HiPACE

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

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Physics in Intense Fields, DESY, July 2013

LAOLA. collaboration
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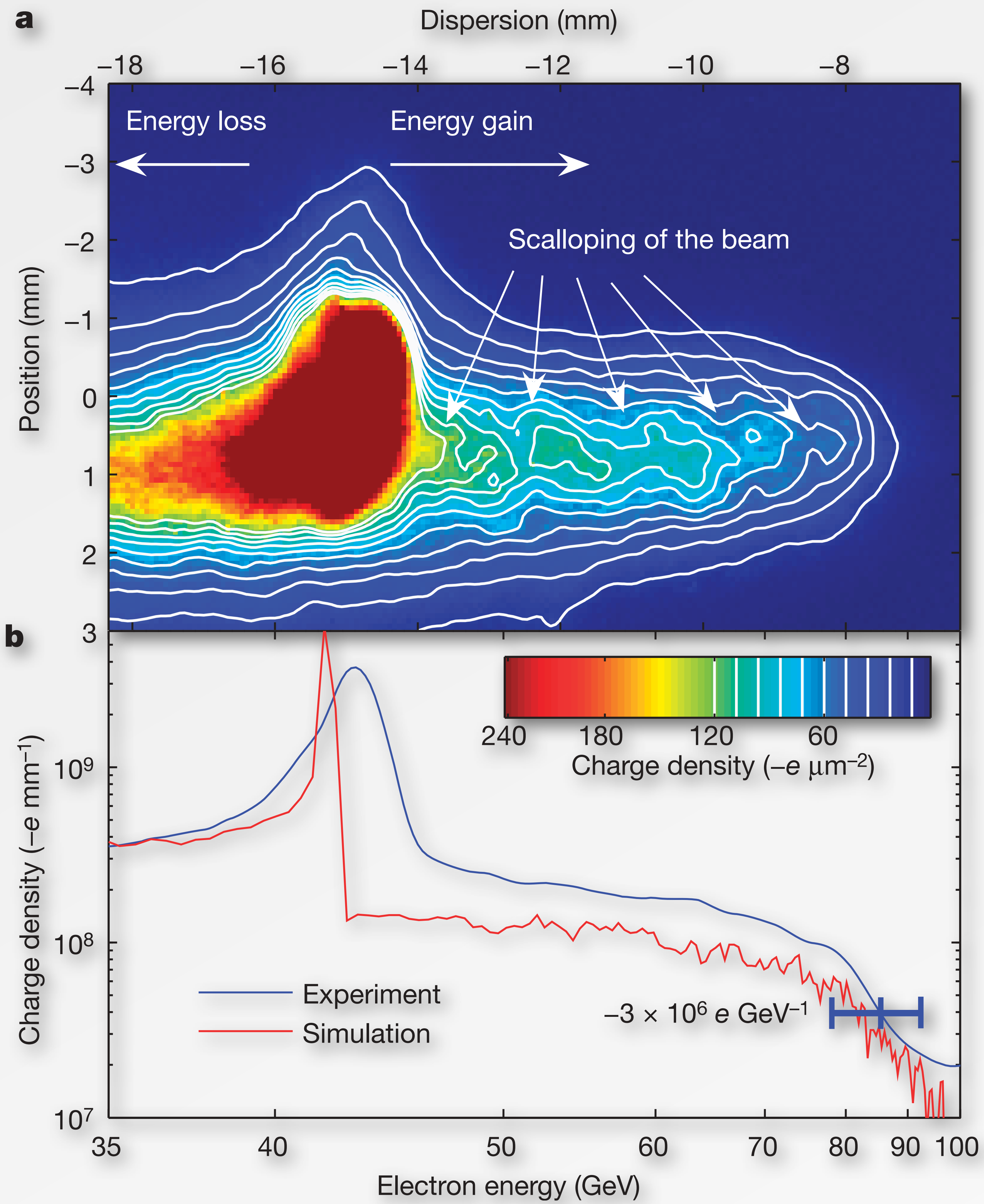
Outline

