Using High Performance Computing To Simulate Cellular Embryogenesis

Kison Osborne, Gerard Vanloo (Morehouse College)
Mentors: Kwai Wong, Ben Ramsey, Dali Wang (UTK)

Abstract

C. Elegans **is a primitive multicellular organism (worm) that shares many important biological characteristics that arise as complications within human beings.[1] It begins as a single cell and then undergoes a complex embryogenesis to form a complete animal. Using experimental data, the early stages of life of the cells are simulated by computers. The goal of this project is to use this simulation to compare the embryogenesis stage of *C. Elegans* cells with that of human cells. Since the simulation involves the manipulation of many files and large amounts of data, the power provided by supercomputers and parallel programming is required.**

1. **https://www.cbs.umn.edu/research/resources/cgc/what-c-elegans**

Objective

- **The objective of this project is to replicate the data of the beginning stages (embryogenesis) of a *C. Elegans* worm cell from experimental data through computer simulation**
- **A preliminary version of simulation was done using the agent based simulation software, NetLogo.**

NetLogo Interface

- **The problem with NetLogo is that it can only run on one computer (serial) and is impractical for large data sets, thus the Netlogo code was ported to RepastHPC, an agent based modeling toolkit made for HPC.**

VisIt

- **Since RepastHPC lacks a visualization component, VisIt is used to show the simulation.**
- **VisIt is capable of reading over 100 different file types and display data in various ways depending on the user.**
- **Different Python scripts were used to convert the files generated by RepastHPC into Point3d files.**

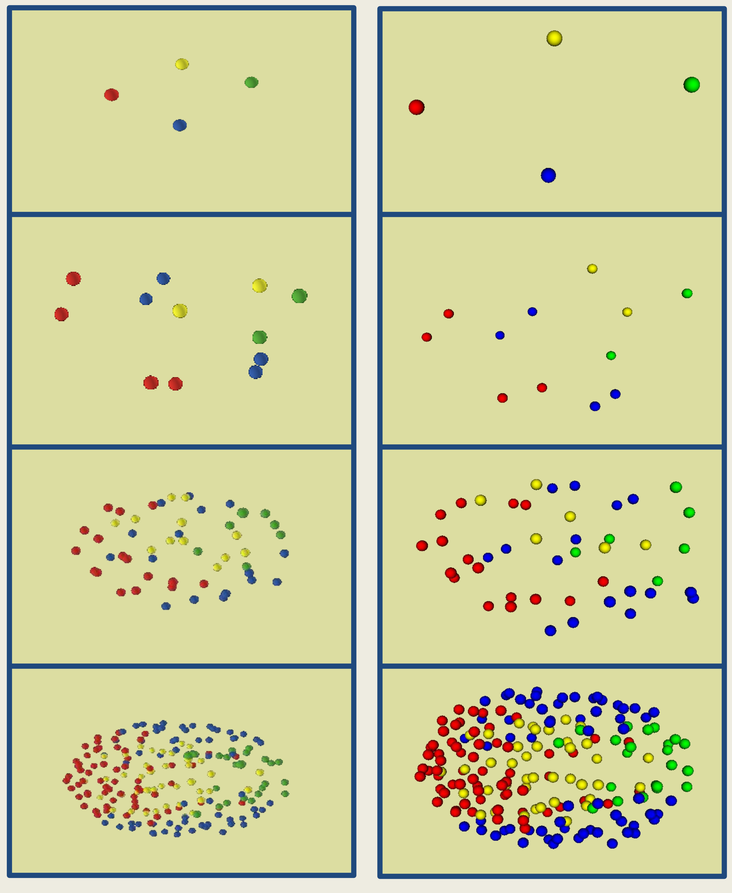
Basic Simulation Algorithms

Every time step, all cells must:

- **Wander**
  - **Move in a linear path**
- **Divide**
  - **If parent cell is ready to divide,**
    - **New cell becomes the first daughter**
    - **Parent cell becomes the second daughter**
  - **If cell has outlived division cycle,**
    - **Stop dividing**
- **Save progress(*)**
  - **X, Y, Z Coordinate**
  - **Name**
  - **Size**
  - **Various IDs**

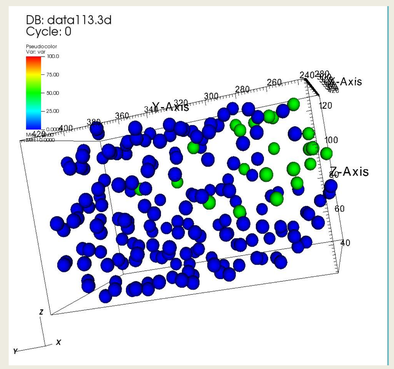
*** = Frequency will change**

Visualization Comparison

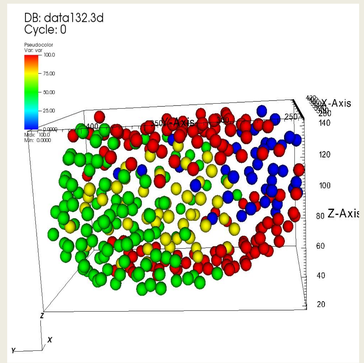


Results

- **Currently, the RepastHPC simulation is able to replicate the NetLogo simulation, with a small degree in error between the placement of cells.**
- **It should be noted that NetLogo simulation was not yet a replica of the actual experimental data.**
- **The visualization component has been completed in VisIt. This includes the single cell tracking and general visualization.**



Cell Tracking



Four Color - General

Next Steps

- **The cell wandering algorithm will be enhanced.**
  - **The current version only allows cells to move linearly.**
  - **A more realistic algorithm would involve a cell using its surrounding neighbors' locations to emulate the actual movement of a cell.**
- **A graphic user interface will be developed to run the RepastHPC simulation and VisIt visualization from one central hub.**

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Vanloo (gerard.vanloo0@gmail.com)
Kison Osborne (ozuboon95@gmail.com)
Kwai Wong (kwong@utk.edu)
Ben Ramsey (bramse10@vols.utk.edu)
Dali Wang (dwang7@utk.edu)
Zhirong Bao (baoz@mskcc.org)