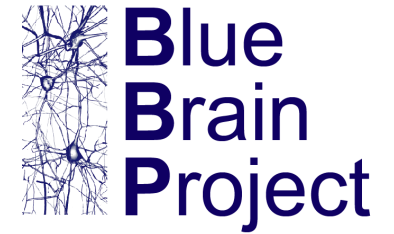


Simulating Morphologically Detailed Neuronal Networks at Extreme Scale

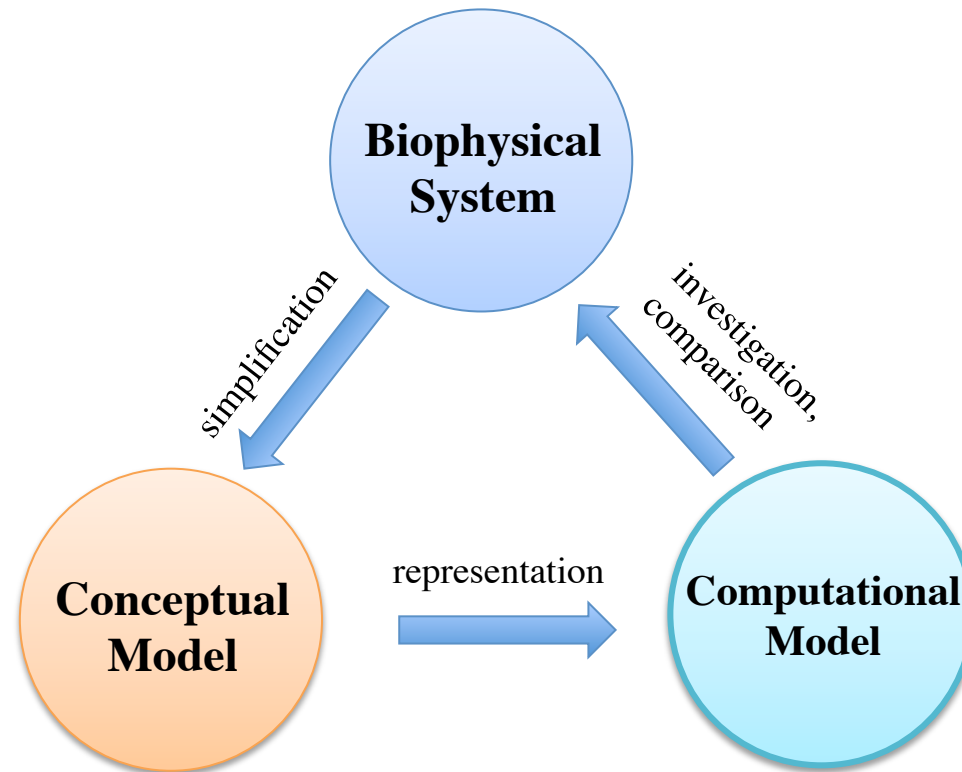
Aleksandr Ovcharenko
(aleksandr.ovcharenko@epfl.ch)

Pramod Kumbhar, Michael Hines, Francesco
Cremonesi, Timothee Ewart, Stuart Yates, Felix
Schuermann and Fabien Delalondre

Blue Brain Project Approach



Constructing virtual brain model by reverse engineering biological components

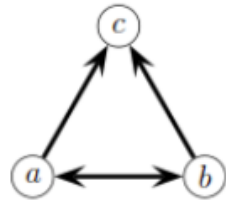


Different Scale ... Different Simulators ...

Nest



A simulator for spiking
neural network models
that focuses on dynamics,
size, structure

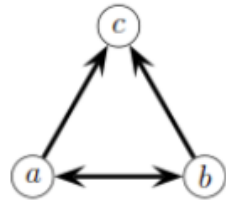


Different Scale ... Different Simulators ...

Nest

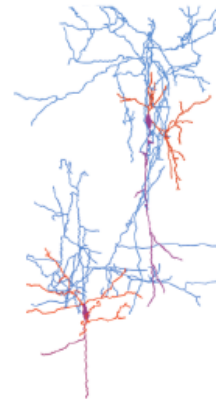


A simulator for spiking neural network models that focuses on dynamics, size, structure



Neuron

A simulator for cells with complex anatomical and biophysical properties.

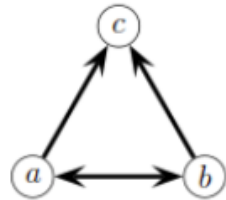


Different Scale ... Different Simulators ...

Nest

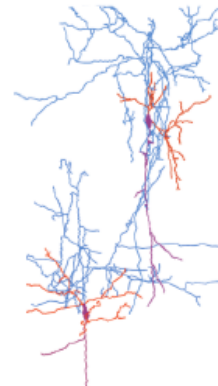


A simulator for spiking neural network models that focuses on dynamics, size, structure



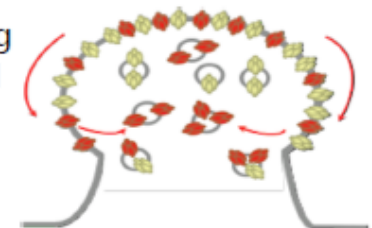
Neuron

A simulator for cells with complex anatomical and biophysical properties.



STEPS

A simulator for detailed models of neuronal signaling pathways at molecular level

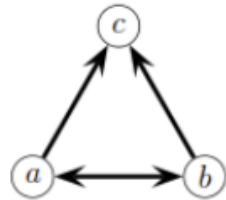


Different Scale of Neuronal Simulators

Nest

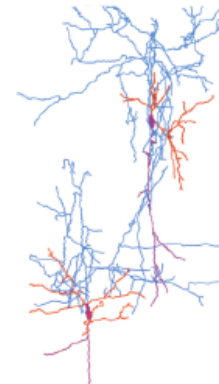


A simulator for spiking neural network models that focuses on dynamics, size, structure



