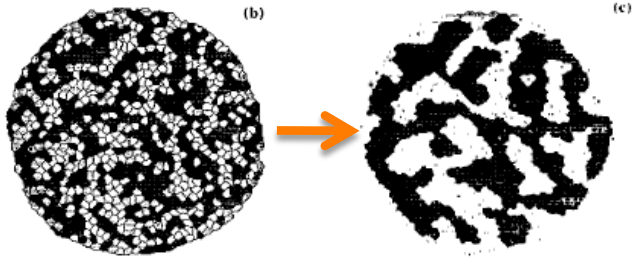
CompuCell3D: what it isn't/is

- Intracellular model
- Genetic mechanisms: genes, proteins, …



from genome.gov

- Intercellular model
- Physical mechanisms: elasticity, mitosis, apoptosis,chemotaxis, …



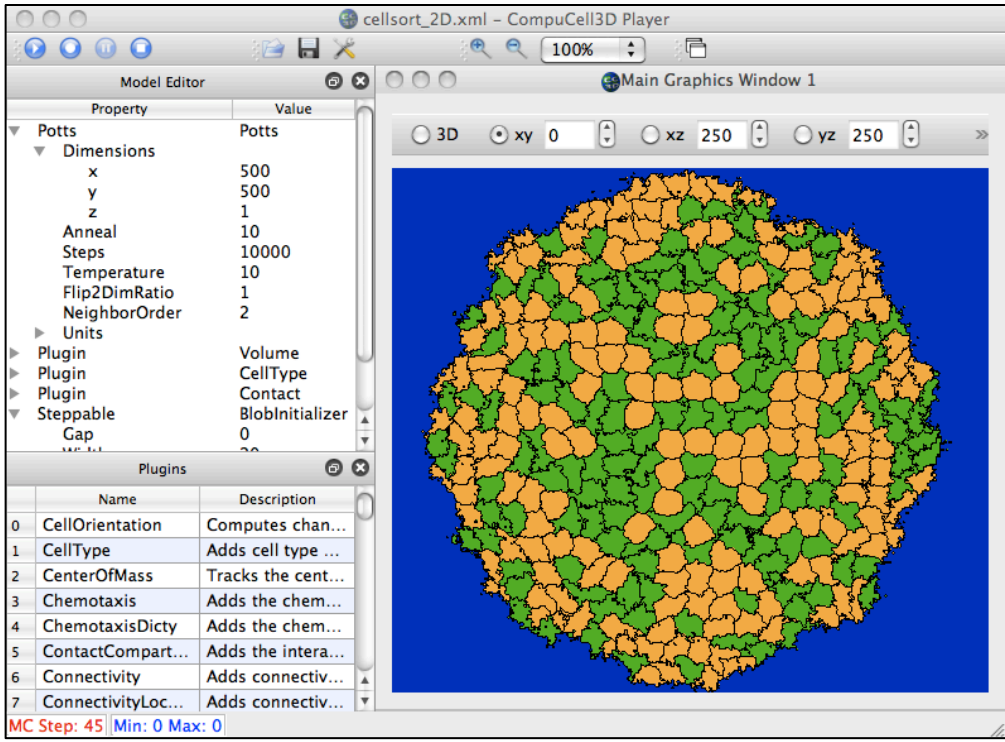
(rf. D'Arcy Thompson: On Growth and Form)

CompuCell3D

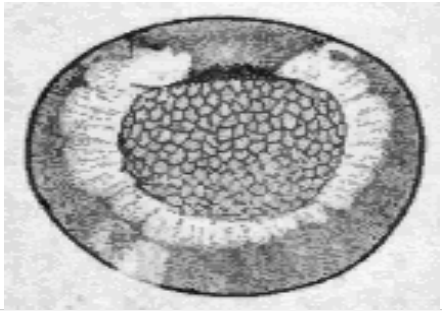
- Origin: Cellular Potts Model

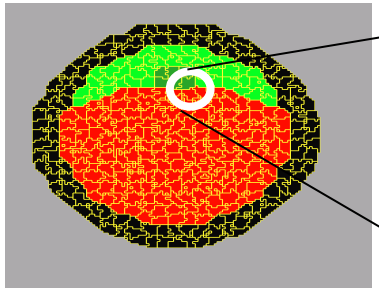
(now Glazier-Graner-Hogeweg model)

- Energy minimization formalism
- Lattice-based domain (2D or 3D)
- Stochastic algorithm
- C++ code base
- Python interface
- Open source
- *Download & try the Demos*

