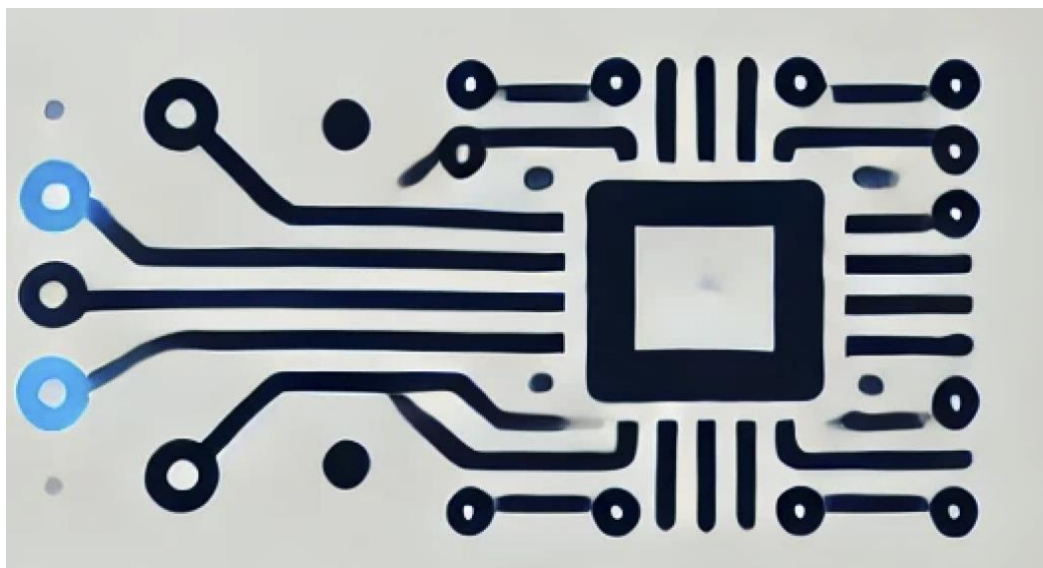


Open software for neural wavefunctions



*July 2 - 4, 2025
CECAM-HQ-EPFL, Lausanne, Switzerland*

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With the support of:



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1. Description

Variational methods based on physically-motivated ansatzes have long been the cornerstone of simulating strongly-correlated quantum systems. However, the field experienced a paradigm shift in 2017 with the introduction of Machine Learning techniques, particularly Neural Networks and advanced optimization schemes, to this domain [1]. This innovation gave birth to Neural Quantum States (NQS), a powerful new class of variational ansatzes that synergizes the physical insight of traditional approaches with the unparalleled function approximation capabilities of Neural Networks.

The impact of Neural-Network based ansatzes on the field has been profound. They have consistently outperformed competing approaches such as tensor networks in simulating spin systems [2], achieved unprecedented numerical precision in ground-state searches for large benchmark problems [3], and enabled the study of long-time dynamics in systems of unprecedented scale [4,5]. The reach of these methods extends beyond spin systems, with state-of-the-art results also reported in Bosonic [6] and electronic systems [7].

This rapid progress can be attributed to two key factors. First, the development of robust, large-scale machine learning libraries such as PyTorch and JAX provided a solid foundation for implementing these complex models. Second, the early development of domain-specific, open-source software packages [8,9] played a crucial role in democratizing these techniques within the quantum physics community.

These open-source initiatives have been instrumental in accelerating research in the field of Machine Learning for quantum physics. They have provided accessible, well-documented libraries that have been widely cited in the literature, lowering the barrier to entry for young researchers and facilitating the reproduction and extension of published work. By centralizing efforts around a core set of libraries, the field as a whole has benefited from continuous algorithmic improvements, creating a virtuous cycle of innovation and implementation.

Objectives

Our primary objective is to bring together leading researchers, software developers, and newcomers to the field to chart the course for the next generation of Neural Quantum States research and supporting open-source infrastructure. In particular, this CECAM Flagship Workshop aims to:

- Identify and address in a collaborative manner challenges originating from software that hamper the development of the field of Machine Learning for Quantum Simulation and Neural Quantum States in particular;
- Kickstart new Open-Source Software efforts, in particular to satisfy the growing need of the community of reproducibility and sharing of Neural Network architectures and trained weights;
- Federate existing Open-Source Software efforts in the domain in an organic manner;
- Recruit new young researchers/students into this effort and make them feel part of the greater community;

We will begin by conducting a comprehensive review of the current state of Neural Quantum States and related open-source software. This will serve as a foundation for identifying critical areas for software improvement and algorithmic implementation. Through collaborative discussions and hands-on sessions, we aim to establish best practices for developing and maintaining open-source quantum physics software, with a particular focus on implementing recent advances and improving code sustainability.

