In the Name of God

Parallel Processing and Simulation in Computational Neuroscience

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HPC workshop, NBML, May 2019

Why We Do Simulations, How We Verify the Results?

- **What is a Model?**
  - Analytical
  - Data Driven

  → Gray Box Modeling

- **Where to Simulate?**
  - We can not measure due to complexity of the system or technical limitations.
  - We can measure, but it is expensive.

Moving on the Boundaries…

- Challenge for biologists
- Challenge for mathematicians, and theory guys!

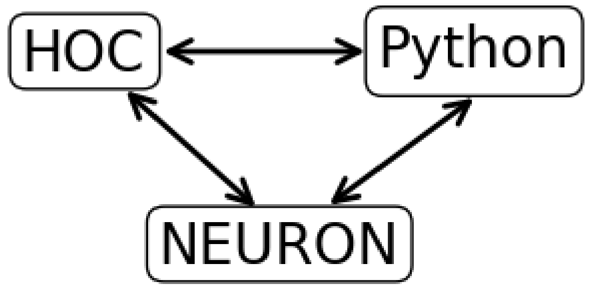
- Simulator vs language…A good simulator?
    - Powerful in computation
    - User friendly

Simulator vs Language

- MATLAB: MAtrix LABoratory

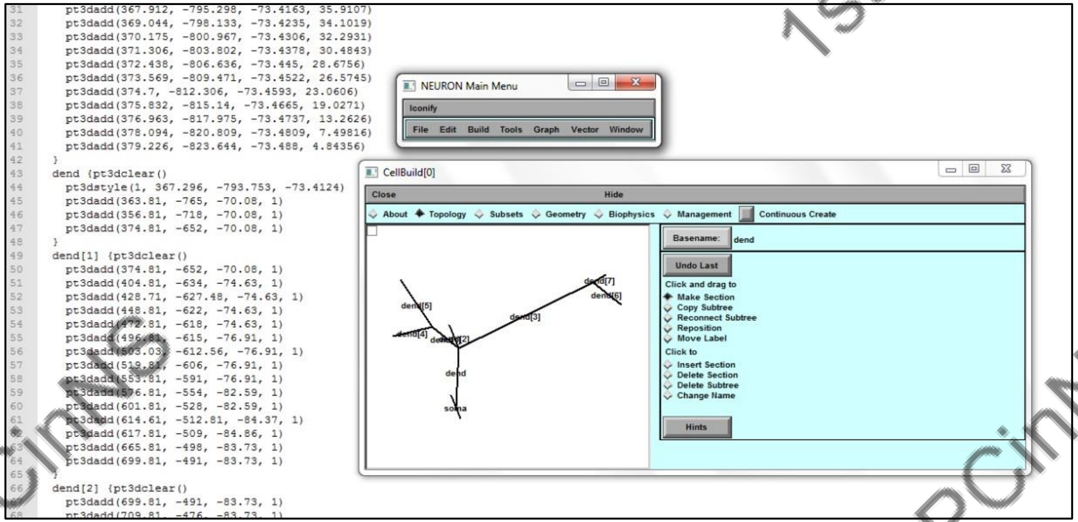
- NEURON: Compartmental Modeling---details, small networks
- Genesis: Compartmental Modeling---details
- BRAIN: Spiking Neural Networks---not for clusters
- NEST: Spiking Neural Networks---large networks

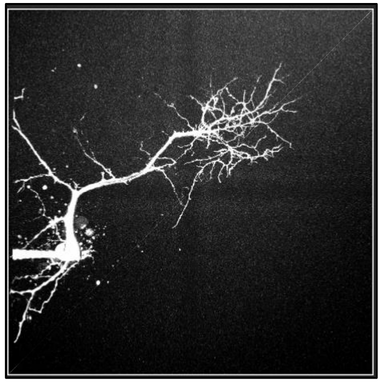
- Python
- C++



HPC in Neuroscience

- Structural connectomics data
- Massive neurophysiology datasets
- Hosting and sharing multimodal data
- Data synthesis through neural circuits simulation