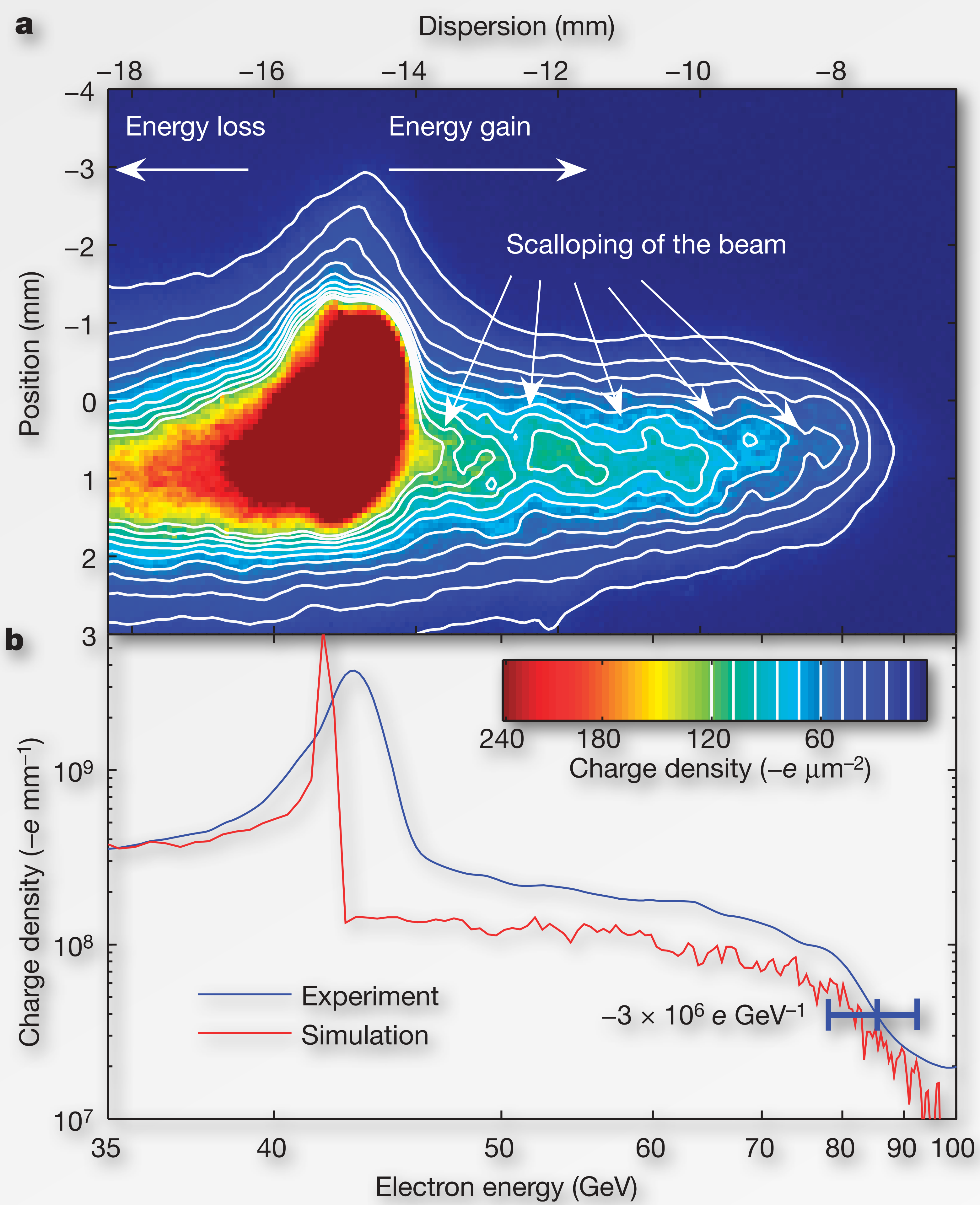
- Introduction and Motivation
- Particle-In-Cell (PIC) Simulations
  - Short introduction and overview over the Particle-In-Cell technique
- The quasi-static PIC code HiPACE
  - Physical basis
  - Numerical implementation
  - Parallelization
  - Benchmark
- Summary and Outlook



Energy doubling of 42 GeV electrons in a metre-scale plasma wakefield accelerator
I. Blumenfeld, et al., Nature 445, 741 (2007).

