

Session 3: FAIR approaches for computational neuroscience

Do we have the tools and resources to develop FAIR large-scale brain circuit models?

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Outline

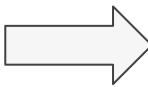
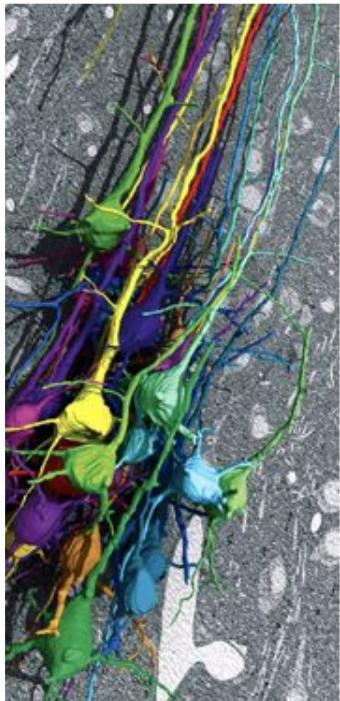
1. Modeling workflow example: large-scale model of motor cortex
2. FAIR tools/resources for each step of the workflow
 - a. Gather and preprocess data
 - b. Implement model
 - c. Tune and validate model
 - d. Experiments and predictions
 - e. Share and disseminate

1

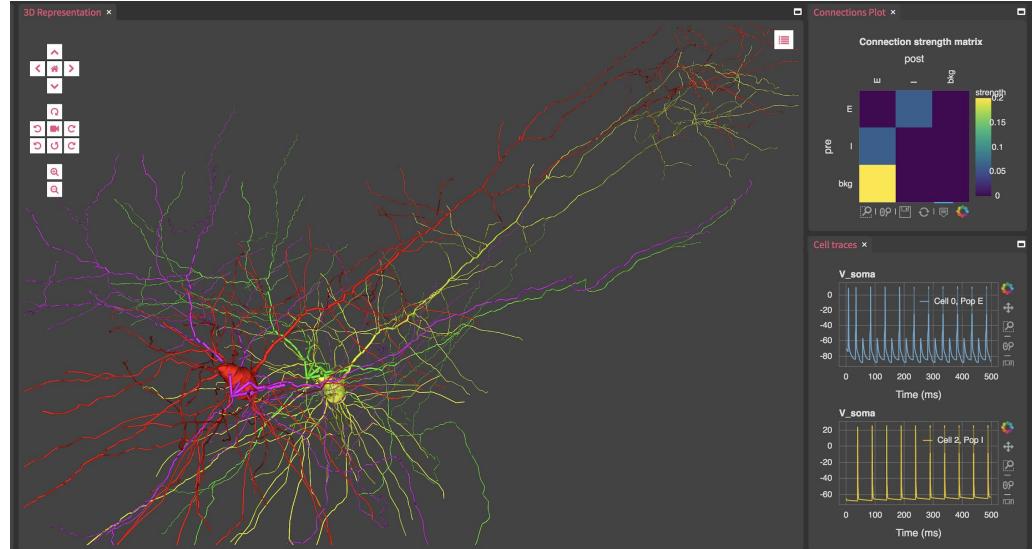
Modeling workflow example:
large-scale model of motor cortex

Computational simulations of the brain

Experiments

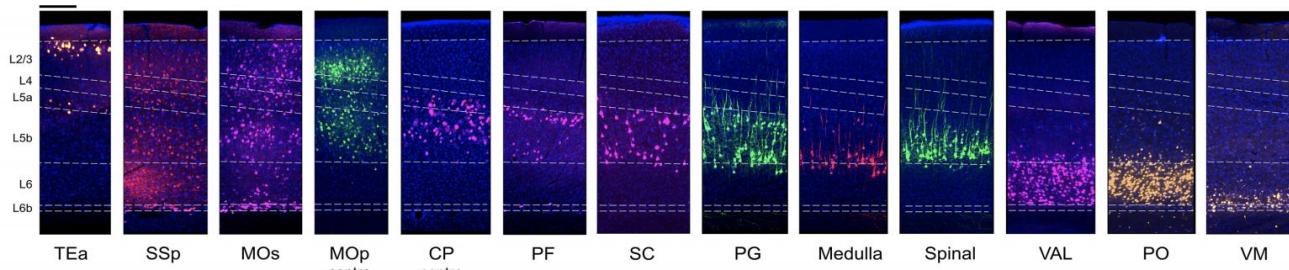


Simulation

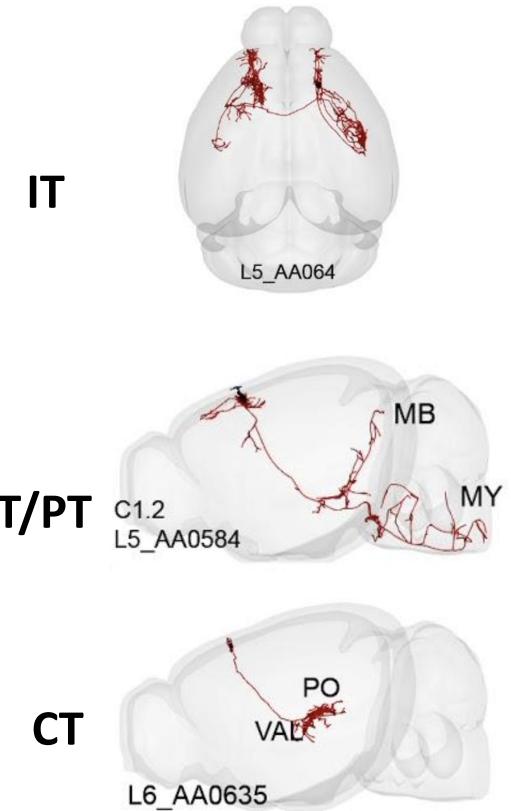
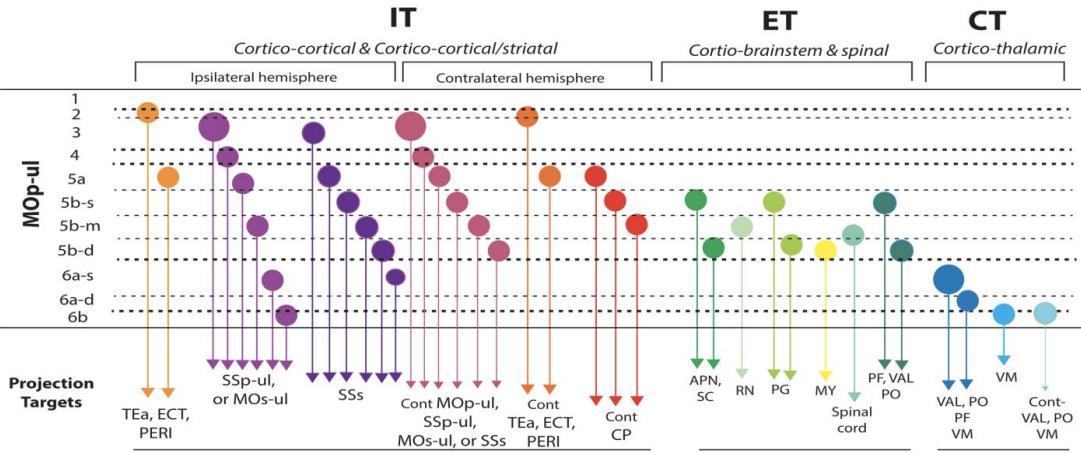