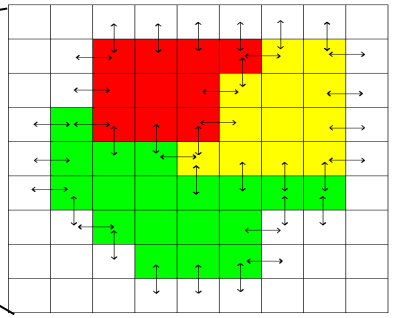


Cell defined on a regular lattice

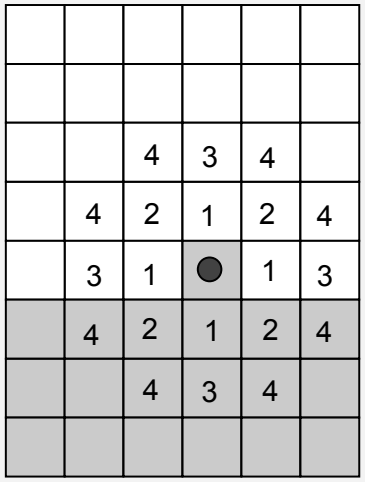


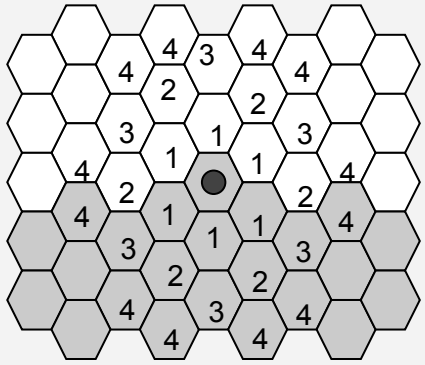


x 20



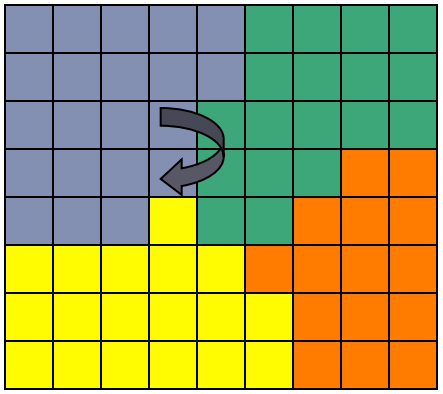
Cell types (colored)



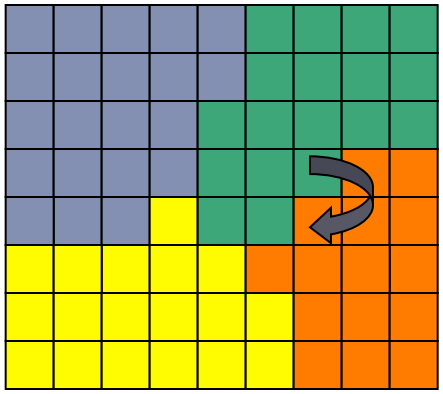


2D: Square or Hex lattice
3D: Cube or Rhombic Dodecahedron
(showing neighbors at different distances)

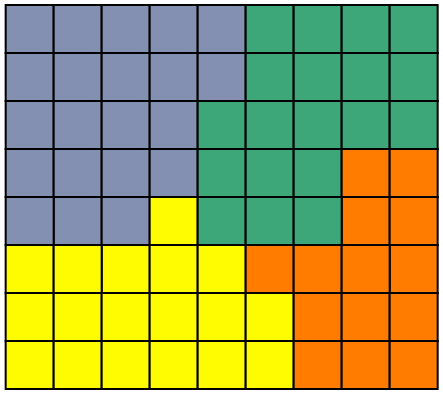
invalid attempt



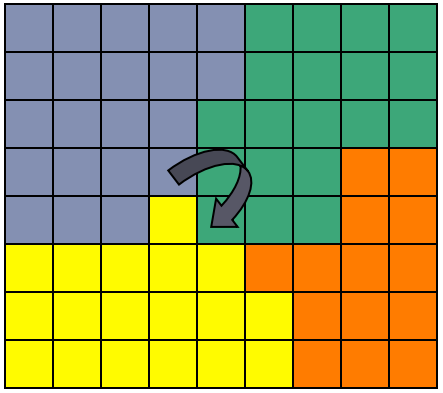
valid attempt



accept



valid attempt



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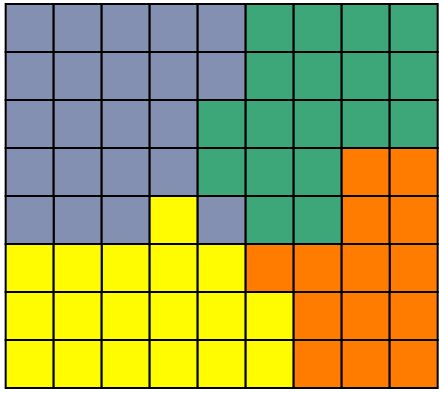
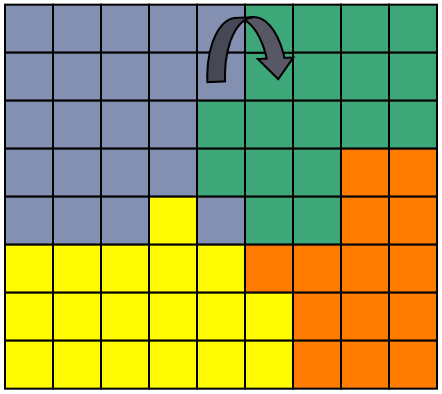
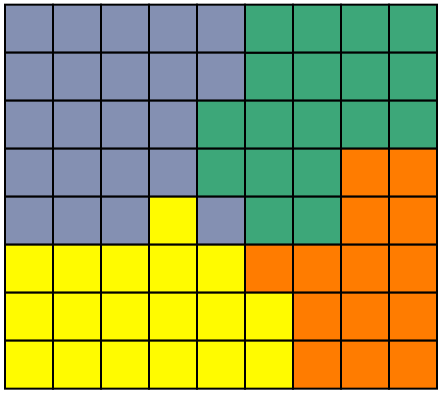