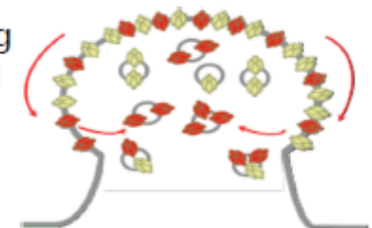
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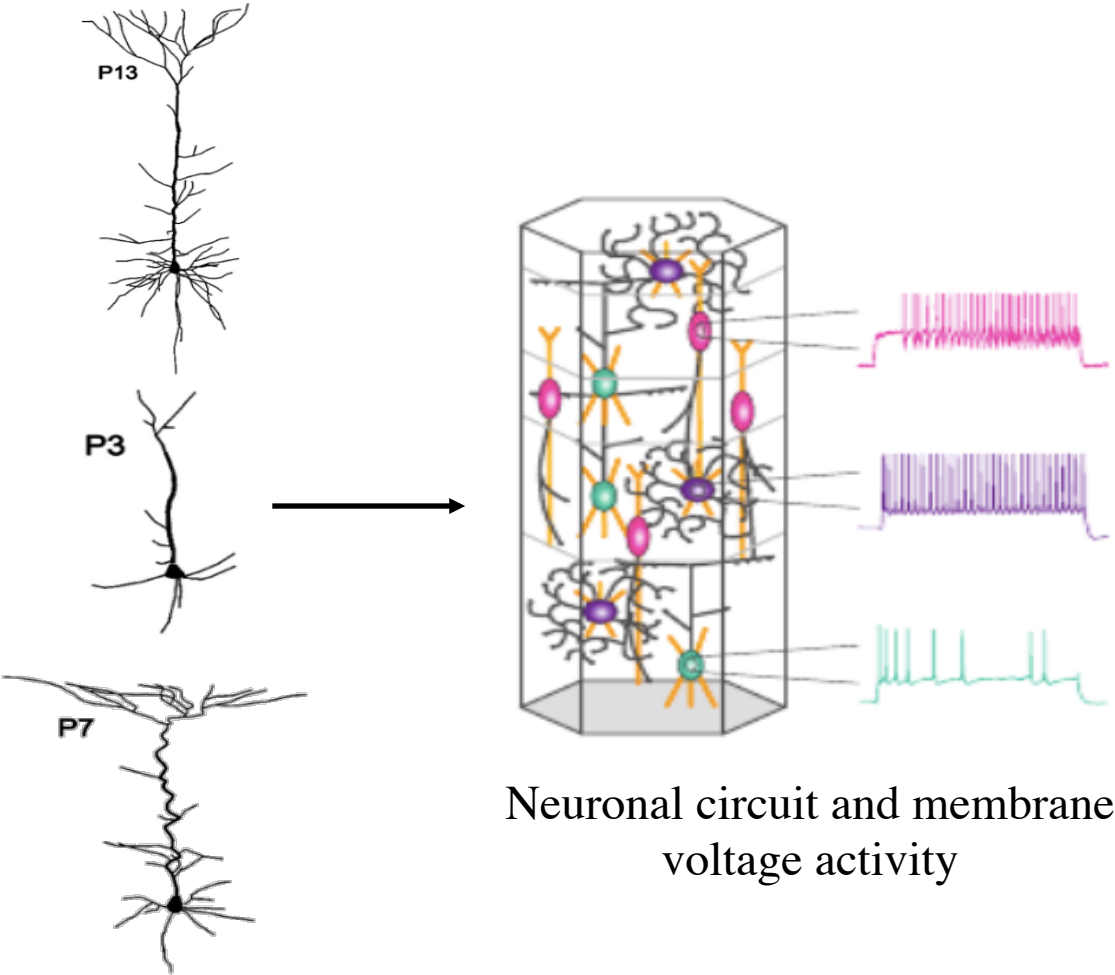


STEPS

A simulator for detailed models of neuronal signaling pathways at molecular level



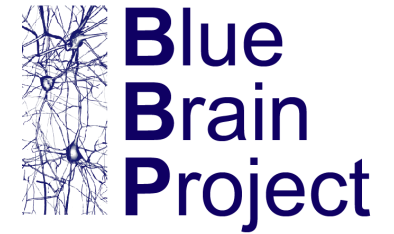
Model Reconstruction



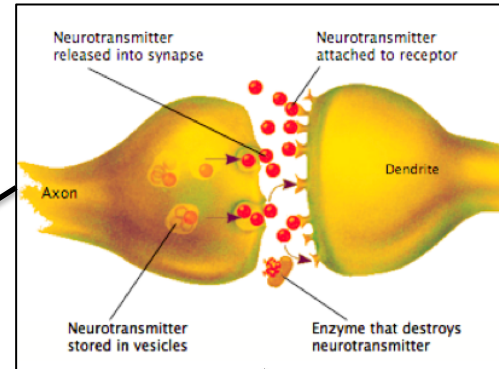
Morphologically detailed neurons

Neuronal circuit and membrane voltage activity

NEURON Modeling

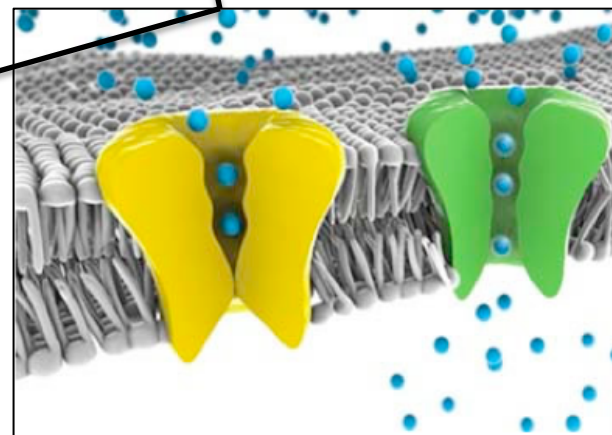
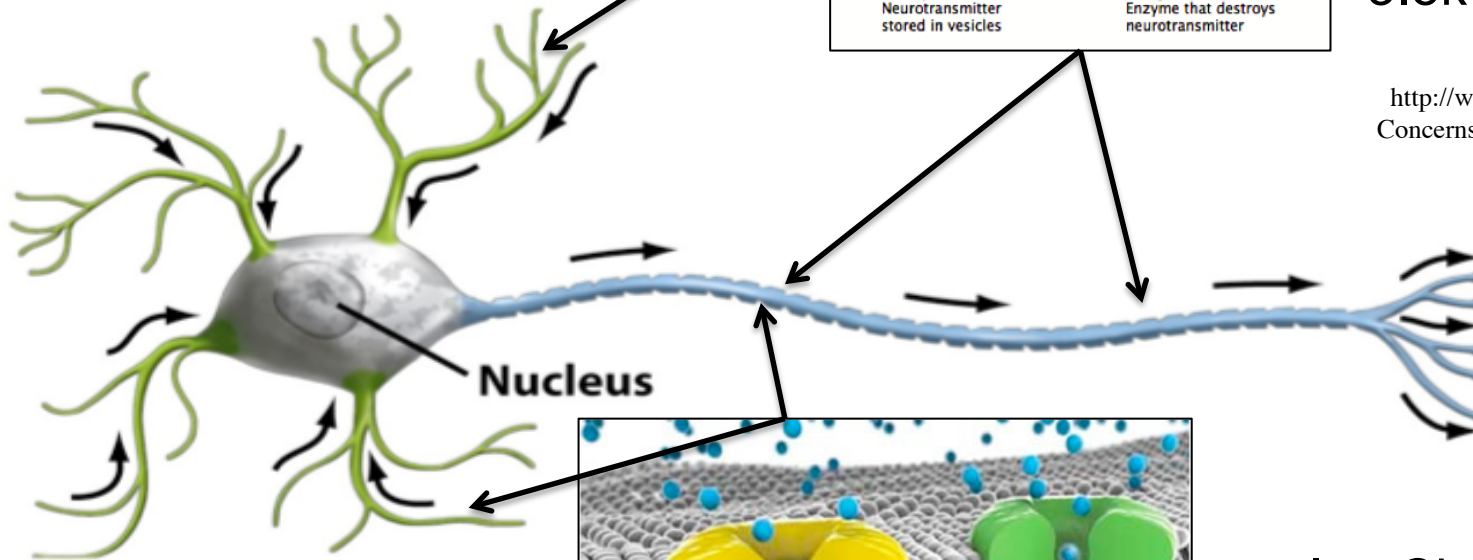


