EBRAINS 2.0

D3.1 EBRAINS Simulation – first release

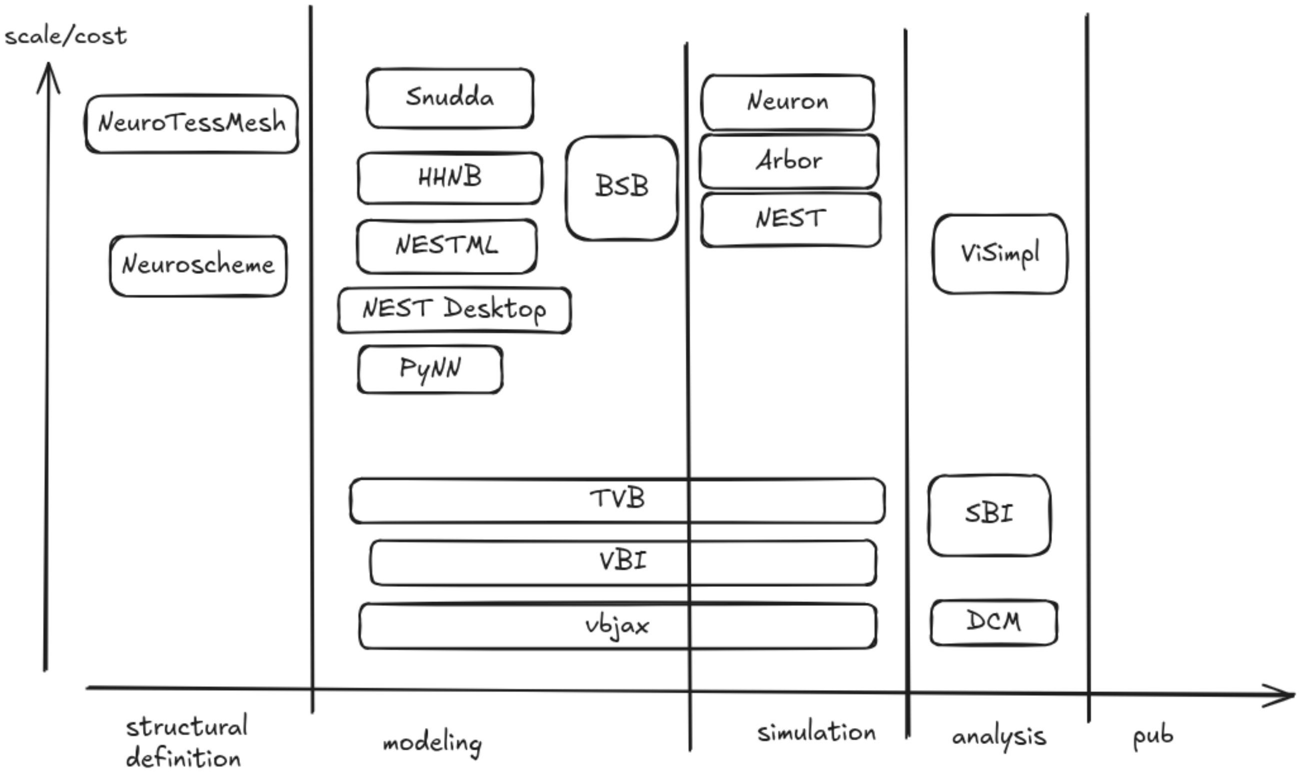

Figure 1: Overview of the different tools and their roles in the data-driven simulations on EBRAINS.

The scientists choose a scale of interest along with resources available appropriate for their data, expressed in the diagram as the vertical axis, then progresses along the stages of their simulation project, expressed as the horizontal axis. The stages are for presentation purposes; in practice, several iterations along the stages may be required in a given project.

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Abstract:	This release of the EBRAINS toolbox provides a foundational platform for future development, offering a functional suite of tools that support complex simulations and research workflows. It integrates tools like NEST, Arbor, HHNB, and TVB, benefiting both experienced researchers and newcomers. The toolbox also supports the EBRAINS project's educational goals, aiding in the training of students and aspiring scientists. Ongoing improvements aim to enhance usability, reduce technical burdens, and foster collaboration, ultimately advancing neuroscience through innovative tools and infrastructure		

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1. List of Abbreviations

Table 1: List of Abbreviations

Abbreviation	Meaning
AI	Artificial Intelligence
API	Application Programming Interface
BOLD	Blood Oxygenation Level Dependent
BSB	Brain Scaffold Builder
CSCS	Swiss National Supercomputing Centre
DCM	Dynamic Causal Modelling
EBRAINS KG	EBRAINS Knowledge Graph
EEG	ElectroEncephaloGraphy
EITN	Fall School in Computational Neuroscience
ERP	Event-Related Potentials
ESD	EBRAINS Software Distribution https://gitlab.ebrains.eu/ri/tech-hub/platform/esd
HBP	Human Brain Project
HHNB	Hodgkin-Huxley Neuron Builder
HPC	High Performance Computing
JSC	Jülich Supercomputing Centre
KG	Knowledge Graph
MCMC	Markov Chain Monte Carlo
MEG	MagnetoEncephaloGraphy
ML	Machine Learning
MPI	Message Passing Interface
NRP	Neurorobotics Platform
NMH	Neuromorphic Hardware
SBI	Simulation-Based Inference
SEEG	Stereoelectroencephalography
T (e.g., T3.1, T3.2)	Task
TVB	The Virtual Brain www.thevirtualbrain.org
VAPT	Vulnerability Assessment and Penetration Test
VBI	Virtual Brain Inference
WP	Work Package
WP3 Gitlab	https://gitlab.ebrains.eu/ri/projects-and-initiatives/ebrains-2/wp3

