### **Breakout Session 2: Track B**

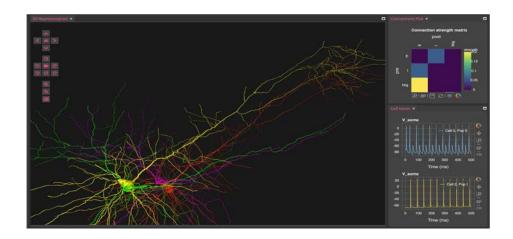
### Dissemination of a Tool for Data-driven Multiscale Modeling of Brain Circuits (U24EB028998)

Dr. Salvador Dura-Bernal Assistant Professor, SUNY Downstate

## Dissemination of a tool for data-driven multiscale modeling of brain circuits (U24EB028998)

Admin Supp: "Exploring cloud GPUs to accelerate multiscale simulations of brain circuits using NetPyNE and CoreNEURON"



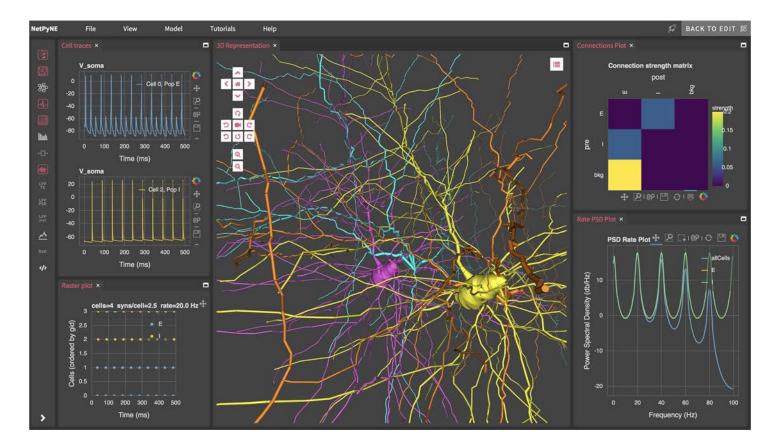


PI: Salvador Dura-Bernal, PhD Assistant Professor, State University of New York (SUNY) Downstate Research Scientist IV, Nathan Kline Institute for Psychiatric Research

Lab web: dura-bernal.org



A python package to facilitate the development, parallel simulation, optimization and analysis of biological neuronal networks using the NEURON simulator.



Funded by:



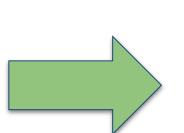
National Institutes of Health

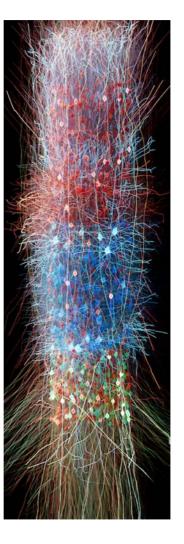
## High level specifications

A standardized, declarative, human-readable Python format to define the model

```
popParams['EXC_L2'] = {
'cellType': 'PYR',
'cellModel': 'simple',
'yRange': [100, 400],
'numCells': 50}
```

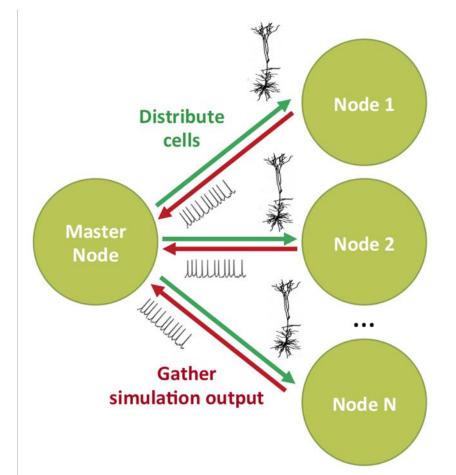
```
connParams['L2->E2'] = {
'preConds': {'y': [100, 400]},
'postConds': {'pop': 'EXC_L2'},
'probability': '1*exp(-dist_3D/200)',
'weight': 0.4,
'delay': 5,
'synMech': 'AMPA'}
```





