Title: NeuroWorkflow: A Node-Based Framework for Scalable Computational Neuroscience with AI-Ready Infrastructure

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Abstract:

Introduction

Computational neuroscience faces significant challenges in model development, reproducibility, and scalability across different simulation platforms. Current tools typically focus on single simulation environments, limiting cross-platform compatibility and collaborative research. We present NeuroWorkflow, a node-based framework that addresses these limitations through a unified, extensible architecture supporting multiple neural simulation paradigms including spiking neural networks (SNNs) and mean-field models. Additionally, the emerging potential of Large Language Model (LLM) agents in scientific workflows remains largely untapped due to the absence of well-structured, AI-ready computational neuroscience code components for AI-augmented and assisted brain modeling. Our well-documented nodes, enabled by our schema system, establish the foundation for organizing computational neuroscience functions, algorithms and tools, ready for AI few-shot learning via protocols such as MCP, enabling future AI-augmented computational neuroscience systems

Methods

NeuroWorkflow implements a modular node-based architecture with three core components: (1) A comprehensive schema system defining standardized node interfaces with input/output ports, parameters, and method definitions; (2) An AI-ready infrastructure featuring machine-readable node designed for LLM comprehension, enabling future integration with Model Context Protocol (MCP) servers where AI agents can autonomously understand, compose, and execute neuroscience workflows; (3) Specialized node libraries including SNNbuilder for detailed spiking neural network construction in NEST and TVB (The Virtual Brain) nodes for brain modeling. The framework employs a port-based connection system enabling type-safe data flow between heterogeneous components. Each node contains structured metadata, semantic descriptions, and usage examples formatted for LLM interpretation, positioning the system as a foundation for AI-augmented scientific computing. We developed automated code generation capabilities that transform high-level workflow descriptions into executable simulation code. The system includes

comprehensive validation mechanisms and error handling, designed to support both human users and AI agents.

Results

We successfully developed NeuroWorkflow with specialized nodes across multiple domains, each equipped with comprehensive machine-readable documentation. The framework operates as a standalone Python library enabling direct node instantiation, port-based connections, parameter configuration, and programmatic workflow execution. SNNbuilder nodes enable construction of detailed cortical microcircuits in NEST. MFbuilder nodes provide seamless access to mean-field models and simulation capabilities in TVB. Nodes communicate through both traditional I/O mechanisms and efficient in-memory object passing, enabling high-performance data flow between components. We developed a comprehensive graphical user interface for intuitive workflow construction and testing, supported by a backend system for workflow management. The system operates in both local standalone mode and distributed client-server configurations, facilitating collaborative research environments. The structured node schema system successfully enables programmatic workflow composition. Preliminary testing with LLM-based workflow generation demonstrates the system's readiness for AI agent integration, with structured node descriptions enabling accurate workflow composition in test scenarios.

Discussion

NeuroWorkflow represents a paradigm shift toward AI-augmented computational neuroscience, enabling both researchers without extensive programming backgrounds and future AI agents to construct sophisticated neural models. The node-based approach with machine-readable schemas facilitates rapid prototyping, systematic parameter exploration, and positions the framework as a foundational component for MCP servers in computational neuroscience. Key innovations include the LLM-comprehensible node documentation system, standardized schema ensuring type safety and AI interpretability, and the unified interface bridging traditionally separate simulation environments. The framework addresses needs for standardization, accessibility, and AI-readiness in computational neuroscience, potentially enabling a new era of AI-augmented brain modeling research where human expertise is amplified by intelligent agents capable of understanding and manipulating complex neuroscience workflows.

Keywords: computational neuroscience, workflow management, spiking neural networks, brain modeling, AI-ready infrastructure, LLM agents, MCP server, node-based programming, automated workflow composition, AI-augmented research