A key focus of the workshop will be exploring the potential of pre-trained models for quantum physics problems [10]. We will work towards developing a framework for creating, sharing, and leveraging these models, potentially revolutionizing how we approach complex quantum systems.

The workshop will also serve as an incubator for new collaborative projects aimed at addressing identified gaps in the current software ecosystem. By bringing together experienced developers with newcomers to the field, we hope to foster knowledge transfer and cultivate the next generation of contributors to open-source quantum physics software.

Ultimately, we aim to produce a community-driven roadmap for the future of open-source software in Neural Quantum States and related fields. This roadmap will serve as a guide for future development efforts and help align the community's efforts towards common goals. By addressing these objectives, we believe this workshop will catalyze the next phase of development in Neural Quantum States and open-source quantum physics software. It will accelerate progress in the field by enabling more researchers to contribute to and benefit from these powerful tools, ultimately advancing our understanding of complex quantum systems.

Key References

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- [3] A. Chen, M. Heyl, *Nat. Phys.*, **20**, 1476 (2024)
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- [6] Z. Denis & Al. , *arXiv:2404.07869* (2024)
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- [9] M. Schmitt, M. Reh, *SciPost Phys. Codebases*, 2 (2022)
- [10] R. Rende, S. Goldt, F. Becca, L. Viteritti, *Phys. Rev. Research*, **6**, 043280 (2024)

2. Program

Day 1 - Wednesday July 2nd 2025

- 09:15 to 09:30 - Welcome & Introduction
- 09:30 to 10:00 - **Yusuke Nomura**
Neural quantum states and many-variable variational Monte Carlo simulations
- 10:00 to 10:30 - **Michael Scherbela**
Fast and accurate VMC using finite-range embeddings
- 10:30 to 11:00 - Coffee break
- 11:00 to 11:30 - **Clemens Giuliani**
JAX for neural quantum states: from autodiff to distributed computing
- 11:30 to 12:00 - **Jonas Rigo**
Fermionic many-body simulations with jVMC
- 12:00 to 12:30 - **Kosuke Nakano**
A new ab initio quantum Monte Carlo package implemented with JAX
- 12:30 to 14:00 – Lunch
- 14:00 to 14:30 - **Werner Dobrautz**
Smoother wavefunctions, smaller bases: transcorrelated approaches for efficient quantum simulations
- 14:30 to 15:00 - **Nicolas Renaud**
QMCTorch: molecular wavefunctions with neural components for force and energy calculations
- 15:00 to 15:30 - Coffee break
- 15:30 to 16:00 - **Javier Rozalén Sarmiento**
Decisional gradient descent: a new optimiser for neural quantum states
- 16:00 to 16:30 - **Gianluca Bertaina**
Time-dependent variational Monte Carlo method for open quantum systems
- 16:30 to 18:00 – Discussion
- 18:00 to 20:00 - Poster session & aperitif

Day 2 - Thursday July 3rd 2025

- 09:30 to 10:00 - **Chris Roth**
Pfaffian NQS for fermion problems
- 10:00 to 10:30 - **Attila Szabó**
Tower-of-states spectroscopy for the Shastry-Sutherland model
- 10:30 to 11:00 - Coffee break
- 11:00 to 11:30 - **Conor Smith**
Neural quantum state prediction of a correlation driven molecular Wigner crystal in a honeycomb moire potential
- 11:30 to 12:00 - **James Keeble**
Neural quantum states for atomic nuclei
- 12:00 to 14:00 - Lunch
- 14:00 to 15:00 - Project Kickstart / Hackathon
- 15:00 to 15:30 - Coffee break
- 15:30 to 18:00 - Project Kickstart / Hackathon
- 19:00 to 21:30 - Social dinner

Day 3 - Friday July 4th 2025

- 09:30 to 10:30 - Project Kickstart / Hackathon
- 10:30 to 11:00 - Coffee break
- 11:00 to 12:30 - Project Kickstart / Hackathon
- 12:30 to 14:00 - Lunch
- 14:00 to 16:00 - Roundtable and Wrap Up

3. Abstracts

A new ab initio quantum Monte Carlo package implemented with JAX

Kosuke Nakano

National Institute for Materials Science (NIMS), Japan

We introduce a new QMC package developed from scratch in Python using JAX. It implements VMC, Lattice Regularized Diffusion Monte Carlo (LRDMC), and their force estimators. By leveraging JAX's just-in-time compilation and vectorized operations, the package achieves high GPU performance while remaining user- and developer-friendly thanks to Python and its packaging ecosystem. These algorithmic and software advances together significantly broaden the applicability of ab initio QMC methods in materials science.