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[1] *For this link to work:*
- the person accessing needs to have an EBRAINS valid account
- with that account login at gitlab.ebrains.eu at least once before
- writing us an email with the username, and we can grant access to the project science@codemart.ro or lia.domide@codemart.ro

2. Overview

EBRAINS is a platform designed to integrate a diverse array of tools and resources for neuroscience research. A recurring issue is that this environment primarily comprises a collection of specialized tools, each addressing specific aspects of the research process, sometimes lacking an overall coherence. While these tools offer substantial capabilities at various scales—from single-neuron modeling to whole-brain dynamics—a key challenge has been establishing clear linkages between data, modeling paradigms, and simulation workflows. This report details the progress made towards addressing this challenge with the first release of a toolbox intended to bridge gaps in the stages of a scientist's progress from FAIR data to high impact simulation results.

The toolbox encompasses a range of tools supporting research across multiple scales and stages of project development. The Brain Scaffold Builder (BSB) facilitates the creation of network architectures, while the Hodgkin-Huxley Neuron Builder (HHNB) enables the construction of detailed neuron models for integration into these networks. The NEST simulator provides a core environment for network dynamics modeling, complemented by Arbor and NEURON for high-resolution simulations of individual neurons. TVB serves as a platform for large-scale whole-brain simulations, and the Virtual Brain Inference (VBI) and Dynamic Causal Modeling (DCM) tools provide crucial inference capabilities for interpreting results within the TVB framework. The toolbox also benefits from the integration of tools like the NEST simulator and the PyNN interface enabling cross-validation across different simulation platforms. This initial release represents a preliminary step toward creating a more cohesive and user-friendly simulation environment, intended to accelerate data-driven discoveries and foster a deeper understanding of brain function.

The list of tools and their corresponding links are presented in Table 2, and the role of these tools are schematized in Figure 1.

Table 2: List of tools with their corresponding links

Tool	Function/Role	Link to the tool on Gitlab
NeuroScheme (0.7.6)	Visualisation allowing the interactive exploration of neural data	Link
NeuroTessMesh (0.5.3)	Visualisation allowing the interactive exploration of neural data	Link
ViSimpl (1.8.12)	Visualisation allowing the interactive exploration of neural data	Link
Virtual Brain Inference	For informed dimensionality reduction	Link
The Virtual Brain (TVB) core packages	For whole-brain simulations	Link1 and Link2
Arbor	Library for high-performance modeling of neurons and neural networks	Link
Hodgkin-Huxley Neuron Builder	For biophysically detailed models of neural cells	Link
NEST	For single-compartment neuron and network models	Link
Brain Scaffold Builder	For network reconstruction	Link

3. Visualization

3.1 NeuroScheme, NeuroTessMesh and ViSimpl

NeuroScheme serves as a crucial initial exploratory tool, providing simplified schematic representations of neural structures and networks to facilitate rapid assessment of network architecture and identify areas of interest for more detailed analysis. The tool utilizes icons and glyphs to encode attributes of neural structures, particularly focusing on the "cortex" and "congen" domains, providing a visual overview of neuron populations and their connections within complex networks. To enhance documentation and collaboration, recent versions (0.7.6) incorporate advanced screenshot and HD video recording capabilities. It is accessible through the EBRAINS environment, leveraging the Spack-based ESD for consistent deployment, and ongoing development efforts are focused on building a new prototype for interactive visualization of complex networks.

NeuroTessMesh is used to visualize the detailed 3D morphology of individual cells, contributing a vital level of detail to overall network analysis. Facilitating detailed analysis of cellular structures and supporting validation of simulation results, it enables visualization of 3D cell morphology based on morphological tracings as input. Recent versions (0.5.3) have prioritized overall stability and performance, with improvements to handling large tracing datasets. Also accessible through the EBRAINS via ESD, NeuroTessMesh contributes significantly to a deeper understanding of neuronal morphology.

ViSimpl allows for the spatio-temporal analysis of simulation data, providing insight into how networks evolve over time and space. It performs spatio-temporal analysis using particle-based rendering, facilitating the visualization of dynamic network behavior and contributing to a broader comprehension of complex neurological processes. Recent versions (1.8.12) focused on performance optimization and improvements to particle rendering capabilities, enabling the visualization of larger and more complex simulations. Also accessible through the EBRAINS via ESD, ViSimpl enables researchers to gain a better understanding of the dynamics generated by simulated neural networks.

Neuroscheme, Neuroteshmesh and ViSimpl provide tools to visually explore models and the resulting data produced. They will support the usage of and integrate into workflows including the standard models generated in T3.2 (INTEGRATE. Provide standard brain models for integrated use in EBRAINS workflows) and the demonstrators developed in T3.4 (DEMONSTRATE. Provide use cases as demonstrators).

