Design Optimization and In Situ Surrogate Modeling Activities in the Beam, Plasma & Accelerator Simulation Toolkit (BLAST)

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The Beam, Plasma & Accelerator Simulation Toolkit (BLAST) is an open source modeling suite of codes for advanced particle accelerators and beam dynamics. In BLAST, novel GPU-accelerated electromagnetic and electrostatic particle-in-cell codes are developed including the DOE Exascale Computing Project code WarpX and the new ImpactX code for s-based beam dynamics. Within this context, we are using AI/ML at several levels, and for several different purposes.

At the "outer-loop" level (i.e. using AI/ML outside of the simulation code), we use AI/ML in design optimization of particle accelerators. In particular, we use Bayesian optimization techniques to reduce the number of expensive simulations to run when trying to find the optimal combination of design parameters. This includes combining codes with different fidelities within the same Bayesian optimization, so that low-cost, low-fidelity simulations can provide guidance on where to most efficiently perform the expensive high-fidelity simulations.

We also present our technical approach to couple AI/ML frameworks and simulations via standards. For instance, we investigate the training of fast ML surrogate models in t-based codes, e.g., for plasma elements, which could be used as fast surrogate elements in s-based beam dynamics codes. For such training workflows, we rely on standardized metadata following the Open Standard for Particle-Mesh Data (openPMD), which we develop. For inference workflows on trained surrogates, we couple into the performance-critical "inner loops" of simulations. For this, we implement Python data interface standards, which enable zero-copy data exchange between GPU-accelerated simulations and GPU-accelerated AI/ML frameworks. We envision that such data standards and interfaces could be used as a basis for a wider, compatible accelerator modeling ecosystem.

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Abstract for 3rd ICFA Beam Dynamics Mini-Workshop on Machine Learning Applications for Particle Accelerators

- https://www.bnl.gov/mlaworkshop2022/
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