The Community Project for Accelerator Science and Simulation 4: Advancing Accelerator Physics through High-performance Computing

Fei Li, Weiming An, Qianqian Su, Jeffrey Larson, Ann Almgren, Warren Mori, Esmond Ng, James Amundson and Stefan Wild

ComPASS4

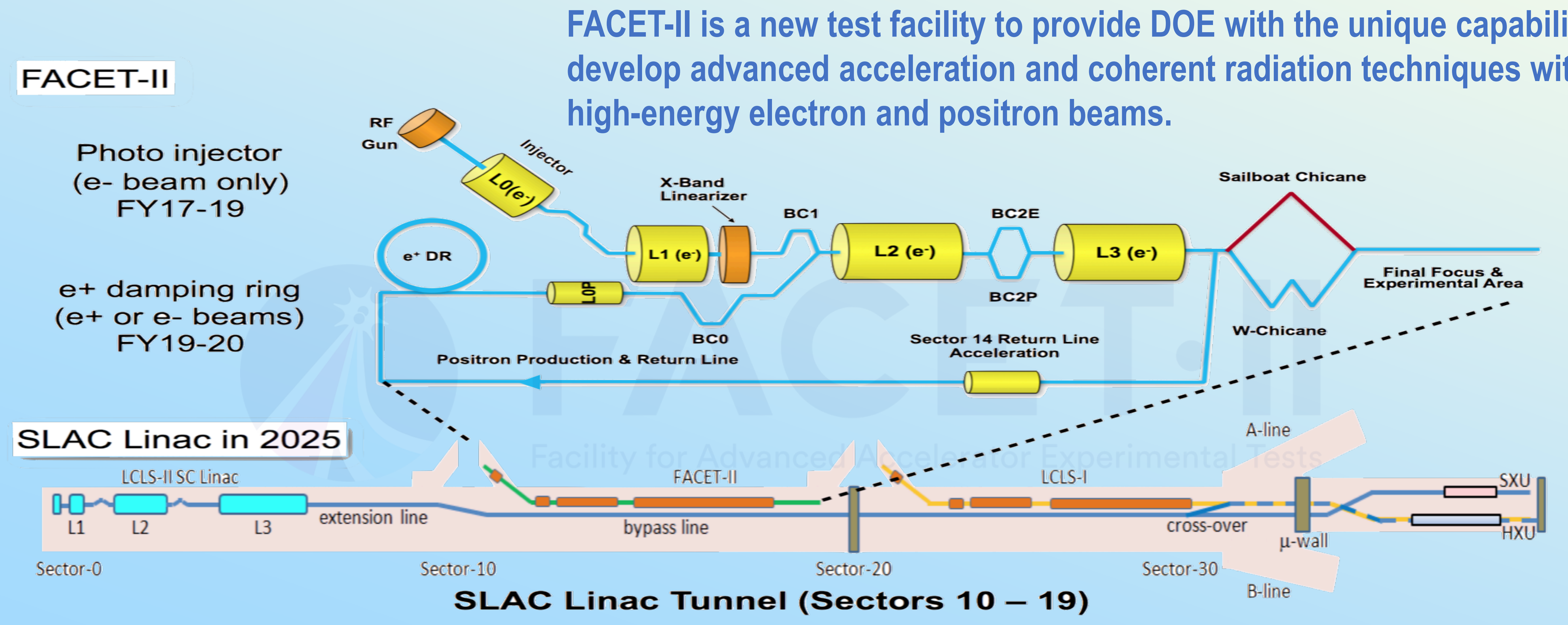
ComPASS4

Introduction

The next ten years of Advanced Accelerator research focuses on addressing common challenges:

- Higher energy staging of electron acceleration with independent drive beams, equal energy, and 90% beam capture.
- Understand mechanisms for emittance growth and develop methods for achieving emittances compatible with colliders.
- Completion of a single electron acceleration stage at higher energy
- Demonstration and understanding of positron acceleration
- Continuous, joint development of a comprehensive and realistic operational parameter set for a multi-TeV collider, to guide operating specifications for Advanced Accelerator.

FACET-II is a new test facility to provide DOE with the unique capability to develop advanced acceleration and coherent radiation techniques with high-energy electron and positron beams.



