cuBNM

GPU-accelerated Biophysical Network Modeling of the Brain

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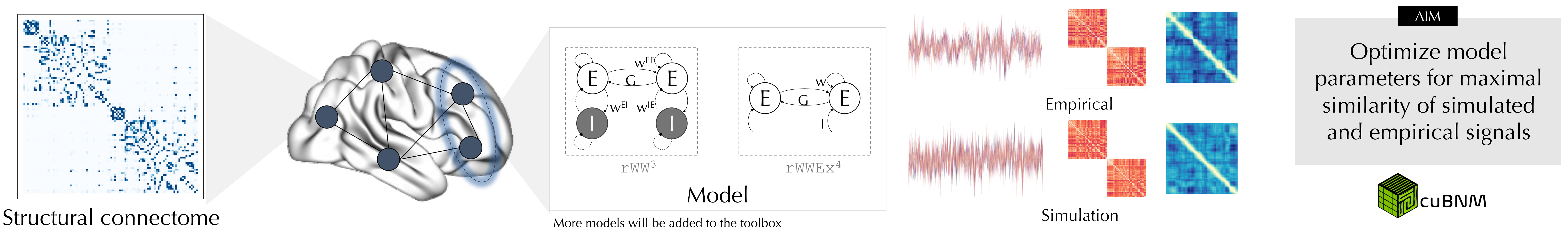
Motivation

Biophysical network modeling (BNM) of the brain is a promising technique to bridge macro- and microscale levels of investigation and enables inferences about latent features of brain activity, such as excitation-inhibition balance. Through this approach, personalized models of the brain can be fitted to the imaging data of individual subjects by parameter optimization[1, 2].
However, this process typically involves running several thousands of simulations for each subject, and therefore is computationally costly. This limits its scalability to a higher number of subjects and more complex models.
Here, we present *cuBNM* (https://cubnm.readthedocs.io), a toolbox for efficient simulation and optimization of BNMs using GPUs (but also supports CPUs).

How does BNM work?



Installation	`pip install cubnm`

Requirements	Linux, Python ≥ 3.7, NVIDIA GPU

Two parameter optimization approaches included:

Evolutionary

```python
from cubnm import datasets, optimize

problem = optimize.BNMProblem(
    model = 'rWW',
    params = {
        'G': (0.5, 2.5),
        'wEE': (0.05, 0.75),
        'wEI': (0.05, 0.75),
    },
    het_params = ['wEE', 'wEI'],
    maps_path = datasets.load_maps('2maps', 'schaefer-100', return_path=True),
    emp_fc_tril = datasets.load_functional('FC', 'schaefer-100'),
    emp_fcd_tril = datasets.load_functional('FCD', 'schaefer-100'),
    duration = 60,
    TR = 1,
    sc_path = datasets.load_sc('strength', 'schaefer-100', return_path=True),
    states_ts = True
)
cmaes = optimize.CMAESOptimizer(popsize=30, n_iter=10, seed=1)
cmaes.setup_problem(problem)
cmaes.optimize()
cmaes.save()
```

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Grid search

```python
from cubnm import datasets, optimize

gs = optimize.GridSearch(
    model = 'rWW',
    params = {
        'G': (0.5, 2.5, 10),
        'wEE': (0.05, 0.75, 10),
        'wEI': 0.21
    },
    duration = 60,
    TR = 1,
    sc_path = datasets.load_sc('strength', 'schaefer-100', return_path=True),
    states_ts = True
)

emp_fc_tril = datasets.load_functional('FC', 'schaefer-100')
emp_fcd_tril = datasets.load_functional('FCD', 'schaefer-100')
scores = gs.evaluate(emp_fc_tril, emp_fcd_tril)
scores.to_csv('scores.csv')
gs.save()
```