4. Modeling

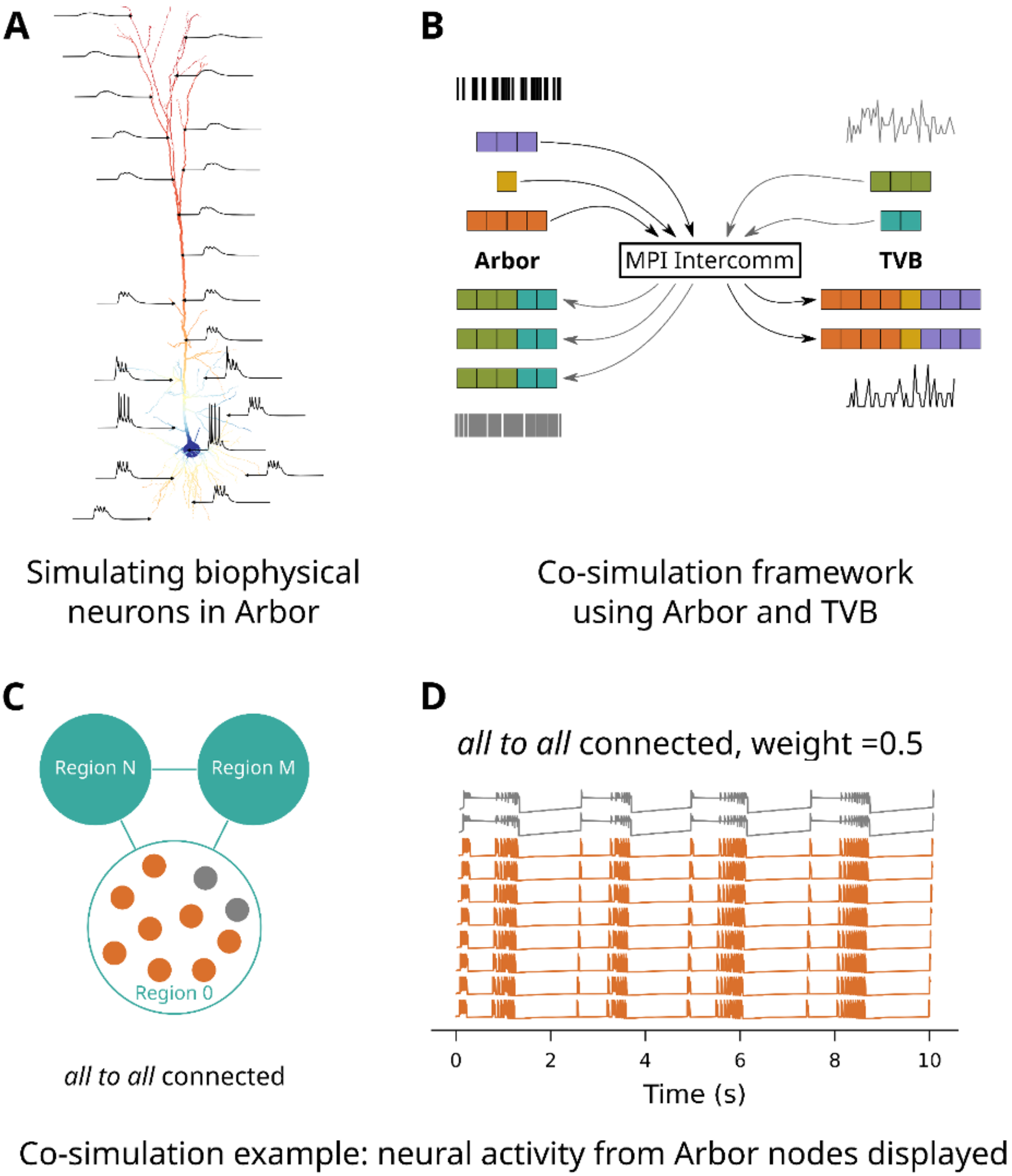
4.1 TVB

The Virtual Brain (TVB) facilitates the simulation of large-scale brain network dynamics using biologically realistic connectivity. As a platform designed for simulating "whole" brain network models, it represents a convergence of clinical, systems, and theoretical neuroscience. TVB's functionality allows for creating personalized brain models using diverse neuroimaging modalities and employs a hybrid approach reducing complexity at the micro level to attain macro-organization, generating EEG, MEG, BOLD, and SEEG signals. TVB enjoys deep integration with the EBRAINS browser-based JupyterLab user interface with several plugins, such as tvb-ext-xircuits, allowing a user to design their simulation visually. TVB has recently undergone several minor releases, to address compatibility upgrades to Python versions 3.11 and 3.12, a transition from OKD to Kubernetes, and the implementation of numerous fixes. This ongoing development has been further enhanced by new versions of the tvb-widgets library, facilitating usability within EBRAINS workflows and JupyterLab, and a migration to JupyterLab for the tvb-ext-xircuits extension. The focus is also on ongoing enhancements to new models and ensuring compatibility with the core organization within TVB.

TVB is a critical component in the demonstrator 3 being developed in T3.4 and in the workflows being built to operate digital twins with focus on personalized predictive medicine being developed in T3.3 (OPERATE. Build workflows to operate DIGITAL TWIN brain models). TVB is also the core simulator supporting standard models for full brain scale developed in T3.2.