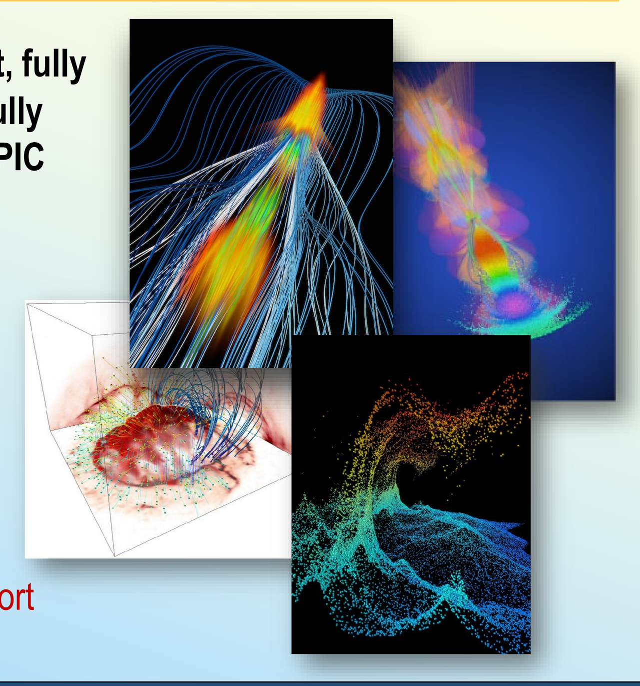
Particle-in-cell Codes: QuickPIC & OSIRIS

QuickPIC is a 3D fully parallelized, fully relativistic, three-dimensional quasi-static PIC code based on the UPIC framework. It was the first and remains the only fully 3D quasi-static PIC code.

- Scalability to ~ 128 K cores
- Pipeline Parallelization in z
- MPI + OpenMP + Vectorization (Intel Phi)
- Laser Module and Field
- Ionization Module
- Open Source on Github

OSIRIS is a state-of-the-art, fully explicit, multi-dimensional, fully parallelized, fully relativistic PIC code.

- Scalability to ~ 1.6 M cores
- SIMD hardware optimized
- Dynamic Load Balancing
- QED module
- Particle merging
- GPGPU and Xeon Phi support

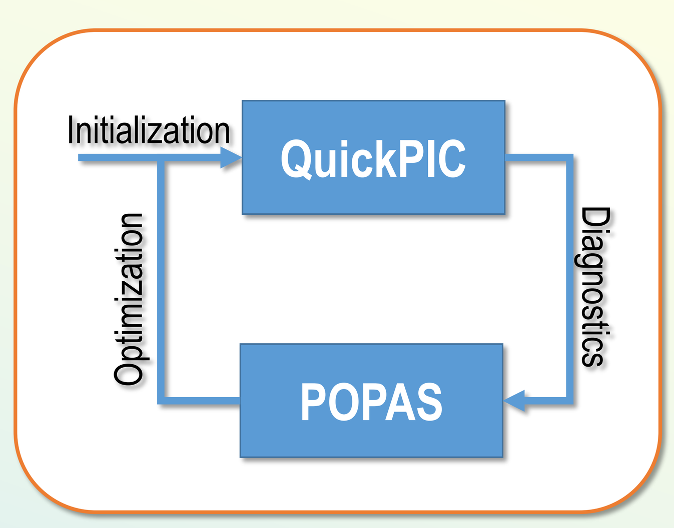


QuickPIC + POPAS

Platform for Optimization of Particle Accelerators at Scale

- **POPAS** will build off the POUNDERS, APOSMM, and LibEnsemble mathematical optimization libraries developed under SciDAC.
- Integrated platform for coordinating the evaluation and numerical optimization of accelerator simulations on leadership-class DOE computers.
- Orchestrate concurrent evaluations of QuickPIC, Synergia, and MARS (or combinations thereof) with distinct inputs/parameter values.