Accumulation of experimental data

Mouse M1 cell types by projection target

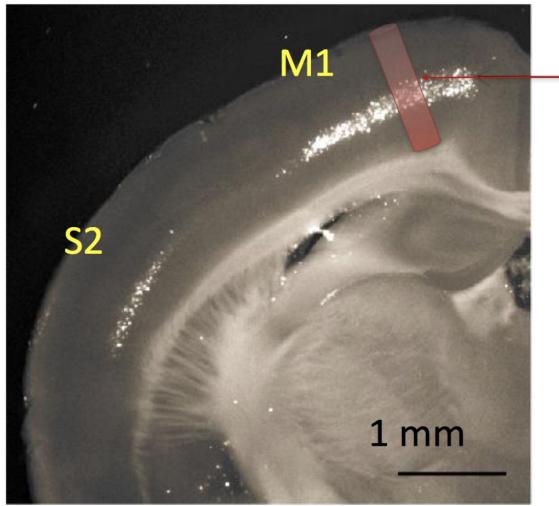


c

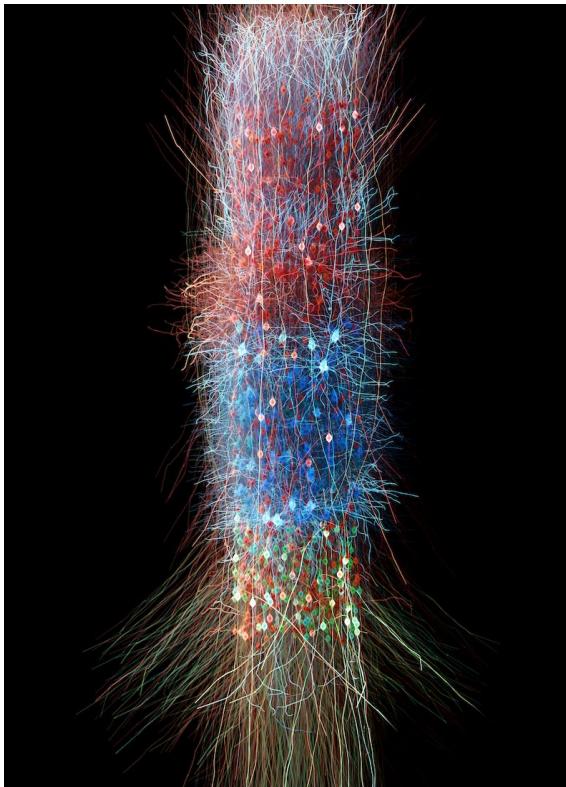


Data-driven model of motor cortex circuits

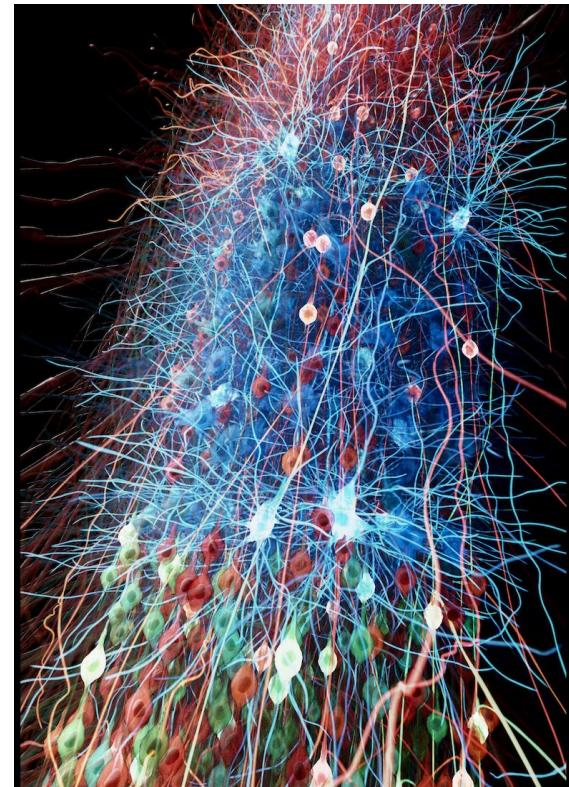
300 um diameter column



10,000 neurons

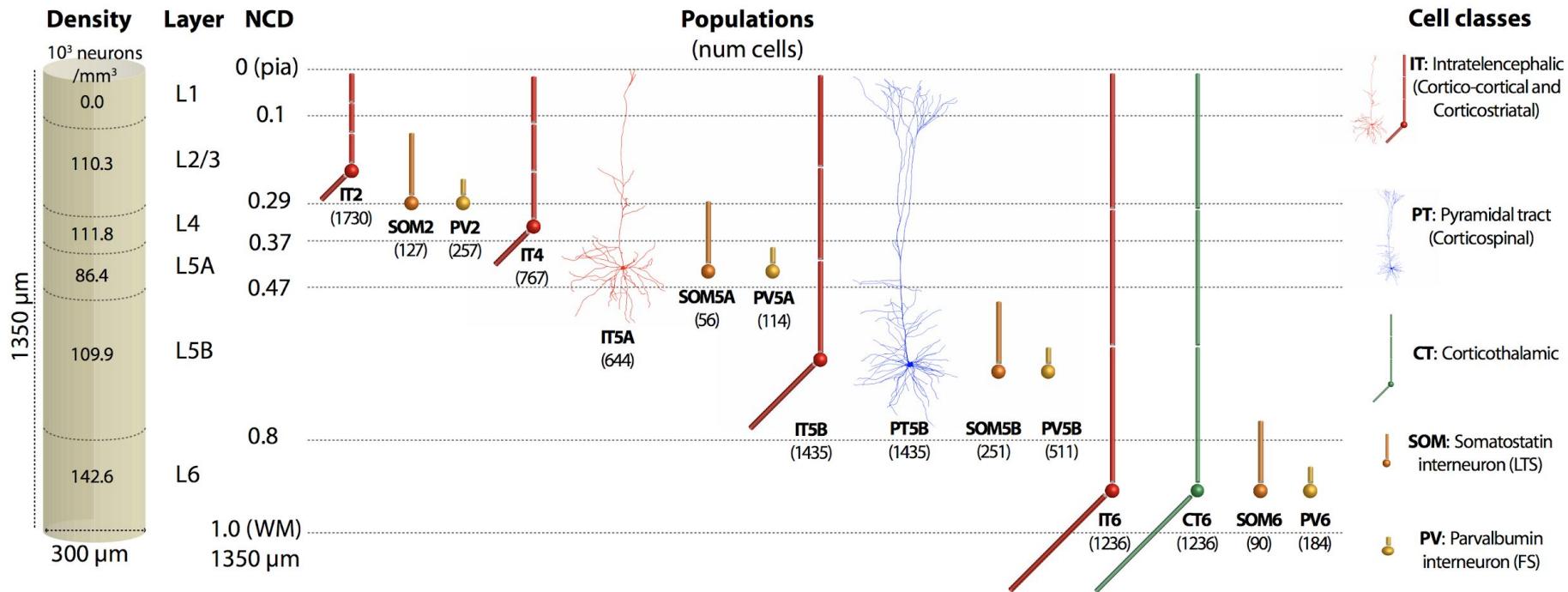


30 million connections

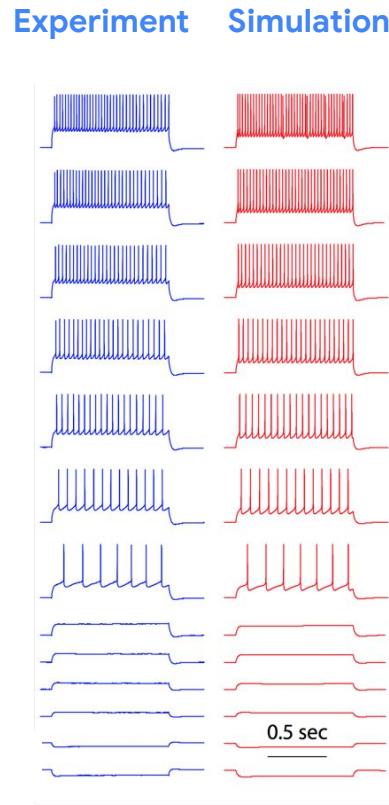
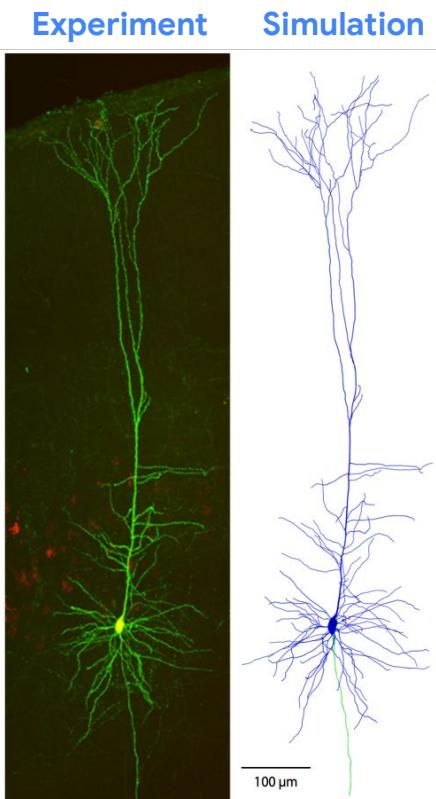


M1 model: cell types and populations

A

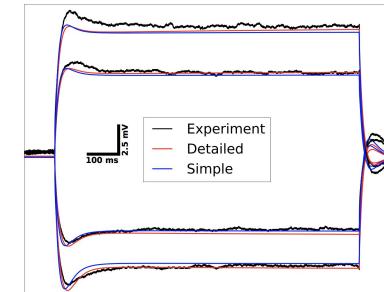
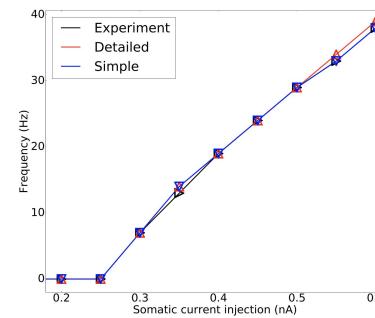


M1 model: single neuron models



Reproduce morphology and physiology of real neurons

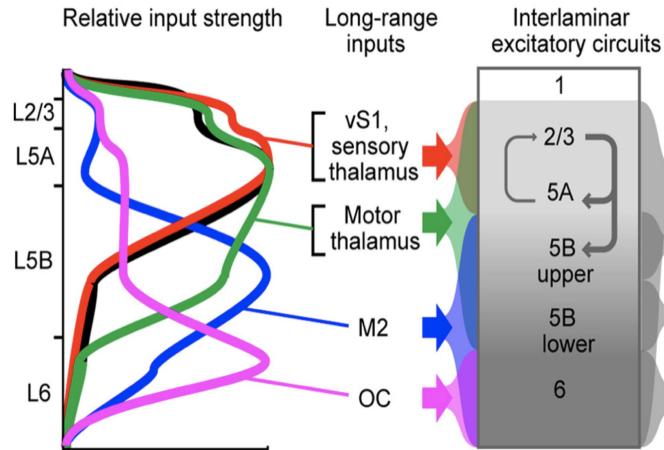
Ionic channel parameters optimized to match data (Na, Kdr, Ka, Kd, HCN, CaL, CaN, KCa)



