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cuBNM: GPU-Accelerated Biophysical Network Modeling

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Biophysical network modeling (BNM) of the brain is a promising technique for bridging macro- and microscale levels of investigation, enabling inferences about latent features of brain activity such as excitation-inhibition balance. This approach allows personalized models of the brain to be fitted to individual subjects' imaging data through parameter optimization. However, the process typically requires several thousand simulations per subject, making it computationally expensive and limiting its scalability to larger subject pools and more complex models.

To address this, we present cuBNM (https://cubnm.readthedocs.io), a toolbox designed for efficient simulation and optimization of BNMs using both GPUs and CPUs. The core of the toolbox operates highly parallelized simulations using C++/CUDA, while the user interface, written in Python, is intuitive and allows for user control over simulation configurations. The toolbox includes parameter optimization algorithms such as grid search and evolutionary optimizers, including the covariance matrix adaptation-evolution strategy (CMA-ES).

Currently, the toolbox supports two types of reduced Wong-Wang models, but its modular design allows for future inclusion of additional models. These models can incorporate global or regional free parameters that are fit to empirical data using the provided optimization algorithms. Regional parameters can be homogeneous or vary across nodes based on a parameterized combination of fixed maps or independent free parameters for each node or group of nodes. This flexibility enables the integration of data, such as the microstructural variability of the brain from the BigBrain project, to enhance the biological realism of large-scale brain simulations.

In this demonstration, we showcase the use of the cuBNM toolbox for running simulations and optimizing parameters in two scenarios: a homogeneous model and a heterogeneous model informed by BigBrain data. Through these examples, we demonstrate the potential of cuBNM to streamline brain simulation research, making it more accessible and scalable for larger studies and more complex modeling tasks.

Primary author: SABERI, Amin (Institute of Neuroscience and Medicine (INM-7), Research Centre Jülich, Jülich, Germany; Otto Hahn Research Group for Cognitive Neurogenetics, Max Planck Institute for Human Cognitive and Brain Sciences, Leipzig, Germany; Institute of Systems Neuroscience, Heinrich Heine University Düsseldorf, Düsseldorf, Germany)

Presenter: SABERI, Amin (Institute of Neuroscience and Medicine (INM-7), Research Centre Jülich, Jülich, Germany; Otto Hahn Research Group for Cognitive Neurogenetics, Max Planck Institute for Human Cognitive and Brain Sciences, Leipzig, Germany; Institute of Systems Neuroscience, Heinrich Heine University Düsseldorf, Düsseldorf, Germany)

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