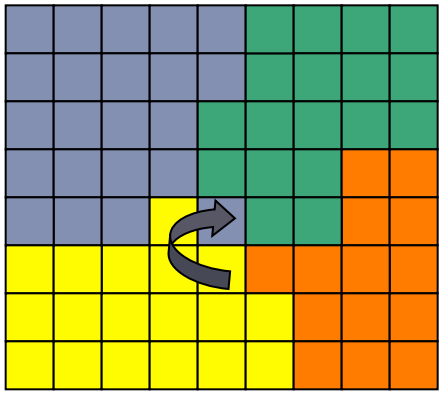
valid attempt



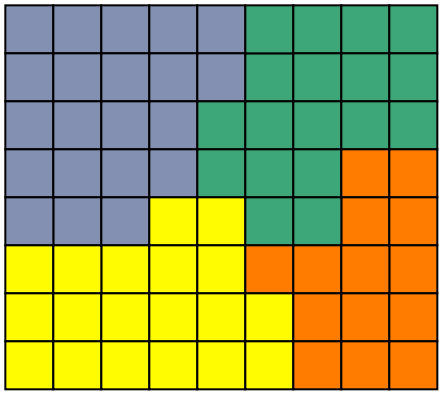
reject



valid attempt

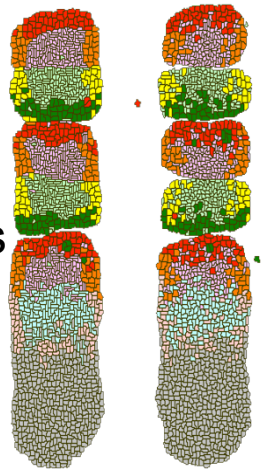


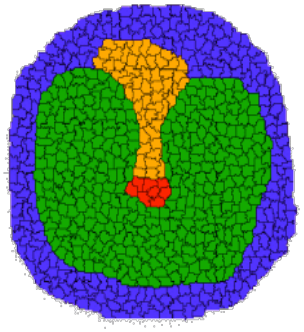
accept



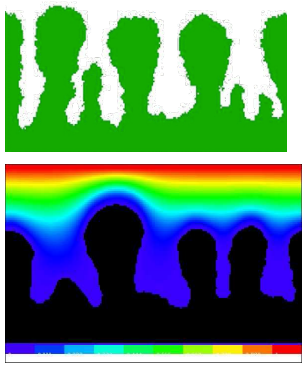
Gallery

somitogenesis

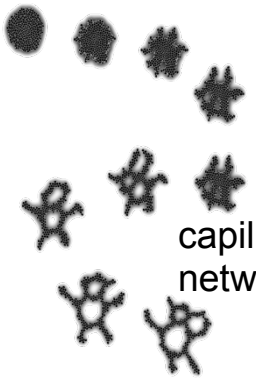




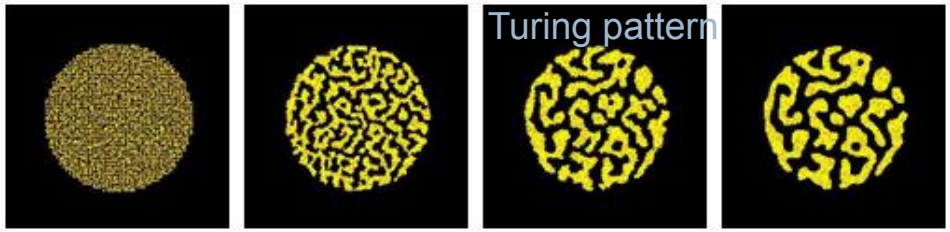
gastrulation



biofilms