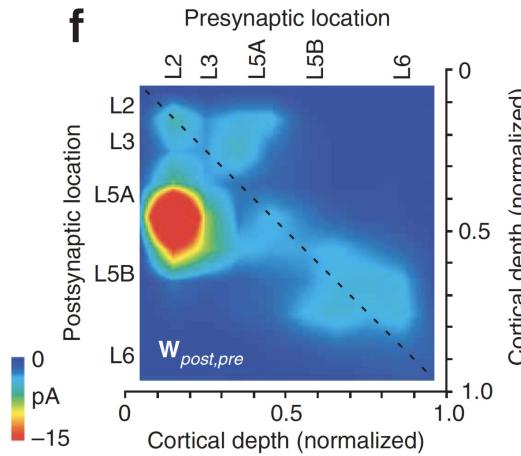
M1 model: connectivity

Incorporates connectivity data at multiple scales

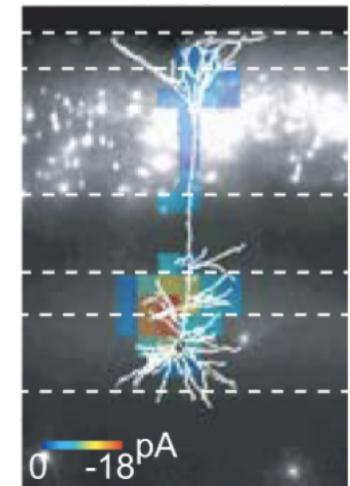
Long-range inputs



Local microcircuits

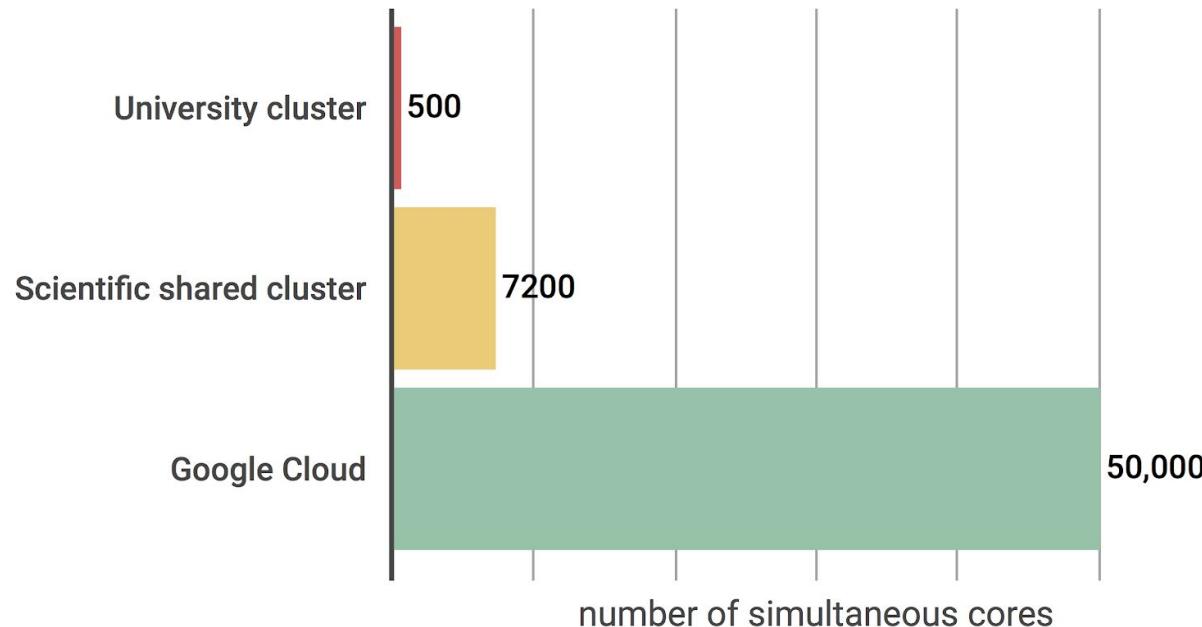


Dendritic inputs

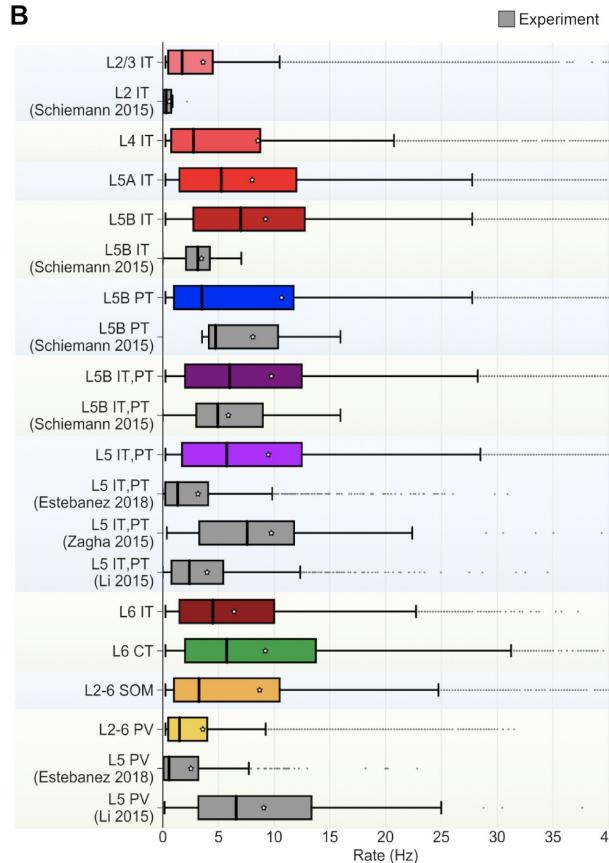
