



Contribution ID: 7

Type: **Contributed poster**

Geometric Optimization in Scientific Machine Learning

Monday, March 2, 2026 6:24 PM (3 minutes)

We discuss an “optimize-then-project” approach for applications in scientific machine learning. The key idea is to design algorithms at the infinite-dimensional level and subsequently discretize them in the tangent space of the neural network ansatz, similar to a natural gradient style ansatz. We illustrate this approach in the context of the variational Monte Carlo method for quantum many-body problems, where neural quantum states have recently emerged as powerful representations of high-dimensional wavefunctions. In this setting, we recover the celebrated stochastic reconfiguration algorithm, interpreting it as a projected Riemannian L^2 gradient descent method. We further explore extensions to Riemannian Newton methods, and conclude with considerations related to the scalability of these schemes.

Author: MÜLLER, Johannes

Co-authors: ZHANG, Hang (ETH Zurich); NYS, Jannes (ETH Zurich); CARRASQUILLA, Juan (ETH Zurich); ZEINHOFER, Marius (ETH Zurich); MISHRA, Siddhartha (ETH Zurich); ARMEGIOIU, Victor (ETH Zurich)

Presenter: MÜLLER, Johannes

Session Classification: Poster blitz, poster session, and welcome reception