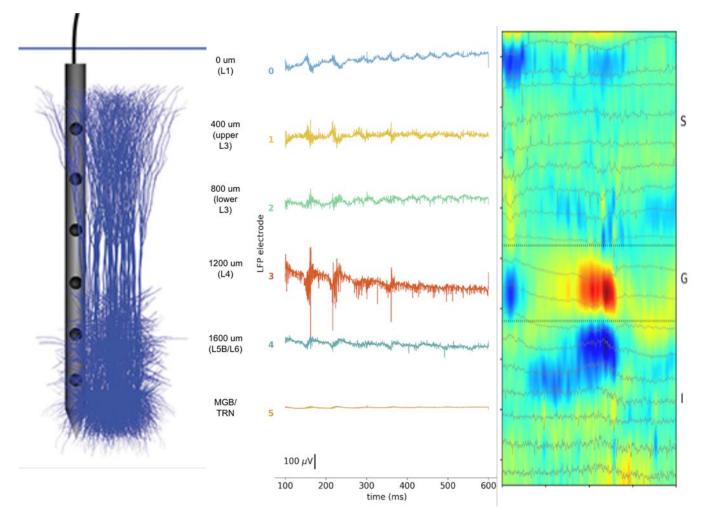
## **Parallel Simulation**

- Set up for MPI parallel simulation across multiple nodes (via NEURON simulator).
- Takes care of balanced **distribution** of cells and **gathering** of simulation output from nodes.