QuickPIC+POPAS workflow

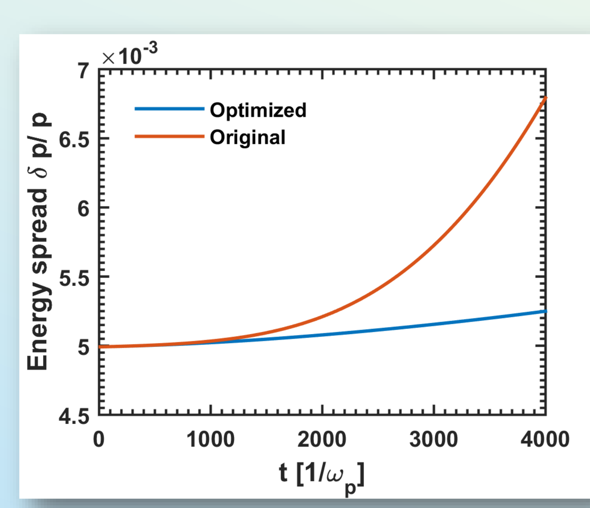


There are five parameters we want to optimize in a plasma based accelerator problem:

- energy spread (minimize)
- energy transfer efficiency (maximize)
- hosing growth rate (minimize)
- emittance growth rate (minimize)
- loaded transformer ratio (maximize or within a range)

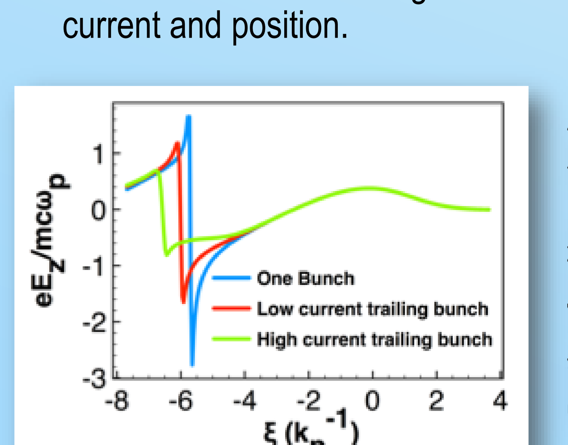
Emittance optimization

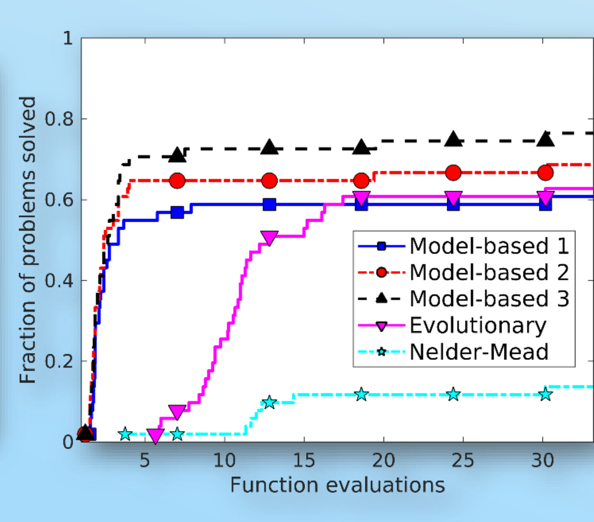
- Optimize witness beam twiss parameter α_0 and β_0.
- Optimized emittance growth as low as 0.1% in 0.5cm.
- Optimized α_0 and β_0 are close to numerical estimation from theory.

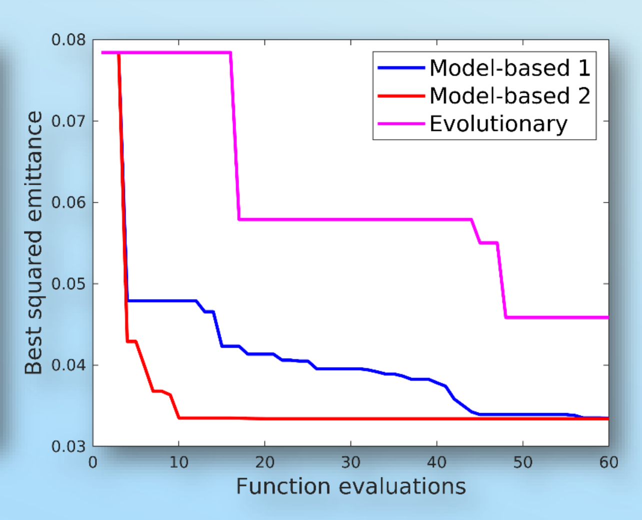


Energy spread optimization

- The energy spread is minimized by seeking the situation where the beam loading effect exactly flattens the E_z field.
- The desired beam loading effect is achieved by optimizing witness beam current and position.