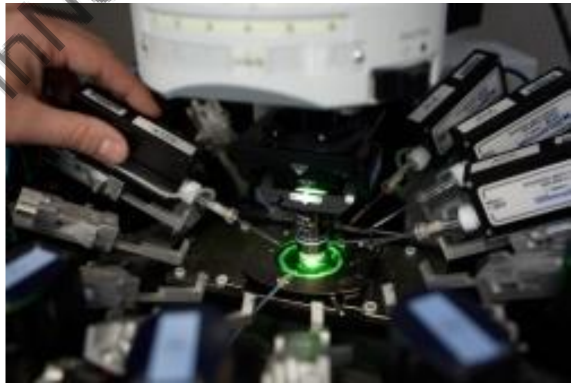
Large Scale Simulations

- Many heterogeneous elements, complex integration,
  different spatio-temporal scales

- Measuring and manipulating neuronal activity, for long period of time and for a large size…

The BLUE BRAIN Project

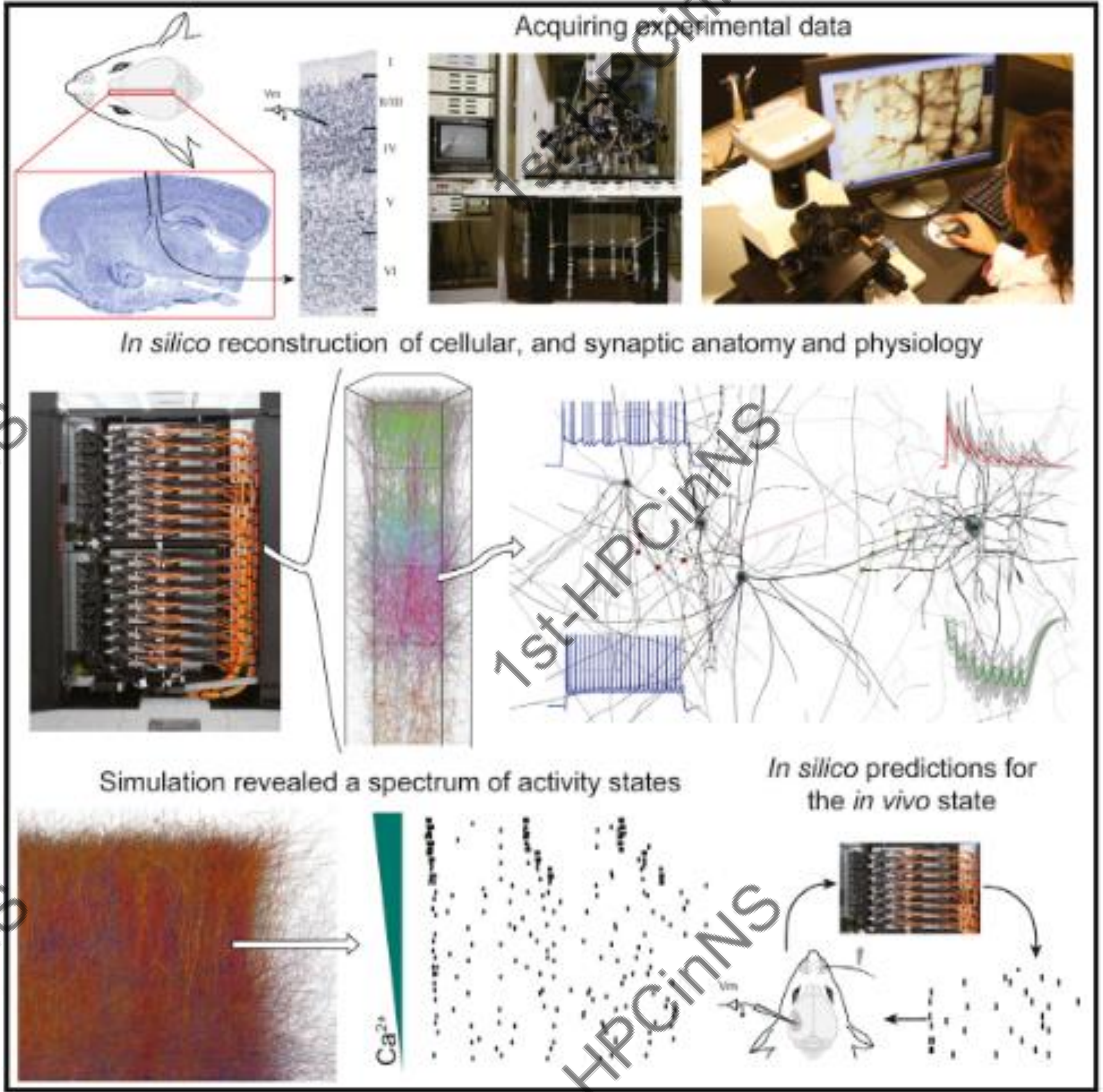
- Founded in 2005 by H.Markram at the EPFL in Lausanne, Switzerland.
- 2023: Cellular-level simulation of the entire human brain!