Decisional gradient descent: a new optimiser for neural quantum states

Javier Rozalén Sarmiento¹, Mehdi Drissi², James Keeble³, Arnau Rios¹

¹Institute of Cosmos Sciences, University of Barcelona, Spain

²TU Darmstadt, Theory Center, Germany

³Bielefeld University, Germany

In this talk, I will discuss the optimisation strategy of NQS, which aims to minimise the energy of the quantum system of choice [1]. Despite the existence of general-purpose numerical optimisers such as Gradient Descent, ADAM, and RMSProp, in NQS there is a preferred choice: Stochastic Reconfiguration (SR) [2,3]. There are two main reasons for this. First, SR can be seen as a second-order optimisation algorithm, and second, it bears information about the geometry of the energy landscape. However, in a recent work it was shown that, when used in a fully-fledged numerical optimisation framework, using adaptive dampening, momentum and re-scaling, SR performed poorly in several scenarios involving Fermionic systems in a continuous Hilbert space [4]. In contrast, it was shown that a tailor-made optimiser leveraging information about the Hamiltonian was better suited for this sort of systems. In this talk, I will present this novel approach to energy minimisation, and show its performance on both continuous and discrete systems. I will also put forth a proposal to incorporate more advanced numerical optimisation techniques in open-source libraries, such as NetKet [5]. Finally, I will bring forward an initiative to develop open-source code to tackle nuclear systems with NQS.

[1] G. Carleo, M. Troyer, *Science*, **355**, 602 (2017)

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Fast and accurate VMC using finite-range embeddings

Michael Scherbela¹, Nicholas Gao²

¹University of Vienna, Austria

²TU Munich, Germany

Neural-network-based Variational Monte Carlo (NN-VMC) in first quantization is among the most accurate methods for computing molecular properties. In several instances NN-VMC has been shown to even outperform computationally costly methods such as CCSD(T). But while NN-VMC has in principle favorable scaling of computational cost with system size, in practice calculations beyond ~100 electrons are prohibitively expensive.

To address this, we propose finite-range embeddings (FiRE), an architecture which limits the range of electron correlations and thereby accelerates VMC by $O(n)$. We demonstrate this acceleration in practice, observing a 10x speed-up over state-of-the-art architectures while still retaining high accuracy for several challenging systems.

[1] Scherbela & Al., *arXiv:2504.06087* (2025)

Fermionic many-body simulations with jVMC

Jonas Rigo, Markus Schmitt

Forschungszentrum Jülich, Germany

The effectiveness of Neural Quantum States (NQS) enables the study of traditionally challenging problems such as two-dimensional superconductors and large quantum impurity systems within dynamical mean-field theory simulations. We approach these problems using the jVMC library, which provides core components for NQS simulations, including multi-GPU accelerated, state-of-the-art time evolution and ground-state optimization for quantum many-body systems. In this talk, I will give an overview of the jVMC library and present recent developments focused on fermionic ground states.

[1] M. Schmitt, M. Reh, *SciPost Phys. Codebases*, 2 (2022)

JAX for neural quantum states: from autodiff to distributed computing

Clemens Giuliani

EPFL, Switzerland

This talk explores the latest developments in utilizing JAX for quantum many-body physics with neural wavefunctions.

I will review advanced applications of automatic differentiation in Stochastic Reconfiguration and kinetic energy computations and discuss recent advances that enable running native JAX distributed code using sharding on CPU (MPI) and GPU (NCCL).

Neural quantum state prediction of a correlation driven Molecular Wigner Crystal in a honeycomb moire potential

Conor Smith

Flatiron Institute/University of New Mexico, United States

Moire materials have received a lot of excitement and attention due to the exotic states found in them and their high tunability. We study a moire system that can in principle be realized on current devices by modeling a two-dimensional electron gas in the presence of a honeycomb potential at various depths. To do so, we use a Message-Passing Neural Quantum State [1] that can do “unbiased” phase discovery [2]. Prior work has explored the triangular potential with NQS [3] and the honeycomb potential with Diffusion Monte Carlo [4]. In both cases, the expected phases were successfully found. In the case of the triangular potential, Molecular Wigner Crystals were observed at high fillings which aligns well with intuition and experimental results [5]. In our simulations, we find an unexpected, novel and highly correlated state at a low filling which we refer to as a correlation driven Molecular Wigner Crystal to distinguish it from the high filling case found in prior simulation and experiment.