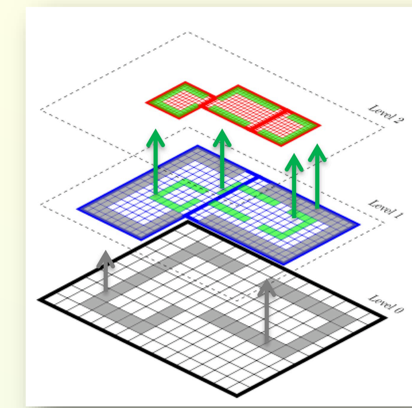


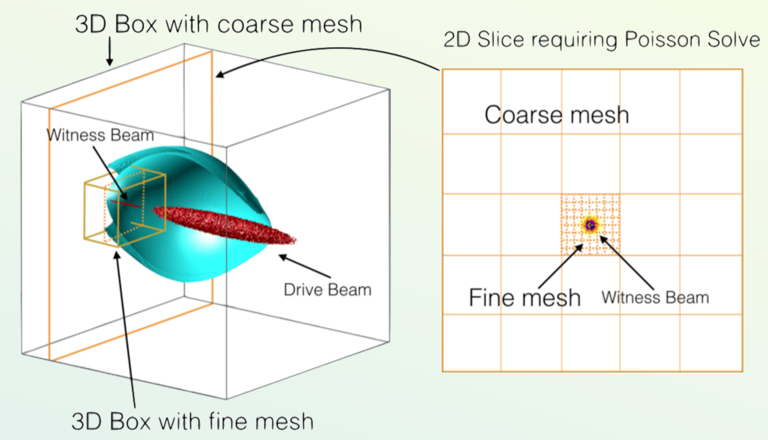




QuickPIC + AMReX

- **AMReX** is a software framework to support the development of block-structured AMR applications for current and next-generation architectures.
- Mesh refinement – both static and adaptive – will be added to QuickPIC to enable faster, more efficient simulation.
- FASTMath support of AMReX provides source code and expertise to enable quick prototyping of multilevel algorithm and eventual optimization on new HPC architectures of the multilevel algorithm in the context of QuickPIC.





Challenging problems: Ion Motion Induced Emittance Growth of Matched Electron Beams in Plasma Wakefields

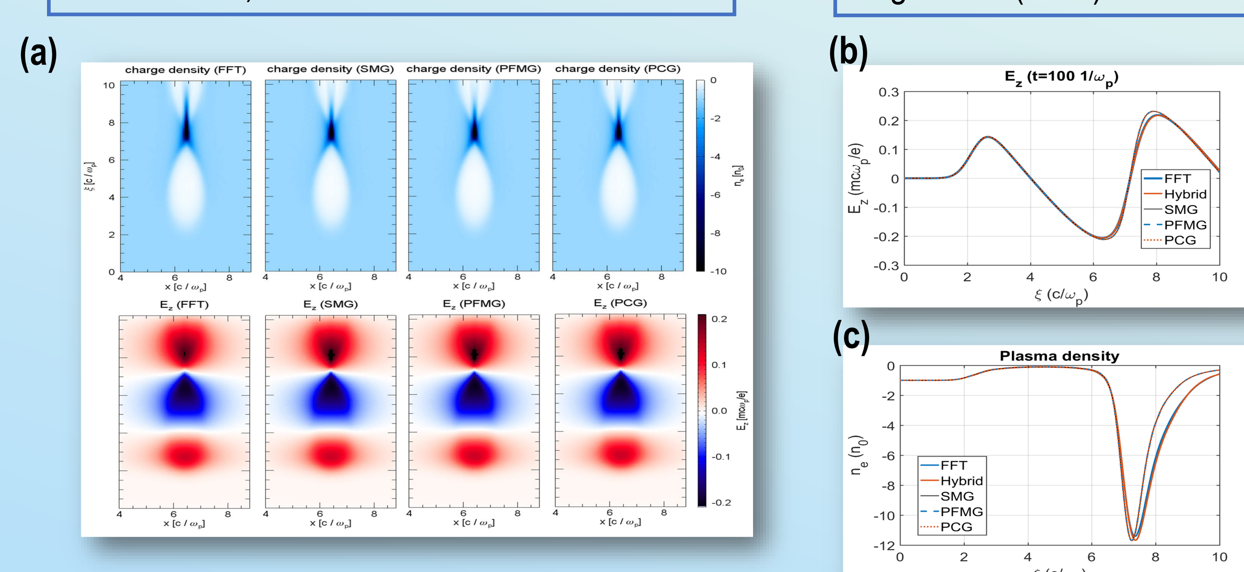
- Extremely tiny beam spot size (σ_r = 0.1 μm)
- Extremely high beam density that will perturbate the background ions. (N = 1.0 x 10^{10}, n_b/n_p = 63500 >> m_{ion}/m_e = 1836)