400 Compartments / Neuron



Synapse
3.5k / Neuron

<http://www.sailhome.org/Concerns/Excitotoxins.html>



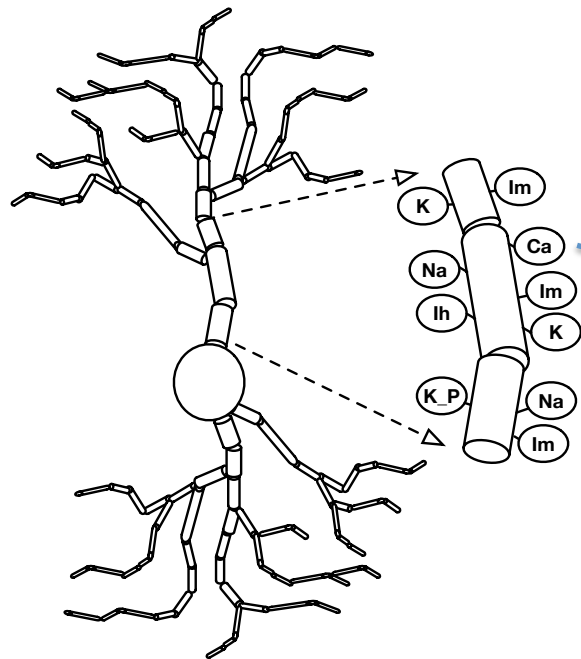
Ion Channel
3-5 / Compartment

Illustration by J.P. Cartailier. Copyright 2007, Symmation LLC

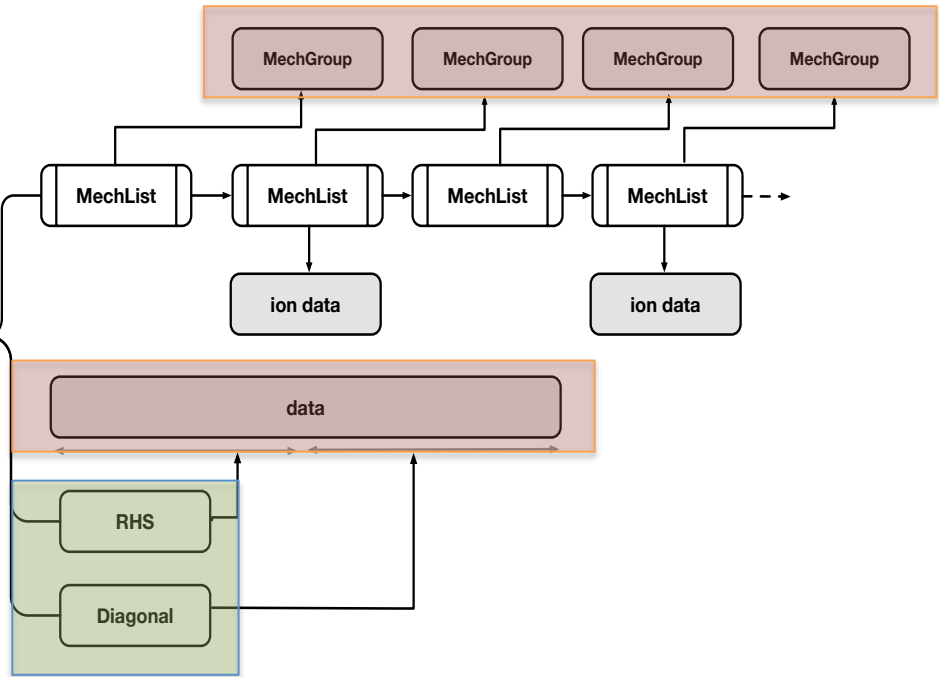
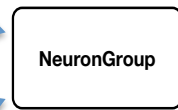
Synapses and Ion Channels referred as mechanisms

Need to solve $O(5k)$ non-linear mechanisms to assemble $O(400)$ dof 3-diagonal sparse matrix

NEURON Data Structures

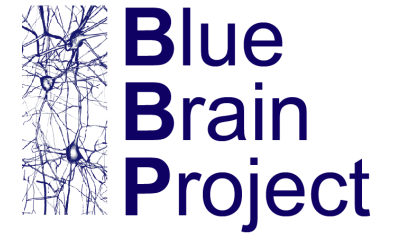


Biologist view:
compartment model

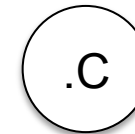
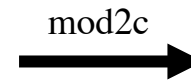


Memory View: In memory
representation of neurons

NModl DSL to .C to Support Scientists



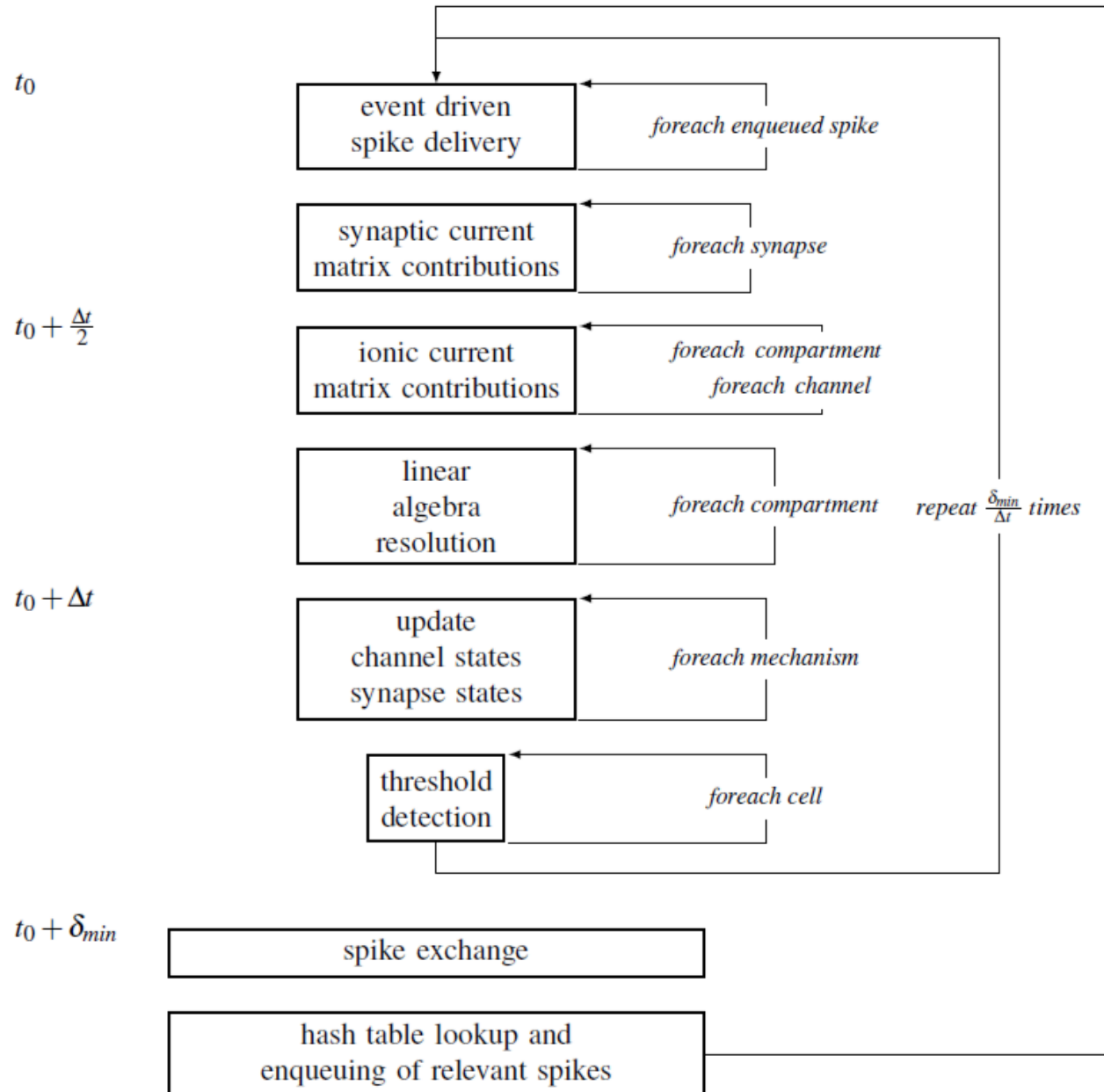
```
DERIVATIVE states {  
    LOCAL mAlpha, mBeta, mInf, mTau, lv, qt  
  
    qt = 2.952882641412121  
    lv = v  
  
    if(lv == -32){  
        lv = lv+0.0001  
    }  
  
    mAlpha = mAlphaf(lv)  
    mBeta = mBetaf(lv)  
    mInf = mAlpha/(mAlpha+mBeta)  
    mTau = (1/(mAlpha+mBeta))/qt  
    m' = (mInf-m)/mTau  
  
    v = lv  
}
```