4.2 Arbor

Arbor functions as a cutting-edge simulator for high-performance modeling of neurons and neural networks, enabling researchers to study biologically plausible neuronal dynamics and their interaction with large-scale brain activity. Its key features include customizable morphology and biophysical properties and, most recently, the implementation of multi-scale modeling that allows seamless integration with TVB. Arbor allows researchers to investigate a wide range of neurological phenomena in health and disease, improving our understanding of complex brain dynamics. As a recent advancement, the implementation of multi-scale modeling introduced in Arbor 0.10.09 now allows seamless co-simulation with TVB (Figure 2). Arbor is available in the ESD and aiming for deployment on next-generation exascale HPC systems such as JUPITER at JSC.



Simulating biophysical neurons in Arbor

Co-simulation framework using Arbor and TVB

all to all connected

Co-simulation example: neural activity from Arbor nodes displayed

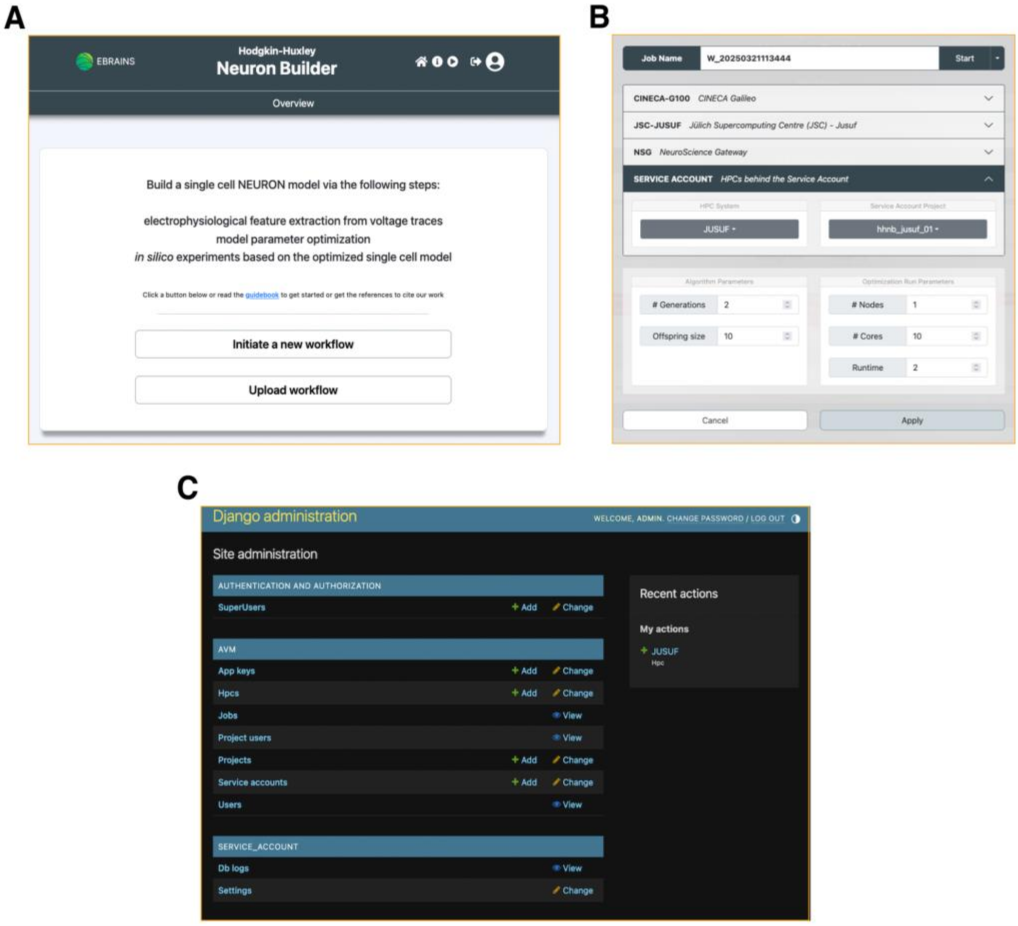
Figure 2: Arbor provides high-fidelity neuronal simulations, complemented by an intercommunicator MPI linking Arbor and TVB.

A) Simulating detailed biophysical neuron models in Arbor, with individual membrane voltage traces shown. (B) Architecture of the co-simulation framework integrating Arbor and The Virtual Brain (TVB) via MPI intercommunication. (C) Schematic of an all-to-all connected network, showing regions with interconnected populations. (D) Example output of the co-simulation.

We have been successfully applying this framework to study seizure propagation in epilepsy through a collaboration with Prof. Thanos Manos at Cergy University, providing insights into how localized seizures influence whole-brain dynamics. Future applications include probing the interaction between network activity and synaptic plasticity in Alzheimer's disease, optimizing brain stimulation protocols, and advancing cognitive modeling.

4.3 Hodgkin-Huxley Neuron Builder

The Hodgkin-Huxley Neuron Builder (HHNB) web application facilitates the construction and optimization of biophysically detailed neuron models implemented in NEURON, enabling researchers to refine models against experimental electrophysiological data [1-2] (Figure 3). This tool provides a user-friendly interface and services for model construction, electrophysiological feature extraction, model optimization on HPC systems, and model simulation, offering a significant benefit for data-driven refinement of neuron models. Recent enhancements to HHNB focus on enabling users lacking direct HPC credentials to submit jobs on national HPC systems at CINECA and JSC. User and project management have been streamlined through an upgraded graphical user interface. Importantly, HHNB maintains a seamless interaction with novel/renewed EBRAINS services, and ongoing work focuses on direct integration with the EBRAINS KG and a tighter relationship with the Hippocampus Hub.



