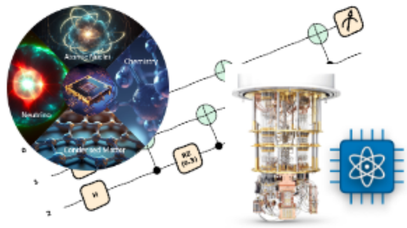

Contribution ID: **37** Type: **Contributed Talk (45min including questions)**

Learning Density Functionals from Noisy Quantum Data

Wednesday, November 19, 2025 10:30 AM (45 minutes)

The search for useful applications of noisy intermediate-scale quantum (NISQ) devices in quantum simulation has been hindered by their intrinsic noise and the high costs associated with achieving high accuracy.
A promising approach to finding utility despite these challenges involves using quantum devices to generate training data for classical machine learning (ML) models.
In this study, we explore the use of noisy data generated by quantum algorithms in training an ML model to learn a density functional for the Fermi-Hubbard model.
We benchmark various ML models against exact solutions, demonstrating that a neural-network ML model can successfully generalize from small datasets subject to noise typical of NISQ algorithms.
The learning procedure can effectively filter out unbiased sampling noise, resulting in a trained model that outperforms any individual training data point.
Conversely, when trained on data with expressibility and optimization error typical of the variational quantum eigensolver, the model replicates the biases present in the training data.
The trained models can be applied to solving new problem instances in a Kohn-Sham-like density optimization scheme, benefiting from automatic differentiability and achieving reasonably accurate solutions on most problem instances.
Our findings suggest a promising pathway for leveraging NISQ devices in practical quantum simulations, highlighting both the potential benefits and the challenges that need to be addressed for successful integration of quantum computing and ML techniques.
This work is recently published in Machine Learning Science & Technology.

[Emiel Koridon et al 2025 Mach. Learn.: Sci. Technol. 6 025020]

Authors: KORIDON;KORIDON, Emiel (Leiden University); POLLA, Stefano (Leiden University)

Co-authors: Mr PREHN, Eric; Dr VAN NIEUWENBURG, Evert (Leiden University); Mr FROHNERT, Felix (Leiden University); Mr TURA, Jordi (Leiden University)

Presenter: KORIDON;KORIDON, Emiel (Leiden University)