HiPACE
Development of a quasi-static Particle-In-Cell code

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HiPACE
Development of a quasi-static Particle-In-Cell code

Physics in Intense Fields, Hamburg 2013

Outline

- Introduction and Motivation
- Particle-In-Cell (PIC) Simulations
  - Short introduction and overview over the Particle-In-Cell technique
- The quasi-static PIC code HiPACE
  - Physical basis
  - Numerical implementation
  - Parallelization
  - Benchmark
- Summary and Outlook
Introduction and Motivation

Potential of beam-driven plasma acceleration

40 GeV in one meter

- Long beam at SLAC injected into plasma target
- Tail of beam is energy-doubled

Energy doubling of 42 GeV electrons in a metre-scale plasma wakefield accelerator

Introduction and Motivation

Potential of beam-driven plasma acceleration

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What’s the lesson?

- Plasma acceleration allows for tens of GeV gradients
- Driver needs to be short compared to plasma wavelength and ...
- ... high degree of control over injection of witness beam needed to produce high-quality beams

Energy doubling of 42 GeV electrons in a metre-scale plasma wakefield accelerator
Introduction and Motivation

FLASHForward

Future-oriented wakefield-accelerator research and development at FLASH

**Driver-beam parameters**
- FEL quality, ≤ 1.6 GeV, 0.1% energy spread, 1 µm transverse emittance
- variable longitudinal beam shape (triangular, Gaussian), 20 to 500 fs long, ~20 pC to 500 pC
- 10 Hz repetition rate with up to three bunches each shot

FF aims at advancing beam-driven novel-accelerator science by exploring
- external injection and in-plasma beam-generation and acceleration techniques to provide high-energy (1.5 to 4+ GeV), low transverse emittance (~100 nm), ultrashort (~ fs), and high current (> 1 kA) electron bunches
- transformer ratios beyond 2
- the application of such beams to assess their potential for free-electron laser gain at photon energies inside and beyond the water window

**Beam-line layout**

FLASH 1
- Extraction
- Driver dump
- Differential pumping
- Plasma cell
- Laser/plasma photon diagnostics
- Witness dump
- Undulator
- X-ray diagnostics

FLASH 2
- Beam matching and focusing section
- Beam diagnostics section

**Driver-beam parameters**

**FLASHForward - technical design, beam properties and goals**

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**FlashForward**
Future-oriented wakefield-accelerator research and development at Flash

**Driver-beam parameters**
- FEL quality, \( \leq 1.6 \text{ GeV}, 0.1\% \text{ energy spread}, 1 \mu \text{m transverse emittance} \)
- variable longitudinal beam shape (triangular, Gaussian), 20 to 500 fs long, \(-20 \text{ pC to 500 pC}\)
- 10 Hz repetition rate with up to three bunches each shot

**FlashForward** aims at advancing beam-driven novel-accelerator science by exploring:

- external injection and in-plasma generation and acceleration techniques to provide high-energy (1.5 to 4+ GeV), low transverse emittance (~100 nm), ultrashort (~fs), and high current (>1 kA) electron bunches
- transformer ratios beyond 2
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See talk tomorrow by Julia Grebenyuk
Particle-In-Cell Simulations

The Particle-In-Cell method

- Typical tool to study highly intense laser or particle beam plasma interactions
  - Successfully used to study a wide range of plasma and gas phenomena
  - Capable of rendering kinetic plasma nature
- Fields defined on a mesh
- Particles with continuous positions and momenta
- Step size given by stability condition for numerical PDE-solvers (CFL-condition)
- Full 3D PIC simulations are computationally expensive
A Highly efficient Plasma Accelerator Emulation

HiPACE

- Quasi-static Particle-In-Cell (PIC) code
- 3D parallelized
- Dynamic time-step adjustment
- Allows for order-of-magnitude speedup for FLASHForward-type simulations
Characteristic time for beam evolution $\sim 1/\omega_\beta$

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

\[ 1/\omega_\beta \simeq \sqrt{2\gamma}/\omega_p \]
Beam is frozen while plasma is evolved over the beam and fields are being solved.