Build a single cell NEURON model via the following steps:

electrophysiological feature extraction from voltage traces
model parameter optimization
in silico experiments based on the optimized single cell model

Click a button below or read the guidebook to get started or get the references to cite our work

Job Name: W_20250321113444

HPC System: JUSUF
Service Account Project: hhnb_jusuf_01

Generations: 2
Offspring size: 10
Nodes: 1
Cores: 10
Runtime: 2

Figure 3: The Hodgkin-Huxley Neuron Builder.

(A) The Neuron Builder homepage guides users through the workflow to construct a single-cell NEURON model. Key steps include electrophysiological feature extraction, model parameter optimization, and in silico experimentation. Users can start a new workflow or upload an existing one. (B) Job configuration panel where users select a high-performance computing backend assign service accounts, and define parameters for optimization and computing resources. (C) Django-based administration interface for managing backend services.

The HHNB is a core component in the single cell to network level modeling, in particular on the standard models using multicompartment neurons developed in T3.2.

4.4 BSB

The Brain Scaffold Builder (BSB), developed by the Department of Brain and Behavioral Sciences at the University of Pavia, functions as a component-based framework for neural modeling, enabling the construction of brain models through the modular connection of predefined components (see Figure 4). Its flexible architecture allows component declarations to be created in various supported configuration languages or directly in Python. The BSB facilitates a wide range of simulation strategies through its capability to parallelize reconstruction and simulation of diverse network topologies, placements, and connectivity strategies. Key to the builder's functionality is the ability to utilize NEURON, NEST and Arbor and integration with the MUSIC interface to perform close-loop simulations with robotic models (e.g. PyBullet). This flexible approach provides researchers with the capability to develop and analyze complex neural network models with enhanced efficiency and reproducibility. Recent enhancements have significantly improved the tool's usability and stability. A major version release (v4) introduced a redesigned user interface focused on core functionalities, ensuring thorough testing, while the implementation of a continuous integration pipeline now streamlines release production. To further enhance accessibility and usability, new tutorials have been developed and interface refinements have been implemented. The BSB is integrated with EBRAINS both in the KG and the ESD.

The BSB is being integrated into Demonstrator 1[2] in T3.4, where it defines hybrid controllers for neurorobotics applications in combination with the NEST simulator and the NRP.

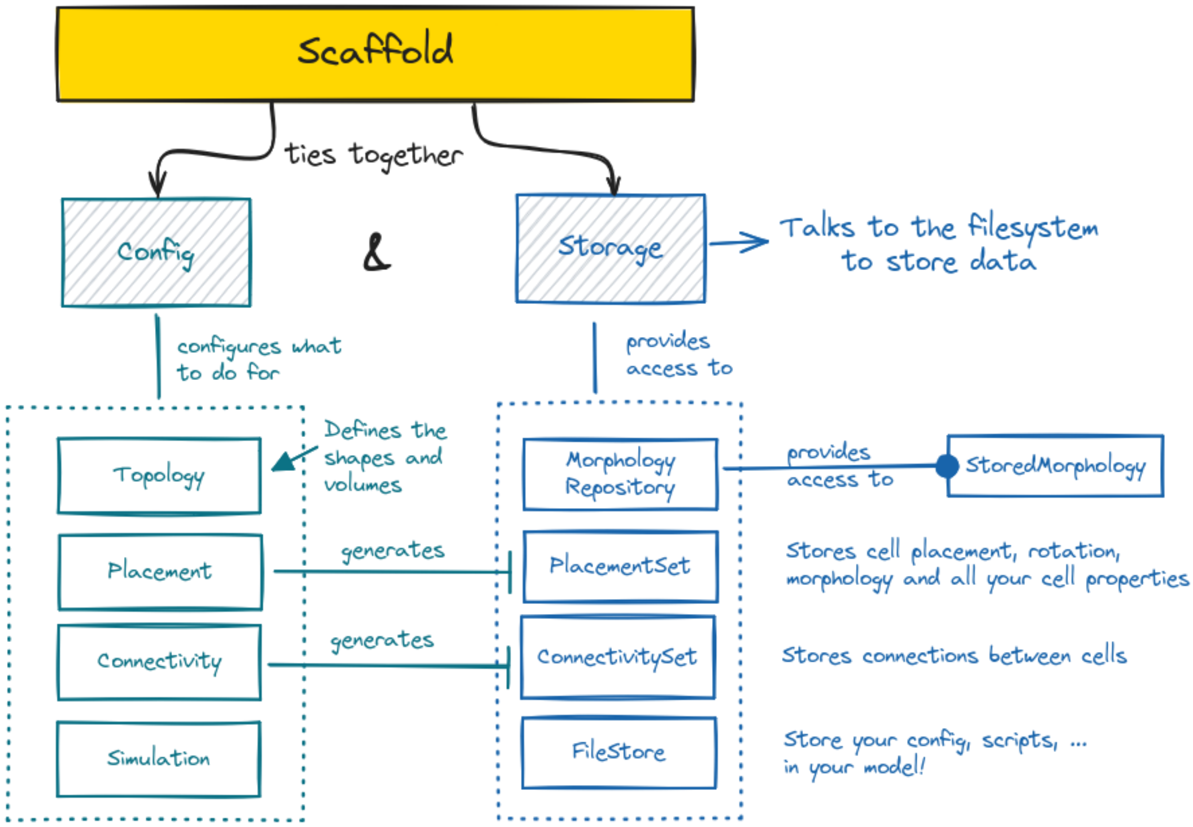


Figure 4: High-level schematic of the BSB interface.