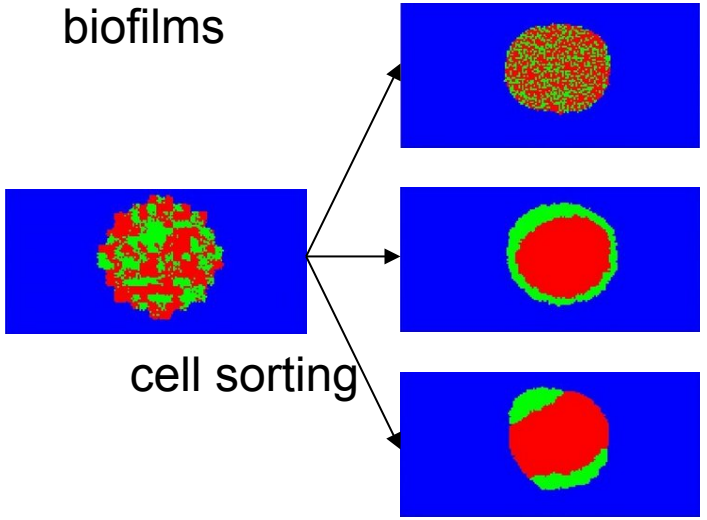


capillary network



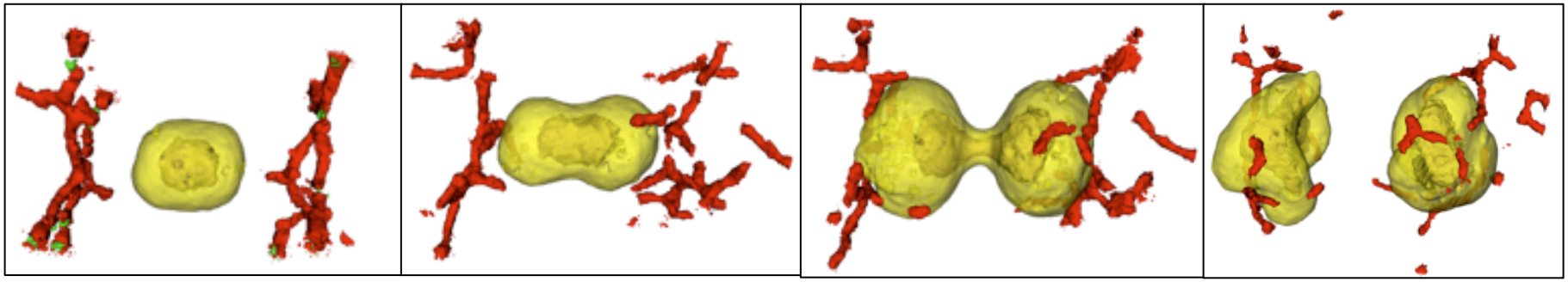
Turing pattern

dictyostelium



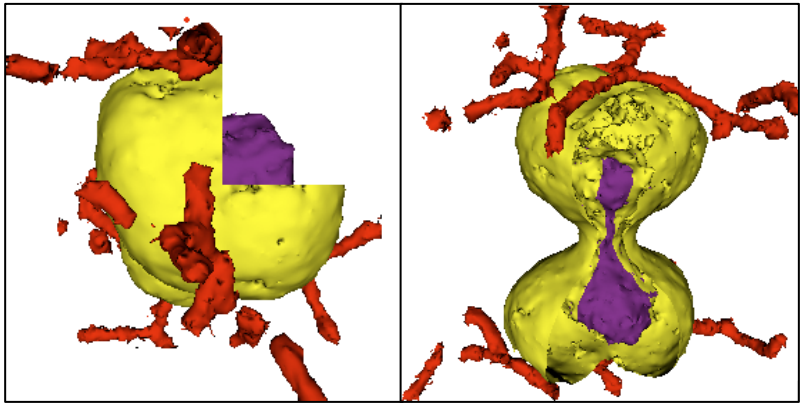
cell sorting

Tumor growth & vascularization



(see accompanying movies)

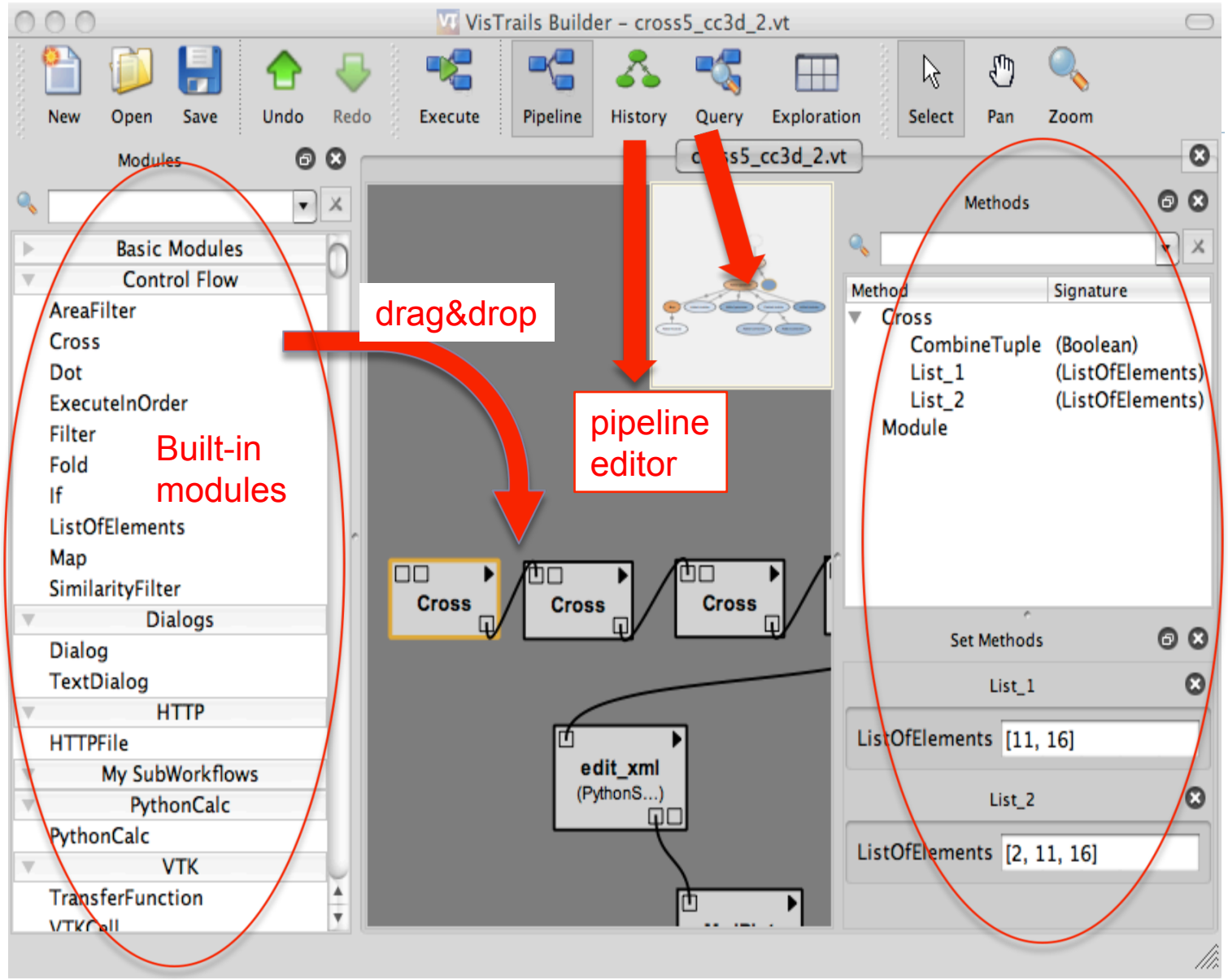
"3D Multi-Cell Simulation of Tumor Growth and Angiogenesis", Shirinifard, Abbas *et al.* *PLoS ONE*, Oct. 2009