Fields are frozen while the beam is advanced.
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Physical basis

Transformation to co-moving frame

\[ \xi = z - ct \]
\[ \tau = t \]
\[ \frac{\partial}{\partial t} = \left( \frac{\partial}{\partial \tau} - c \frac{\partial}{\partial \xi} \right) \cdot \frac{\partial}{\partial z} = \frac{\partial}{\partial \xi} . \]

Quasi-Static Approximation (QSA) for properties of plasma particles and field configuration

\[ \frac{\partial}{\partial \tau} \ll c \frac{\partial}{\partial \xi} . \]
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Physical basis

Hamiltonian of a relativistic charged particle
\[
\mathcal{H} = \gamma mc^2 + q\phi
\]

Application of the QSA to the Hamiltonian

\[
\frac{d\mathcal{H}}{dt} = \frac{\partial \mathcal{H}}{\partial t} - c \frac{\partial \mathcal{H}}{\partial \xi} = -c \frac{\partial \mathcal{H}}{\partial z} = c \frac{dP_z}{dt}
\]

Yields an invariant of motion

\[
\frac{d}{dt} (\mathcal{H} - cP_z) = \frac{d}{dt} (\gamma mc^2 + q\Psi - cp_z) = 0
\]

Where the wake-potential is introduced

\[
\psi = \frac{e\Psi}{mc^2} = \frac{e}{mc^2} (\Phi - A_z)
\]

For particle which was at rest and no field initially

\[
\gamma - \psi - u_z = 1
\]

\[
\gamma = \frac{1 + u_{\perp}^2 + |\hat{a}_f|/2 + (1 + \psi)^2}{2(1 + \psi)}
\]

Mora and Antonsen, Phys. Plas. 4, 217 (1997)

Esarey et al., Phys. Fluids B 5 (7), July 1993
Transformation to co-moving frame

$$\xi = z - ct \quad \frac{\partial}{\partial t} \cdot = \left( \frac{\partial}{\partial \tau} - c \frac{\partial}{\partial \xi} \right) \cdot \quad \frac{\partial}{\partial z} \cdot = \frac{\partial}{\partial \xi} \cdot$$

Quasi-Static Approximation (QSA) for properties of plasma particles and field configuration

"Ingredients" for plasma particle advance

$$\partial_\xi \mathbf{u}_\perp = \frac{\gamma}{1 + \psi} \left( \frac{E_x - B_y}{E_y + B_x} \right) + \left( \frac{B_y}{-B_x} \right)$$

$$\partial_\xi \psi = \frac{\mathbf{u}_\perp}{1 + \psi} \left( \frac{E_x - B_y}{E_y + B_x} \right) - E_z$$

Adams-Bashforth backward integrator used
Field equations from Maxwell equations and QSA

\[ \partial_\xi \left( \frac{E_x - B_y}{E_y + B_x} \right) = J_\perp \]

\[ \nabla_\perp^2 E_z = \nabla_\perp J_\perp \]

\[ \nabla_\perp^2 B_x = - \partial_y \left( J_z - \partial_\xi E_z \right) \]

\[ \nabla_\perp^2 B_y = \partial_x \left( J_z - \partial_\xi E_z \right) \]

Solving Poisson-eqns with a fast Poisson solver using FFTW3

\[ \frac{d^2 U}{dx^2} = F(x), \quad a \leq x \leq b \]

\[ \frac{u_{k-1} - 2u_k + u_{k+1}}{\Delta x^2} = f_k \equiv F(x_k), \quad k = 1:n-1. \]

\[ \begin{pmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} f_1 - \alpha/h^2 \\ f_2 \\ f_3 \\ f_4 - \beta/h^2 \end{pmatrix} \]

\[ \lambda_j = -4\sin^2 \left( \frac{j \pi}{2n} \right) \]

for \( j = 1:n-1 \), then

\[ V^{-1} \Sigma_{n-1} V = \text{diag}(\lambda_1, \ldots, \lambda_{n-1}) \]

Computational Frameworks for the Fast Fourier Transform, Charles Van Loan

Field equations from Maxwell equations and QSA

\[ \partial_\xi \left( \frac{E_x - B_y}{E_y + B_x} \right) = J_\perp \]

\[ \nabla_\perp^2 E_z = \nabla_\perp J_z \]

\[ \nabla_\perp^2 B_x = -\partial_y (J_z - \partial_\xi E_z) \]

\[ \nabla_\perp^2 B_y = \partial_x (J_z - \partial_\xi E_z) \]