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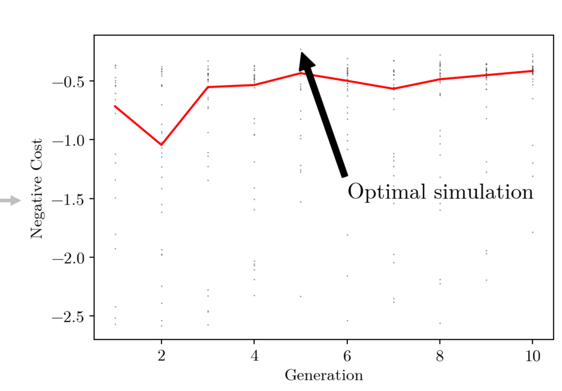
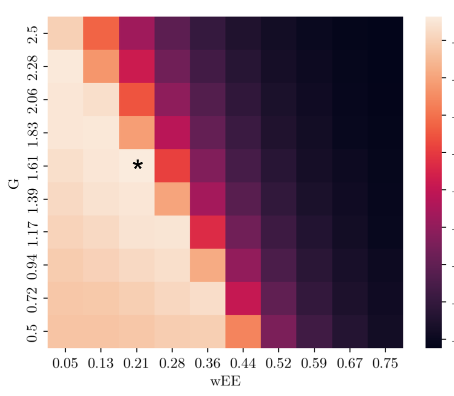
FEATURES

- ✓ Modular design
- ✓ Simulation + FC and FCD on GPU
- ✓ Extensive options for simulations
- ✓ Regional parameter heterogeneity
- ✓ Supports *pymoo* optimizers