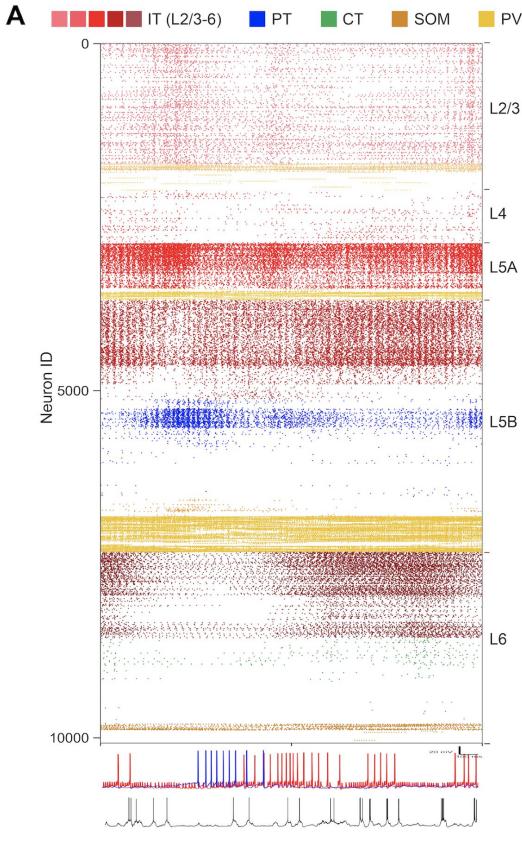


Parallel Simulation on Supercomputers

1 simulated second → 1 hour on 100 computer cores



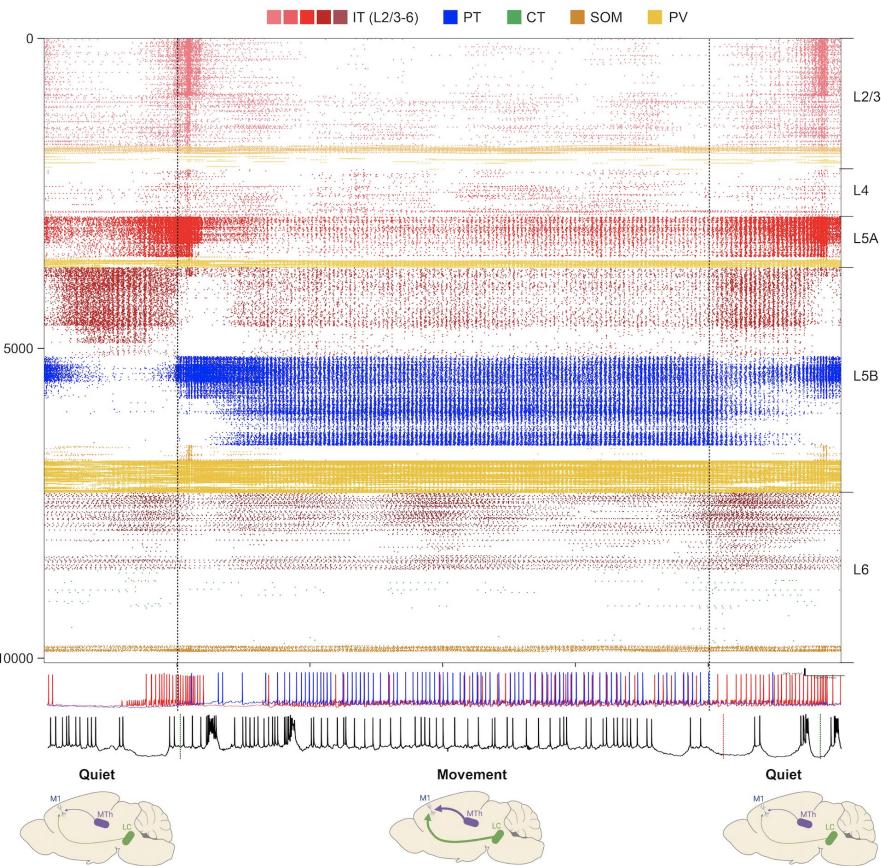
Motor cortex model results: spiking



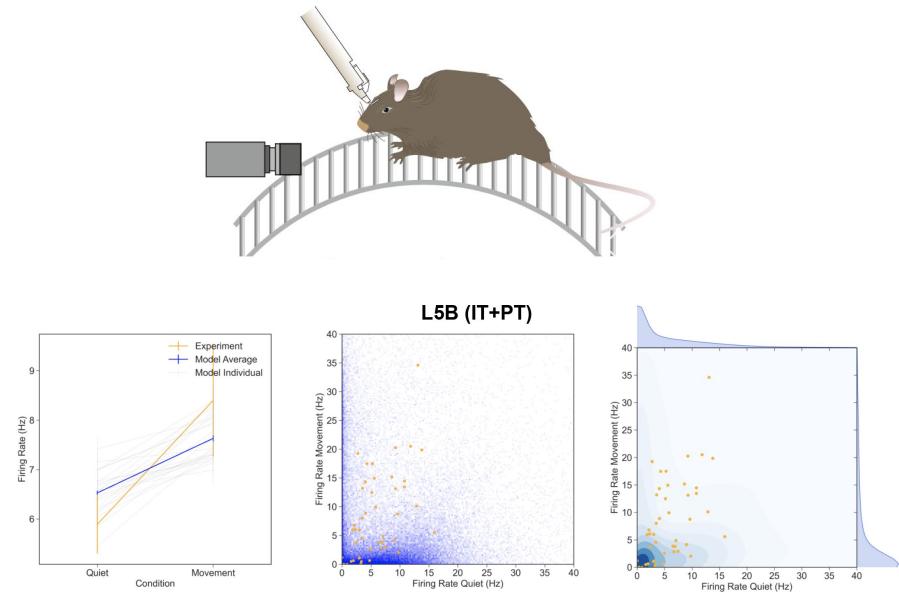
- Activity depends on cell type and layer
- Firing rate stats match experimental data