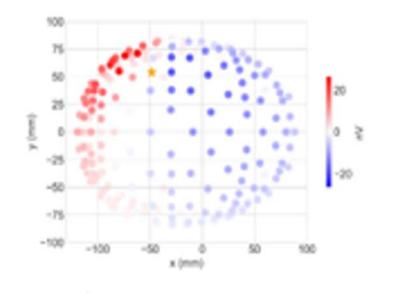


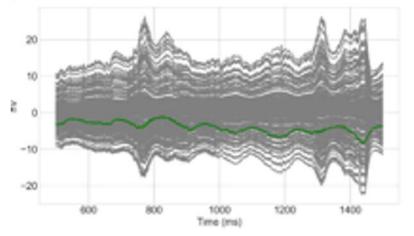
### Multiscale measures

### LFP / CSD



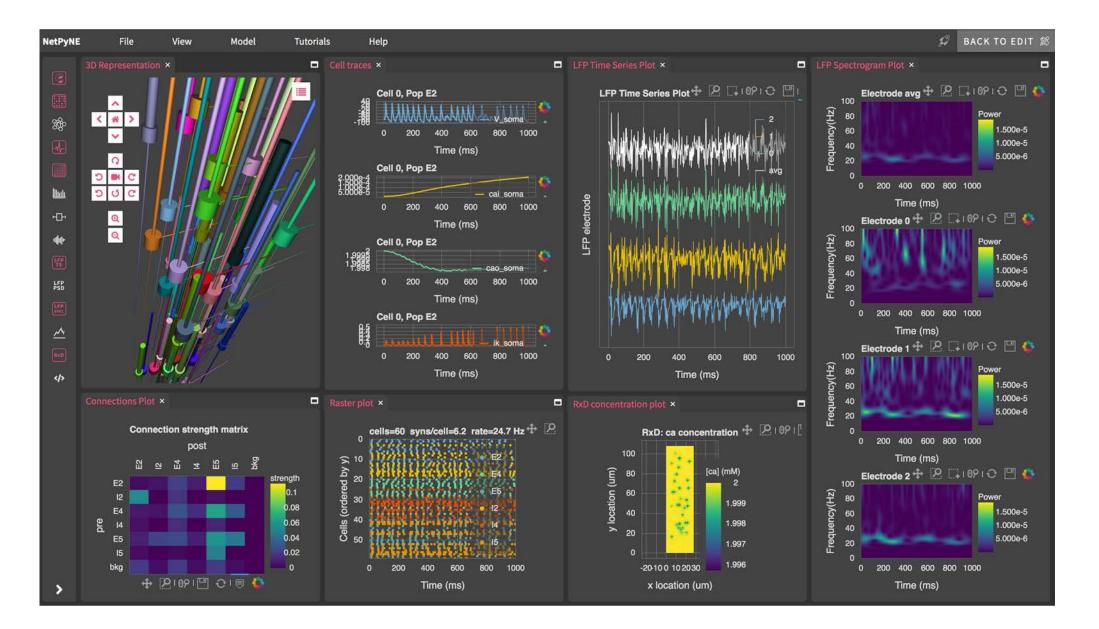
### **EEG / Current Dipoles**





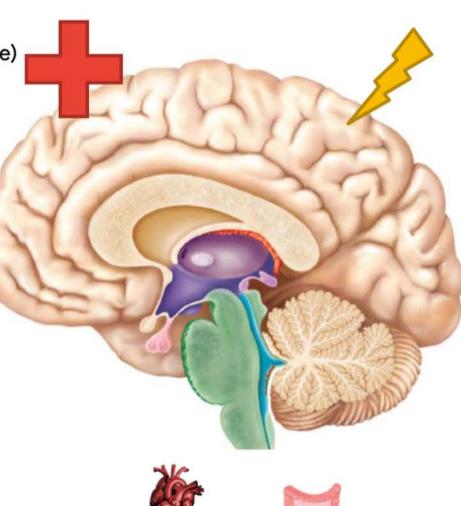
Dura-Bernal et al, 2019, eLife

## **GUI** for Development, Simulation, Analysis



# Growing <u>MetPyNE</u> ommunity: >50 Labs, >90 models

- Schizophrenia (TU Berlin, Brown)
- Ischemic stroke (Yale, Downstate)
- Epilepsy (Cincinatti, Brown, Downstate)
- Chronic Pain (Okinawa, Downstate)
- Depression (Brown)
- Parkinson's (Edinburgh)
  - PFC (Sao Paulo)
  - Thalamus (UCL, Missouri)
  - Olfactory Bulb (Palermo)
  - Striatum (Dublin)
  - Amygdala (Princeton)
  - Hippocampus (Sao Paulo)
  - Cardiac circuits (Jefferson, Downstate, Pavia)



- TMS / tDCS / tACS (Duke, Toronto)
- Optogenetics (Sydney)
- Electrical stimulation (Downstate)
- Ketamine (Brown)
- EEG/MEG (Puerto Rico, Brown, Rice)
- fMRI (Linkopig)
  - M1 and S1 (Downstate)
  - A1 (NKI)
  - V1 (Queensland, Sao Paulo)
  - Claustrum (Singapore)
  - Cerebellum (Sao Paulo)
  - Spinal Cord (Northeastern)
- Enteric / gastrointestinal circuits (Melbourne)



### **NetPyNE** used in >30 publications

#### Schizophrenia

ARTICLE OPEN

Check for updates

#### The effect of alterations of schizophrenia-associated genes on gamma band oscillations

Christoph Metzner<sup>[0]</sup><sup>1,2⊠</sup>, Tuomo Mäki-Marttunen<sup>3</sup>, Gili Karni<sup>1,4</sup>, Hana McMahon-Cole<sup>1,4</sup> and Volker Steuber<sup>[0]</sup>



Neurobiology of Disease Volume 179, April 2023, 106059



Biophysical characterization and modelling of *SCN1A* gain-of-function predicts interneuron hyperexcitability and a predisposition to network instability through homeostatic plasticity

Géza Berecki <sup>a 1</sup> A 🖾 , Alexander Bryson <sup>a b 1</sup>, Tilman Polster <sup>c</sup>, Steven Petrou <sup>a d e</sup> A 🖾

#### A Hippocampal-Entorhinal Cortex Neuronal Network for Dynamical Mechanisms of Epileptic Seizure

IEEE TRANSACTIONS ON NEURAL SYSTEMS AND REHABILITATION ENGINEERING, VOL. 31, 2023

Ying Yu<sup>0</sup>, Fang Han, and Qingyun Wang<sup>0</sup>



Communications in Nonlinear Science and Numerical Simulation Volume 117, February 2023, 106918

#### Research paper

Optogenetic stimulation of primary motor cortex regulates beta oscillations in the basal ganglia: A Computational study

