

# **BIODYNAMICS MODELLER**

#### **CERN openlab Technical Workshop**

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### Help Life Scientists Understand (Patho)physiological Processes







### **Agent-based simulations**

#### Simulation object = *Agent*



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Simulation object = *Agent* 

Local region





• Modular system that supports different specialities



- Modular system that supports different specialities
- Support large-scale biological simulations



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- Hide complexity of distributed computing



- Modular system that supports different specialities
- Support large-scale biological simulations
- Hide complexity of distributed computing
- Promote reproducibility of results



### **Large-scale Simulations**

The cerebral cortex consists of ~16 billion neurons

- Scale up
  - Efficient use of modern hardware (multi-core CPUs and accelerators)
- Scale out
  - Distributed runtime

### **Preliminary Performance Results**

#### Cell grow and divide Speedup: 25x

### 35000 -25000 -25000 -15000 -10000 -5000 -Cortex3D BioDynaMo

#### Soma clustering Speed-up: 31x



### Preliminary Performance Results

#### AOS vs SOA memory layout

#### cell grow and divide

#### soma clustering



### Mechanical Interactions on GPU or FPGA



### **Retinal Mosaics Use Case**



## Research performed by Jean de Montigny at the University of Newcastle, UK

### **Current Status**

- Modular simulation engine
- Fully parallelized with OpenMP
- GPU & FPGA implementation for mechanical interactions using CUDA and OpenCL
- First version of **distributed runtime** based on the framework Ray
- ROOT I/O for storage of simulation results and snapshots
- Visualization using ParaView and ROOT Eve









### Future Work: Distributed Runtime

### **Domain-Decomposition**



Hauri, Andreas. *Self-construction in the context of cortical growth* . Diss. 2013.











### Prototype based on Ray



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#### Ray: A Distributed Framework for Emerging AI Applications

🖋 ROBERT NISHIHARA / 🋗 DECEMBER 20, 2017 /

The next generation of AI applications will continuously interact with the environment and learn from these interactions. These applications impose new and demanding systems requirements, both in terms of performance and flexibility. In this paper, we consider these requirements and present Ray---a distributed system to address them. Ray implements a dynamic task graph computation model that supports both the task-parallel and the actor programming models. To meet the performance requirements of AI applications, we propose an architecture that logically centralizes the system's control state using a sharded storage system and a novel bottom-up distributed scheduler. In our experiments, we demonstrate sub-millisecond remote task latencies and linear throughput scaling beyond 1.8 million tasks per second. We empirically validate that Ray speeds up challenging benchmarks and serves as both a natural and performant fit for an emerging class of reinforcement learning applications and algorithms.

#### Published On:

Link: https://arxiv.org/pdf/1712.05889.pdf

Authors: Philipp Moritz, Robert Nishihara, Stephanie Wang, Alexey Tumanov, Richard Liaw, Eric Liang, William Paul, Michael Jordan, Ion Stoica

#### developed by our summer student Nam Nguyen

### Challenges

- Alleviate the overheads of distributed execution
  - e.g. (De)serialization
- Performance issues in the cloud
  - Inferior network performance compared to supercomputers
  - Load balancing (heterogeneous computing, runtime variance)
- Fault-tolerance
  - Long running simulations with large number of nodes Will checkpointing be enough?



### **QUESTIONS?**

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