A quasi-static particle-in-cell code

T. Mehrling¹, C. Benedetti², J. Grebenyuk¹, A. Martinez de la Ossa¹, C.B. Schroeder², J. Osterhoff¹
¹ DESY, Notkestrasse 85, 22603 Hamburg, Germany
² Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

Laser and Plasma Accelerators Workshop - Goa, September 2013
Outline

Introduction and Motivation

The quasi-static PIC code HiPACE
- Physical basis - Quasi-static approximation
- Numerical implementation
- Benchmark
- Parallel scaling
- Strengths and drawbacks of quasi-static PIC codes

Hybrid simulations
- Hybrid simulations of down-ramp-injection for FACET experiment E215

Summary and Outlook
Introduction and Motivation

The Particle-In-Cell method

- Particle-in-cell (PIC) codes are a widely used tool for laser- and beam-plasma interactions
- Time-step size $dt$ is limited by stability condition for explicit partial differential equation (PDE) solvers (CFL-condition)
- $dt < dx$, where $dx$ is determined by smallest resolved features
- Full 3D PIC simulations are computationally expensive
Introduction and Motivation

Disparity of timescales in plasma wakefield acceleration

Characteristic time for beam evolution $\sim 1/\omega_\beta$

Characteristic time for plasma particle evolution $\sim 1/\omega_p$

$1/\omega_\beta \approx \sqrt{2\gamma}/\omega_p$
HiPACE

A Highly efficient Plasma Accelerator Emulation

- Quasi-static Particle-In-Cell (PIC) code
- 3D MPI parallelized
- Fully Electrodynamic and relativistic
- Dynamic time-step adjustment
- Allows for order-of-magnitude speedup for PWFA simulations compared to full PIC codes
- Tailored for clusters with a moderate number of nodes (~1k)
HiPACExx | Physical basis

Quasi-static approximation (QSA)

$$\xi = z - ct$$
$$\tau = t$$

Quasi-Static Approximation (QSA) for field configuration

$$\frac{\partial F}{\partial \tau} \ll c \frac{\partial F}{\partial \xi}$$

Beam is frozen while plasma is evolved over the beam and fields are being solved

Fields are frozen while the beam is advanced


Mora and Antonsen, Phys. Plas. 4, 217 (1997)
Field solver - strategy

Field equations from Maxwell equations in Coulomb gauge and using QSA

\[ \partial_\xi \left( \frac{E_x - B_y}{E_y + B_x} \right) = J_\perp \]
\[ \nabla^2_\perp E_z = \nabla_\perp J_\perp \]
\[ \nabla^2_\perp B_x = -\partial_y (J_z - \partial_\xi E_z) \]
\[ \nabla^2_\perp B_y = \partial_x (J_z - \partial_\xi E_z) \]

Fastest way of solving poisson equations: “fast poisson solver” using FFTs

2D grid with N\times N points

Fast poisson sover: \( \mathcal{O}(N^2 \log(N)) \)

Any other method: \( \geq \mathcal{O}(N^3) \)

Poisson-equations are solved with a fast Poisson solver using FFTW3-MPI

Computational Frameworks for the Fast Fourier Transform, Charles Van Loan

**Plasma routine**

- Charge & current deposition
- Pushing plasma particles using a linear multistep method

Computing fields

---

**HiPACE**

---

Plasma routine

- Pushing plasma particles using a linear multistep method
- Computing fields
- Iterate with new B-fields and check convergence

Charge & current deposition
Plasma routine

Advancing plasma particles in -\(\xi\) direction and solving field equations in next slab
Comparison between a full PIC code and HiPACE:

\[ k_p z = 450 \quad \frac{k_\beta}{\sqrt{2\gamma}} \quad \gamma = 2000 \quad k_\beta z = 7.1 \]

Full PIC code: 19968 core hrs \quad \text{Factor: 42} \quad \text{HiPACE: 474 core hrs}
Comparison between a full PIC code and HiPACE:

\[ k_p z = 450 \quad \text{Factor: 42} \quad k_\beta z = 7.1 \]

Full PIC code: 19968 core hrs  HiPACE: 474 core hrs
Comparison between a full PIC code and HiPACE:

- Transverse field
- Longitudinal field

Field configurations in HiPACE are close to those obtained from the full PIC code.