The Scaffold module orchestrates configuration (left) and storage (right) components. Configuration defines shapes, volumes, and simulation parameters via modules for topology, placement, connectivity, and simulation. These generate model elements that are then stored using the storage

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[2] Demonstrator 1 will illustrate a use case in neurorobotics integrating spiking neural networks (SNNs) and AI modules to construct cognitive brain scaffolds

system, which provides access to morphology data, cell placement, connectivity, and filesystem storage.

4.5 NEST

The NEST Simulator forms the core infrastructure within the EBRAINS ecosystem for simulating network dynamics at a single-neuron resolution. Providing a low-threshold entry point for researchers of all levels, the NEST Simulator can be used via a web-interface (NEST Desktop) allowing users to quickly build and execute simulations without requiring any prior programming experience. As a next step, users with a deeper programming background can leverage a convenient "code translation" feature to transfer their developed simulations directly into EBRAINS JupyterLab, where they can then perform more complex experiments and analyses within a Python environment. Model customization and reusability are significantly streamlined by the NEST modeling language (NESTML), a key component of EBRAINS that translates theoretical mathematical descriptions into loadable simulation modules. The system further supports research through compatibility with the simulator-independent PyNN interface, facilitating cross-validation across various simulations and the incorporation of network connectivity data from SONATA files. Deployed on EBRAINS through the ESD, with NEST Desktop operating as a service on the cloud infrastructure, and with a wealth of models accessible through the KG, the NEST Simulator provides a versatile and robust platform for network neuroscience investigations.

NEST is used to simulate the standard models at the mesoscale level developed in T3.2, and is the core simulation engine for Demonstrator 1 in T3.4.

5. Inference

The OPERATE task (T3.3) focuses on developing inference tools that are interoperable and applicable across scales, datasets, and species. These tools leverage data features and model parameters to enable informed dimensionality reduction, bridging the gap with state-of-the-art machine learning and classification toolboxes. To maximize the predictive power of personalized brain models, we develop automated tools that quantify predictive outcomes along with their associated uncertainty regarding adaptive or maladaptive responses (degeneration and dedifferentiation, and degeneracy). These probabilistic AI/ML tools can be seamlessly integrated with other tools in EBRAINS.

To achieve these objectives, we have built automated and flexible inference tools integrated into EBRAINS. These tools enable Bayesian inference of latent and observed states within systems influenced by input stimuli, such as noise and/or network effects. Such a probabilistic approach quantifies all possible solutions within the parameter space to quantify the uncertainty (Figure 5A). Hence, they deal with non-identifiability and its geometrical counterpart known as degeneracy, i.e., the existence of multiple equivalent solutions in the parameter space [3]. This has been accomplished through two primary inference pipelines (likelihood-based, and likelihood-free inference) presented in the following.

5.1 Dynamic Causal Modeling

Dynamic Causal Modelling (DCM) provides a powerful framework for analyzing the causal relationships between brain regions and their responses to experimental manipulations, addressing the challenge of efficient and automated model inversion. The implementation leverages advanced probabilistic programming languages, including Stan, PyMC, and NumPyro, enabling efficient benchmarking and incorporating state-of-the-art machine learning techniques for model comparison. This framework allows researchers to investigate the direction and strength of influences between brain areas and evaluate the plausibility of various model configurations (see Figure 5B), achieving reliable MEG and

EEG event-related potential (ERP) analyses in under one minute on the EBRAINS platform, with inference carefully monitored using convergence diagnostics. To facilitate user adoption and learning, notebooks with example workflows are available in the repository, a tutorial is offered at the EITN School to enable students within the EBRAINS environment (see code here, and here), and detailed information is accessible through the EBRAINS wiki here.

Task 3.3 “Operate” provides a concrete use case of this tool, in its application to High-Gamma Activity observed in MEG and intracranial sEEG data, following the work of Chen *et al.* [4]. The tool’s data-driven approach streamlines the analysis, allowing researchers to rapidly evaluate the plausibility of different model configurations, exemplified by the successful application to data from 8 subjects reported by Brovelli *et al.* [5]. This allows for a fast and accessible means of investigating causal interactions within brain networks.