Motor cortex model results: molecules to behavior

A

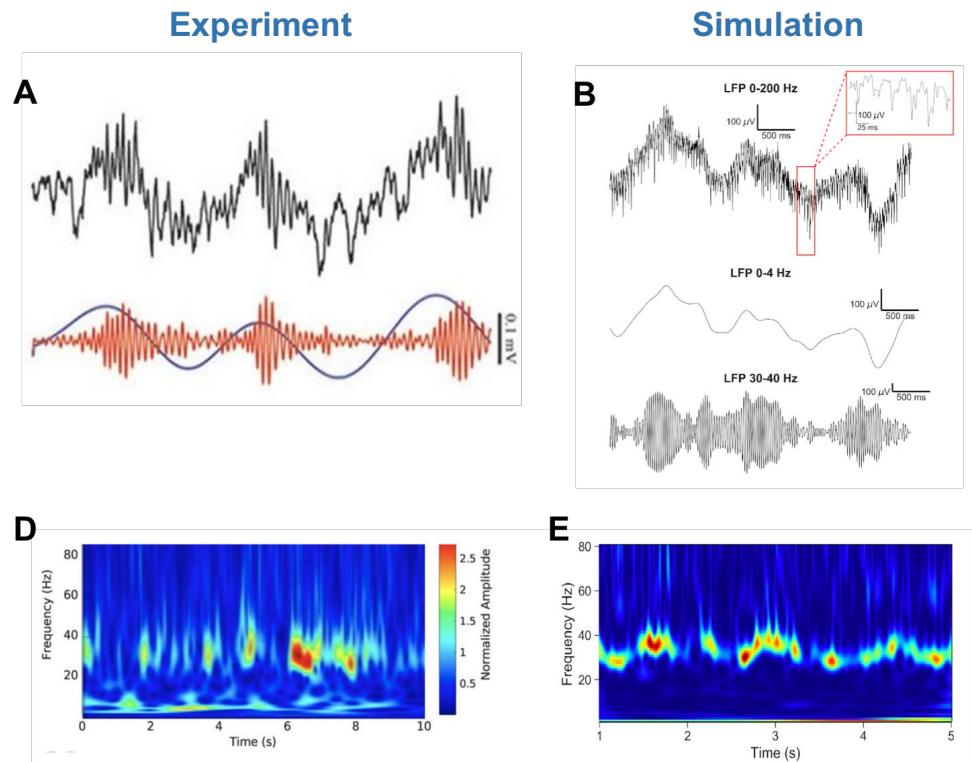
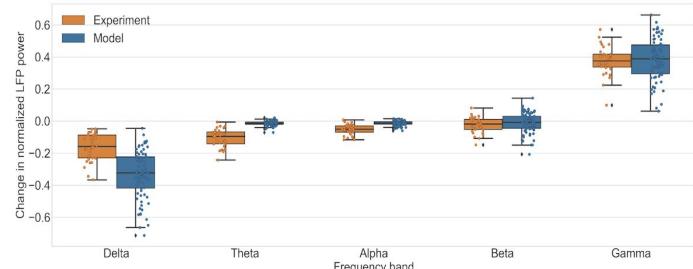


- Reproduces dynamics related to *in vivo* changes in behavior



Motor cortex model results: oscillations

- Reproduces LFP oscillations
- Phase-amplitude coupling
- Behavior-related changes in LFP

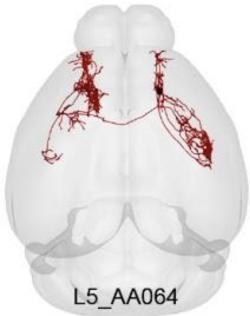


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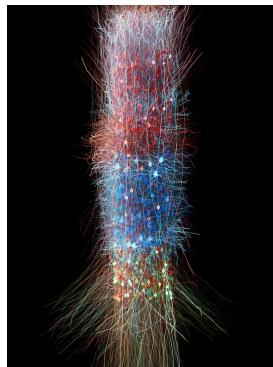
FAIR tools/resources for each step of the workflow