Solving Poisson-eqns with a fast Poisson solver using FFTW3

\[ \frac{d^2 U}{dx^2} = F(x), \quad a \leq x \leq b \]

\[ (u_{k-1} - 2u_k + u_{k+1})/h^2 = f_k = F(x_k), \quad k = 1:n - 1. \]

\[ \frac{1}{h^2} \begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} f_1 - \alpha/h^2 \\ f_2 \\ f_3 \\ f_4 - \beta/h^2 \end{bmatrix} \]

\[ \lambda_j = -4 \sin^2 \left( \frac{j\pi}{2n} \right) \]

\[ \text{for } j = 1:n - 1, \quad V^{-1} \Sigma_{n-1} V = \text{diag}(\lambda_1, \ldots, \lambda_{n-1}) \]

Computational Frameworks for the Fast Fourier Transform, Charles Van Loan

**HiPACE**

Numerical implementation

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**main loop**
- beam density deposition
- plasma routine
- beam pusher

**plasma routine**
- advance plasma particles
- deposit plasma charge & currents
- compute $E_z$
- compute $B_x$ and $B_y$

**compute $B_x$ and $B_y$**
- advance plasma particles $(n-1)$
- deposit plasma currents $(n-1)$
- compute $E_z$ $(n-1)$
- update $B_x$ and $B_y$ $(n)$
- check convergence
Numerical implementation

PLASMA ROUTINE
Plasma particle subroutine

Pushing particles → Computing fields

Current deposition

HiPACE
PLASMA ROUTINE

Plasma particle subroutine

Advancing plasma particles in $-\xi$ direction and solving Poisson equations in next slab.
**HiPACE**

- **Numerical implementation**

**main loop**

- $t + \Delta t$

**plasma routine**

- $\xi - \Delta \xi$

  - advance plasma particles
  - deposit plasma charge & currents
  - compute $E_z$, $Ex-By$ and $Ey+Bx$
  - compute $B_x$ and $B_y$

**compute $B_x$ and $B_y$**

- advance plasma particles ($n-1$)
- deposit plasma currents ($n-1$)
- compute $E_z$ ($n-1$)
- update $B_x$ and $B_y$ ($n$)
- check convergence
HiPACE

Parallelization

schematic parallel main loop flow

beam current depos.

plasma routine and field solver

beam pusher

e.g. exchanging current values at borders

proc-slab i

idle

proc-slab i+1

e.g. exchanging current values at borders

passing plasma information etc.

time

...
Parallelization

Showcase domain decomposition:
Four processes in propagation-direction

collective, global communication

proc-slab0  proc-slab1  proc-slab2  proc-slab3

idle  idle

node 1  node 2  node 1  node 2

slabs 0  1  2  3
Parallelization

Point-to-point-communication only

Showcase domain decomposition:
Four processes in propagation-direction

Slabs 0 1 2 3
Parallelization

“backward” directed communication only

Showcase domain decomposition:
Four processes in propagation-direction

slabs 0 1 2 3
Comparison between the full PIC code OSIRIS and HiPACE:
1 GeV gaussian electron beam, nb/n0 = 2.0
Comparison between the full PIC code OSIRIS and HiPACE: 1 GeV gaussian electron beam, nb/n0 = 2.0
Comparison of long. field: HiPACE and OSIRIS

nb/n0 = 0.1

nb/n0 = 1.0

nb/n0 = 2.0
FACET at SLAC
20 kA, 23 GeV

HiPACE simulation with dynamical time-step adjustment

Propagating the beam over a 15cm long gas cell

OSIRIS: 1.25e5 core hrs
HiPACE: 7.2e3 core hrs
Summary and Outlook

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

  Studies with FLASHForward and FACET beams ongoing

» Fully 3D electrodynamic quasi-static PIC code HiPACE functional

» First benchmarks show order-of magnitude speedup compared to full PIC codes

» Beams can be initialized from tracking codes or full PIC codes

» Code is currently improved in speed, functionality and stability

  Implementation of plasma fluid routine
Summary and Outlook

Thanks for listening!