40 GeV in one meter

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



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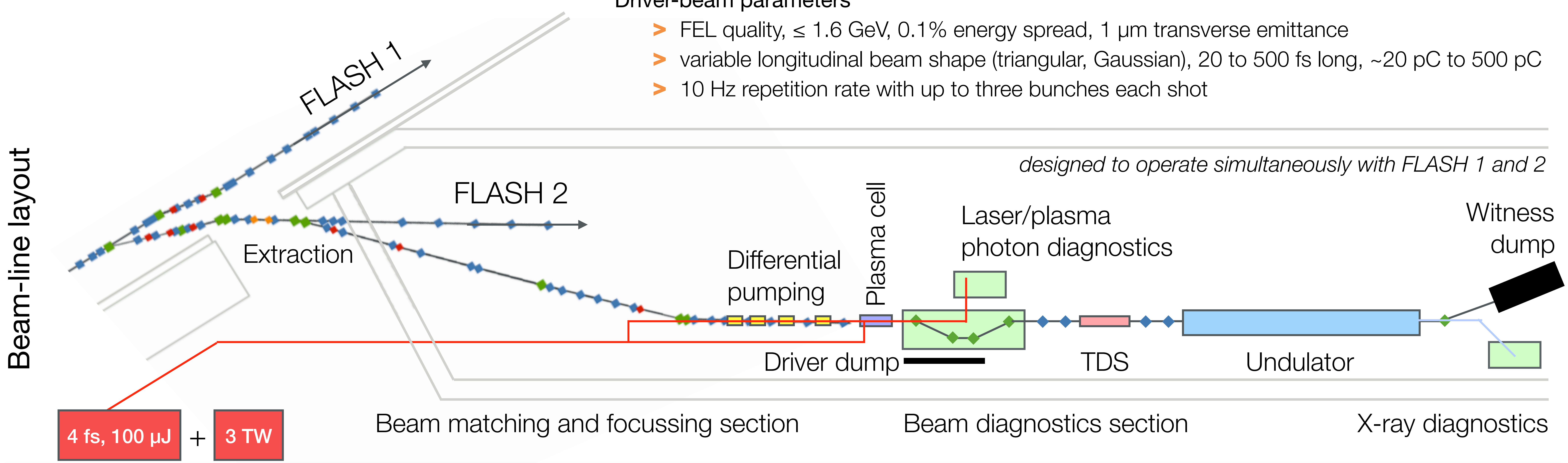
What's the lesson?

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

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

FLASHForward▸▸

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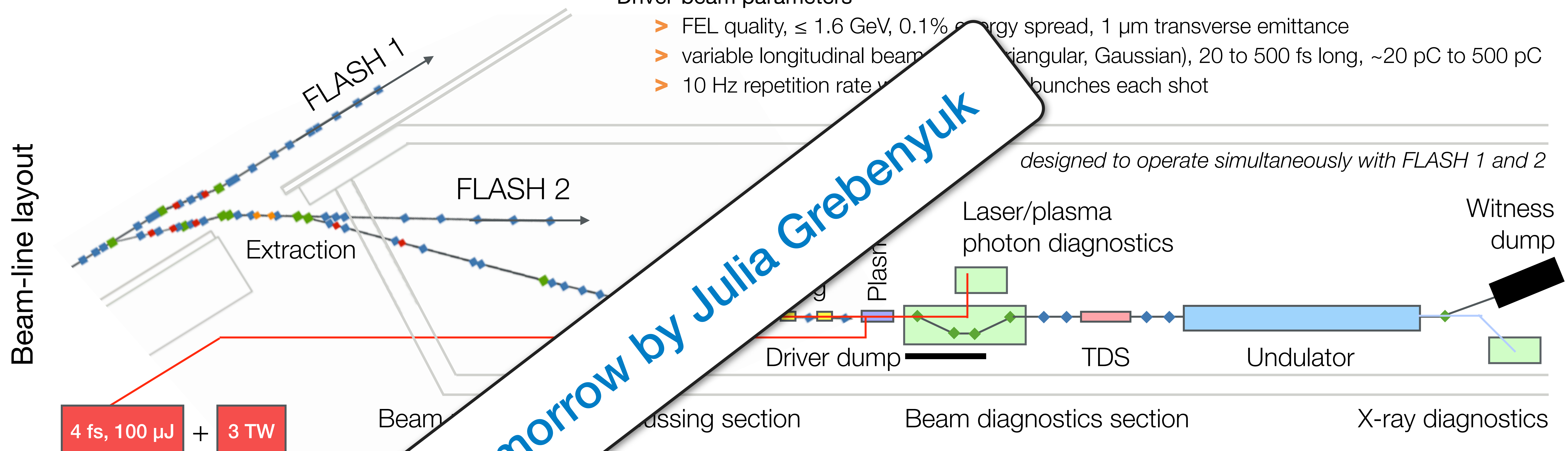