Modeling workflow

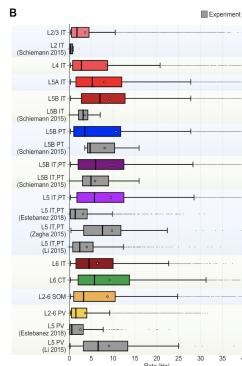
1. Gather and preprocess data



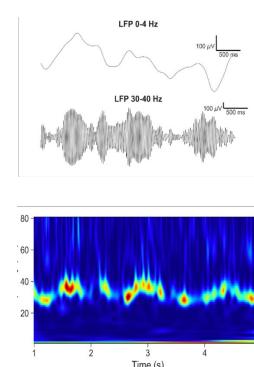
2. Implement model



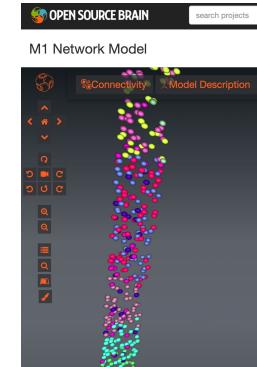
3. Validate model



4. Experiments + predictions

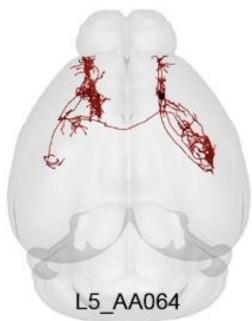


5. Share and disseminate

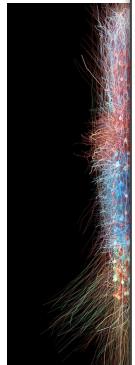


Modeling workflow

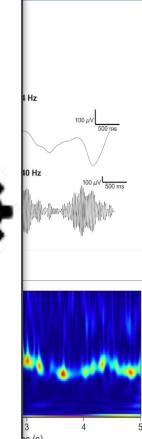
1. Gather and preprocess data



2. Integrate data



3. Experimentations
and validations



5. Share and disseminate

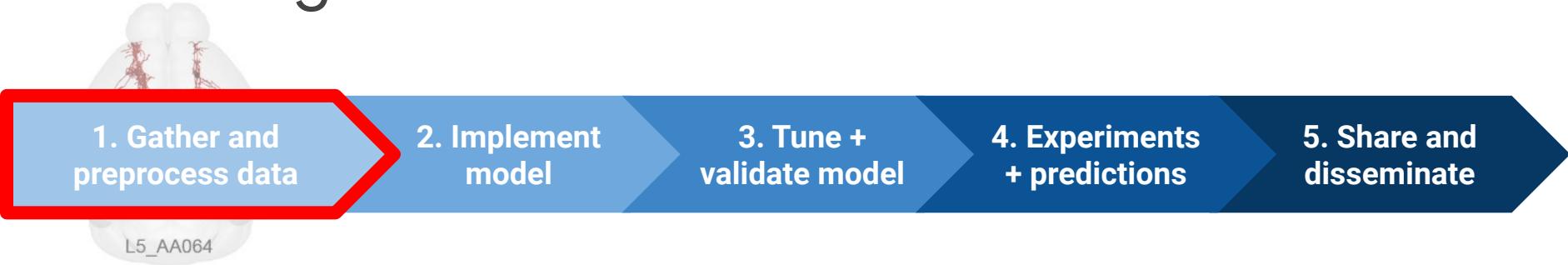
OPEN SOURCE BRAIN search projects

M1 Network Model

Connectivity Model Description

The interface shows a 3D brain model with colored dots representing nodes or neurons. A legend on the left indicates node types: blue for 'Connectivity' and orange for 'Model Description'. A sidebar on the left contains various search and filter icons.

Modeling workflow



Collect experimental data required for model

- Google Scholar
- ModelDB
- OSB + NeuroML DB
- NeuroElectro
- NeuroMorpho
- CRCNS
- Allen Brain Map



- Paperpile
- Google Drive / Sheets
- E-notebook (VScode + org-mode)
- WebPlotDigitizer

Modeling workflow



1. Gather and preprocess data

2. Implement model

3. Tune + validate model

4. Experiments + predictions

5. Share and disseminate

Collect experimental data required for model

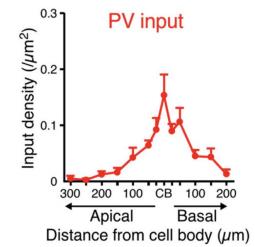
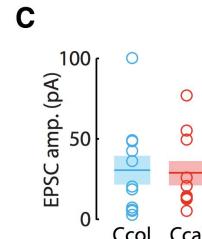
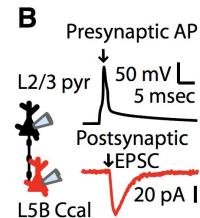
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Preprocess data so can be used in model

- Python



Store provenance of data used in model

- Python

Modeling workflow: what is missing?



1. Gather and preprocess data

2. Implement model

3. Tune + validate model

4. Experiments + predictions

5. Share and disseminate

L5_AA064

Tools for automated search/extraction/preprocessing of data

- Specific queries: "unitary connection EPSP amplitudes (in mV) between L5B PT cells and L2/3 PV cells in mouse primary motor cortex during spontaneous activity"
- Returns data in a standardized format
- Potential existing tools/resources:
 - <http://g-node.github.io/nix/>
 - <https://knowledge-space.org/>
 - <https://bluebrainnexus.io/>



Modeling workflow

1. Gather and preprocess data

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Backend simulator

- NEURON

Network model building tool

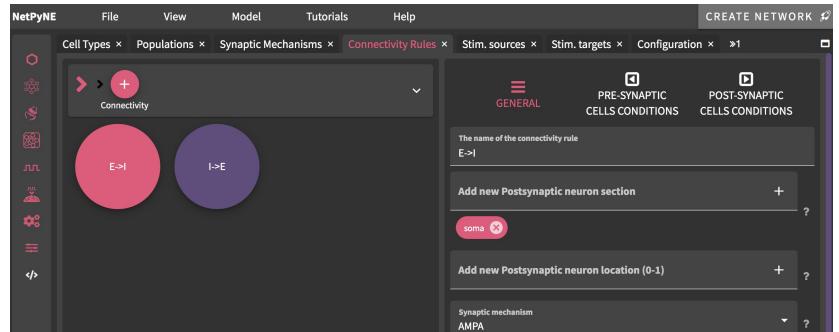
- NetPyNE
- Others: BMTK Bionet, PyNN

Tracking/managing model versions

- NetPyNE
- Github
- E-notebook (VScode + org-mode)



```
## Cell connectivity rules
netParams.connParams['S->M'] = {
    'preCnds': {'pop': 'S'},
    'postCnds': {'pop': 'M'},
    'probability': 0.5,
    'weight': 0.01,
    'delay': 5,
    'synMech': 'exc'}
```



Modeling workflow

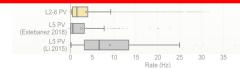
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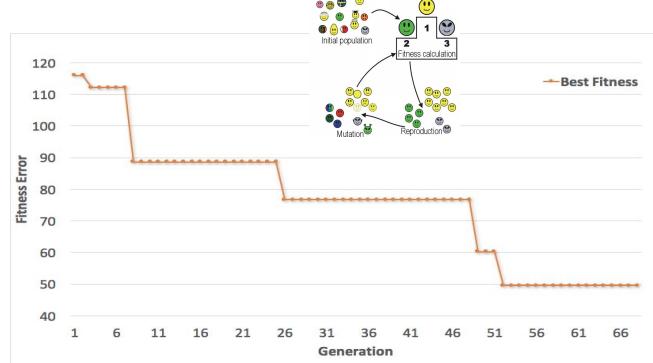
4. Experiments + predictions

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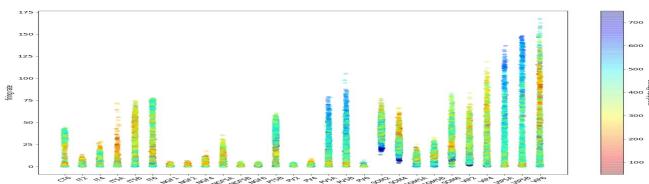
Tune model parameters to match experimental data

- Modeling: NEURON / NetPyNE
- Optimization: Inspyred, Optuna (others: BluePyOpt, NeuroTune)
- HPCs: NSG, XSEDE, GCP, E-BRAINS



Tracking/managing model version and simulations

- NetPyNE
- Github
- E-notebook (VScode + org-mode)



Modeling workflow

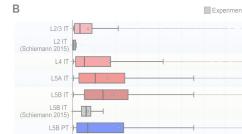
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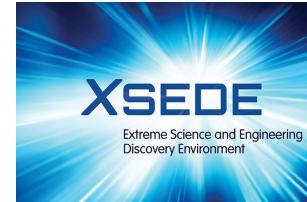
4. Experiments + predictions

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EBRAINS

Tracking/managing model version and simulations

- NetPyNE
- Github
- E-notebook (VScode + org-mode)



Google Cloud Platform

Modeling workflow

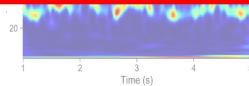
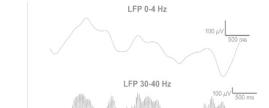
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Tune model parameters to match experimental data

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```
* VERSIONS
** v7 - Added template for connectivity
** v8 - Added cell types
** v9 - Added local connectivity
** v10 - Added thalamic populations from prev model
** v11 - Added thalamic conn from prev model
** v12 - Added CT cells to L5B
** v13 - Added CT cells to L5A
** v14 - Fixed L5A & L5B E cell densities + added CT5A & CT5B to 'Epops'
** v15 - Added cortical and thalamic conn to CT5A and CT5B
```

Tracking/managing model version and simulations

- NetPyNE
- Github
- E-notebook (VScode + org-mode)