•4,096 quad-core nodes (16,384 cores in total)
•Each core is 850 MHz
•16 terabytes of memory
•1 PB of disk space (1000 TB)
•Operating system: Linux SuSE SLES 10

•Morphology, electrophysiological behavior, location, population density.

•One second of simulated time takes five minutes to complete (300X)



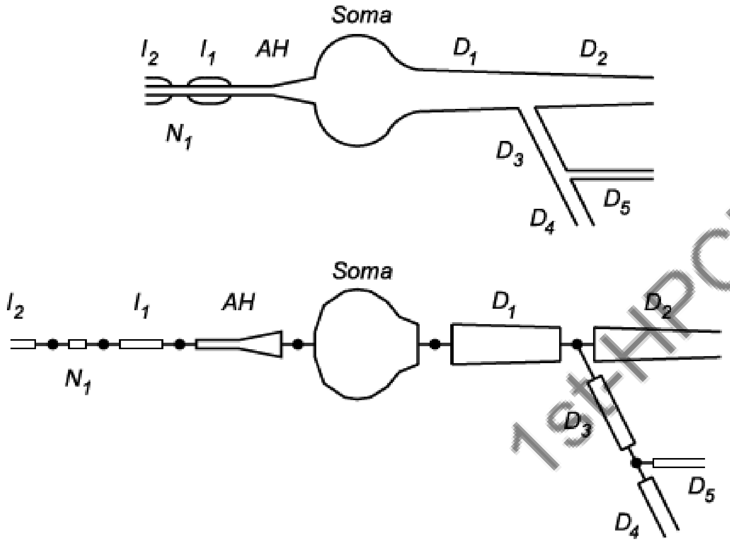
Acquiring experimental data
In silico reconstruction of cellular, and synaptic anatomy and physiology
Simulation revealed a spectrum of activity states
In silico predictions for the in vivo state
Ca²⁺
Vm

NEURON

- John Wilson Moore, famous for TTX, Duke University, 1984, first concepts of "computational neuroscience", Yale University
- Michael Hines (Mathematics), Ann Stuart (Biology), Gordon Shepherd, Zach Mainen (Champalimaud Neuroscience Program) , Ted Carnevale, Peter Davison (CNRS)
- Up to 2008: more than 700 papers by NEURON

Building up a Model…

- Defining the morphology of the network
- Defining the “sections”:
  - Geometry, biophysics
- Inserting point process
- Stimulating and Recording



- Customizing the mechanisms of the sections:
  - Channels and conductance
  - Diffusion of Ions

Building up a Model

- Theoretical frame works:

  - Electrical Circuits, Cable theory
    - Solving the equation:
    - Constraints, numerical methods

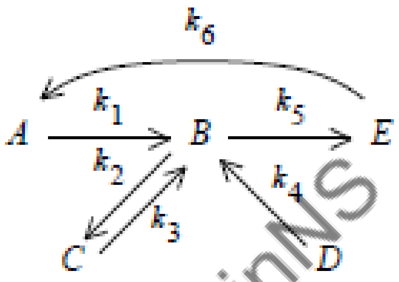
$$\frac{\partial V}{\partial T} + F(V) = \frac{\partial^2 V}{\partial X^2}$$

