RateML: A Code Generation Tool for Brain Network Models

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Motivation

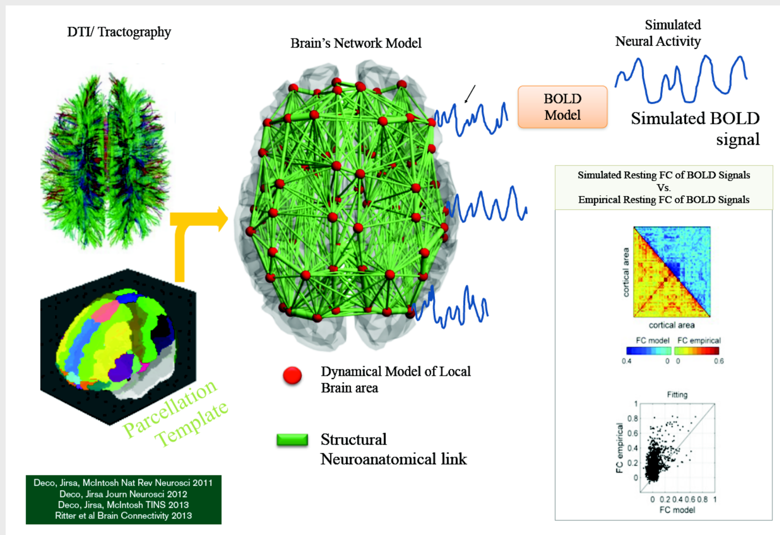
Challenges:

- Relieve neuroscientific modeling from engineering expertise
- Hardware agnostic implementation of models
- Standard for Neural Field/Mass models

Achievements:

1. Automatic code generation for TVB models
2. GPU simulator tuned to model for parameter exploration
3. Linked to L2L [1] for Hyper Parameters optimization
4. Using LEMS [2] for neuroscientific standard

Target: The Virtual Brain (TVB) [3]



Features:

- Whole brain simulation using neural mass models and detailed connectomes
- Connectome has spatial and temporal aspects
- Simulation core in Python, JIT backends in development
- Scripting and GUI interface
- Platform includes data management

RateML [4]: Code generation for TVB

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<ComponentType name="derivatives">
    <Parameter name="global_speed" dimension='1.0, 2.0'/>
    <Parameter name="global_coupling" dimension='1.0, 2.0'/>
    <DerivedParameter name="rec_speed_dt"
    value="1.0f / global_speed / (dt)"/>
    <DerivedParameter name="nsig" value="sqrt(dt) * sqrt(2.0 * 1e-5)"/>

    <Constant name="omega" value="60.0 * 2.0 * 3.1415927 / 1e3"
    dimension=""
    description="base line frequency Kuramoto oscillator [rad/ms]"/>

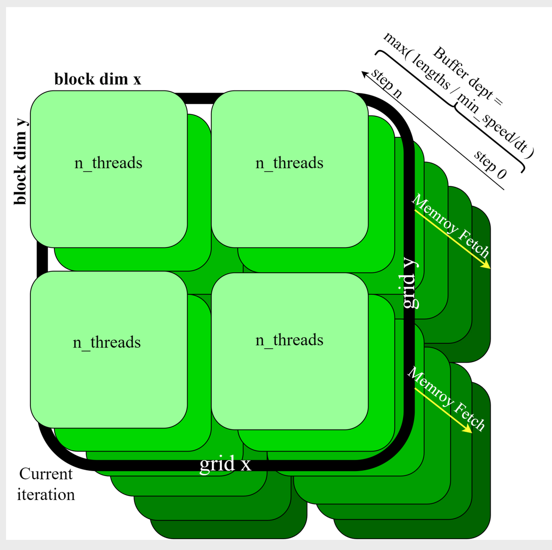
    <Exposure name="theta" dimension="" />

