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Multi-task Bayesian optimization of laser-plasma accelerators

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When designing a laser-plasma acceleration setup, it is common to explore the parameter space (plasma density, laser intensity, focal position, etc.) with Particle-In-Cell (PIC) simulations in order to find an optimal configuration that, for example, minimizes the energy spread or emittance of the accelerated beam. However, PIC simulations can be computationally expensive. Various reduced models (e.g., reduced-model simulation codes, ML surrogates) can approximate beam behavior at a much lower computational cost. Although such models do not capture the full physics, they could still suggest promising sets of parameters to be simulated with a full PIC code and thereby speed up the overall design optimization.

In this work, we automate such a workflow with a Bayesian multitask algorithm, where the different tasks correspond to simulations making different approximations. This algorithm learns from past simulation results with different fidelities, and dynamically chooses the next parameters to be simulated. The libEnsemble library is used to orchestrate this workflow on a modern GPU-accelerated high-performance computing system.

Primary Keyword

bayesian optimization

Secondary Keyword

ML-based optimization

Tertiary Keyword

MLOps

Primary author: LEHE, Remi (LBNL)

Presenter: LEHE, Remi (LBNL)

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