  - Conceptual models, dynamic of conductance, Ionic pumps, exchangers…
  - Flux and kinetic schemes

$$Ca_i \underset{k_d}{\overset{k_d}{\rightleftarrows}} Ca_{bulk}$$

$$Ca_i + Pump \underset{k_2}{\overset{k_1}{\rightleftarrows}} Ca\,Pump$$

$$Ca\,Pump \underset{k_4}{\overset{k_3}{\rightleftarrows}} Ca_o + Pump$$

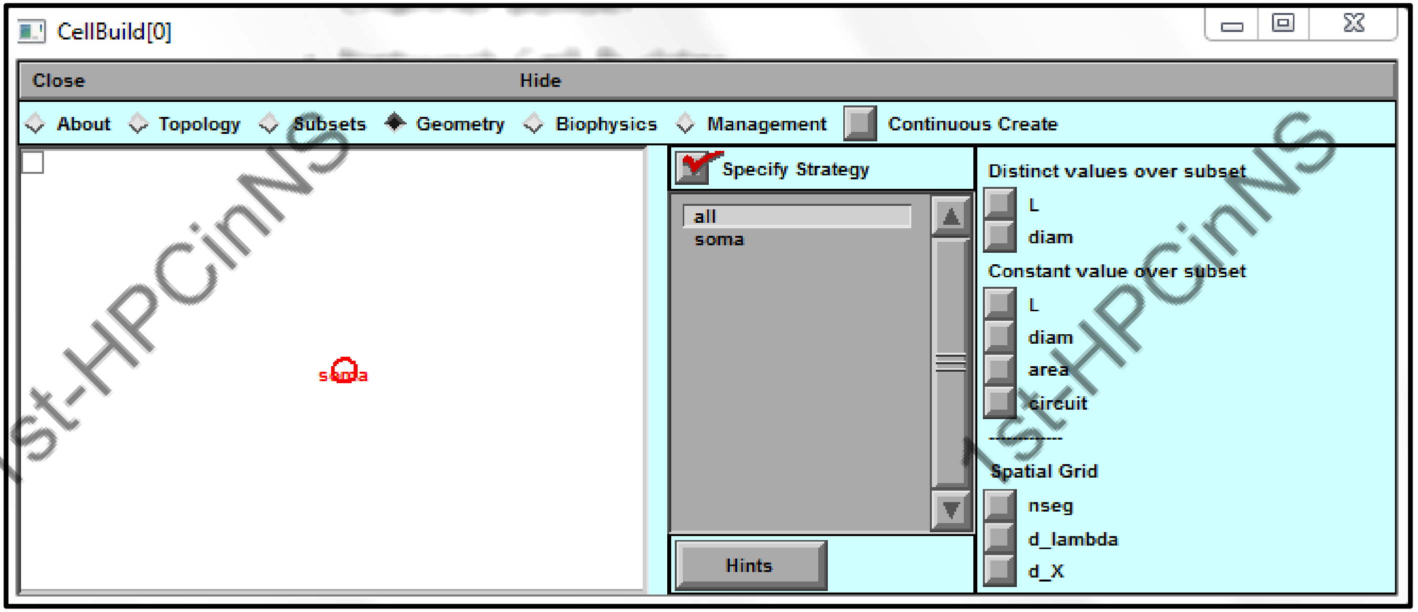


$$A + B \underset{k_b}{\overset{k_f}{\rightleftarrows}} C$$

$$\frac{dA}{dt} = -k_f\,AB + k_b\,C$$

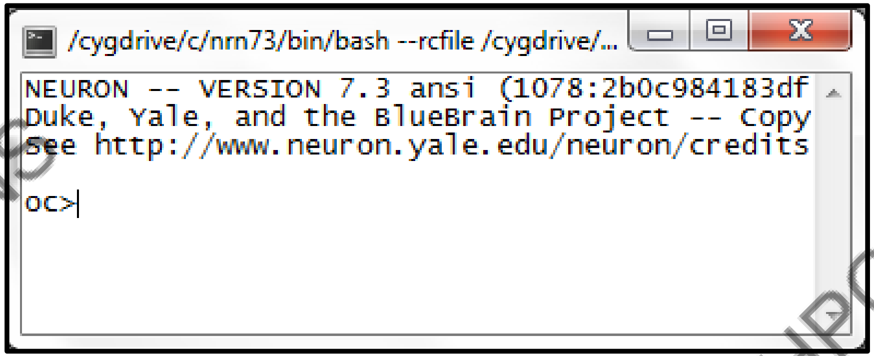
NEURON Environment

- Programing Language: hoc, an orphan language…
- Cross-Platform: Win, Linux, Mac