<u>Ying Yu</u><sup>a</sup>, <u>Yubo Fan</u><sup>b</sup>, <u>Songan Hou</u><sup>c</sup>, <u>Qingyun Wang</u><sup>c d</sup> ♀ ⊠

#### Cell Reports Open access

ARTICLE I VOLUME 42, ISSUE 6, 112574, JUNE 27, 2023

Multiscale model of primary motor cortex circuits predicts *in vivo* cell-type-specific, behavioral state-dependent dynamics

Open Access • Published: June 09, 2023 • DOI: https://doi.org/10.1016/j.celrep.2023.112574 •

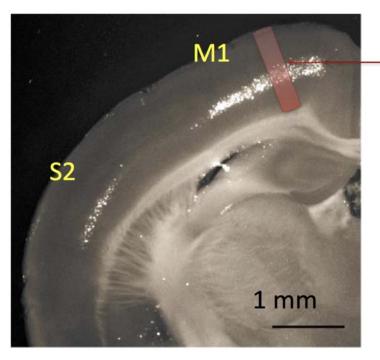
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### Active Grants using NetPyNE (US-based)

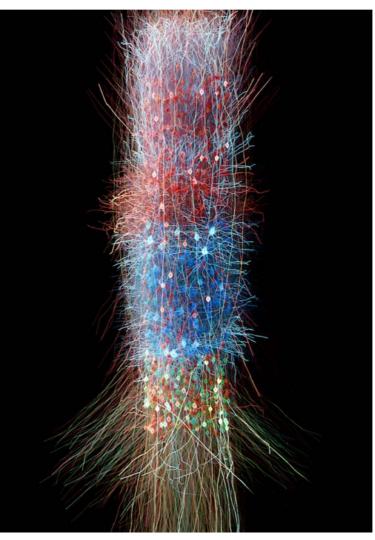
- 2023-2028; \$18M; NIH Conte Center P50: "Neurobiology and Cognitive Role of Slow Brain Network Fluctuations"
- 2023-2028; \$4.5M; NIH R01: "Neural Recording and Simulation Tools to Address the Mesoscale Gap"
- 2023-2028; \$3.5M; NIH R01: "Dynamic circuit motifs underlying multimodal interactions in primate auditory cortex"
- 2023-2028; \$300k; NYS DOH : "Restoring motor function after spinal cord injury using multiscale modeling to decode neural latent dynamics from motor cortex EEG"
- 2023-2027; \$3.7M; NIH U24: "Advancing Bio-Realistic Modeling via the Brain Modeling ToolKit and SONATA Data Format"
- 2023-2026; \$300k; The Hartwell Foundation: "Utilizing neuronal simulations to tailor therapies for children suffering from channelopathy related neurodevelopmental disorders"
- 2022-2026; \$2M; NIH R01: "Extension of NEURON simulator for simulation of reaction-diffusion in neurons"
- 2022-2025; \$3.5M; NIH R01: "Secondary analysis of resting state MEG data using the Human Neocortical Neurosolver software tool for cellular and circuit-level interpretation"
- 2021-2023; \$330k; NIH R21: "Combined EEG and in silico modeling to investigate the mechanisms of ketamine's sustained antidepressant effect in patients"
- 2019-2023; \$3.4M; NIH R01: "Cortical and thalamic mechanisms of selective auditory attention"
- 2019-2023; \$1.5M; NIH U24: "Dissemination of a tool for multiscale modeling of brain circuits"
- TOTAL: >\$40M; (+6 grants under review > \$20M)