See talk tomorrow by Julia Grebenyuk

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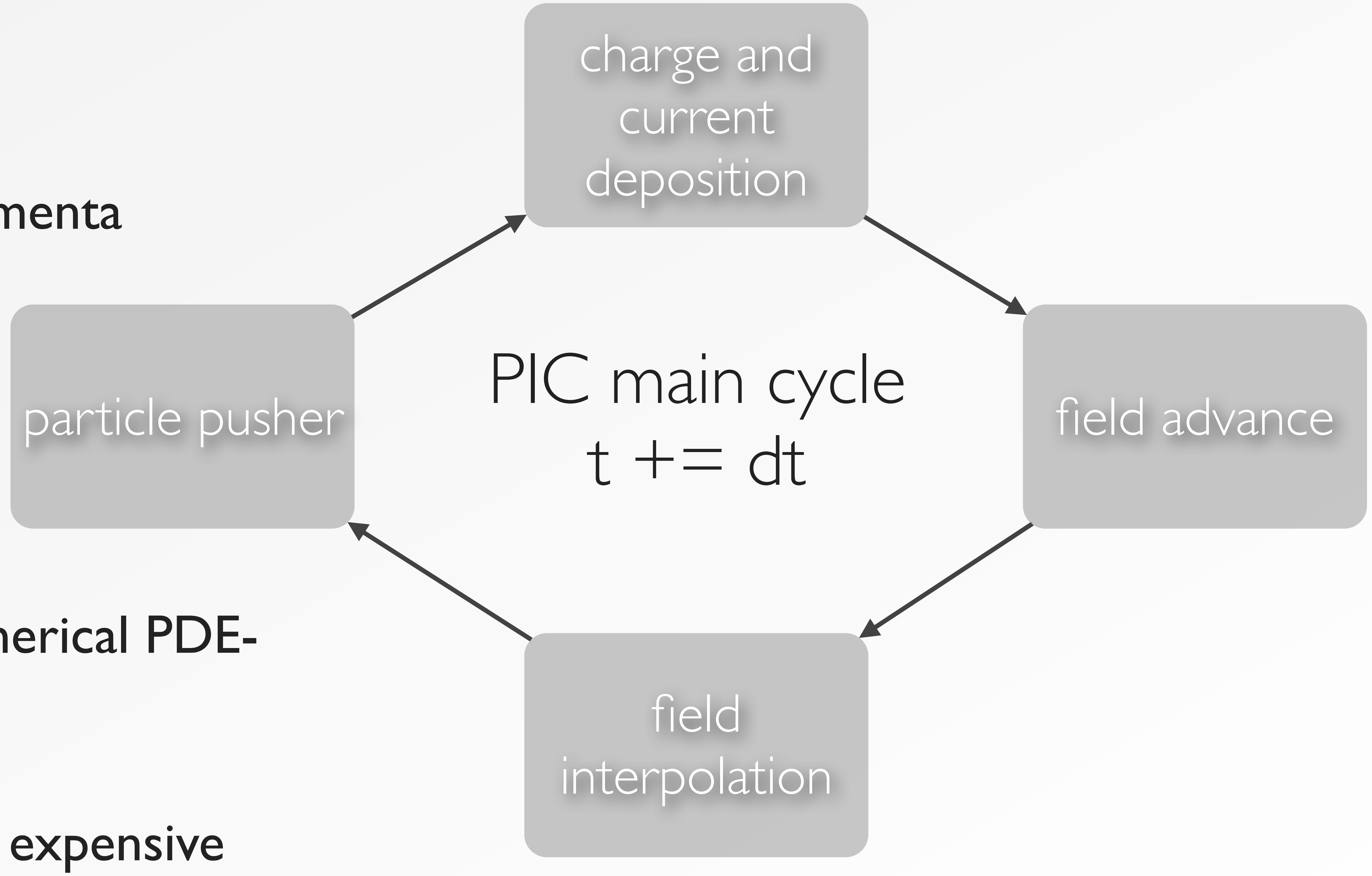
The Particle-In-Cell method