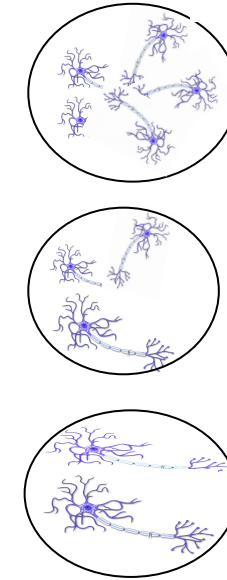
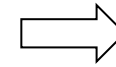
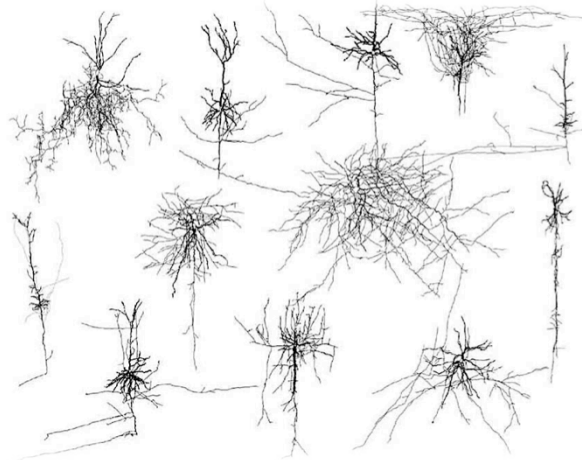
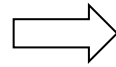
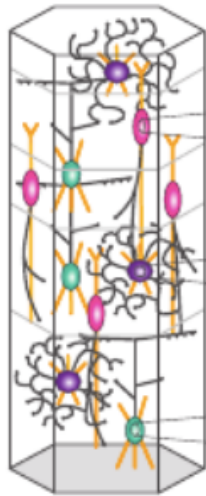
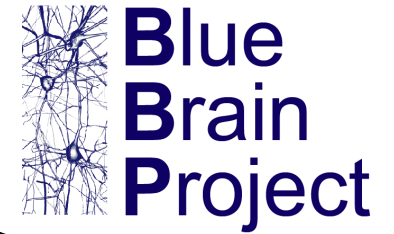
Scientists use domain specific
language NModl

Each .mod mechanism
file is converted to .c

NEURON Workflow



Static Load Balancing Workflow



Circuit Building

Neuronal problem domain created by neuroscientists

Cell Computational Complexity

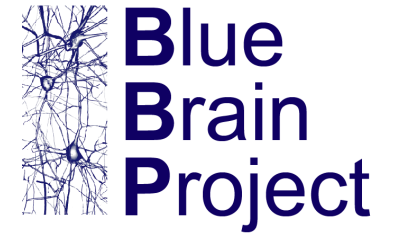
LPT algorithm calculates number of compartments & channels and their computational complexity

Neuron Groups

Construct neuron groups based on complexity factors

Less than 2% load imbalance on IBM Blue Gene/Q

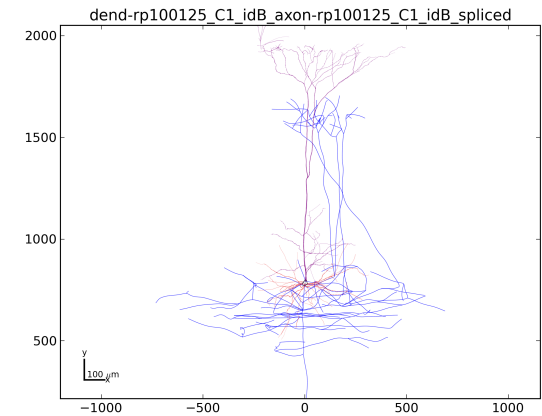
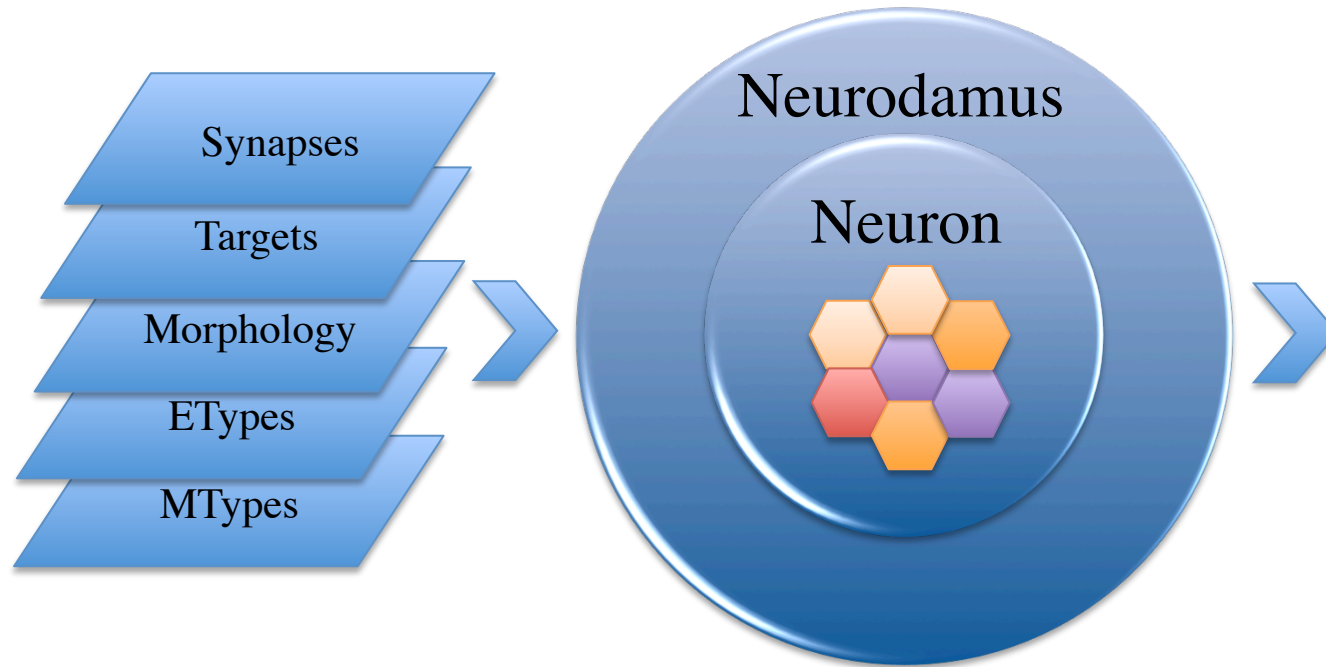
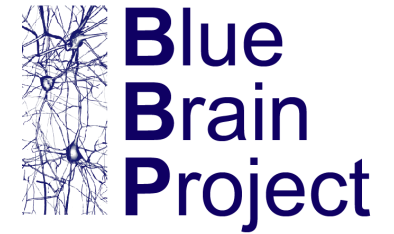
Going Further in Scale