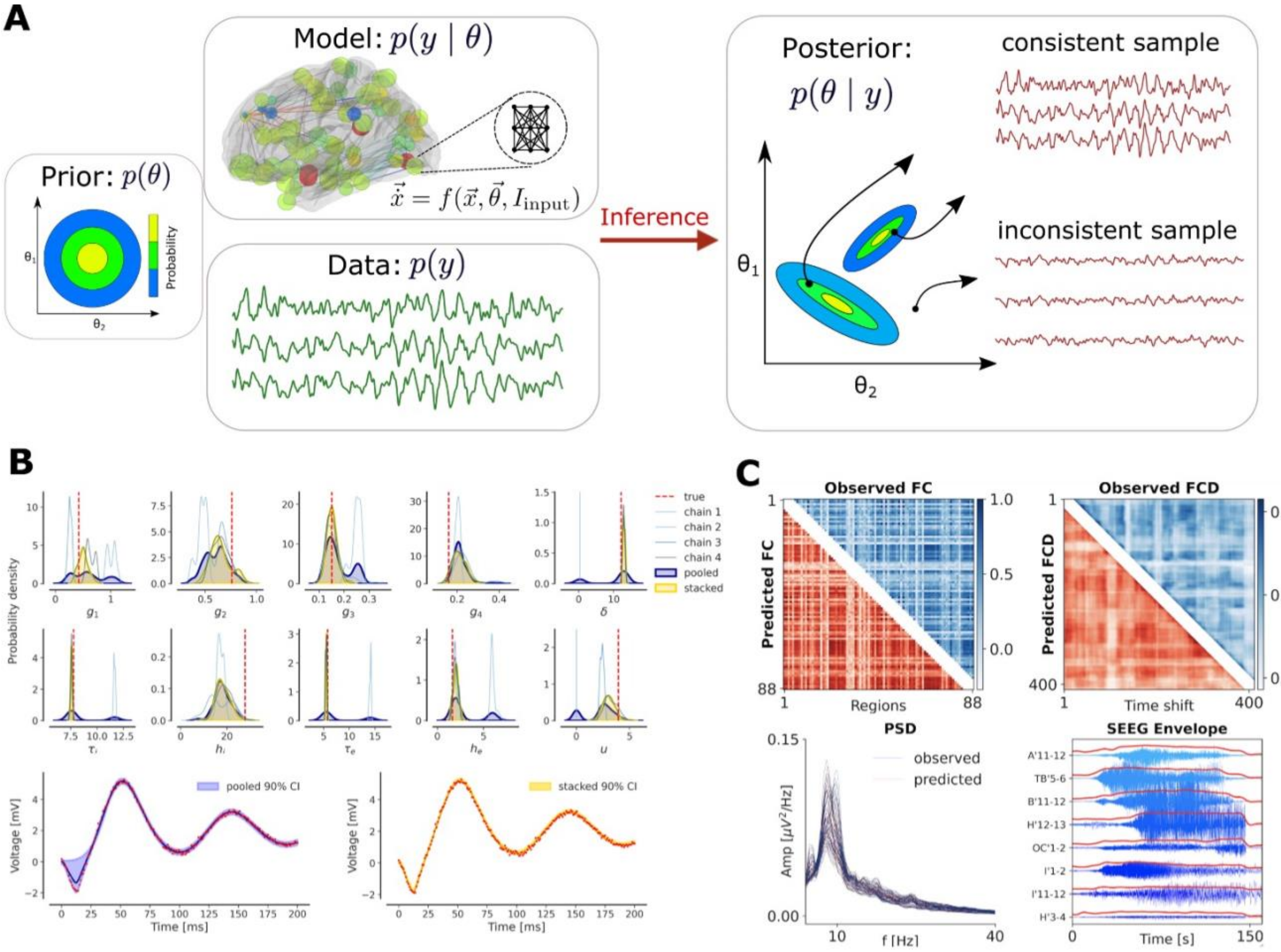

Figure 5: Bayesian inference framework for brain network modeling and validation with empirical data

Based on Bayes’ theorem, background knowledge about parameters is combined with information from observed data (in the form of a likelihood function) to determine the posterior distribution. MCMC algorithms directly sample from the posterior distribution, while SBI algorithms transform a simple distribution (prior) into any complex target (posterior). Both methods inform us about degeneracy by providing all possible solutions in parameter space that best explain the data. (B) Automatic DCM address the issue of degeneracy by weighted stacking of multimodal posteriors. (C) Examples of the observed and predicted data features, such as functional connectivity, functional connectivity dynamics, power spectral density, and SEEG envelope

5.2 Simulation-based Inference

Simulation-Based Inference (SBI) offers an efficient method for estimating posterior distributions when the likelihood function becomes intractable, allowing researchers to draw inferences about model parameters even when traditional analytical solutions are not available. This powerful approach utilizes deep neural density estimators to approximate an invertible function between parameters and data features, supporting inference from a wide range of non-invasive and invasive recordings. To support its use, a taxonomy of machine learning tools has been developed for feature extraction (see Figure 5 panel C) and example workflows are available in provided wikis (see code here). These capabilities have been demonstrated in various settings, including providing inference on spiking neurons in human and monkey [6], mean-field of spiking neurons [7], whole-brain simulations [8], modeling a virtual multiple sclerosis patient [9], and assessing focal interventions [10]. Virtual Brain Inference (VBI) specifically serves as a TVB-oriented application of SBI, providing fast simulations, a taxonomy for feature extraction, efficient data storage and loading, and provides an accessible means of applying the SBI framework to complex neuroscientific investigations. We have demonstrated SBI in several cases, providing inference on spiking neurons in human and monkey (see wiki here), mean-field of spiking neurons (see wiki here), whole-brain (see wiki here), virtual multiple sclerosis patient, and focal intervention. While these examples are primarily TVB oriented, they are applicable to other modeling scenarios with NEST or Neuron. The integration of SBI with EBRAINS in the ESD ensures continued accessibility and advancement of this powerful tool for the broader research community.