- >> 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



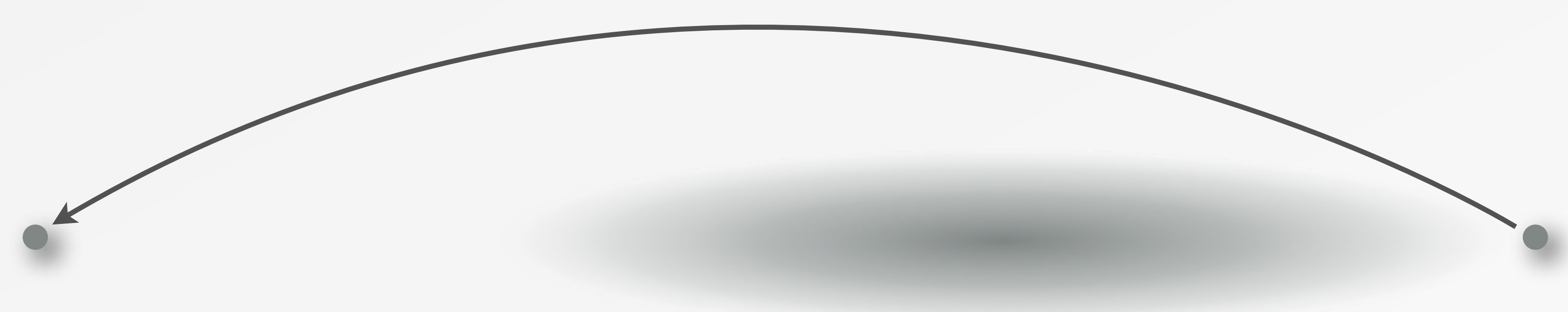
- >> Step size given by stability condition for numerical PDE-solvers (CFL-condition)
- >> Full 3D PIC simulations are computationally expensive

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

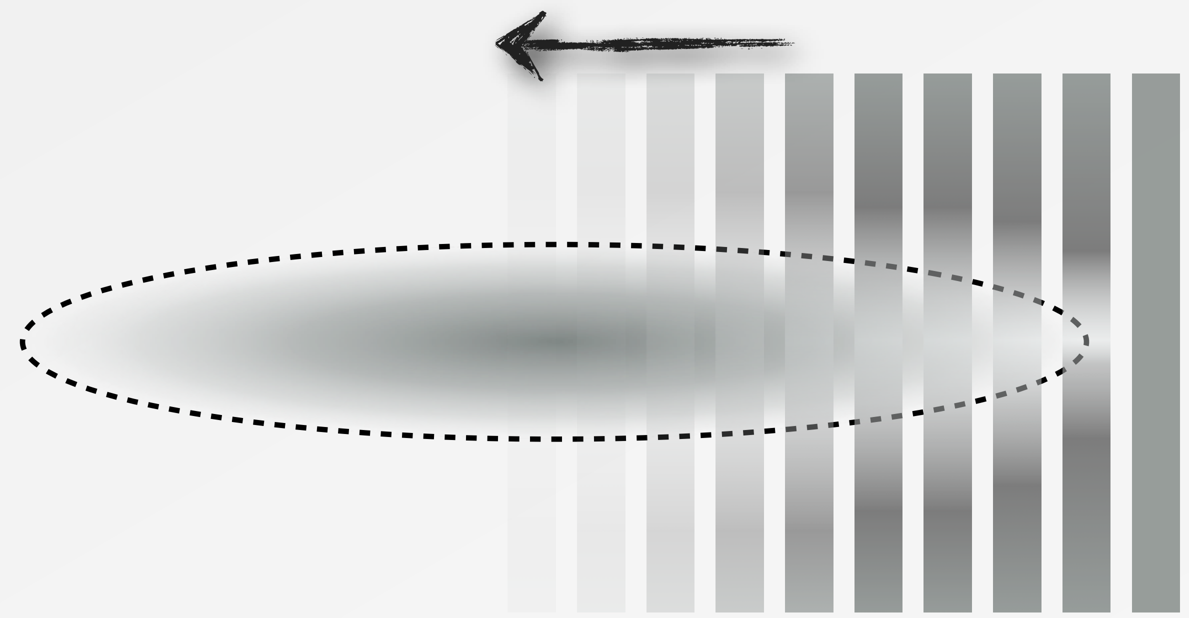
Characteristic time for beam evolution $\sim\ 1/\omega_\beta$