Problem size and memory requirements for future simulations

parameters / brain type	rat	monkey	human
number of neurons	1×10^8	1×10^9	8×10^{10}
number of synapses	5×10^{11}	1×10^{13}	1×10^{15}
number of state variables	3.3×10^{12}	6.3×10^{13}	6×10^{15}
estimated size in memory	100 TiB	1 PiB	80 PiB

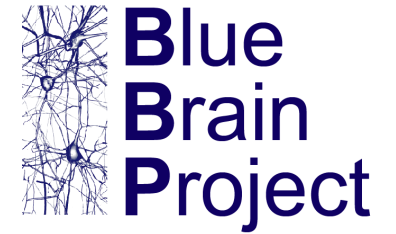
NEURON/Neurodamus: 12 MiB/Neuron



Fails at 756k neurons
Every process stores
900 MiB of global
information

2008	2010	2012
IBM Blue Gene/L	IBM Blue Gene/P	IBM Blue Gene/Q
8,192 cores	65,536 cores	65,536 cores
10k neurons	217k neurons	756k neurons

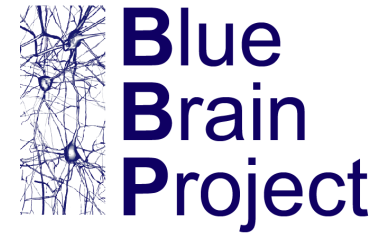
CoreNeuron Development Decision



Why?

- Simulate bigger models
- Decrease time to solution
- Support scalability at extreme scale
- Portability & extensibility on any HPC platform

CoreNeuron Development Decision



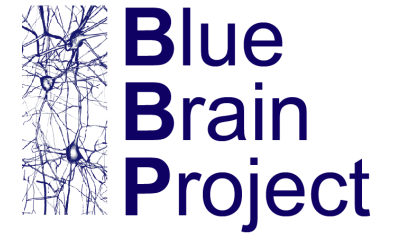
How?

- Have reduced & optimized data structures
- Vectorization using autovectorization
- Hybrid MPI / OpenMP with single MPI process per node
- Code reduction
 - Model configuration data structured are removed
 - Support of interpreter languages is not included
 - 15k lines vs 300k lines in NEURON

Highlights of CoreNeuron

- Simulation functionality of NEURON
- Reduced memory footprint (2MB/neuron vs 12MB/neuron)
- Three levels of parallelism
 - Nodes: collection of cell groups
 - Threads: each cell group has its (OpenMP) thread
 - Vectorization: computed mechanisms per cell group
- Spike delivery is done via `MPI_Allgather(v)`

Where is CoreNeuron in Scale

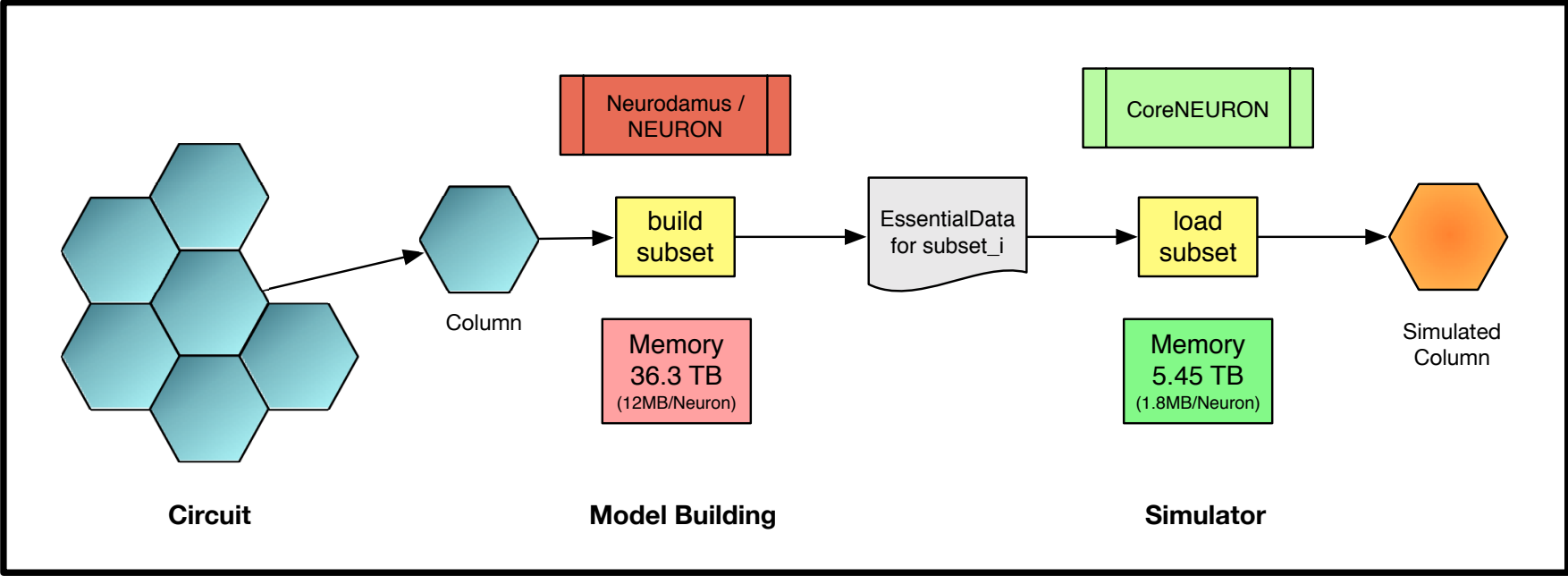
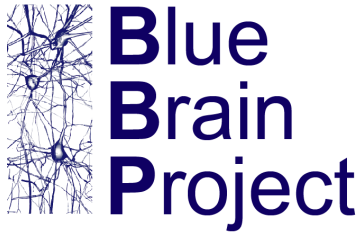


