

A Comprehensive Framework for Computational Neuroscience: Exploring Descriptive, Mechanistic, and Interpretive Models with Analysis

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Abstract: This paper introduces a groundbreaking framework for computational neuroscience, uniting Descriptive, Mechanistic, and Interpretive models. Tailored to unravel the complexities of the brain, our framework categorizes and establishes a dynamic platform for real-time comparative analysis, offering insights into individual model strengths and weaknesses. Descriptive models (Neural Firing Rate, Population Rate, Neural Field) quantitatively capture neural phenomena without an explicit focus on underlying mechanisms. Mechanistic models (Hodgkin-Huxley, Synaptic, Biophysical) delve into intricate biological processes, simulating neural activity with detailed mechanisms. Interpretive models (Integrate-and-Fire, Generalized Linear) prioritize conceptual understanding, offering insights into the principles governing neural processes.

Index Terms - computational neuroscience, descriptive model, framework, interpretive model, mechanistic model

I. INTRODUCTION

Computational Neuroscience has made significant strides in recent years, utilizing the power of computation to unravel the dynamic mechanisms of the brain. In this work, we present a comprehensive framework for the same, encompassing descriptive, mechanistic, and interpretive modeling types. Our framework is designed to bridge the gap between theoretical understanding and empirical data, providing a unified approach to simulating brain functions.

A literature revealed a rich tapestry of computational models employed to dissect various aspects of the neuronal processes. However, a recurrent observation was the lack of a comprehensive framework that systematically categorized and emphasized each modeling type based on their criteria. Existing studies often applied computational models collectively, without explicitly highlighting the distinct characteristics of each type and their specific contributions to the field.

In unveiling this framework, we aim to empower researchers and practitioners in the field to navigate the intricate landscape with clarity and purpose.

Computational neuroscience utilizes mathematical models, computer science techniques, theoretical analysis, and abstract representations of the brain to explore the principles governing the

development, structure, physiology, and cognitive functions of the nervous system.

Current trends in computational neuroscience include challenges in understanding the brain, highlighting the complexity of higher brain functions and the limitations of studying individual neurons. The emergence of properties at higher levels of organization is emphasized, necessitating advances in techniques for probing distributed processing in the brain. It also mentions ongoing developments in experimental methods, including simultaneous recording from multiple single units, optical recording of cortical organization, and large-scale measurements of brain structure and activity. Despite the advancements, these techniques have limitations in spatial or temporal resolution, prompting the need for new approaches to understanding distributed processing.

The importance of computational modeling in addressing conceptual issues related to information processing in the brain is emphasized. The advantages of brain models are outlined, including their ability to make complex systems more accessible, predict experimental outcomes, and simulate experiments that may be challenging in living tissue. A literature delves into the

question of what kind of computer the brain is, drawing a distinction between mechanical and computational explanations. Unlike digital computers, the brain is described as a collection of specialized, efficient systems with constrained flexibility due to its evolutionary nature.

Researchers in neuroscience have turned to computational modeling as an essential tool in their toolkit. By creating and simulating models that mimic the neural processes observed in the brain, researchers can gain insights into the algorithms underlying brain function. Computational neuroscience models serve as a bridge between experimental observations and theoretical understanding, allowing researchers to explore hypotheses, make predictions, and test the consequences of complex, nonlinear systems. These models are particularly valuable for investigating emergent properties at higher levels of brain organization, providing a complementary approach to experimental techniques in unraveling the mysteries of the mind.

In the study of complex systems like the brain, it is argued that neuroscience should begin by examining the specific computations a system aims to accomplish. The emphasis is placed on studying particular computations rather than focusing solely on theories of the system. Various approaches and methods for modeling can be employed in this context. Descriptive models aim to characterize observed phenomena without specifying underlying mechanisms, providing a comprehensive portrayal. In contrast, mechanistic models delve into the detailed processes and interactions that generate the observed outcomes, offering a deeper understanding of the underlying mechanisms at play.

II. APPROACH

The objective of this research is to develop an integrated and versatile computational framework that combines descriptive, mechanistic, and interpretive models in the field of neuroscience. The aim is to investigate the interplay between these diverse model types, providing a holistic understanding of neural processes and their implications. Additionally, the research seeks to analyze the performance and validity of the models, offering insights into the emergent properties of complex neural systems. Ultimately, this study aims to contribute to the advancement of computational neuroscience methodologies and deepen our understanding of the brain's functionality. Several studies have focused on descriptive models, offering insights into observed neural phenomena without delving into the underlying mechanisms. A study developed a descriptive model elucidating the temporal dynamics of membrane potential in specific neural circuits. Conversely, mechanistic

models aim to untangle the intricate processes and interactions with neural systems and processes. A researcher pioneered a mechanistic model investigating the input-output transformations of neurons, offering a detailed understanding of the underlying psychological mechanisms. Interpretive models, emphasizing the broader implications of neural processes, have also been prevalent in a literature employing an interpretive model to analyze the cognitive implications of observed neural patterns, linking neural activity to higher-order cognitive functions.