[1] Gabriel Pescia et al., *Phys. Rev. B* 110, 035108 (2024)

[2] C. Smith, Y. Chen et al., *Phys. Rev. Lett.* 133, 266504 (2024)

[3] Y. Yang et al., *Phys. Rev. Lett.* 133 266501 (2024)

[4] Xiang Li et al., *arxiv:2406.11134* (2024)

[5] Hongyuan Li et al., *Science* 385,86 (2024)

Neural quantum states and many-variable variational Monte Carlo simulations

Yusuke Nomura

Tohoku University, Japan

We will discuss that artificial neural networks used in machine learning can be useful for analyzing quantum many-body systems, in particular, strongly correlated electron systems.

Motivated by the seminal work by Carleo and Troyer [1], we have continuously worked on the development of the neural-network wave function method for zero-temperature and finite-temperature simulations (for a review paper, see, e.g., [2]).

Through various extensions, the neural-network wave functions are beginning to be applied to challenging problems in physics, such as frustrated quantum spin problems and strongly correlated fermion problems. We show such a successful application to the frustrated J1-J2 Heisenberg model on

the square lattice, revealing the existence of quantum spin liquid [3]. We may also touch upon our extension to finite-temperature simulations [4], made possible by integrating deep learning models with the physical concept of “purification.”

Given that one of the workshop’s themes is open-source software, we will introduce mVMC, an open-source software package for many-variable variational Monte Carlo simulations [5]. mVMC supports Pfaffian wave functions combined with various correlation factors, including the conventional Gutzwiller and Jastrow forms, as well as neural-network-based correlation factors. It also implements a range of quantum projection techniques, such as spin and momentum projections. We will provide an overview of the software’s implementation details during the talk.

[1] G. Carleo, M. Troyer, *Science*, **355**, 602 (2017)

[2] Y. Nomura, *J. Phys.: Condens. Matter*, **36**, 073001 (2023). Y. Nomura, M. Imada, *J. Phys. Soc. Jpn.*, **94**, (2025)

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Neural quantum states for atomic nuclei

James Keeble¹, Caroline Robin¹, Alessandro Lovato²

¹Universität Bielefeld, Germany

²Argonne National Laboratory, United States

Atomic nuclei present large degrees of quantum complexity, including large-scale multi-body entanglement and non-stabilizerness (quantum magic). In this talk, I will explore to what extent Neural Quantum States (NQS) can capture this quantum complexity. In particular, I will use the nuclear shell model, specifically focusing on light nuclei, as a benchmark to quantify the expressibility of a NQS via its non-stabilizerness, which holds a direct connection to quantum resource theory.

Pfaffian NQS for fermion problems

Chris Roth¹, Ao Chen², Antoine Georges¹, Anirvan Sengupta¹

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Neural quantum states (NQS) offer a promising path towards understanding strongly correlated phases of matter. I will discuss progress on simulating the Fermi-Hubbard model, a model that can realize high-temperature superconductors and fractionalized phases, using NQS wavefunctions. We use an Ansatz which we call hidden fermion Pfaffian states (HFPS), which generalizes the hidden fermion determinant states to wavefunctions with pairing. I will show that starting with a paired mean-field allows us to stabilize superconducting phases that have lower energy than their non-superconducting counterparts, which we have used to determine where the Fermi-Hubbard model superconducts. Finally, I'll discuss software progress that has allowed us to simulate systems of more than 200 electrons.

QMCTorch: molecular wavefunctions with neural components for force and energy calculations

Nicolas Renaud

Netherlands escience Center, Netherlands

In this talk, I will present results obtained using QMCTorch, our modular framework for real-space Quantum Monte Carlo (QMC) simulations of small molecular systems. Built on the popular deep learning library PyTorch, QMCTorch is GPU-native and enables the integration of machine learning-inspired components into the wave function ansatz, such as neural network backflow transformations and Jastrow factors, while leveraging efficient optimization algorithms. QMCTorch interfaces with two widely used quantum chemistry packages - PySCF and ADF - which provide initial values for atomic orbital exponents and molecular orbital coefficients. QMCTorch provides a modular and extendable platform for rapidly prototyping new wavefunction ansätze, evaluating their performance, and analyzing optimization outcomes.

Smoother wavefunctions, smaller bases: transcorrelated approaches for efficient quantum simulations

Werner Dobrautz

Helmholtz-Zentrum Dresden-Rossendorf, Germany

Accurate and resource-efficient simulation of quantum many-body systems remains a fundamental challenge in electronic structure theory. In this talk, I will present recent advances based on the **transcorrelated (TC) method**, which incorporates the **electron-electron cusp condition** directly into the Hamiltonian via a similarity transformation using a Jastrow factor. By explicitly regularizing the short-range divergence of the wavefunction, this transformation yields **results much closer to the complete basis set (CBS) limit** even in **significantly reduced basis sets**, enabling smoother and more compact wavefunction representations and substantial savings in computational and hardware resources.