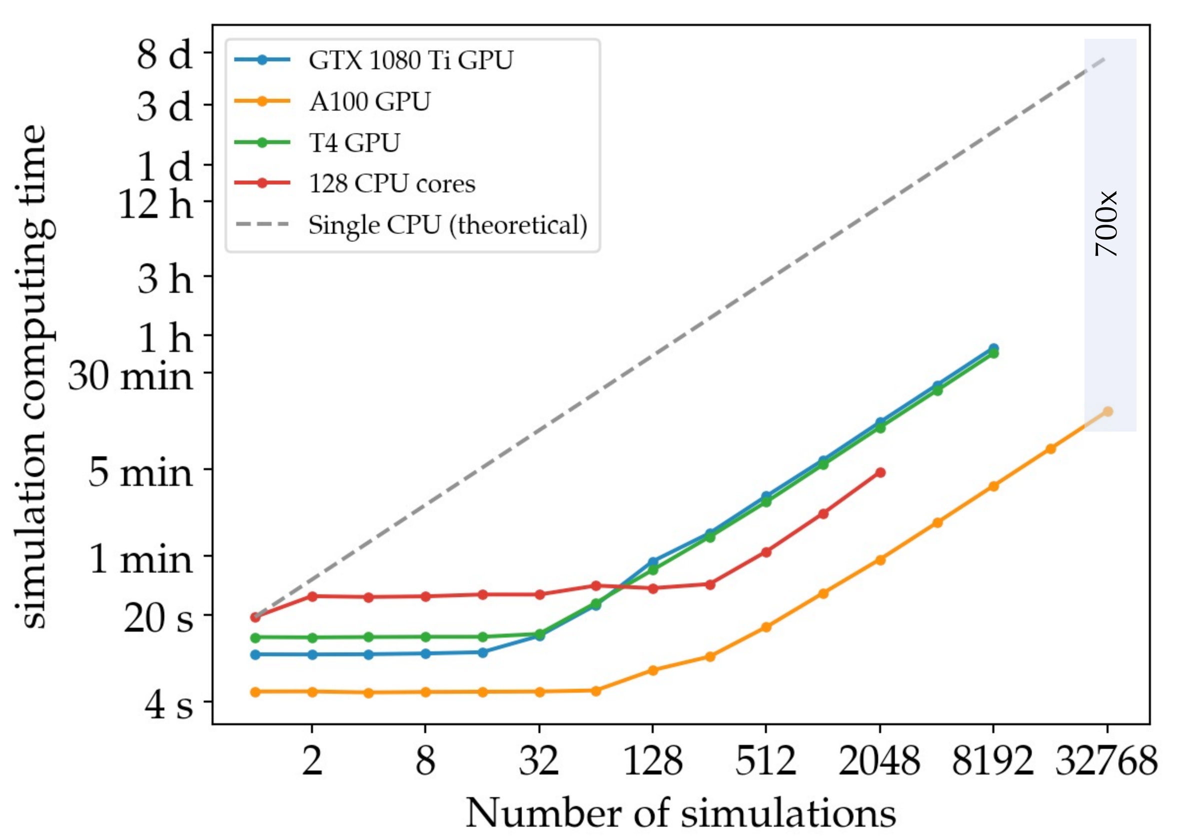




PLANS

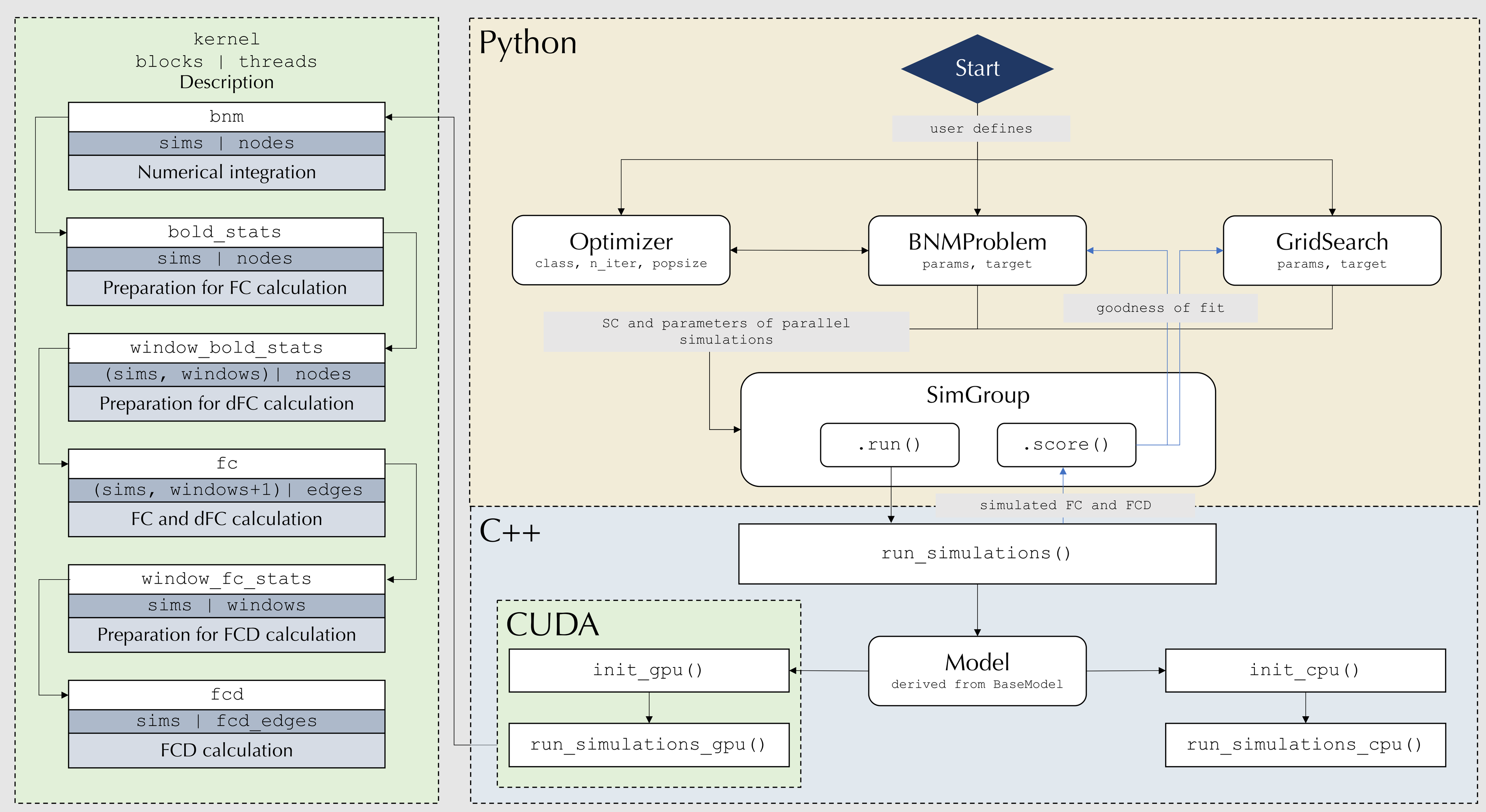
- ✓ New models
- ✓ Improve documentations and add tutorials
- ✓ Command-line interface
- ✓ Docker container

Contact us if you're interested to contribute :)



A100 GPU up to 700x faster than a CPU

Program flowchart



References:
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