In light of the fragmented nature of existing literature, our research seeks to address the gap between collection and problem by proposing a comprehensive framework that harmonizes descriptive, mechanistic, and interpretive models. Through systematic analysis and validation, our research endeavors to pave the way for a more cohesive and insightful exploration of computational neuroscience.

For creating this framework the aforementioned models: Descriptive, Mechanistic, and Interpretive are implemented and evaluated based on:

- **Speed of information processing:** The rate of information processing in biological neural systems is comparatively faster than digital processing, the nervous system overwhelmingly prefers parallel computation over serial ones in time-critical applications.
- **Robustness:** A model is robust if it continues to produce the same set of outputs under variations of inputs or new parameters are introduced, nonetheless the model should be steady and robust no matter what.
- **Gain control:** The principle behind the response of a nervous system should stay within certain bounds even when the inputs from the environment change drastically. The producing outputs should follow the constraints provided while building the model.
- **Linearity vs nonlinearity:** A linear system is one type of modeling that follows a specific unit of measure, the set of inputs will be considered at once. Linear systems are easier to analyze mathematically and are a persuasive assumption in many models. Whereas nonlinear models are generally assumed to be parametric and are described in a nonlinear equation.

To commence the process of benchmarking and creating the framework, we systematically employed a variety of models and modeling types representing different paradigms within computational neuroscience. Within Descriptive models, we utilized mathematical and computational representations of

models including the Linear-Nonlinear-Poisson model (LNP) and Rectified Linear unit model (ReLU), which allowed us to explore the relationship between inputs and outputs without modeling detailed biophysical processes. Population rate models and Neural field models were also used, providing insights into spatiotemporal dynamics within the process. In parallel, we integrated Mechanistic models such as the Hodgkin-Huxley model, Synaptic models such as the Tsodyks-Markram model, and Biophysical models, incorporating detailed properties such as dendritic compartments and ion channels. To provide a comprehensive and conceptual understanding, Interpretive models were also included. Models such as the Integrate-and-fire models, representing neurons as passive electrical circuits, and generalized linear models (GLMs), combine linear filters with nonlinear transformations. Our framework also considered other specialized models and modeling paradigms, including the Kuramoto model, point process models, hidden Markov models, FitzHugh-Nagumo oscillator, neuromuscular models, cellular automata models, spiking neural network models, reaction-diffusion models, place cell models, population vector models, Bayesian models, and information theory models. By integrating these diverse models, our approach aimed to create a robust and versatile framework for computational neuroscience, facilitating a more holistic exploration of neural processes.

III. METHODOLOGY

The methodology adopted for this research focuses on creating a versatile framework for simulating diverse brain behaviors. The integration of multiple computational models is a key feature, ensuring a comprehensive representation of neural dynamics. A pivotal aspect involves the development and implementation of algorithms designed to convert raw spikes into excitatory and inhibitory signals, bridging the gap between raw data and meaningful neural representations. The parameterization and calibration process fine-tuned model parameters to align with experimental observations, enhancing simulation fidelity. Sensitivity analysis further explores the impact of input parameter variations on model outputs, providing insights into critical parameters influencing simulated neural activity. This methodology collectively enables researchers to gain valuable insights into different computational methods for understanding brain structure and function.

Descriptive Models:

Descriptive models are mathematical and computational representations that aim to describe and replicate observed neural phenomena or data without focusing on underlying mechanisms.

These models may not provide insights into the detailed biophysical processes occurring within neurons or neural networks. Instead, they are used to capture and replicate specific features of neural activity or behavior.

Neural Firing Rate Models: Utilizing the average firing rate of neuron populations offering a high-level description of neural activity.

Population Rate Models: Focusing on the aggregate firing rate of neuronal populations capturing the overall activity patterns.

$$R(t) = \frac{1}{N} \sum_{i=1}^N r_i(t)$$

Neural Field Models: A population-level approach concentrating on the non-linear dynamics of neurons.

$$\frac{\partial u(x,t)}{\partial t} = -au(x,t) + \int_{\Omega} w(x,y)f(u(y,t))dy + I(x,t)$$

Mechanistic Models:

Mechanistic models are essential for understanding the fundamental biological processes underlying neural function. They are used to simulate and predict neural activity and explore how neural mechanisms can lead to others. Unlike descriptive models, they delve into the details of how neurons are functioning.