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

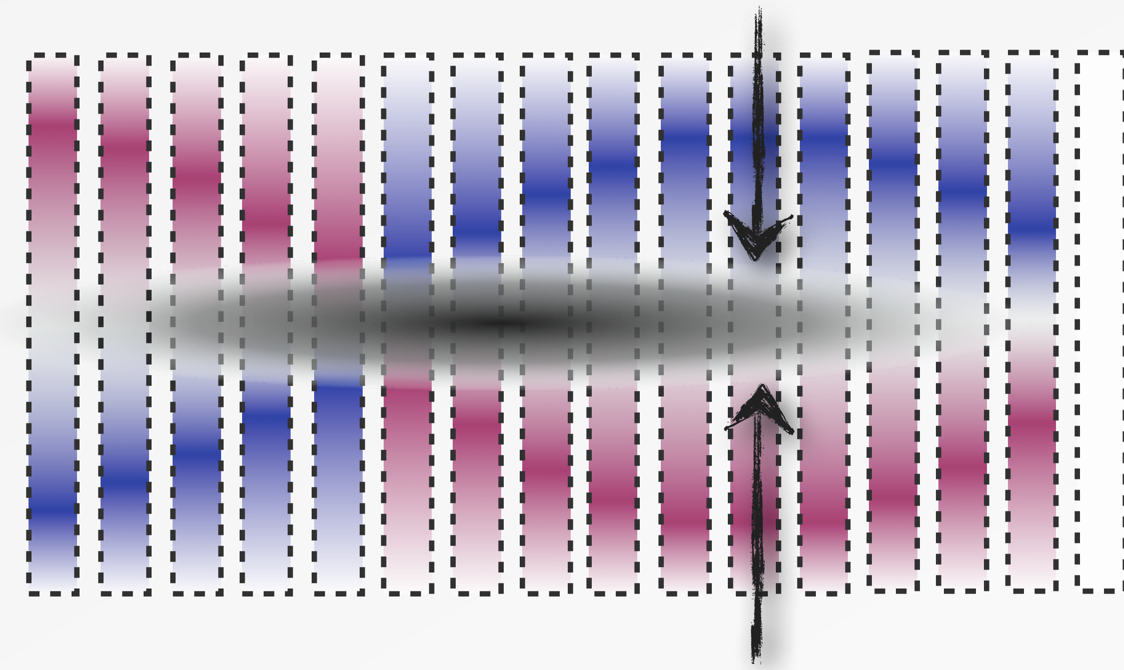


$$1/\omega_\beta \simeq \sqrt{2\gamma}/\omega_p$$

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



Fields are frozen while the beam is advanced



Transformation to co-moving frame

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

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

$$\boxed{\frac{\partial}{\partial \tau}\cdot \ll c\,\frac{\partial}{\partial \xi}\cdot}$$

Hamiltonian of a relativistic charged particle

$$\mathcal{H} = \gamma mc^2 + q\phi$$

Application of the QSA to the Hamiltonian

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

Yields an invariant of motion

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

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

Where the wake-potential is introduced

$$\psi = \frac{e\Psi}{mc^2} = \frac{e}{mc^2}\left(\Phi - A_z\right)$$

For particle which was at rest and no field initially

$$\gamma - \psi - u_z = 1$$

$$\longrightarrow \gamma = \frac{1 + u_\perp^2 + \left|\hat{a}_f\right|/2 + (1+\psi)^2}{2(1+\psi)}$$

Esarey et al., Phys. Fluids B 5 (7), July 1993

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

$$\boxed{\frac{\partial}{\partial \tau}\cdot \ll c\,\frac{\partial}{\partial \xi}\cdot}$$

"Ingredients" for plasma particle advance

$$\partial_\xi \mathbf{x}_\perp = -\frac{\mathbf{u}_\perp}{1+\psi}$$

$$\partial_\xi \mathbf{u}_\perp = \frac{\gamma}{1+\psi}\begin{pmatrix} E_x - B_y \\ E_y + B_x \end{pmatrix} + \begin{pmatrix} B_y \\ -B_x \end{pmatrix}$$

$$\partial_\xi \psi = \frac{\mathbf{u}_\perp}{1+\psi}\begin{pmatrix} E_x - B_y \\ E_y + B_x \end{pmatrix} - E_z$$