In order to efficiently modeling the physical problems of interest, the current QuickPIC code needs modification to be compatible with AMReX framework.

EM-field solver

- Fast Poisson solver based on FFT. Fast and accurate.
- Requires global data communication among processors,only allowing for 1D partition.
- Only have simple boundary conditions (homogeneous Dirichlet & Neumann conditions)

- Hybrid schemes with FFT solver for coarse mesh and FD solver for fine mesh.
- FD solvers are fully local, allowing for 2D partition.
- Capable of treating complicated boundary conditions.
- Several types of FD solvers in conjunction with multigrid method have been implemented, including semi-coarsening method (SMG, PFMG) and preconditioned conjugate gradient (PCG).



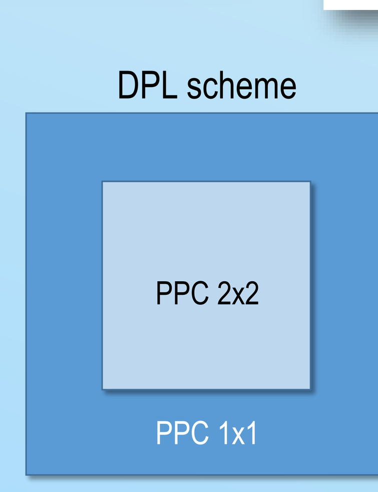
(a) Comparison of electron density and Ez field between FFT and FD multigrid solvers.

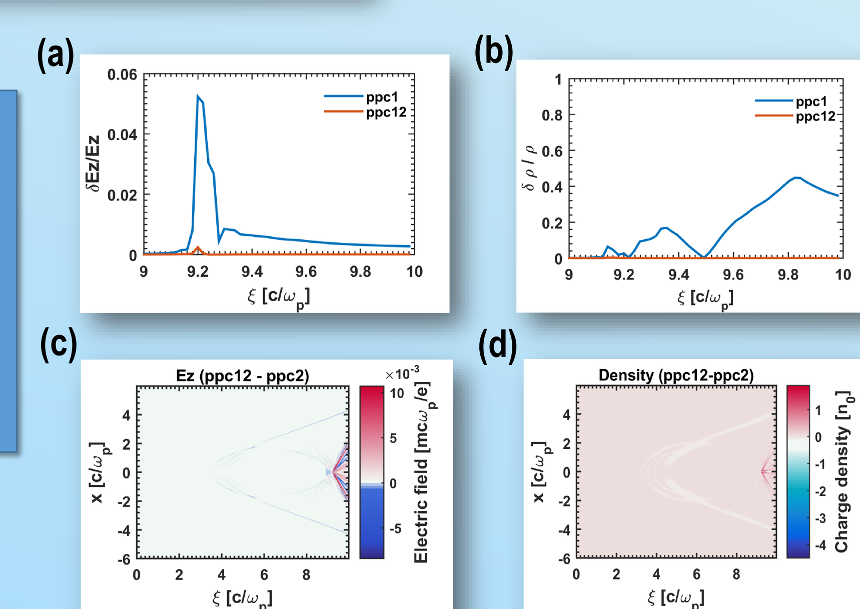
(b)-(c) Axial E_z field and plasma density comparison between FFT and FD multigrid solvers.