Problem size & memory requirements for future simulations

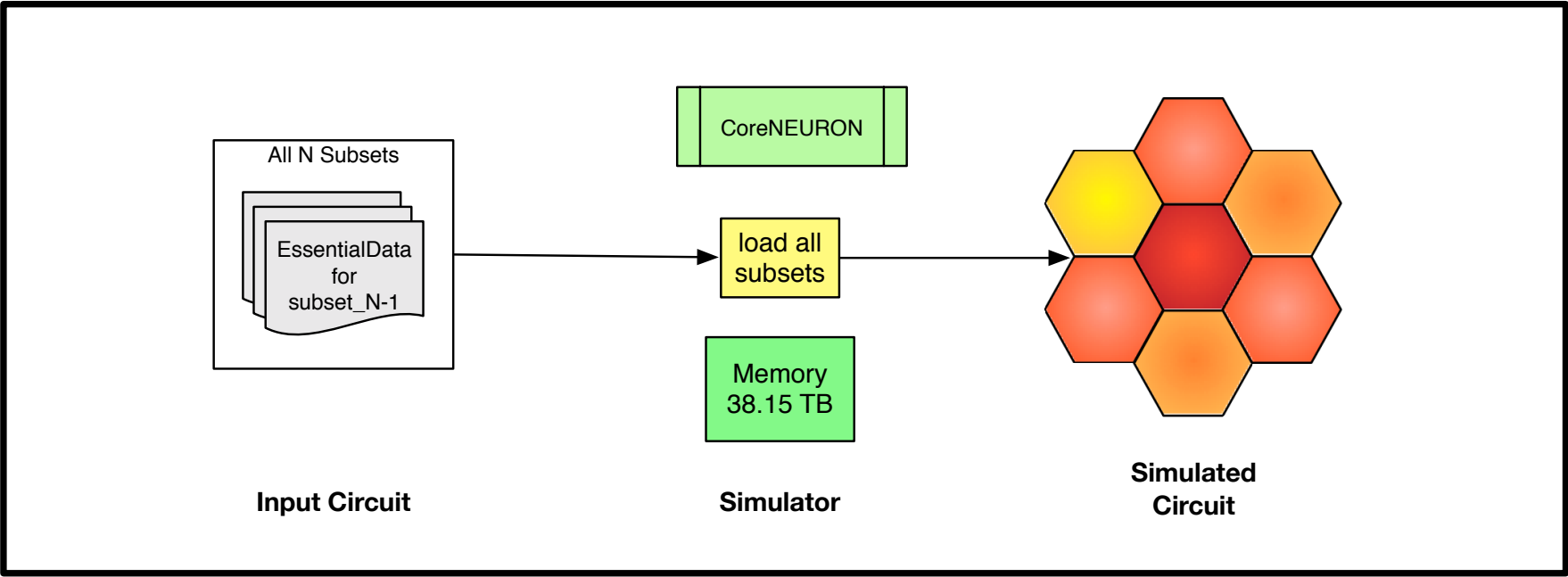
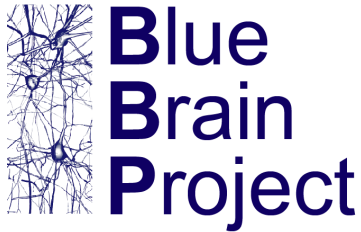
parameters / brain type	rat	monkey	human
number of neurons	1×10^8	1×10^9	8×10^{10}
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number of state variables	3.3×10^{12}	6.3×10^{13}	6×10^{15}
estimated size in memory	100 TiB	1 PiB	80 PiB