Cut-away view to reveal the necrotic core

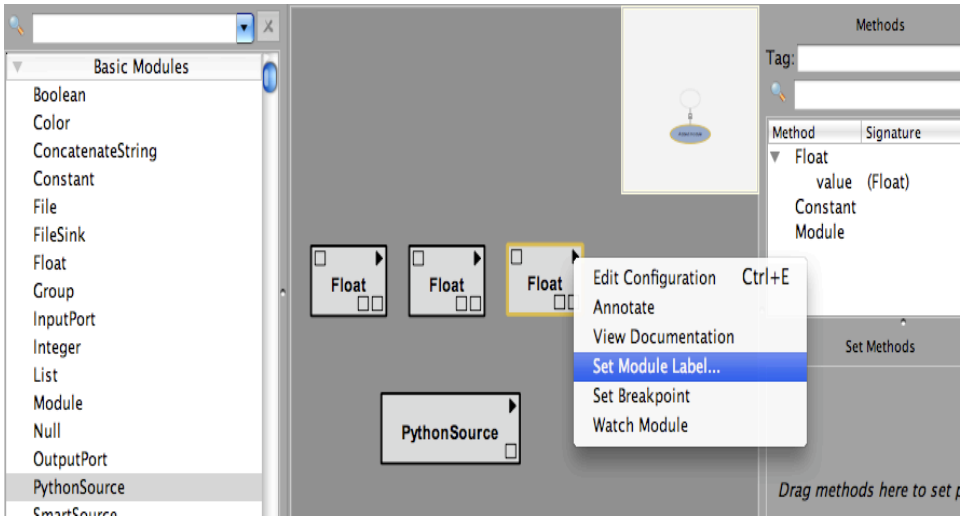
Workflows: VisTrails

- Scientific workflow and provenance mgmt system
  - Workflow: visual representation (pipeline) of dataflow
  - Provenance: recording/annotating data
- Drag & drop pipeline editor, built-in modules (visualization, control, etc)
- Written in Python
- Open source (vistrails.org)
- University of Utah (SCI Institute)

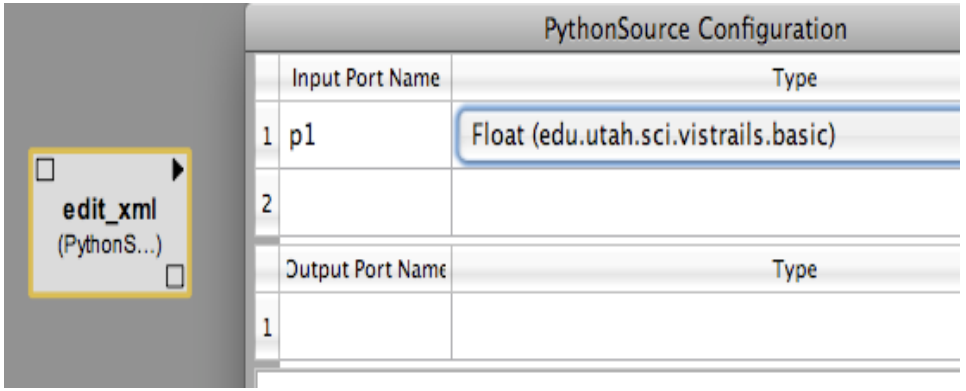


VisTrails GUI

VisTrails: Easy to use and Extensible



Can create/edit
Input/output ports



VisTrails → parameter sweeps → CC3D

- Models have many parameters
- Not uncommon to have single simulation run several hours on a workstation
- Let's farm out the simulations to a distributed compute resource
- Where/How?

TeraGrid

- Distributed resources (HPC, storage, etc) w/ high-speed networking
- Common software stack
- NSF-funded
- Open science

- Overkill for our purpose, but convenient

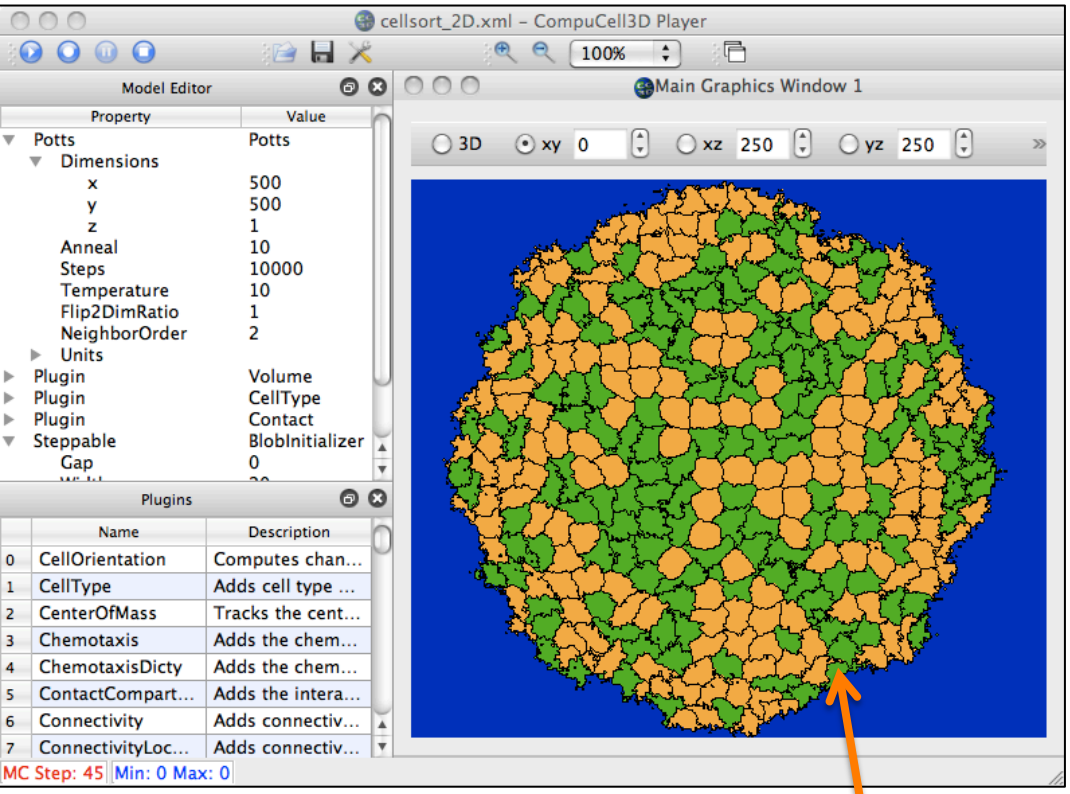
Indiana Univ: a TeraGrid Resource Provider