Hodgkin-Huxley Models: Describing the biophysical mechanisms of action potential generation in neurons by modeling the behavior of voltage-gated ion channels.

$$C \frac{dv}{dt} = I - g_{Na} m^3 h (V - E_{Na}) - g_K n^4 (V - E_K) - g_L (V - E_L)$$

Synaptic Models: Entailing a mathematical description of the transformation of a presynaptic action potential into a postsynaptic response, such as an ionic current.

STDP (Spike-Timing Dependent Plasticity):

$$\Delta w = A_+ \exp\left(-\frac{\Delta t}{\tau_+}\right), \text{ for } t_{post} > t_{pre}$$

$$\Delta w = -A_- \exp\left(\frac{\Delta t}{\tau_-}\right), \text{ for } t_{post} < t_{pre}$$

Tsodyks-Markram Model:

$$\frac{du}{dt} = -\frac{u}{\tau_f} + \sum_j w_j s_j$$

$$\frac{ds}{dt} = -s \frac{s}{\tau_d} + U(1-s) \sum_j \delta(t - t_j^{spike})$$

Biophysical Models: Simulating the interactions between neurons with detailed biophysical properties such as dendritic compartments and multiple ion channels.

$$v' = 0.04v^2 + 5v + 140 - u + I$$

Izhikevich Model: $u' = a(bv - u)$

FitzHugh-Nagumo Model:

$$v' = v - \frac{v^3}{3} - w + I$$

$$w' = \frac{v + a - bw}{\tau}$$

Interpretive Models:

Interpretive models focus on explaining or interpreting specific neural phenomena. These models are designed and used to provide insights into the underlying mechanisms or principles governing neural processes, providing the relationships between neural activity and external stimuli. Though they provide insights, unlike mechanistic models they may not necessarily aim to capture all the intricate details of neural biology, they just prioritize conceptual understanding.

Integrate-and-Fire Models: Operating on the principle of accumulating input until a threshold is reached, providing a simplified yet powerful interpretation of neuron behavior.

$$C \frac{dV}{dt} = I(t) - g(v - E_{leak})$$

Spike condition: If $V(t) \geq V_{threshold}$ rest V and add a spike

Generalized Linear Models: Encompassing various subtypes such as temporal filtering, Bernoulli, and logistic regression, these models offer a flexible framework for capturing relationships between stimuli and neural responses.

Temporal Filtering

$$y(t) = \sum_{\tau=0}^T h(\tau) x(t-\tau) + \varepsilon(t)$$

Bernoulli GLM:

$$P(y=1) = \sigma(w \cdot x + b)$$

Logistic Regression:

$$P(y=1) = \frac{1}{1 + \exp(-(w \cdot x + b))}$$

For the diverse set of neural models used in the framework, optimal parameters were selected through a combination of literature reviews.

The goal was to ensure that each model accurately captured essential characteristics observed in experimental data.

Parameters such as transfer functions, connectivity kernels, activation functions, and external inputs were carefully chosen for descriptive and mechanistic models. These decisions were informed by the desire to replicate realistic firing rate patterns, spatial and temporal dynamics, and synaptic plasticity observed in neural systems. The models were evaluated by running them against randomly sampled arrays simulating various input conditions, to ensure the adaptability and robustness of each model across diverse neural scenarios.

IV. LITERATURE SURVEY

In crafting a comprehensive computational neuroscience framework, a survey of foundational literature reveals key insights across various modeling paradigms. The integration of Python into the NEURON [1] simulation program signifies a significant leap in computational neuroscience, empowering researchers with the flexibility and extensive analysis tools of Python alongside NEURON's traditional Hoc interpreter. This collaboration not only grants access to established engineering and scientific tools but also propels ongoing NEURON software development. Existing models seamlessly transition into Python, exemplified by the utilization of Python's XML module in NEURON's Import 3D and CellBuild tools for reading MorphML and NeuroML model specifications. This seamless interoperability enhances NEURON's adaptability, providing a modern and robust programming environment for intricate neural simulations. Simultaneously, The Virtual Brain (TVB) [2] emerges as a neuroinformatics platform, featuring a simulation environment supporting model-based inference of neurophysiological mechanisms. TVB's Python core, data management framework, and support for personalized brain configurations make it a versatile tool for macroscopic neuroimaging signal generation. As neuroscience experiences rapid experimental growth, a pragmatic perspective emphasizing the distinct roles of descriptive, mechanistic, and normative models guides neuroscientific practice [3], offering methodological insights for advancing modeling approaches. The collaborative potential of Python in NEURON and TVB's comprehensive simulation capabilities collectively contribute to the evolving landscape of sophisticated neuroscientific methodologies.

V. RESULTS

Incorporating the models into the framework facilitated the seamless exploration of neural phenomena at various scales, emphasizing the versatility and adaptability of our approach. The analyses were not only informative but also visually compelling, with the framework’s visualization tools allowing for a nuanced interpretation of simulated neural activities.