## Detailed model of motor cortex (M1) circuits

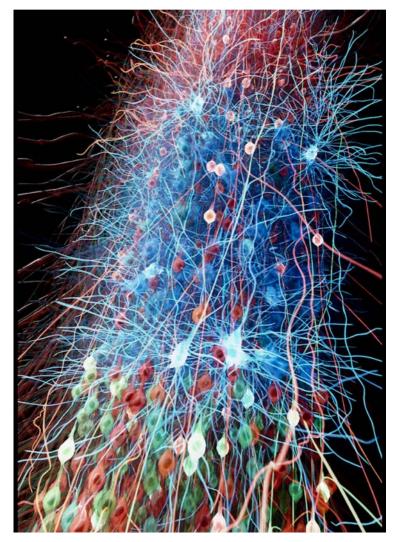
#### 300 um diameter column



10,000 neurons

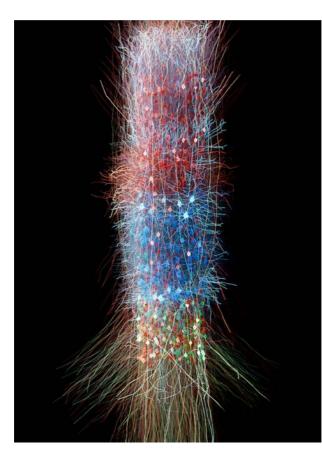


#### **30** million connections



### A simulation requires a lot of computing power

1 second simulation

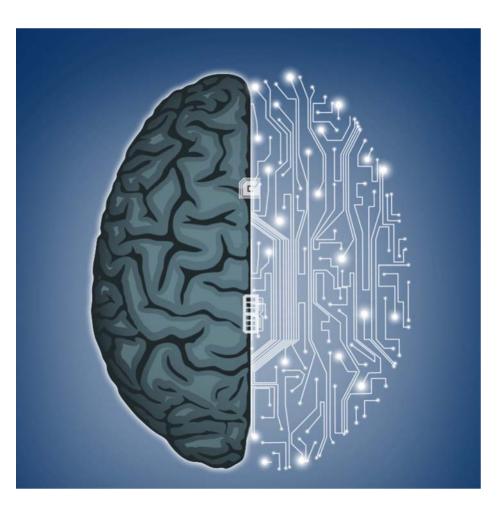


100 cores 3 hours



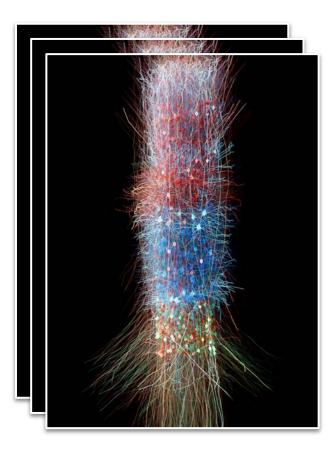
## Need to run 1000s of simulations

- 1) Find model parameters that reproduce real brain activity
- 1) Experiment with simulated brain

