





CERN

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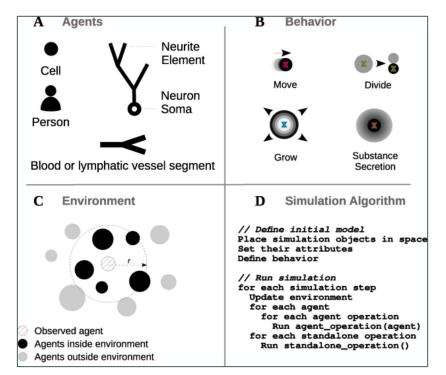
## What is BioDynaMo



#### Open-source, high performance, general purpose, agent-based modeling for studying complex biological systems.

- □ Solves some of the problems *In silico simulations* have due to
  - Moore's law
  - Dennard Scaling
  - Developed for a specific use
- BioDynaMo system properties:
  - Agent-based
  - General Purpose
  - □ Large Scale
  - Easily Programmable
  - Quality Assured

- □ BioDynaMo Platform Use:
  - 1. Formulate Problem
  - 2. Assemble Simulation
  - 3. Execute Simulation
  - 4. Analyze Results
  - 5. Publish and Contribute
  - 6. Add New Modules and Use

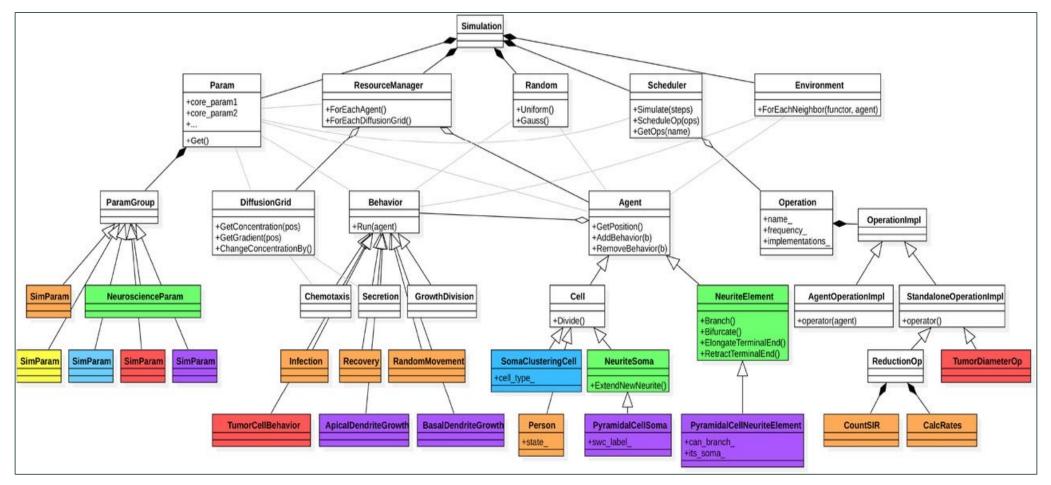


*Figure 1: BioDynaMo core simulation concepts* 





### What is BioDynaMo



*Figure 2: BioDynaMo software design and modularity* 







#### <u>Neuroscience</u>

Use of BioDynaMo to model neurite growth of pyramidal cells using chemical cues.

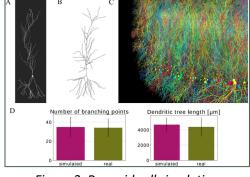


Figure 3: Pyramid cell simulation

#### **Epidemiology**

Use of BioDynaMo to model two behaviors of cell clustering.

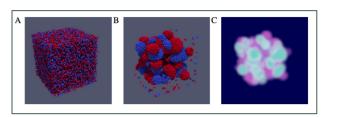


Figure 4: Soma clustering simulation

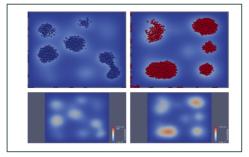
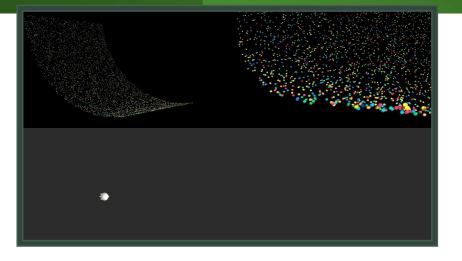
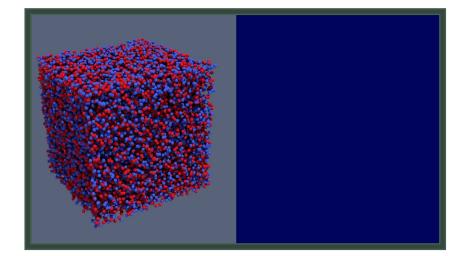