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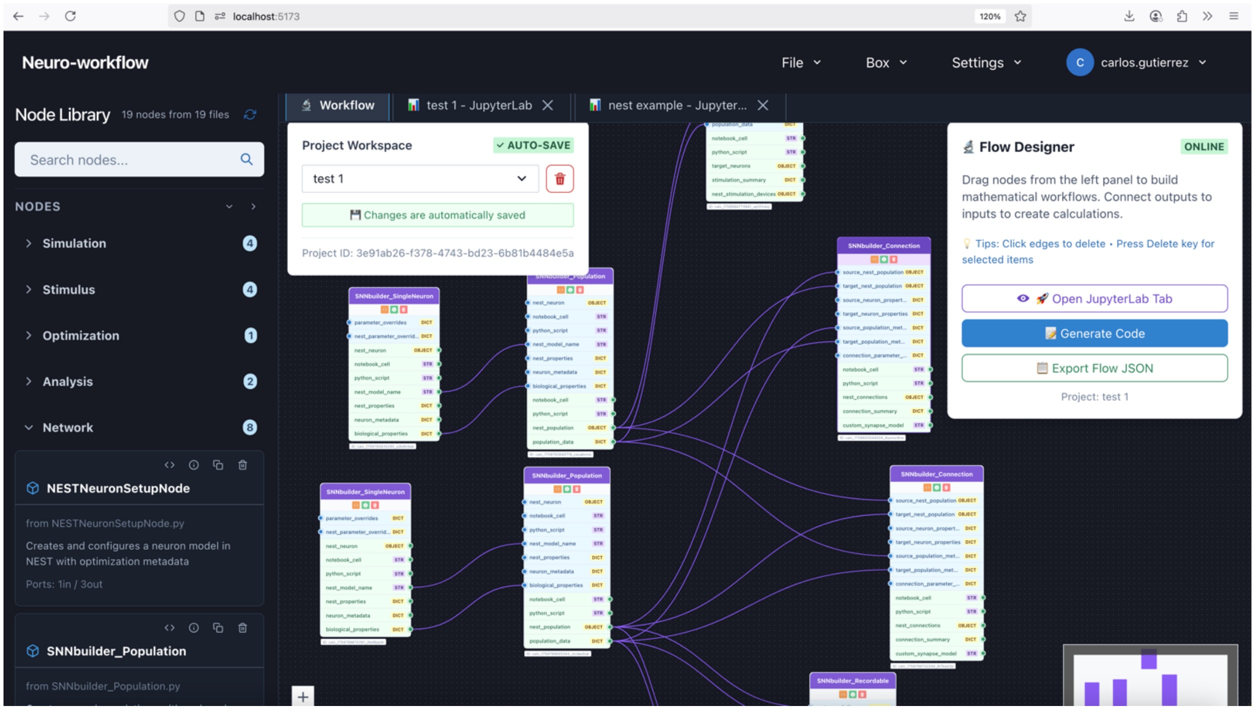

Figure 1. Neuroworkflow includes a graphical user interface for intuitive workflow construction and testing.

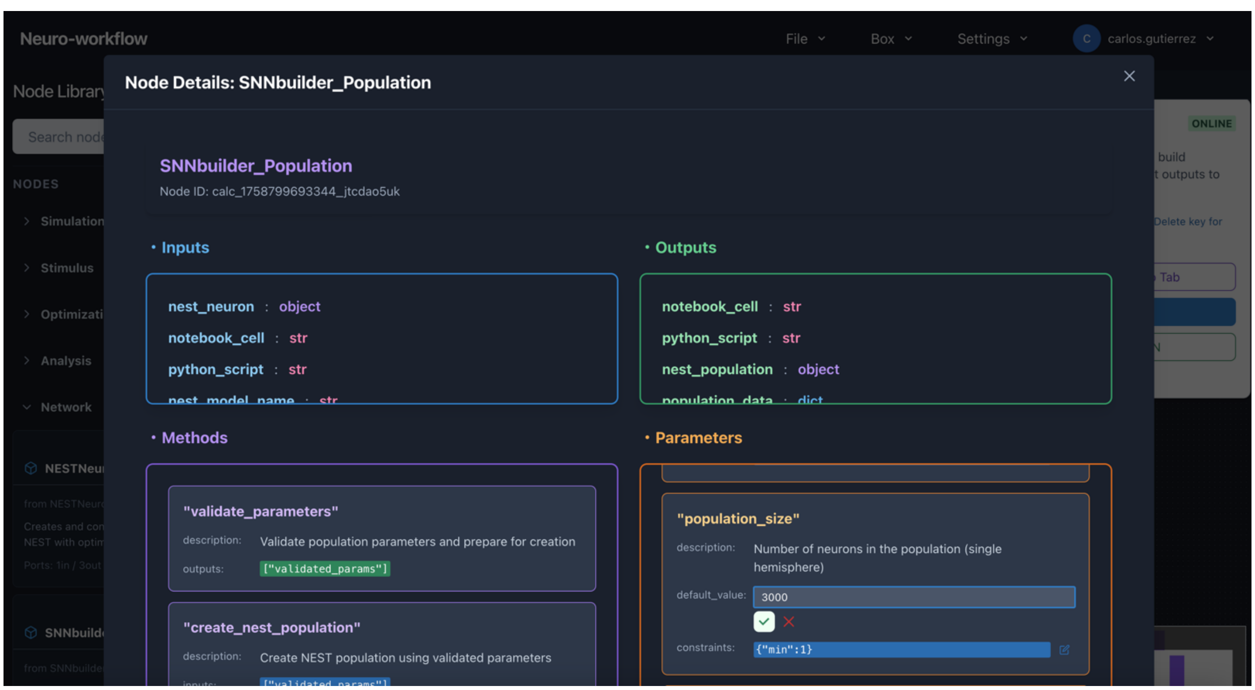

Figure 2. Schema defining standardized node interfaces with input/output ports, parameters, and method definitions.