Today: the order of the rat brain size on a full JUQUEEN

NEURON & Neurodamus vs CoreNeuron

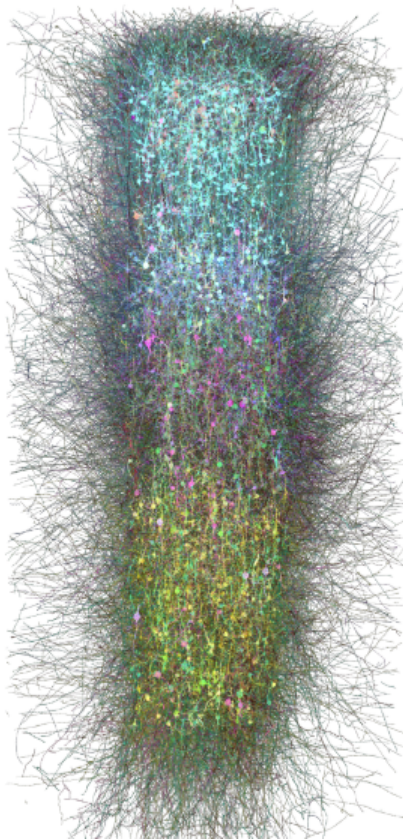


NEURON & Neurodamus vs CoreNeuron

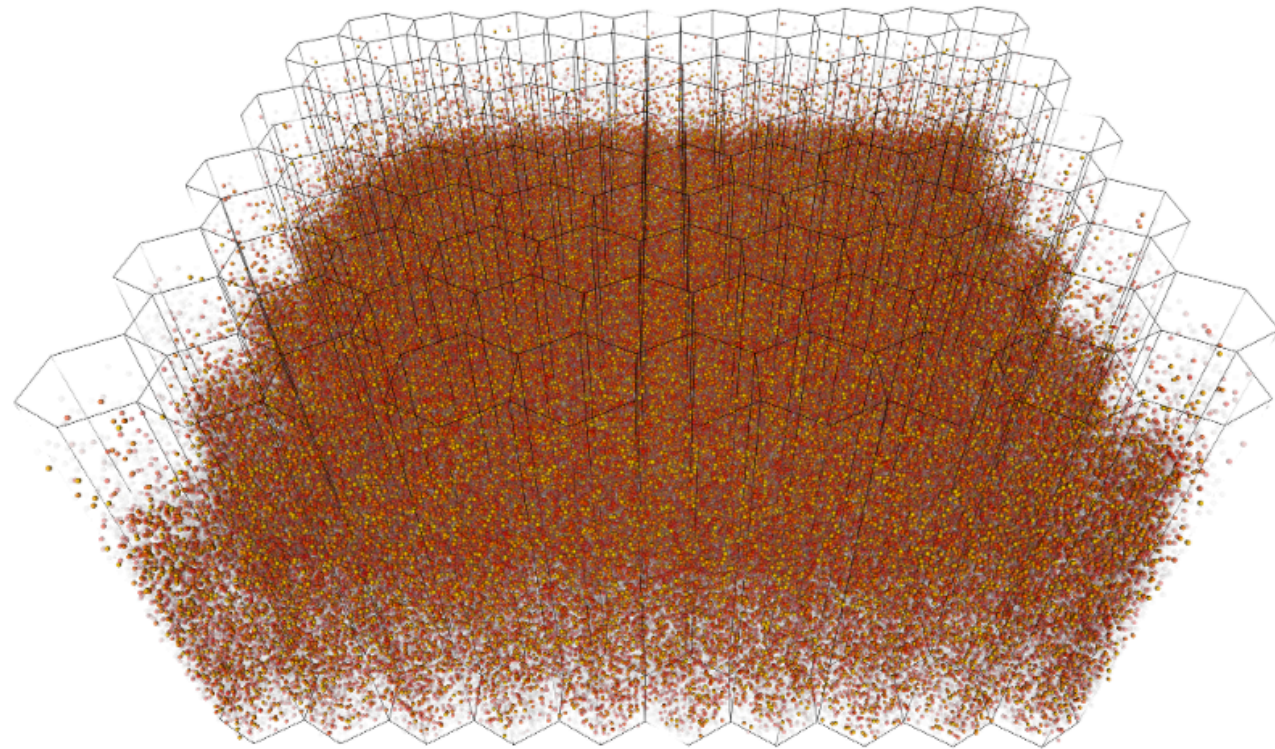


Use Case Description

Single column

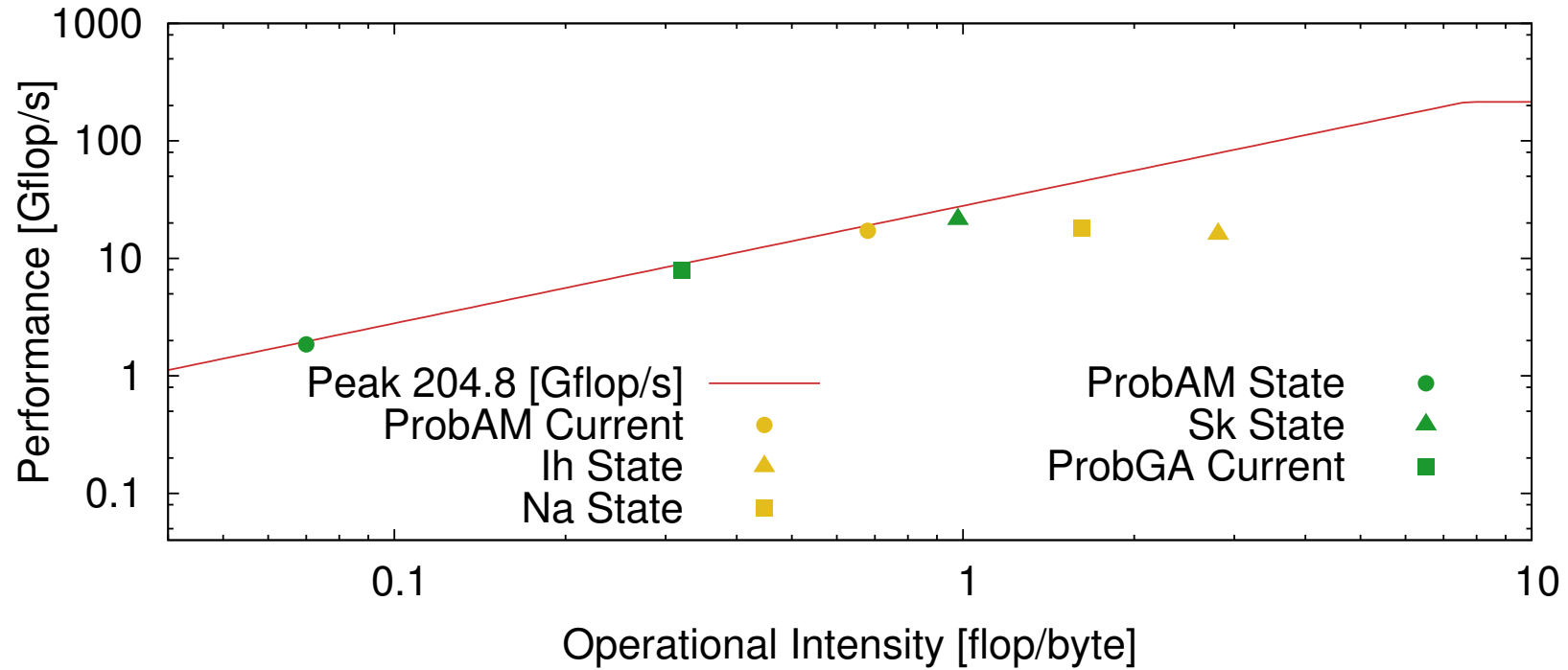
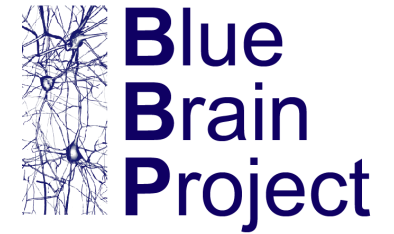


Top-side view of the circuit, 100 columns



- Initial circuit: 3 million neurons and 9 billion synapses
- Ready for in-memory duplication. Default size: 24 million neurons
- I/O size to read: 5 TB

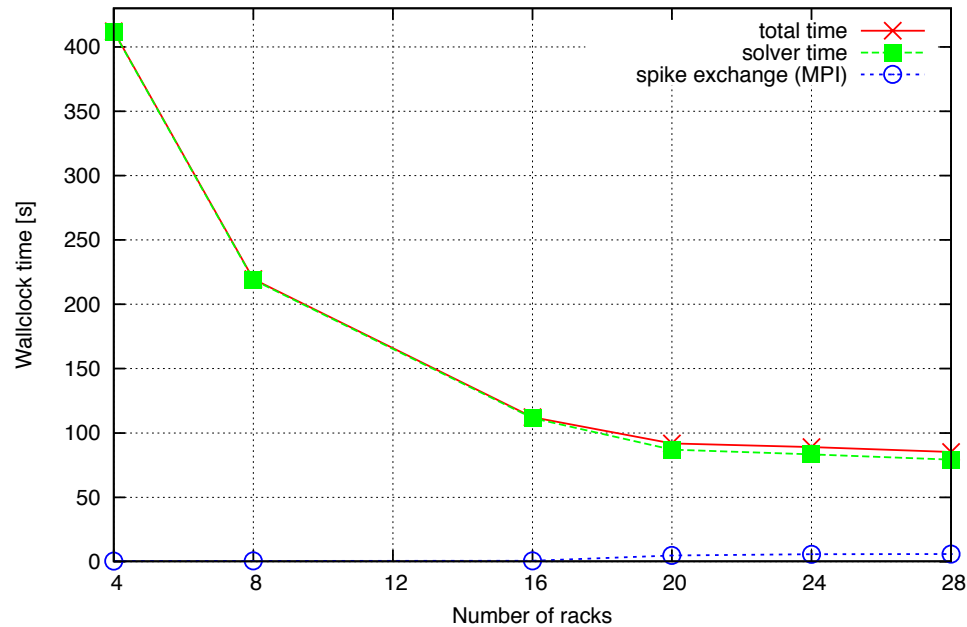
IBM Blue Gene/Q Node Performance Analysis