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

Adams-Bashforth backward integrator used

Field equations from Maxwell equations and QSA

$$\partial_\xi \begin{pmatrix} E_x - B_y \\ E_y + B_x \end{pmatrix} = \mathbf{J}_\perp$$

$$\nabla_\perp^2 E_z = \nabla_\perp \mathbf{J}_z$$

$$\nabla_\perp^2 B_x = -\partial_y \left(J_z - \partial_\xi E_z\right)$$
$$\nabla_\perp^2 B_y = \partial_x \left(J_z - \partial_\xi E_z\right)$$

Solving Poisson-eqns with a fast Poisson solver using FFTW3

$$\frac{d^2U}{dx^2} = F(x), \qquad a \le x \le b$$

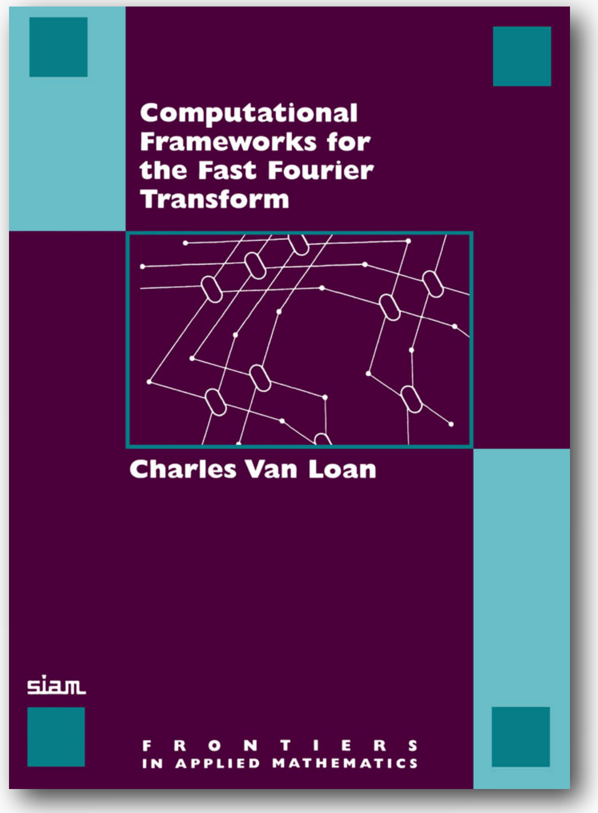
$$(u_{k-1} - 2u_k + u_{k+1})/h^2 = f_k \equiv F(x_k), \qquad k = 1{:}n-1 .$$

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

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

for $j = 1{:}n-1$, *then*

$$V^{-1}\mathcal{T}_{n-1}V = \mathrm{diag}(\lambda_1, \ldots, \lambda_{n-1}) .$$



Computational Frameworks for the Fast Fourier Transform, Charles Van Loan

FFTW3: M. Frigo and S. G. Johnson, Proc. IEEE **93** (2), p. 216 (2005)

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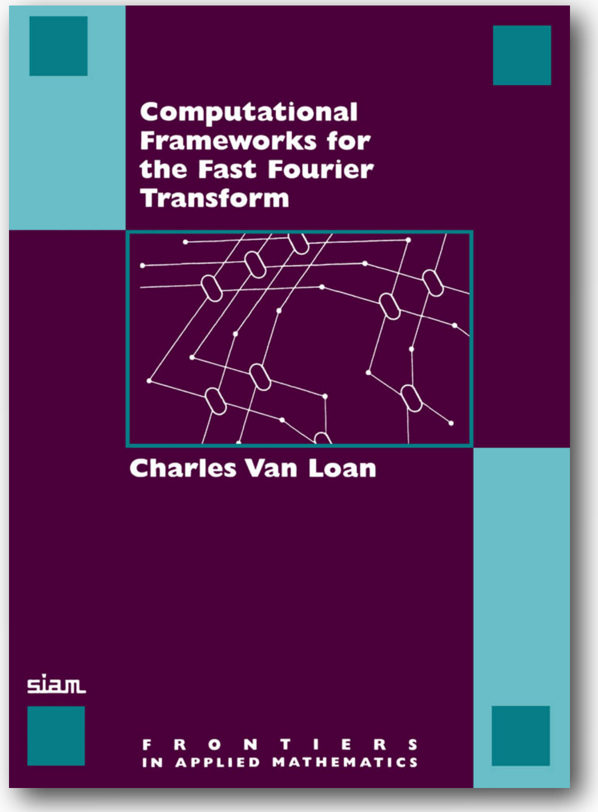