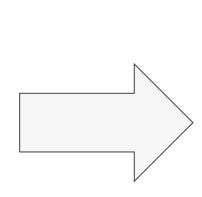


### 1000s of simulations require massive power

## 1000 x 1 second simulations

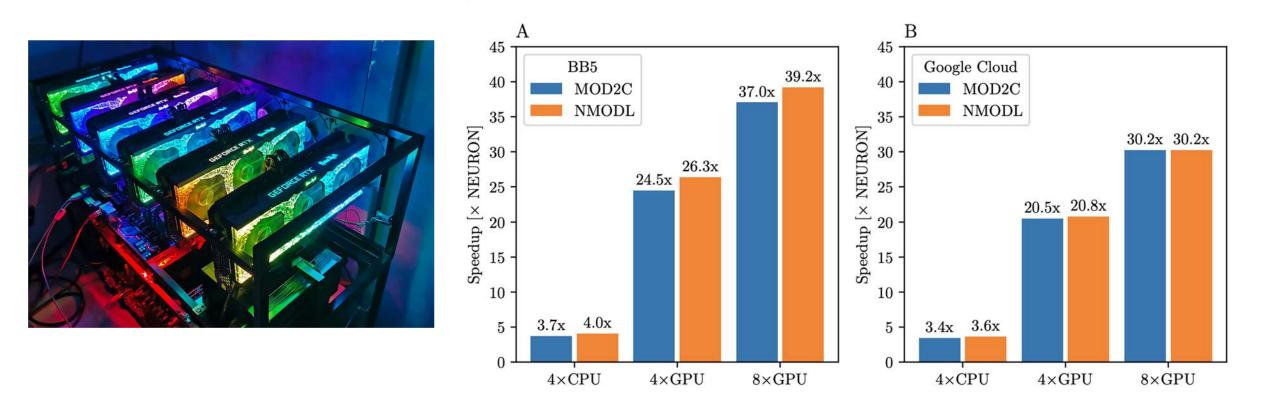


#### 100,000 cores 3 hours





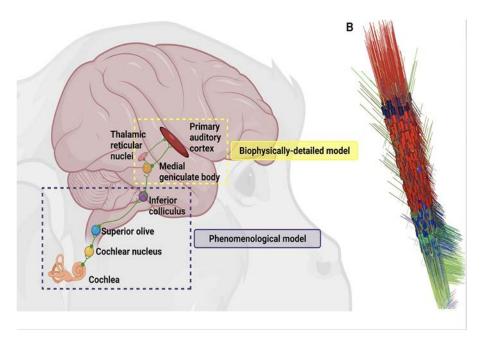
### Up to 40x speedup using GPUs

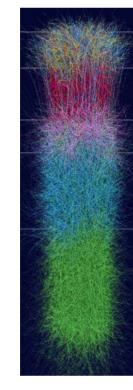


Aim 1: Evaluate cloud GPUs to simulate large-scale brain circuit models

Auditory thalamocortical model (14k neurons)

Somatosensory cortical model (37k neurons)



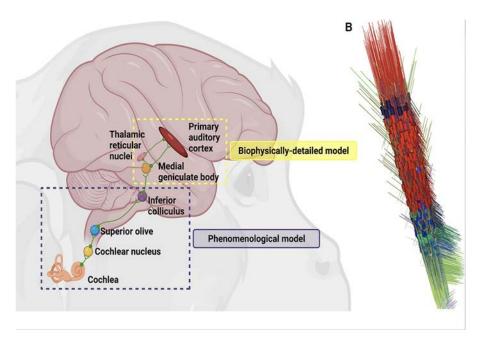


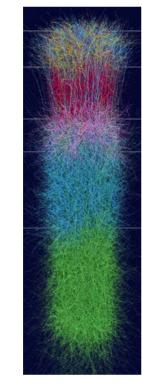
Aim 1: Evaluate cloud GPUs to simulate large-scale brain circuit models

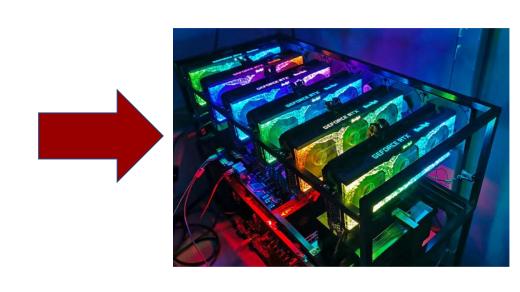
Auditory thalamocortical model (14k neurons)

Somatosensory cortical model (37k neurons)

### **Cloud GPUs**

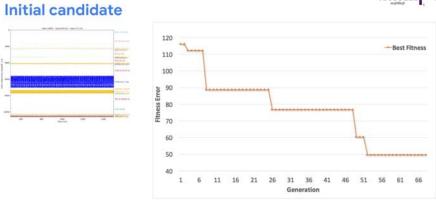


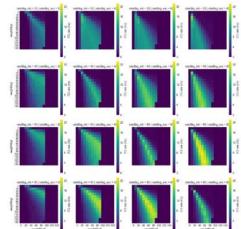




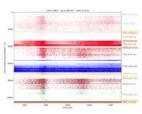
**Aim 2.** Evaluate clusters of GPUs to explore and optimize the parameters of large-scale brain circuit models.

Large-scale parameter exploration and optimization



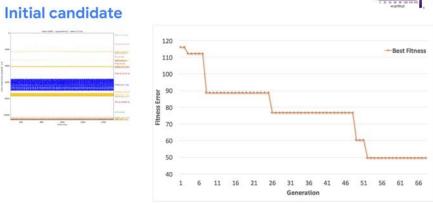


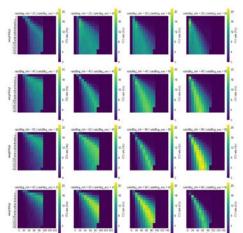
**Final candidate** 



**Aim 2.** Evaluate clusters of GPUs to explore and optimize the parameters of large-scale brain circuit models.

Large-scale parameter exploration and optimization





**Final candidate** 