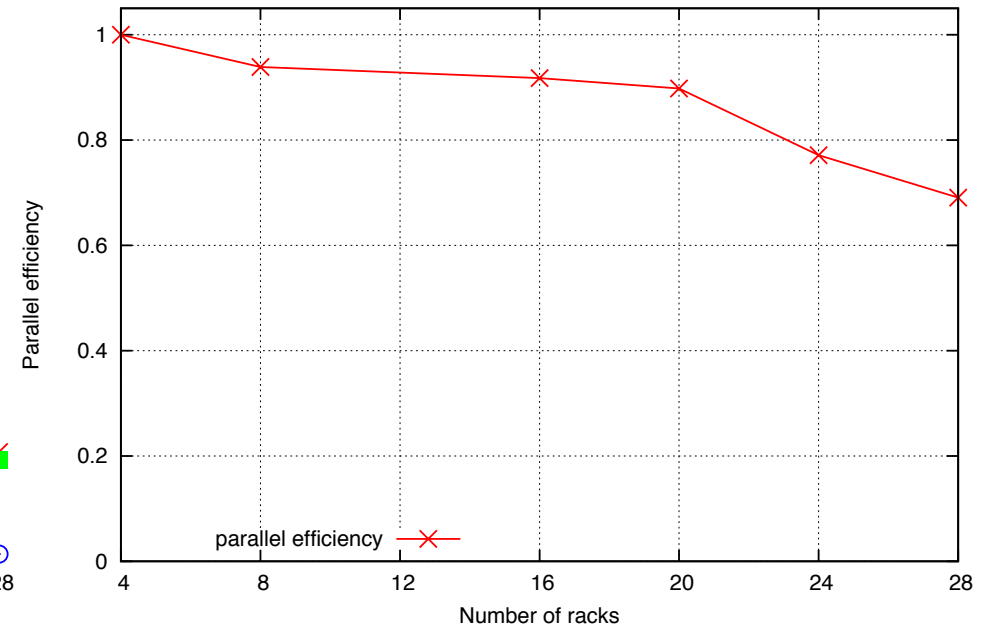
- Most kernels (ProbAM Current, etc.) memory bandwidth limited
- Some (*Ih State*, *Na State*) can be vectorized to get better performance

Strong Scaling Studies

Time breakdown for the strong scaling studies



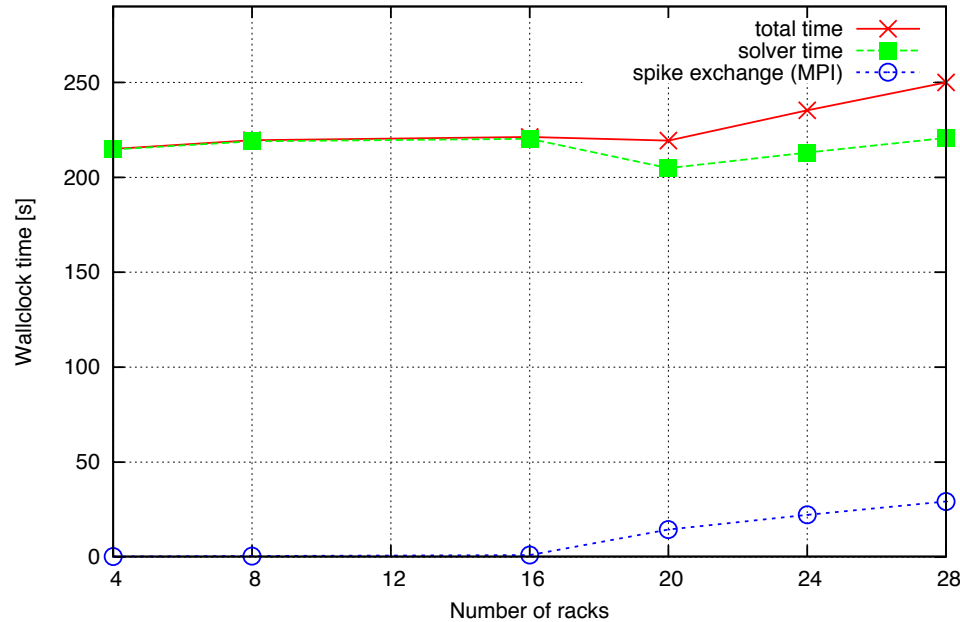
Strong scaling



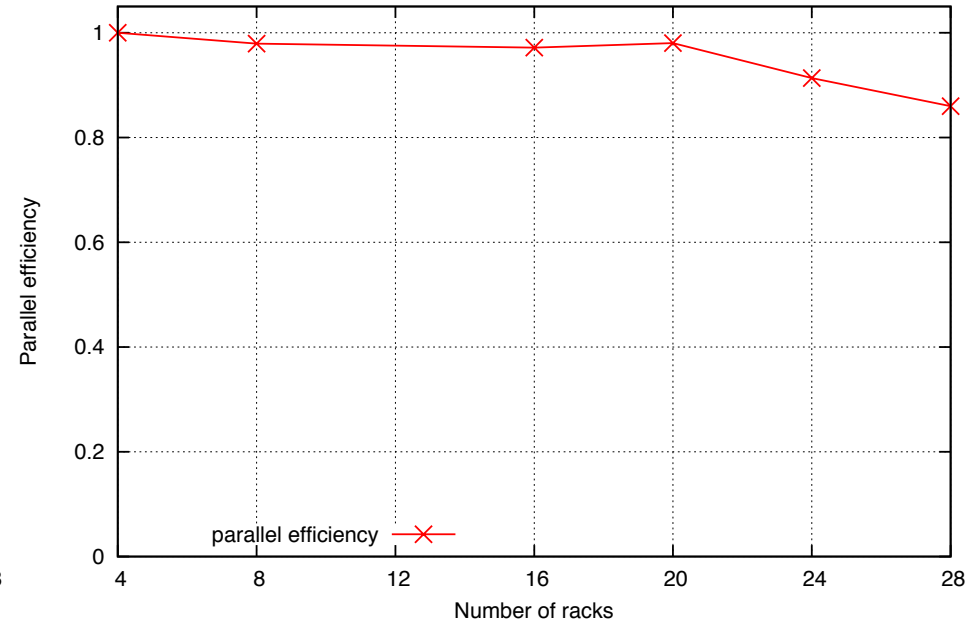
- 1 MPI task per node, 64 OpenMP threads per node
- 10 milliseconds of biological time
- 24 million neurons for each run (from ~90% of DRAM to ~10% of DRAM)
- No uniform distribution of data across 20, 24, 28 racks \Leftrightarrow artificial load imbalance
- Up to 16 racks: 10% of strong scaling efficiency loss

Weak Scaling Studies

Time breakdown for the weak scaling studies



Weak scaling



- 1 MPI task per node, 64 OpenMP threads per node
- 10 milliseconds of biological time
- 2906 neurons per node: from 12 million to 82 million neurons (~50% of DRAM)
- Parallel efficiency is nearly optimal up to 20 racks

Closing Remarks

- Full JUQUEEN machine simulation
 - 28 racks, utilizing all 1,835,008 threads
 - 15.9 GB of node DRAM, 155 million neurons (duplicated circuit)
- Memory reduction 6-8 times comparing to NEURON
- Improved on-node performance, ready for larger scale

Further Steps

- Ongoing reduction of memory footprint
- Disk-to-memory data management: utilize HDF5
- Implementation simplification
- Introduction of clear C++ API
- Light-weight python interface for high-level API
- Exposing more parallelism in mechanisms & spike exchange