We apply this framework within the **Full Configuration Interaction Quantum Monte Carlo (FCIQMC)** method to both **ab initio molecular systems** and **strongly correlated lattice models**, such as the Hubbard model. The TC transformation leads to faster convergence and a significant reduction in the size of the determinant space needed. These capabilities are implemented in the **open-source NECI code**, which supports the non-Hermitian and three-body operators arising from the TC formalism.

Building on this foundation, we demonstrate how the TC approach enables more efficient **quantum algorithms**, specifically through its integration with **variational imaginary time evolution (VarQITE)** on near-term quantum hardware. The reduced basis requirements directly translate into **fewer qubits** and **shallower circuits**, making chemically accurate simulations more tractable on current noisy devices.

Finally, I will discuss the potential of combining **transcorrelated Hamiltonians** with **neural quantum states (NQS)**. The TC approach could similarly improve NQS accuracy by enabling meaningful results at smaller basis sizes, while also enhancing **trainability** through the more compact and regular structure of the transformed wavefunctions—opening promising directions for machine-learned wavefunction methods in strongly correlated systems.

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[2] A. Cohen, H. Luo, K. Guthrie, W. Dobrautz, D. Tew, A. Alavi, *The Journal of Chemical Physics*, **151**, (2019)

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Time-dependent variational Monte Carlo method for open quantum systems

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We extend the time-dependent variational Monte Carlo (tVMC) method to simulate the dynamics of open quantum systems governed by the Lindblad master equation. Our approach combines quantum trajectory techniques with tVMC in a unified and efficient framework for tackling many-body open quantum dynamics [J. D'Alberto, PhD thesis, Università degli Studi di Milano (2024), paper in preparation]. In contrast to previous methods [1-3], we unravel the Lindblad equation into an ensemble of stochastic Schrödinger equations and introduce a variational formulation, overcoming the exponential complexity of density matrix evolution. This formulation accommodates both highly expressive neural-network wavefunctions and compact, efficient Jastrow wavefunctions. We carefully derive the stochastic equations of motion for the variational parameters, in nonlinear trajectory formulation, and design suitable stochastic solvers to ensure numerical stability and accuracy. We validate our method, open time-dependent variational Monte Carlo (otVMC), by simulating quantum quenches in the one-dimensional long-range Ising model in a transverse field and with local dissipation. This system is experimentally relevant to quantum metrology, trapped ions, and Rydberg atom arrays. Our results show that otVMC accurately captures non-equilibrium features such as spin squeezing dynamics, while remaining computationally efficient and scalable to large system sizes, thanks to its compatibility with massively parallel high-performance computing. This work opens the door to simulating complex open quantum systems in higher dimensions, also with continuous variables and quantum optics platforms,

with broad implications for quantum technologies and fundamental quantum science. The method can be readily integrated into existing tVMC implementations, greatly extending their applicability to realistic, dissipative quantum systems.

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Tower-of-states spectroscopy for the Shastry-Sutherland model

Attila Szabó

University of Zürich, Switzerland

The Shastry-Sutherland Hamiltonian is a simple model of magnetic frustration, realised by several materials. It has a remarkably rich phase diagram featuring an exactly solvable dimer phase, a valence-bond solid (VBS), and conventional Néel order. Recently, a quantum spin liquid (QSL) phase has also been observed [1,2], and an adiabatic connection between the phase diagrams of the Shastry-Sutherland and the square-lattice J_1 - J_2 models has been proposed [2].

In this talk, I will explore these rich phase diagrams through their signatures in the low-energy spectrum, known as the (Anderson) tower of states [3]. These towers are accessible in variational Monte Carlo using ansätze restricted to different symmetry sectors: I will discuss how to construct such ansätze using NetKet's group convolution infrastructure.

In the Shastry-Sutherland model, similar to the square-lattice J_1 - J_2 model [4], the relative energy gaps of the Néel and VBS towers of states can be used to accurately locate the Néel-QSL-VBS transitions. Furthermore, both spectra and order parameters paint a picture of the VBS phase that is consistent with other theoretical studies but not with experiment. I will finally comment on the nature of the VBS phase of the square-lattice J_1 - J_2 model.

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[3] A. Wietek & Al., *arXiv:1704.08622* (2017)

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