Contribution ID: **72** Type: **Poster**

Optimization Methods for Material Science

Friday 6 December 2024 13:45 (3 hours)

Optimization Methods for Material Science

The Setup for LOw-energy Positron Experiments (SLOPE) at the MLL creates a state-of-the-art monoenergetic positron beam, tailored to the needs of (near-) surface positron annihilation spectroscopy. [1]
The beam is guided by a series of magnetic coils and electrostatic lenses onto the sample, where the positrons annihilate with electrons inside the material. The Doppler broadening of the 511 keV line then reveals the local electronic structure.

The electromagnetic guidance system needs to be precisely optimized in order to focus the beam onto the sample. We showcase an implementation of Bayesian Optimization, which outperforms more conventional algorithms (e.g. downhill simplex), offering greater robustness and improved efficiency for the Beam optimization.

Additionally, we show that deep learning techniques can greatly reduce the number of measurements taken during beam width and position optimizations, while maintaining good accuracy. This results in faster optimization compared with traditional least squares fitting.

[1] L. Mathes, M. Suhr, V. V. Burwitz, D. R. Russell, S. Vohburger, and C. Hugenschmidt, "Surface and near-surface positron annihilation spectroscopy at very low positron energy," arXiv preprint, arXiv:2409.07952, Sep. 2024.

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Presenter: ALAM, Saad

Session Classification: Poster Session

Track Classification: Positrons