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AI/ML Coupling & Surrogates in BLAST Accelerator Modeling Codes

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Detailed modeling of particle accelerators can benefit from parallelization on modern compute hardware such as GPUs and can often be distributed to large supercomputers. Providing production-quality implementations, the Beam, Plasma & Accelerator Simulation Toolkit (BLAST) provides multiple modern codes to cover the widely different time and length scales between conventional accelerator elements and advanced, plasma-based elements. The Exascale code WarpX provides electromagnetic and -static, t-based particle-in-cell routines, advanced algorithms and is highly scalable. For beam-dynamics, the s-based ImpactX code provides an efficient implementation for tracking relative to a nominal reference trajectory, including space charge. Yet, integrated modeling of "hybrid" beamlines integrating both detailed plasma models and large-scale transport at full detail require exchange between both codes and are limited by the computational speed of the most-detailed element, usually the plasma element.

In this work, we present an alternative approach to coupling particle-in-cell models and codes beyond direct data exchange or reduced details for accelerator modeling. In particular, we investigate and demonstrate detailed data-driven modeling based on high-quality WarpX simulations that were used to train surrogate models for the beam transport code ImpactX. We describe new workflows, illuminate predictive quality, performance and applicability to central research topics in advanced accelerator research, such as staging of laser-wakefield accelerators.

Primary Keyword

surrogate model architecture

Secondary Keyword

MLOps

Tertiary Keyword

digital twins

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