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A Graph-Based, In-Memory Workflow Library for Brain/MINDS 2.0 –The Digital Brain Project

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The Brain/MINDS 2.0 Digital Brain Project aims to develop an open, interoperable software platform dedicated to digital brain construction. This platform targets seamless integration of neuroscience simulation tools—including TVB, NEST, BMTK, —via their Python APIs, allowing researchers to build comprehensive and detailed brain models. As brain modeling and simulation research evolves, there is a growing need for digital infrastructures that can efficiently handle heterogeneous data while supporting scalable simulation workflows.

Current workflow systems like Snakemake and Nextflow are well-suited for linear data-processing pipelines but are inherently dependent on serialized, I/O-bound data exchanges. This makes them less effective for in-memory data structures typical of neural simulations, posing challenges for constructing understandable and reusable workflow modules.

To address this gap, we introduce a graph-based workflow framework where brain modeling tasks are encapsulated as modular, reusable nodes. These nodes communicate using direct memory references, enabling rapid in-memory propagation of complex neural data (e.g., neuron states, connectivity matrices) and eliminating the overhead of serialization and disk I/O. Workflows are defined as node-edge graphs, fostering flexible, composable scientific pipelines.

In addition, to leverage the benefits of traditional tools, our implementation analyzes data exchange patterns to identify optimal process boundaries, grouping tightly coupled in-memory tasks while enabling file-based I/O modularity where appropriate. This hybrid model aims to support distributed workflow execution with Nextflow and Snakemake under the hood, while maintaining the modularity, clarity, ease of use, and reusability needed for scientific users and collaborative research.

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References

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