CDCS
CENTER FOR DATA AND COMPUTING
IN NATURAL SCIENCES

OPENING SYMPOSIUM 2022

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

DESY.

TUHH

Contribution ID: **121** Type: **Poster**

Bayesian optimization of plasma accelerators with concurrent particle-in-cell simulations

The design and study of plasma-based accelerators greatly relies on numerical simulations with particle-in-cell codes. These simulations accurately model the interaction between plasmas, lasers, and charged particle beams, but are often computationally expensive. Thus, given the wide range of physical parameters involved, optimizing the accelerator performance requires efficient methods that reduce the number of simulations needed. In this context, Bayesian optimization has proven to be a particularly successful technique. It generates a surrogate model of the objective function, which is then used to guide the optimization by suggesting the most promising function evaluations. The model is iteratively updated with the new observations, leading to improved suggestions. Typically, this process is carried out sequentially, i.e., by performing only one simulation (of the most promising evaluation) per model iteration. Here, we present the development of a new library for Bayesian optimization capable of handling the concurrent evaluation of multiple simulations. This capability, enabled by the libEnsemble library, allows the optimization to take full advantage of high-performance computing clusters and results in a significant speedup of the process.

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Session Classification: Poster session with buffet

Track Classification: CDL4 (Control of Accelerators)