No current/field smoothing required - FFT field solvers do the job.
HiPACE

>> Parallel scalings

Strong scaling

>> Simulated problem:
   Plasma is advanced over homogeneous distribution of beam-electrons and -positrons

>> Fixed total problem size:
   2x8 beam particles and 4 plasma particles per cell,
   4,194,304 cells

>> Scaling from 1 to 1024 cores

>> The code efficiency is 84% @ 64 cores, dropping to
   44% @ 128 cores and 22% @ 256 cores

>> Reason for decaying efficiency can be investigated with
   a weak scaling
HiPACE

Parallel scalings

Weak scaling

Simulated problem:

Plasma is advanced over homogeneous distribution of beam-electrons and -positrons

Fixed problem size per core:

2x8 beam particles and 4 plasma particles per cell, 16^3 cells

Longitudinal scaling from 1x1x1 to 1024x1x1 cores

Transverse scaling from 1x1x1 to 1x32x32 cores

The performance is limited by the overhead of the 2D-FFTs which are performed in transverse slices

Good performance expected as long as transverse slices are within one CPU
Strengths and drawbacks of quasi-static PIC codes

Strengths of quasi-static PIC codes

+ High energetic particle beam - plasma interactions are correctly modeled with high computational efficiency
+ Beams can consistently be initialized in the plasma
+ No current or field smoothing required
+ Implementation of quasi-static codes allow for a reduced memory usage

Drawback of quasi-static PIC codes compared to full PIC codes

- Less versatile: Particles must either be highly-relativistic (beam) or non-/ mildly-relativistic (plasma)
- Plasma particle injection cannot be modeled consistently
- Radiation effects (Raman instabilities, betatron radiation etc.) cannot be modeled intrinsically
- Field solvers in quasi-static PIC codes are not as easily parallelizable as in full PIC codes
- More subtleties need to be taken care of for stable simulations (e.g. time and spatial resolution)
Strengths and drawbacks of quasi-static PIC codes

**Strengths of quasi-static PIC codes**

+ High energetic particle beam - plasma interactions are correctly modeled with high computational efficiency
+ Beams can consistently be initialized in the plasma
+ No current or field smoothing required
+ Implementation of quasi-static codes allow for a reduced memory usage

**Drawback of quasi-static PIC codes compared to full PIC codes**

- Less versatile: Particles must either be highly-relativistic (beam) or non-/ mildly-relativistic (plasma)
- Plasma particle injection cannot be modeled consistently
- Radiation effects (Raman instabilities, betatron radiation etc.) cannot be modeled intrinsically
- Field solvers in quasi-static PIC codes are not as easily parallelizable as in full PIC codes
- More subtleties need to be taken care of for stable simulations (e.g. time and spatial resolution)
Hybrid simulations

- Simulating internal injection, e.g. density down-ramp or ionization injection using a full 3D PIC code
- After the injection process, particles of driver-beam and injected beam are imported to a 3D HiPACE simulation and propagated further
- Dynamic time-step adjustment ensures for best efficiency while rendering motion of all beam particles
Hybrid simulations of down-ramp-injection for FACET experiment E215

- FACET-type driver-beam traverses short plasma density transition
- Plasma particles are injected and subsequently accelerated

**Result of example simulation**: Longitudinal phase space of driver and witness beam after 1.7 meters propagation in a plasma target.
Hybrid simulations

Hybrid simulations of down-ramp-injection for FACET experiment E215

FACET-type driver-beam traverses short plasma density transition

Plasma particles are injected and subsequently accelerated

Result of example simulation: Longitudinal phase space of driver and witness beam after 1.7 meters propagation

FACET-type beam

Injected beam

Energy (GeV)

Charge per energy and length (a.u.)

Down-ramp-injection for FACET experiment E215

injected beam
Quasi-static PIC codes are an appropriate tool to study relativistic beam-plasma interactions.

Order-of magnitude speedup compared to full PIC codes for adequate problems.

3D quasi-static PIC code HiPACE shows good parallelization.

Beams can be initialized before or in the plasma from results of tracking codes or full PIC codes.

Studies for FLASHForward (see talk by J. Dale) and FACET experiments ongoing.

Code is currently improved in speed, functionality and stability.

- Improvements on the parallel FFTs
- Implementation of a laser-envelope model
- Adding more features (e.g. fluid plasma)
Thanks for listening!