Proposal for a Postdoctoral / PhD Position
AI for Correlated Quantum Materials (AICQM)

Keywords: optimization, machine learning, computational quantum physics, surrogate models

Abstract. We are recruiting a postdoc/PhD to work on optimization and machine learning aspects of some surrogate models used in computational quantum physics for the study of materials. The project will be conducted in continuous collaboration with physicists. The objective is to develop a theoretical framework to analyze the optimization and machine learning components of the simulations, in order to provide rigorous guarantees for the simulation output and to suggest algorithmic improvements. It is not essential to have prior experience in quantum physics to apply.

Context. The ANR project *AICQM* (*Artificial Intelligence for Correlated Quantum Materials*) combines machine learning, optimization, and computational quantum physics to accelerate and improve Dynamical Mean-Field Theory (DMFT) [1] computations for strongly correlated materials. DMFT is a foundational computational method in condensed-matter physics, but it requires solving many coupled high-dimensional quantum embedding problems—a computational bottleneck that severely limits its practical applicability. This challenge presents a prime opportunity for machine learning: training surrogate models to approximate expensive quantum computations, developing neural network ansätze as replacements for traditional numerical solvers like Quantum Monte Carlo [2], and applying modern optimization theory to improve the stability and efficiency of variational algorithms. From an ML perspective, these are inverse problems with complex input-output mappings in high-dimensional spaces, offering rich opportunities for the application and development of optimization, architecture design, and uncertainty quantification techniques.

The project brings together researchers from Inria, Ecole Polytechnique (CPHT), and Collège de France, including **Raphael Berthier** (Inria), **Filippo Vicentini** (CPHT), **Antoine Georges** (Collège de France), and **Michel Ferrero** (CPHT). The project develops next-generation impurity solvers based on Neural Quantum States (NQS) for multi-orbital systems, trains ML-based surrogate models on Quantum Monte Carlo datasets to accelerate DMFT computations, and produces open-source software and datasets for the community.

Position Description

The Inria postdoc will work on the foundational machine learning and optimization aspects of the AICQM project, contributing to three interconnected research areas.

Theory of Optimization for Neural Quantum States. This involves developing a rigorous theoretical framework for optimizing Neural Quantum States (NQS) using advanced stochastic optimization techniques. We address inherent biases and inefficiencies in gradient estimation by investigating sampling strategies beyond conventional Metropolis-Hastings schemes, variance reduction techniques (including a novel SAGA variant), and systematic comparison of natural gradient methods with higher-order optimization techniques [3, 4]. The goal is to bridge the gap between stochastic optimization theory and scalable, reliable neural-network-based quantum solvers.

Architectures and Learning Biases in Neural Quantum States. This involves systematically investigating how neural network architectures and physical priors affect the accuracy and stability of multi-orbital impurity solvers. We design specialized architectures exploiting impurity-bath structure (inspired by recurrent neural networks), explore symmetry-preserving approaches, and characterize the inductive biases emerging from overparameterization in quantum systems. The focus is on finding optimal architectural choices that balance expressivity and computational efficiency for realistic multi-orbital systems.

Theoretical Understanding and Error Estimation. This involves analyzing supervised-learning surrogates developed for DMFT, gaining theoretical understanding of their learning properties, biases, and limitations [5, 6]. We perform analytical studies on simplified impurity models to uncover dominant learned features, and develop confidence scoring mechanisms using Bayesian neural networks and Gaussian process-based approaches to estimate predictive uncertainties. The objective is to establish when ML solvers can be used confidently versus when exact solvers from WP1 are necessary.

Methodologically, the postdoc will work at the intersection of modern optimization (stochastic methods, implicit regularization), scientific machine learning, and computational quantum physics. Contributions will include implementations in open-source softwares `NetKet` [7] and `TRIQS` [8].

The position is based at Inria and will be under the direct supervision of **Raphael Berthier**, with close collaboration with the other project members: Filippo Vicentini (CPHT), Antoine Georges (Collège de France), and Michel Ferrero (CPHT). This collaborative structure ensures multidisciplinary expertise and frequent interactions across optimization, machine learning, and quantum many-body physics.

Who Should Apply

Candidates with a PhD (or expected PhD defense before start date) in applied mathematics, machine learning, computational physics, or a closely related field. Strong candidates currently finishing a Master degree are also encouraged to apply.

Desired background (required): A solid background in optimization, statistics, or machine learning theory is essential. **Background appreciated but not necessary:** Experience in quantum many-body physics and condensed matter theory, scientific computing and numerical methods, and strong programming skills (Python/JAX/PyTorch/C++) are valuable but not required.

Practical Information

Host institution: Inria (France). **Planned start date:** flexible, with a target around Fall 2026. **Duration:** up to 3 years. **Research environment:** close interactions with collaborators at Inria, CPHT (Ecole Polytechnique), and Collège de France.

To apply, send an email to `raphael.berthier@inria.fr`.

References

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