```
* SIMS
** v21_batch3 - Param sweep 6 conn params; adjusted EEGain and IIGain; fixed bug IEGain...
** v21_tune - adjusting bkg weights...
** v22_batch1 - bkg weights for all pops (E+I 40 hz) ...
** v22_batch2 - bkg weights for all pops (only E 40hz) ...
** v22_batch3 - bkg weights for all pops (E 20hz apicdend, I 40 Hz perisom) ...
** v22_batch4 - bkg weights for all pops (E 20hz apicdend 2*weight, I 40 Hz perisom) ...
** v22_batch5 - bkg weights for all pops (E 40hz apicdend, I 40 Hz perisom 2*weight) ...
** v22_batch6 - bkg weights for all pops (E 40hz apicdend, I 40 Hz perisom) ...
```

Modeling workflow: what is missing?

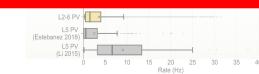
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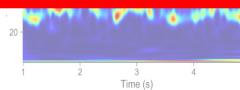
2. Implement model



3. Tune + validate model



4. Experiments + predictions



5. Share and disseminate

Tune model parameters to match experimental data - more standard methods/formats

- SciUnit / SciDash
- OSB NWB Explorer

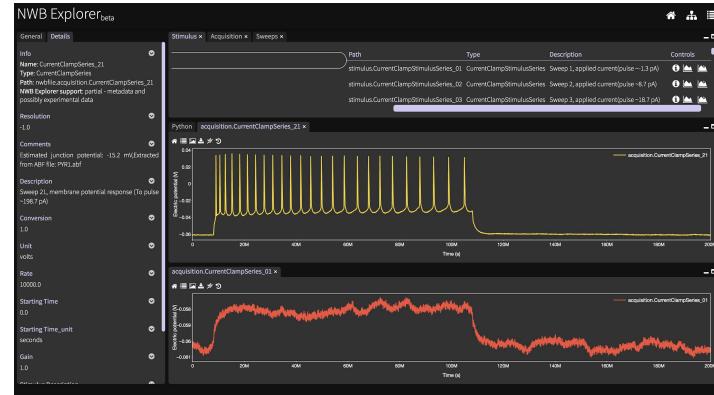


SciUnit

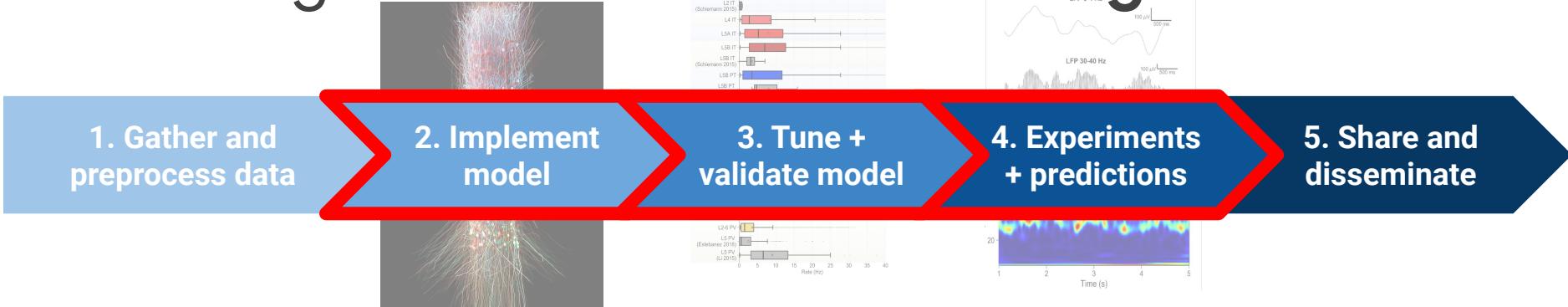


NeuronUnit

Name	Score	Score Type	Model
InputResistanceTest	0.296		ReducedModel(QuickModel)
InputResistanceTest	0.296		ReducedModel(QuickModel)
InputResistanceTest	0.296		ReducedModel(QuickModel)
InputResistanceTest	78.634		ReducedModel(QuickModel)



Modeling workflow: what is missing?



More standard methods/formats to tune model parameters to match experimental data

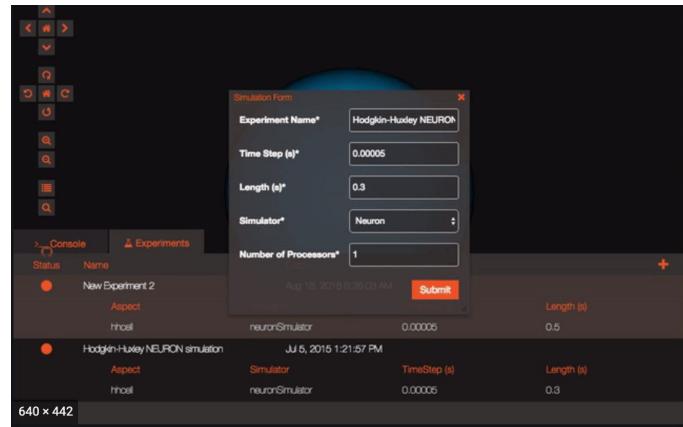