Figure 5: Soma clustering cross seciton



Video Demo





## **Performance Analysis**



#### □ Performance improvements against established agent-based simulators(Cortex3D)

- BioDynaMo and Cortex3D use the same method to determine mechanical forces between agents and the same model to grow neural morphologies.
- □ Significant speedup between 18 and 78×.
- Runtime of 1 hour 37 minutes, 6 hours 49 minutes, and 3 hours 54 minutes with respect to neuroscience, oncology, and epidemiology use cases.

#### □ Scalability of BioDynaMo

- □ Increased the number of agents used in the comparison with Cortex3D and reduced the number of simulation timesteps to 10.
- □ The maximum speedup ranged between 65× and 75×, which corresponds to a parallel efficiency of 0.90 and 1.04.
- □ Performance improved even after all physical cores were utilized and hyper-threads were used.

#### □ Impact of calculating the mechanical forces on the GPU using soma clustering simulations.

- □ The benchmarks were executed on System C, comparing an NVidia Tesla V100 GPU with 32 CPU cores (64 threads).
- □ We observed a speedup of 1.27 × for cell growth and division, and 5.04 × for soma clustering.



### **Results and Discussions**



BioDynaMo is more than three orders of magnitude faster than Cortex3D.

U With enough memory, BioDynaMo is capable of supporting hundreds of billions of agents.

#### BioDynaMo allows researchers to:

- Develop models in computational biology field in a modular architecture manner,
- □ Collect results fast thanks to the parallelized execution engine,
- □ Model billions of agents on a single server,
- Produce results that correspond to validated experimental data.

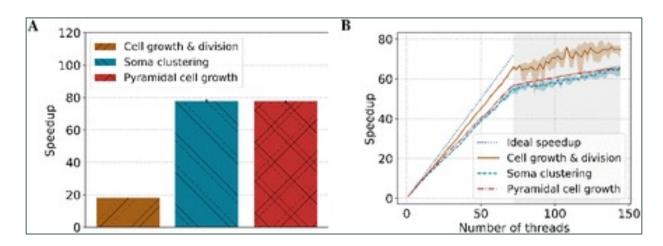


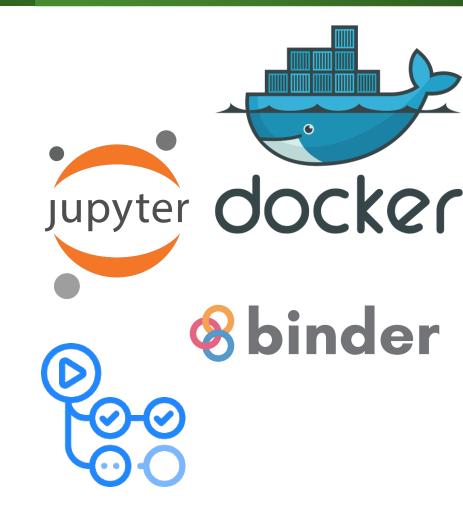
Figure 6: BioDynaMo performance analysis





# Making BioDynaMo More Accessible

- □ BioDynamo Container Available on Docker-hub with all Prerequisites Installed .
- □ Easy To Run Jupyter Notebooks Available on BioDynamo Website.
- □ Notebooks can be executed in Browser using My-Binder.
- GitHub Actions build and push Latest BioDynamo Version to Docker-hub





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Preprint of the BioDynaMo paper:

https://www.biorxiv.org/content/10.1101/2020.06.0 8.139949v2

# Thank You



Supplementary information:

https://doi.org/10.5281/zenodo.4501515

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BioDynaMo webpage:

https://biodynamo.org