Particle loading

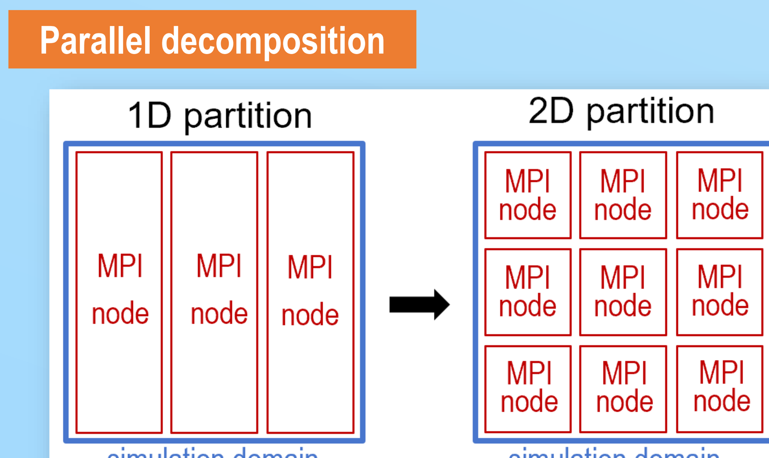
Static particle loading. Particle # per cell (PPC) is fixed within the entire simulation domain.

Dynamic particle loading (DPL). Allow for set up different PPC at different regions.





Parallel decomposition



(a)(b): Axial E_z field and charge density errors (PPC 1x1)-(PPC 2x2) (blue) and (DPL)-(PPC 2x2) (red).
(c)(d): 2D plots for E_z field and charge density errors (DPL)-(PPC 2x2).
With DPL scheme, obtain 2x speedup without much loss of accuracy compared to static particle loading.

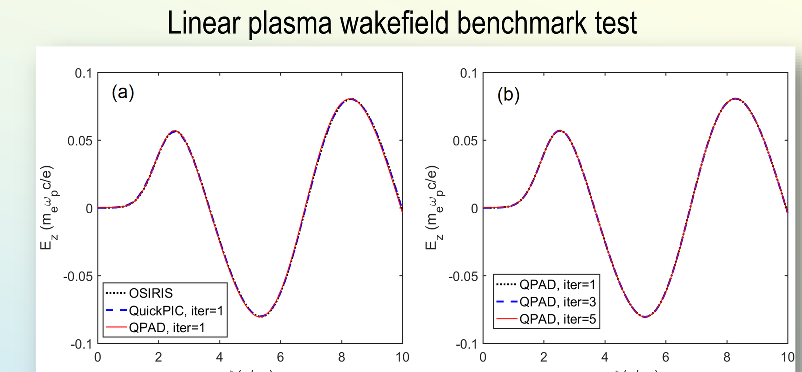
QPAD

QuickPIC with Azimuthal Decomposition

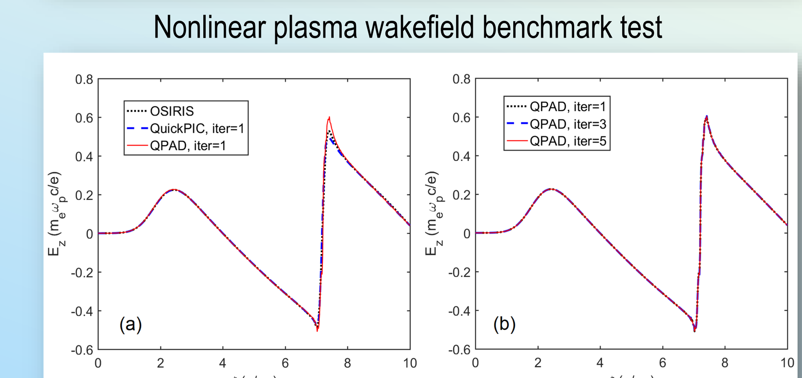
- QPAD is a new PIC code developed by UCLA based on the workflow and structure of QuickPIC.
- QPAD is the first quasi-static PIC code combining with Fourier azimuthal decomposition, a speedup technique that expands the fields, charge and current density into azimuthal harmonics and truncates the expansion.
- The complex amplitudes of fields are solved on a r-z grid using multigrid finite difference solvers. The beam and plasma particles are advanced in 3D space in the cylindrical geometry.
- QPAD could be orders of magnitude faster than QuickPIC.

QPAD has naturally 1D partition for fields and particles and simpler particle management routines, which makes it easier to incorporate with AMR.

Linear plasma wakefield benchmark test



Nonlinear plasma wakefield benchmark test



Fermilab UCLA Argonne NATIONAL LABORATORY BERKELEY LAB