WarpX: Toward Exascale Modeling of Plasma Particle Accelerators on GPU

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Goal

Particle accelerators are a vital part of the DOE-supported infrastructure of discovery science and applications, but we need game-changing improvements in the size, scale, and cost for future accelerators. Plasma-based particle accelerators stand apart in their potential for these improvements. Turning this from a promising technology into mainstream scientific tools depends critically on high-performance, high-fidelity modeling of complex processes.

Solution

WarpX is an open-source particle-in-cell (PIC) code supported by the Exascale Computing Project (ECP) that combines advanced algorithms with adaptive mesh refinement to allow challenging simulations of a multi-stage plasma-based TeV acceleration relevant for future high-energy physics discoveries.

Application domain: plasma accelerators

- A multi-TeV plasma-based particle accelerator would be based on multiple plasma stages.
- Each stage is computationally intensive.
- Need for × 100 stages × 100 ensemble.
- Need most advanced algorithms + Exascale

10-year problem: modeling of 20-100 consecutive stages.

OpenPMDF standard in WarpX

OpenPMDF is a naming and attributes standard for self-describing file format for particle and mesh-based data, from scientific simulations and experiments.

- high-level description
- human and machine readable particle and mesh
- based data general unit system
- file format agnostic
- Portable
- scalable from desktop to HPC forward-updatable

OpenPMDF-compliant HDF5 I/Os are currently implemented in WarpX. For performance reasons, ADIOS data format is under development.

WarpX code structure and distribution: Open Source

- Warp
  - Python coupling
  - Problem setup
  - Loop control
  - Data processing
  - Extra physics
- AMReX
  - Mesh refinement
  - Data structures
  - Adaptive mesh
  - Communications
  - Load balancing
- PICSAR
  - Optimized subroutines
  - Field gather
  - Particle push
  - Current deposition
  - Maxwell solver

WarpX combines most advanced algorithms

Lower # time steps:
- optimal Lorentz boosted frame

Higher accuracy:
- Adaptive Mesh Refinement
- Arbitrary order & pseudo-spectral
- Analytical Maxwell solvers
- Sub-cycling

Higher stability:
- Galilean T. to suppress
- Numerical Cherenkov Instability

Higher scalability:
- FFT Maxwell solvers on local domains + domain decomposition
- Dynamic load-balancing

WarpX fulfills and performances

Wakefield simulations with mesh refinement
First wakefield acceleration simulation with MR.
Convergence tests for multi-stage accelerators
Convergence tests for 3-stage accelerators on Cori KNL, without MR

Scalings on Summit up to half-machine
Weak and strong scaling for uniform plasma on Summit up to half-machine
- CUDA managed memory
- Whole PIC loop on the GPU
- Uses Thrust library (through AMReX for portability)
- amrex::ParallelFor (similar to Kokkos, RAJA) calls CUDA kernels

Perspectives

- WarpX is the first electromagnetic particle-in-cell code combining adaptive mesh refinement and pseudo-spectral methods.
- WarpX shows good weak and strong scalings on Summit after 3-year development, and current active efforts are dedicated to improving production-quality capabilities on GPU-accelerated machines.