- IBM PowerPC “Big Red” cluster

Fall 2006 – Mar. ~~2010~~ 2011

- s/w stack includes Globus
  - Grid certificate
  - Remote job submission

Use case: 2D biological cell sorting



CompuCell3D

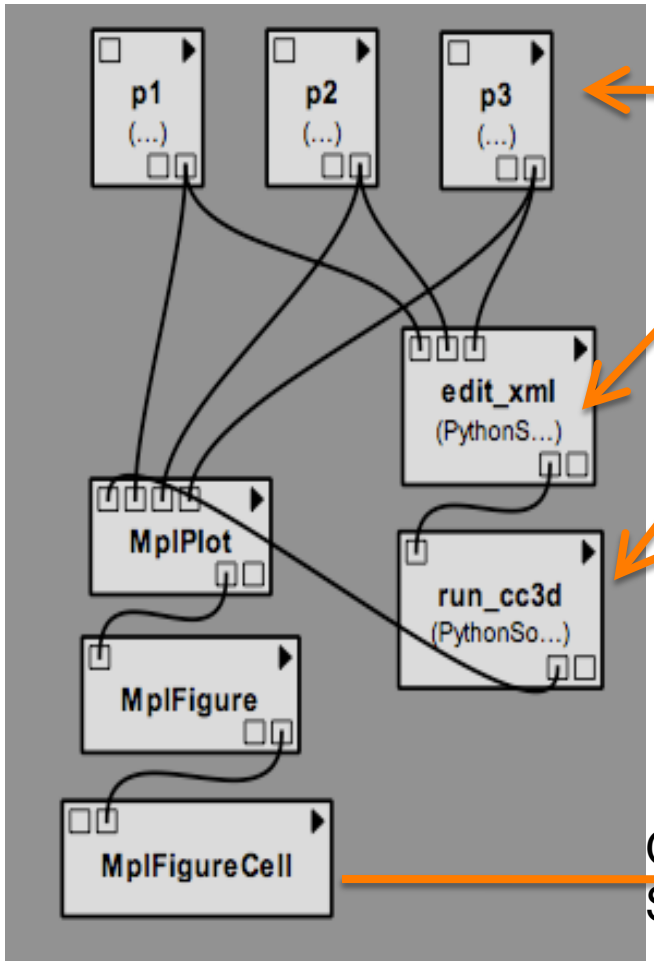
- Different cell types tend to adhere (or not) to neighbor cells