This research opens avenues for further research and application, demonstrating the framework’s potential as a valuable tool for researchers and practitioners in the field of computational neuroscience.

TABLE 1

Parameters and variables

Type	Model	Input		
		Stimulus	Rate	Time Steps
Descriptive	Neural Firing Rate	[0.1,0.3,0.6,0.3,0.1]	100	5
	Population Rate	20	5	100
	Neural Field	[1.5,0.5]	2	20
Mechanistic	Hodgkin-Huxley	10	400	500
	STDP	[11,25,47]	3	100
	Tsodyks-Markram	[11,25,47]	3	1
	Izhikevich	[0,0,0,0,10,10,10,10]	0.1	700
	Fitzhugh Nagumo	[0.02,0.1,0.9]	0.9	10000
Interpretive	Integrate-and-Fire	[0,0,0,0,1,1,1,1,0,0,0,0]	10	10
	Temporal Filtering	[0.1,0.3,0.6]	1000	5
	Bernoulli GLM	[0.5,-0.2,0.8]	1000	5
	Logistic Regression	[0.5,-0.2,0.8]	1000	5

From the above table, diverse neural response patterns were obtained across the implemented models, with all other variables chosen in accordance with their respective equations.

VI. CONCLUSION

We began by recognizing the challenges inherent in modeling neural phenomena across scales and proposed a unified framework to encompass various modeling approaches. The significance of our finding lies in the framework’s ability to seamlessly unite Descriptive, Mechanistic, and Interpretive models showcasing the underlying properties of neural systems. The simulations yielded a rich variety of outputs, including the adaptability and versatility of our approach. Each model is chosen for its appropriateness to specific aspects of neural dynamics.

Our framework addresses the challenge of unifying disparate modeling approaches, providing a cohesive environment for researchers to investigate and infer neural phenomena.

The contributions of our work extend beyond individual models offering insights for future investigations and advancements in

computational neuroscience methodologies. In summary, our research marks a significant step towards advancing and fostering a deeper comprehension of the facets of neural dynamics.

REFERENCE

- [1] D. Levenstein et al., “On the Role of Theory and Modeling in Neuroscience,” *The Journal of Neuroscience*, vol. 43, no. 7, pp. 1074–1088, Feb. 2023, doi: 10.1523/jneurosci.1179-22.2022.
- [2] E. M. Izhikevich, “Simple model of spiking neurons,” *IEEE Transactions on Neural Networks*, vol. 14, no. 6, pp. 1569–1572, Nov. 2003
- [3] S. H. Koslow and S. Subramaniam, *Databasing the Brain*. 2005.
- [4] N. M. Grzywacz, “The Computational Brain.Patricia S. Churchland , Terrence J. Sejnowski,” *The Quarterly Review of Biology*, vol. 68, no. 3, pp. 457–457, Sep. 1993, doi: 10.1086/418250.
- [5] M. Hines, “NEURON and Python,” *Frontiers in Neuroinformatics*, vol. 3, 2009
- [6] P. Sanz-Leon et al., “The Virtual Brain: a simulator of primate brain network dynamics,” *Frontiers in Neuroinformatics*, Jan. 01, 2013.
- [7] A. Gillies and G. Arbutnott, “Computational models of the basal ganglia,” *Movement Disorders*, vol. 15, no. 5, pp. 762–770, Sep. 2000, [Online]. Available: [http://dx.doi.org/10.1002/1531-8257\(200009\)15:5<762::aid-mds1002>3.0.co;2-2](http://dx.doi.org/10.1002/1531-8257(200009)15:5<762::aid-mds1002>3.0.co;2-2)
- [8] J. Harbecke, “The methodological role of mechanistic-computational models in cognitive science,” *Synthese*, vol. 199, no. S1, pp. 19–41, Feb. 2020, doi: 10.1007/s11229-020-02568-5.
- [9] M. Tsodyks and S. Wu, “Short-term synaptic plasticity,” *Scholarpedia*, vol. 8, no. 10, p. 3153, 2013, doi: 10.4249/scholarpedia.3153.
- [10] J. Sjöström and W. Gerstner, “Spike-timing dependent plasticity,” *Scholarpedia*, vol. 5, no. 2, p. 1362, 2010, doi: 10.4249/scholarpedia.1362.
- [11] J. Vreeken, "Spiking neural networks, an introduction," 2003
- [12] T. B. Williams, C. J. Burke, S. Nebe, K. Preuschoff, E. Fehr, and P. N. Tobler, “Testing models at the neural level reveals how the brain computes subjective value,” *Proceedings of the National Academy of Sciences*, vol. 118, no. 43, Oct. 2021, doi: 10.1073/pnas.2106237118