The ability to amortize inference highlights the potential for a more stratified and efficient approach to data-driven simulations. Specifically, a future workflow could involve assembling a pool of pre-built simulations, training a Simulation-Based Inference (SBI) estimator, and applying it to data. In the most advanced scenario, SBI estimators could be pre-trained, reducing the data analysis process to feature computation and estimator application. Recognizing the potential to significantly lower the cost of data-driven simulations on EBRAINS and substantially improve scientist productivity through the utilization of pre-built simulations, we believe a deeper integration into the platform is warranted. This could involve developing APIs and client libraries to automate this process, fostering a more streamlined and accessible data-driven simulation ecosystem within EBRAINS.

6. Discussion

6.1 Interoperability

The core strength of the EBRAINS toolbox lies not just in the collection of individual simulation tools – NEST, Arbor, BSB, HHNB, and others – but in their capacity to function as a unified and interconnected ecosystem. This interconnectedness extends beyond simple co-location; it represents a deliberate effort to establish theoretical interoperability and standardization, ensuring that data and models can flow seamlessly between tools. A central element of this design is the EBRAINS Software Distribution (ESD), which provides a standardized and accessible platform for deploying and managing these tools. This approach minimizes installation complexity and ensures consistency across various HPC environments, dramatically reducing friction for users. The ESD also brings significant benefits related to data management – allowing for the strategic placement of data, particularly large or sensitive datasets, closer to computational resources, alleviating load on the central EBRAINS cloud infrastructure.

Interoperability is demonstrated in several practical examples. For instance, a research workflow might begin with datasets accessed from the Knowledge Graph or WP1 Atlas services, then leverage the Brain Scaffold Builder to construct complex network architectures. Following that, the Hodgkin-Huxley Neuron Builder (HHNB) can be used to build detailed neuron models, which can then be integrated into the network architecture defined by the Brain Scaffold Builder. Similarly, the ability to load network connectivity from SONATA files allows for a data-driven approach, commonly used for simulations on finer scales, to be incorporated into larger-scale network simulations. Furthermore, tools like the NEST simulator and the PyNN interface enable cross-validation across different simulation platforms, strengthening the reliability of results. Tasks such as T3.2 (focused on neuromodulation across multiple scales) and T3.4 (involving Demonstrator 1 and Demonstrator 3[3]) contribute to this integrated workflow by leveraging the toolbox's capabilities to address complex research questions, demonstrating the power of this interconnected environment.

6.2 Future work

For the next EBRAINS Simulation toolbox release our main goals are to:

- make it easier for EBRAINS users to run models at different scales, integrating these tools further with other EBRAINS services e.g. Collaboratory access, HPC support and different storage tiers, access to multimodal data, automated testing and workflow execution, etc.,
- have a more uniform access to HPC and NMH to support whole workflows where needed, and
- further support for interoperability and standards, addressing new use cases and making it easier for users to move easily through different tools.

Looking ahead, further enhancing the platform’s functionality involves integrating Simulation-Based Inference (SBI) as a readily available service. This would provide an accessible “frontline” for master’s and PhD students, allowing them to rapidly build and test hypotheses before embarking on more resource-intensive simulations. The prospect of an API facilitating amortized SBI inference, drawing on a pool of existing simulations, presents a particularly promising avenue for accelerating data-driven discoveries while managing storage costs. The ongoing discussion with Task 3.5 (CURATE. Maintain, upgrade and enhance the usability, robustness, reliability and performance of the workflow software) and WP5 aims to refine this vision and explore innovative ways to make the toolbox even more accessible and powerful for the research community, continually supporting a collaborative and impactful research environment.

6.3 Conclusions

This release marks a significant milestone in the development of the EBRAINS toolbox, representing a foundation upon which future iterations will build. While this is considered a first release, the integrated suite of tools provides a functional and valuable environment for supporting ongoing demonstrations and facilitating a range of research workflows. The toolbox’s ability to streamline complex simulations, as evidenced by the interconnectedness of tools like NEST, Arbor, and HHNB, as well as whole brain modeling tools like TVB, provides a valuable platform for both experienced researchers and those newer to the field.

Beyond direct research applications, this release contributes to the broader pedagogical goals of the EBRAINS project. The accessible nature of tools like the NEST simulator and the integrated workflow supports the onboarding of students and aspiring scientists, helping them develop the skills and knowledge needed to contribute to the neuroscience community. Moreover, the ongoing efforts to enhance integration and usability are designed to improve the overall quality of life for researchers by reducing technical burdens and fostering a more collaborative research environment. We anticipate that this foundation will be built upon to offer an even more robust and user-friendly experience in future

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[3] Demonstrator 3 will use WP2 data to highlight the application of virtual brain twins to epilepsy surgery.

releases, continuing to advance the field of neuroscience through innovative simulation tools and integrated research infrastructure.

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List of Wiki:

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2) https://wiki.ebrains.eu/bin/view/Collabs/inference-mfm/
3) https://wiki.ebrains.eu/bin/view/Collabs/sbi-vbms/
4) https://wiki.ebrains.eu/bin/view/Collabs/sbi-brunel-se/

Link to the notebooks:
https://wiki.ebrains.eu/bin/view/Collabs/ebrains-task-3-3/Drive#notebooks