  → cell sorting

- Parameter study of "contact energies" between cells

2 cell types
surrounded by ECM

Cell sorting workflow: version 1

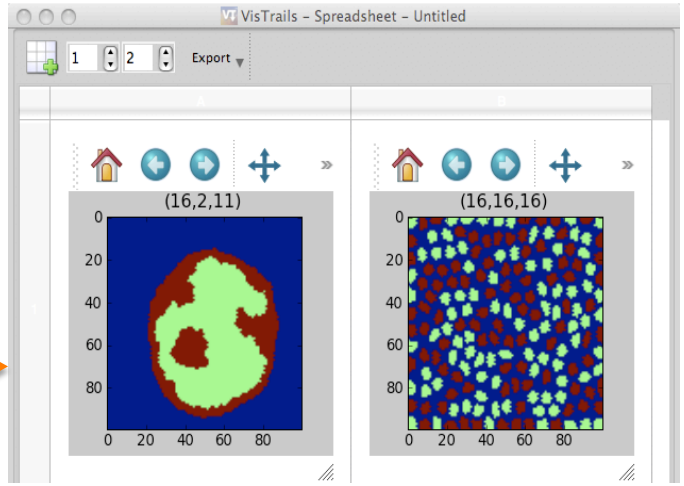


Manually enter 3 param values

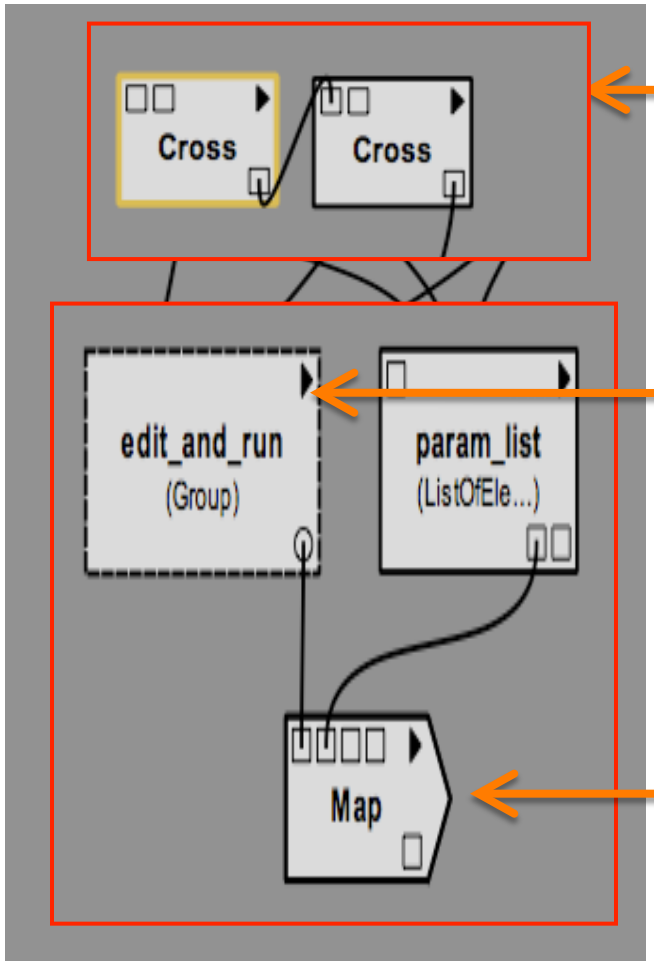
Python script to edit XML input

Run locally

Output to Spreadsheet



Cell sorting workflow: version 2 (part A)



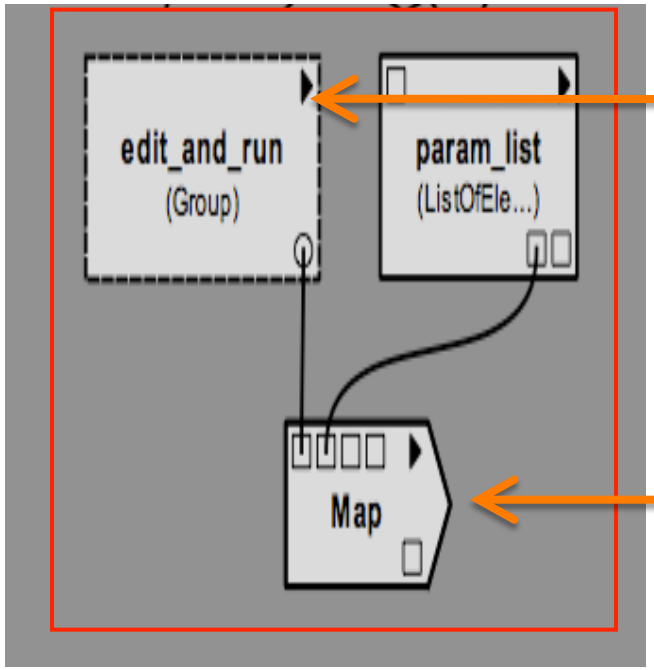
Use Cross product modules for params

Python script to edit XML input and

Submit remote jobs (via Globus cmds)

Use Map module: param set → job

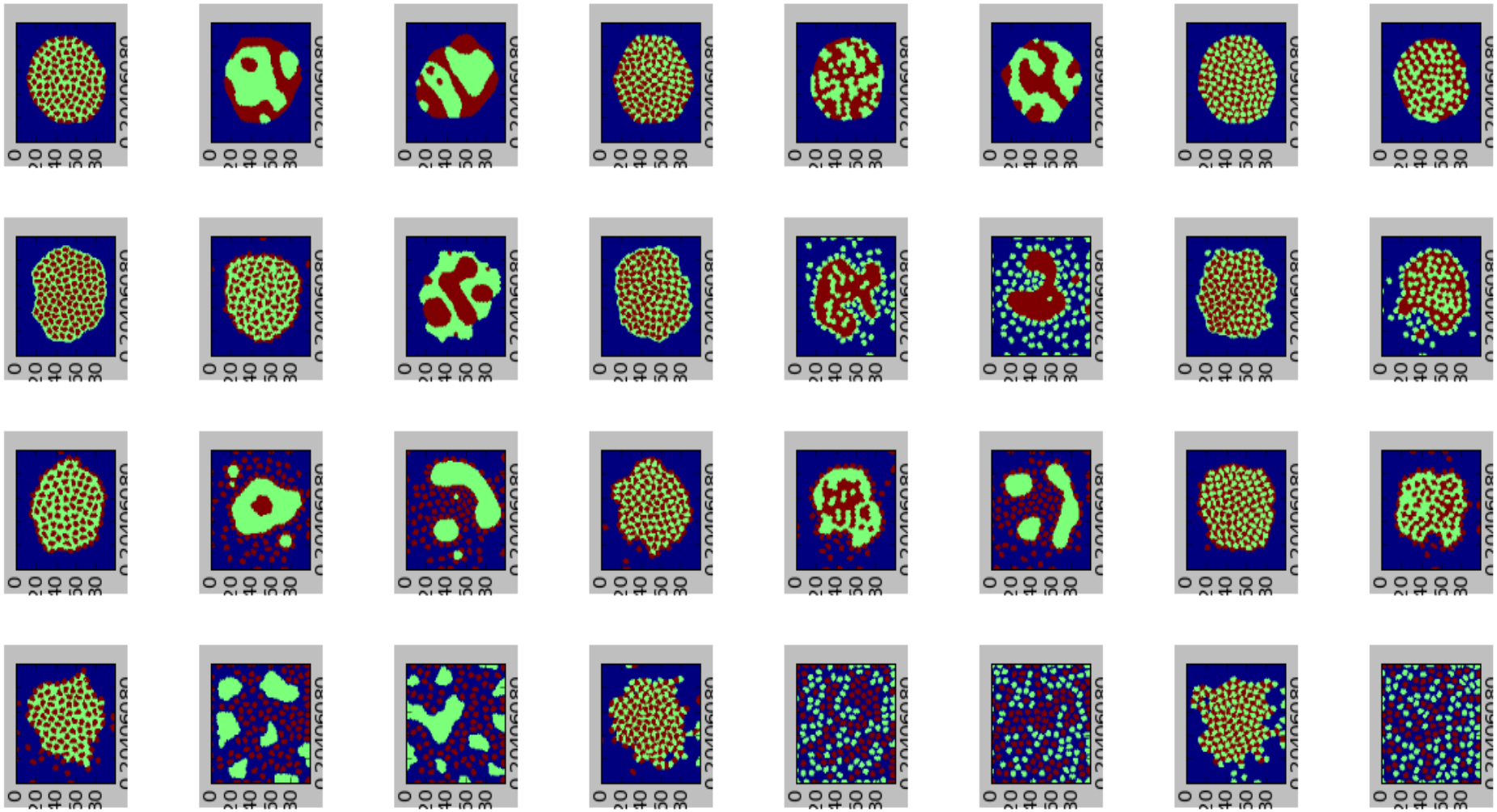
Cell sorting workflow: version 2 (part B)