    <Dynamics>
        <StateVariable name="theta" dimension="0.0, 1.0"
        exposure="0.0, numpy.pi * 2.0"/>
        <TimeDerivative variable="dV" value="omega + c_pop0"/>
    </Dynamics>
</ComponentType>
```

Features:

- Domain specific language LEMS
- Uses Mako templating
- Human readable eXtensible Markup Language (XML)
- Python (Numba) regular TVB model
- CUDA Parameters space exploration on GPU

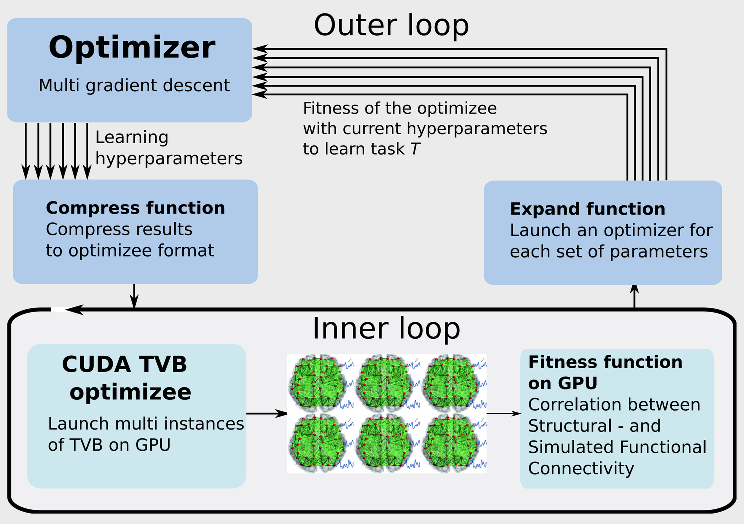
CUDA state space specification



Properties

- Each RateML conversion produces model specific GPU simulator
- Each thread is a TVB simulation with different parameters
- States are stored corresponding to buffer depth
- Parameter ranges are set in XML
- Parameter resolution is set from command line

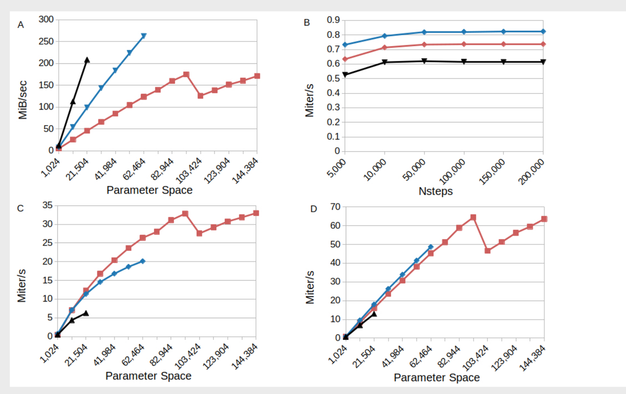
Learning to Learn [5] (L2L)



Properties

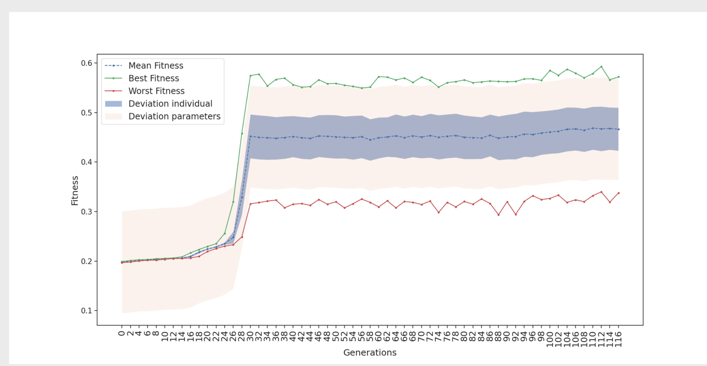
- Hyper-parameters optimization framewor with RateML interface
- Parameter fitting to match patient EEG/fMRI
- TVB Python optimizee
- TVB CUDA multi-instance optimization (left figure)
- Relating functional connectivity to structural connectivity
- Population based optimizer for HPC
- No node communication overhead
- Not limited to TVB use cases

Performance



Kuramoto (r), Montbrió (bu) and Epileptor (bl):

A. Memory bandwidth consumption
B. Iterations/s fixed parameter space size of 1,024
C. Iterations/s 4,000 integration steps (0.4 s sim time)
D. Iterations/s 100,000 integration steps (10 s sim time)



L2L TVB results for function to structure comparison

1. Best fitness after 30 generations
2. Parameter size of 1,024 explored in a single generation
3. 4,000 TVB integration steps (0.4 s sim time)

References

[1] Alper Yegenoglu et al. "Exploring hyper-parameter spaces of neuroscience models on high performance computers with Learning to Learn (in review)". In: *Frontiers In Computational Neuroscience* (2022).

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[3] Paula Sanzleon et al. "The virtual brain: A simulator of primate brain network dynamics". In: *Frontiers in Neuroinformatics* 7.MAY (2013). ISSN: 16625196. DOI: 10.3389/fninf.2013.00010.

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[5] Sebastian Thrun and Lorien Pratt. *Learning to learn*. Springer Science & Business Media, 2012.

Acknowledgements

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