- GUI
  - Cell Builder
  - Channel Builder
  - Network Cell Builder
  - Simulation and Recording

- Scripting Environment
  - hoc
  - NMODL



NEURON Environment: Scripting

- hoc: Built-in interpreter, C-like syntax, added features object oriented syntax

- NMDL: Adding new mechanisms in form of physical model by
  nonlinear algebraic equations, differential equations or kinetic schemes

  Hocmodl translator --> C --> Dynamically load shared object, executable

NEURON…

`L`	section length	[µm]
`Ra`	cytoplasmic resistivity	[Ω cm]
`nseg`	discretization parameter	[1], i.e. dimensionless

Name	**Meaning**	**Units**
`gna_hh`	conductance density of open Hodgkin-Huxley sodium channels	[S/cm^2]
`ina`	net sodium current density (i.e. produced by *all* mechanisms in a section that generate sodium current)	[mA/cm^2]
`rs`	series resistance of an `SEClamp`	[10^6 Ω]
`gmax`	peak conductance of an `AlphaSynapse`	[µS]
`i`	total current delivered by an `SEClamp` or an `AlphaSynapse`	[nA]

HPC in NEURON

- ParallelNetworkManager, Since 2005
- Based on MPI

- Joint with Python

- NetCon Object: Connecting Target and Source, Connecting Networks

HPC in Neuron

- Allocating Gids to the hosts
- Load Balance…
- Python interface for MPI, mpi4py

Simple Sample

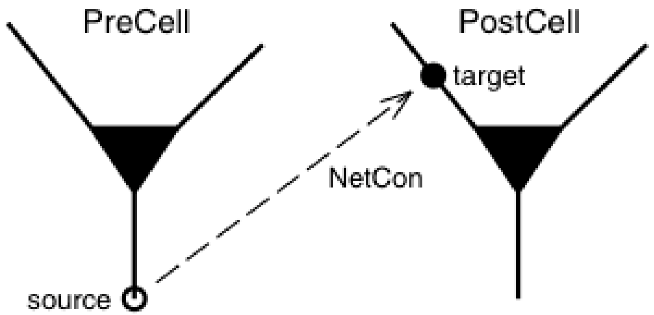


Figure 2.1. A NetCon attached to the presynaptic neuron PreCell detects spikes at the location labeled source, and delivers events to the synapse target which is attached to the postsynaptic neuron PostCell.

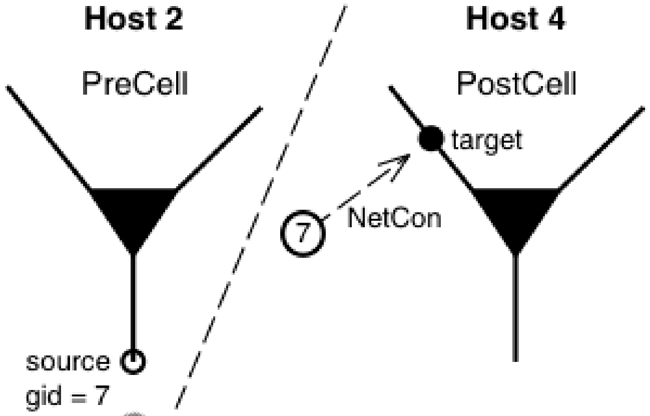


Figure 2.2. A presynaptic spike source PreCell with gid = 7 is on host 2, but its target is a synapse attached to PostCell on host 4. If PreCell spikes, a message is passed to all hosts so that NetCons that have gid 7 as their source will deliver events to their targets.