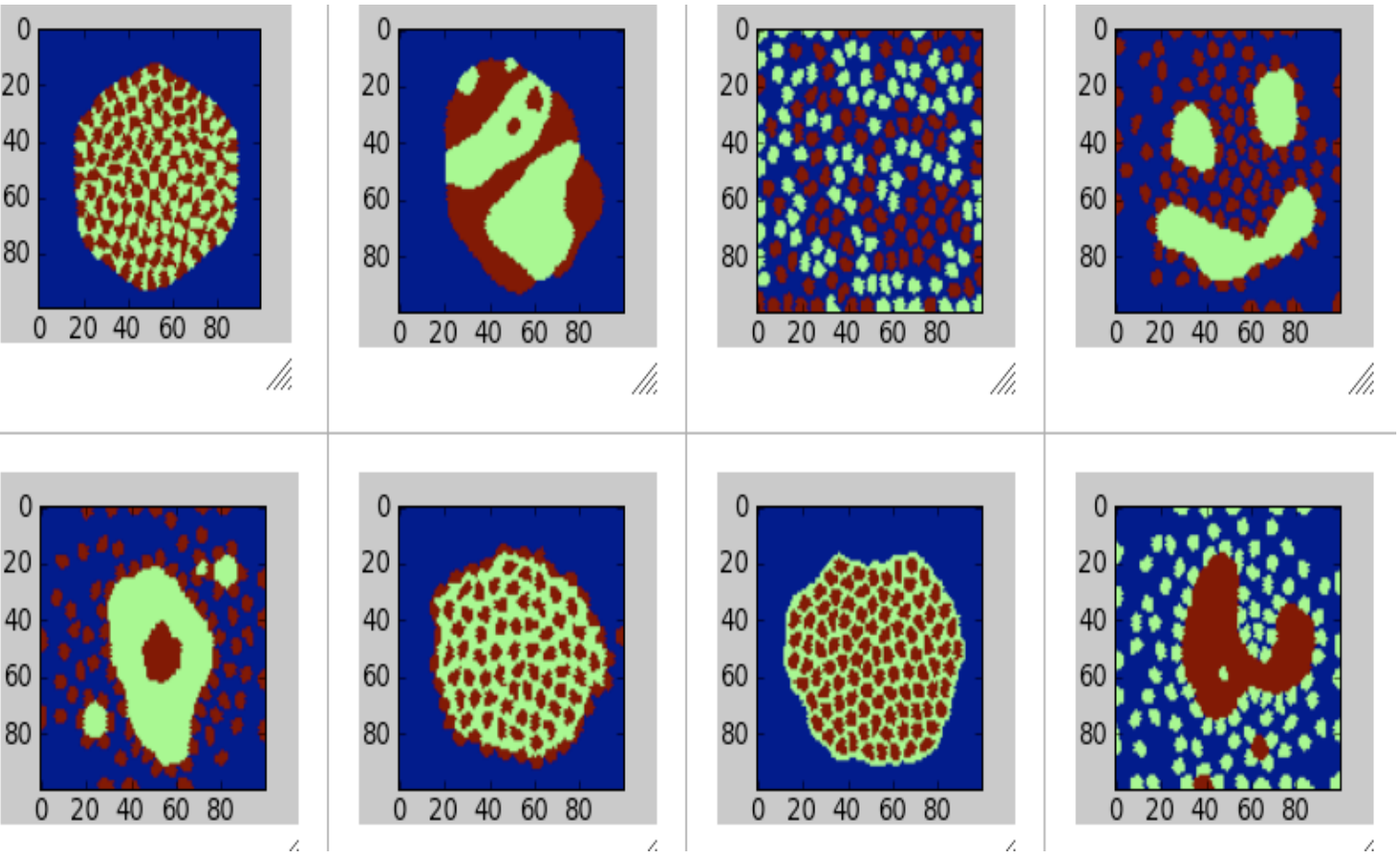
Retrieve remote results

Map module: output file → render

Subset of cell sorting results (32/72)



Qualitatively different outcomes



Caution:
NOT steady-state solutions, but…

Summary: Basic recipe

in 6 EASY steps!

1. Install VisTrails (on your workstation)
2. Get TeraGrid/Big Red account and Grid certificate
3. Install CompuCell3D (remotely; locally for local tests)
4. Install Globus client s/w on your workstation
5. Workflow for parameter sweep (remotely via Globus)
6. Workflow to retrieve results and display in VisTrails

Credits

- NIH NIGMS 1R01 GM076692-01
- Biocomplexity Institute, Indiana University
- Pervasive Technology Institute, Indiana University
- Lilly Endowment, Inc.

Thanks for your attention!

(If anyone has interest/experience in bifurcation analysis of stochastic processes, please email me)