- SciUnit / SciDash
- OSB NWB Explorer

Tracking/managing model version and simulations

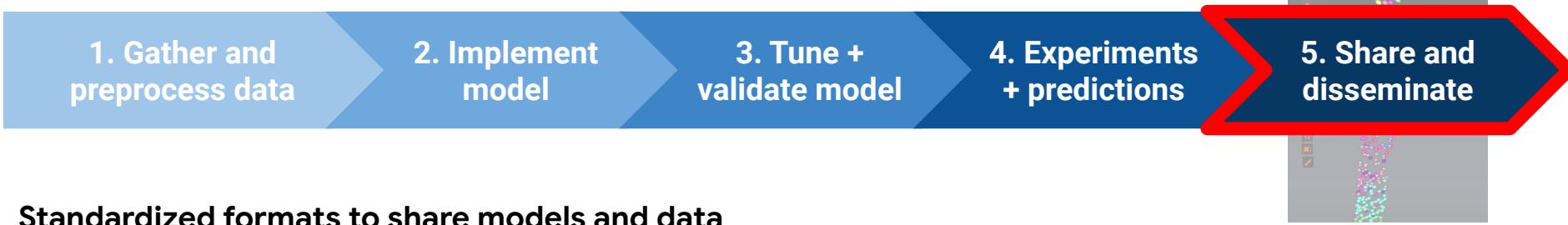
- Integrated / systematic tool and standard format:

e.g. SimTracker, OSB, NetPyNE GUI

- model version and list of changes
- provenance of model parameters
- simulation parameters, associated results



Modeling workflow

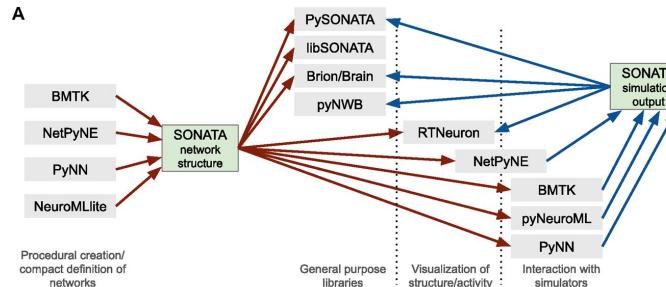


Standardized formats to share models and data

- NetPyNE
- NeuroML
- SONATA
- NWB (in progress)

Platforms/tools to share models and data

- ModelDB
- OSB
- GitHub
- E-BRAINS



Modeling workflow: what is missing?



1. Gather and preprocess data

2. Implement model

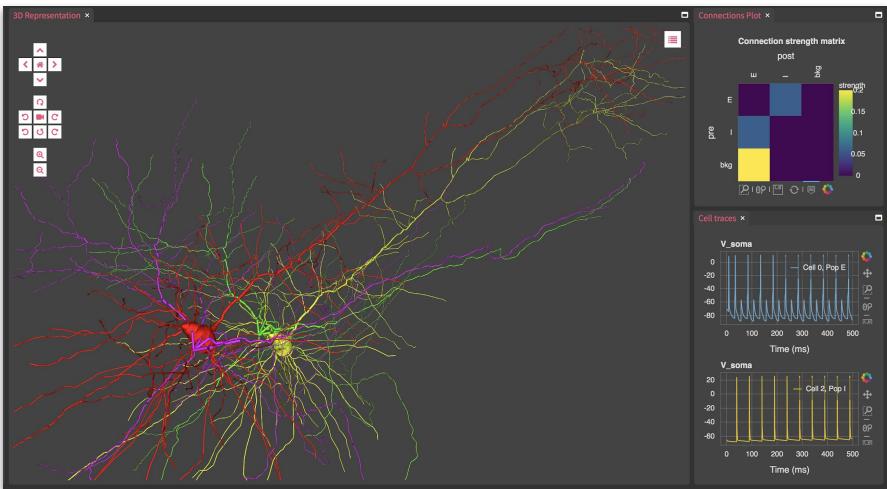
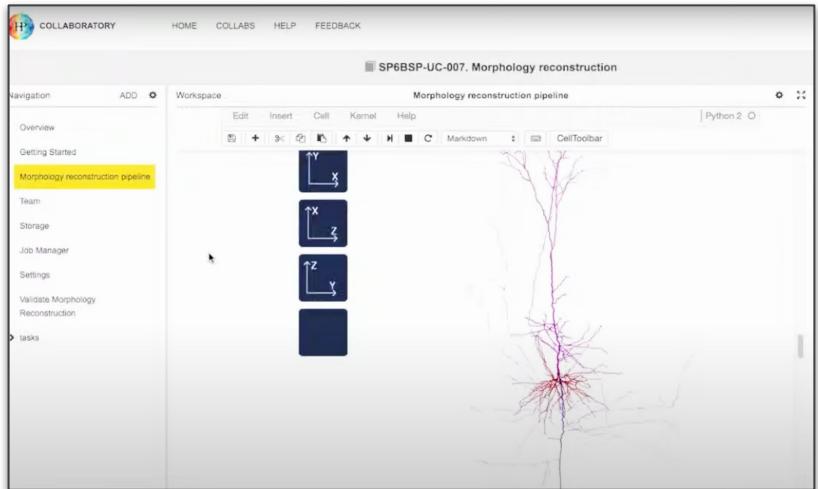
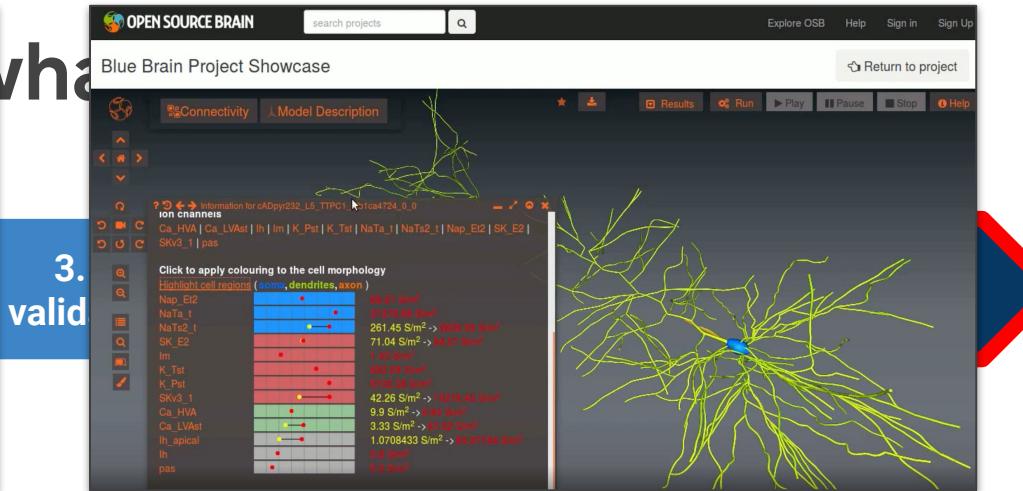
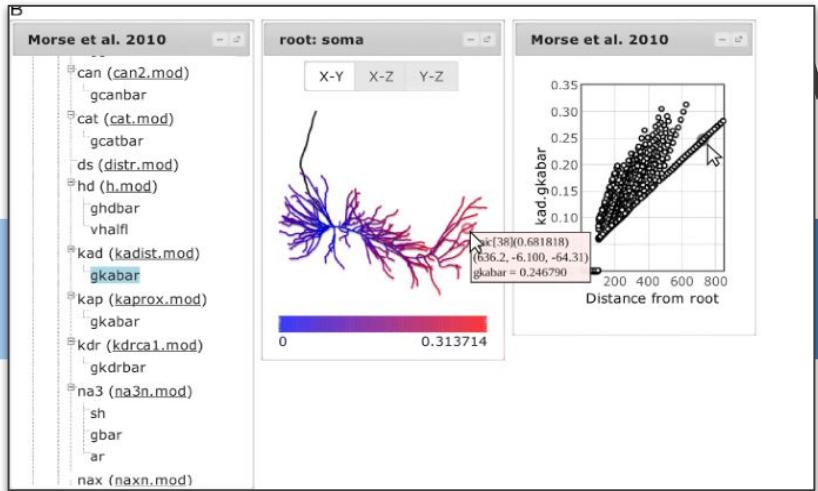
3. Tune + validate model

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Standardized formats to share models and data

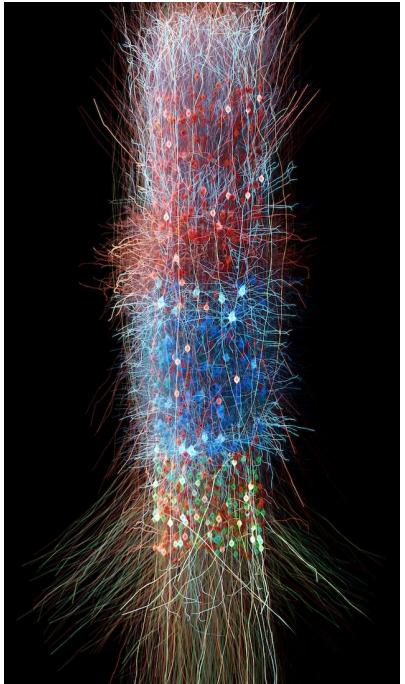
- Standards/tools for provenance of model parameters
- Standards for high-level specification of networks (in progress: NetPyNE, NeuroMLLite, NEST?)
- Robust and easy-to-use online platforms to run, visualize and analyze existing models (in progress: ModelDB, OSB, E-BRAINS, NetPyNE GUI)
- Adoption of standards and tools by the community



Thank you!



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DOWNSTATE
Medical Center



Lab web: dura-bernal.org

Software tool web: netpyne.org