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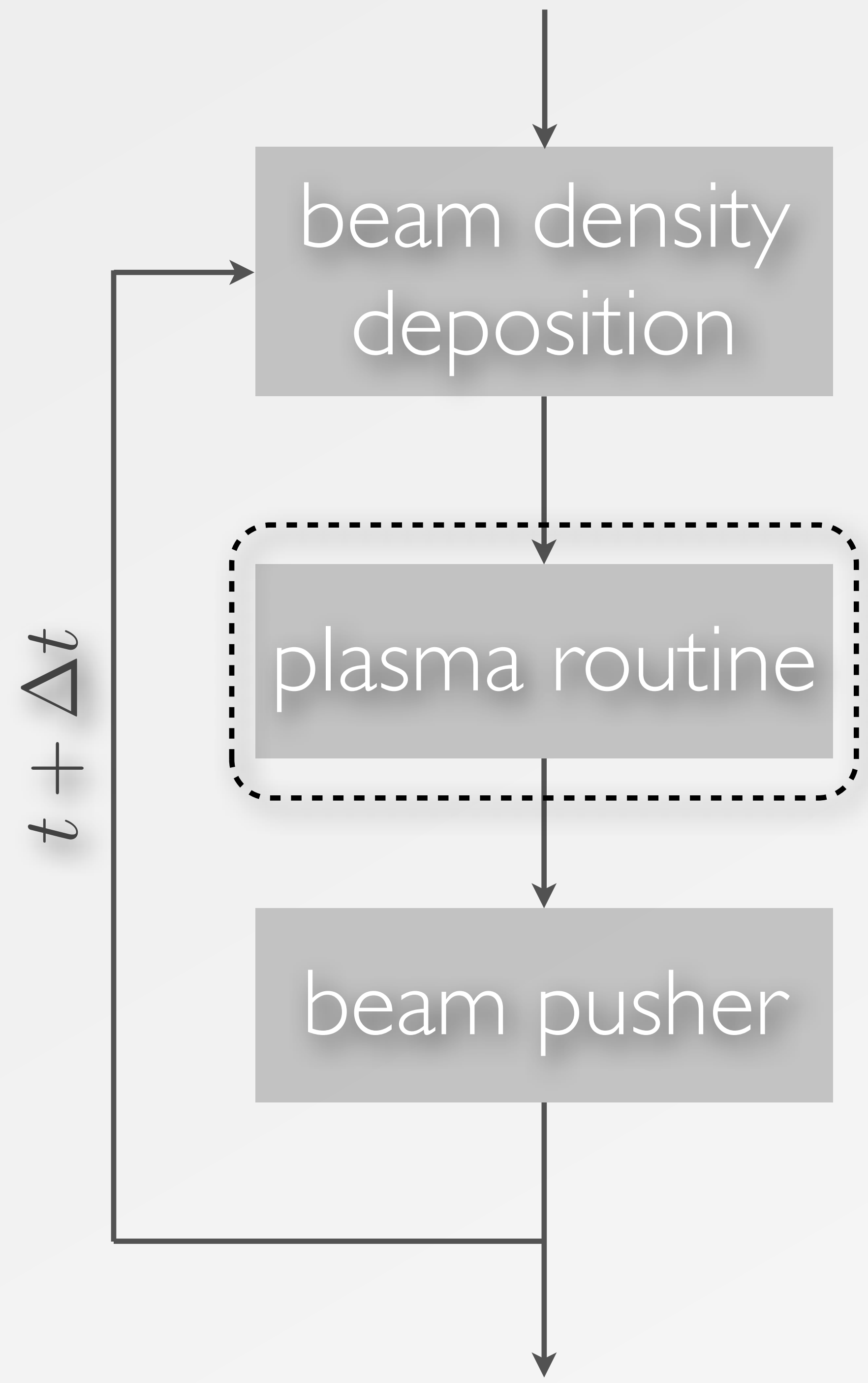
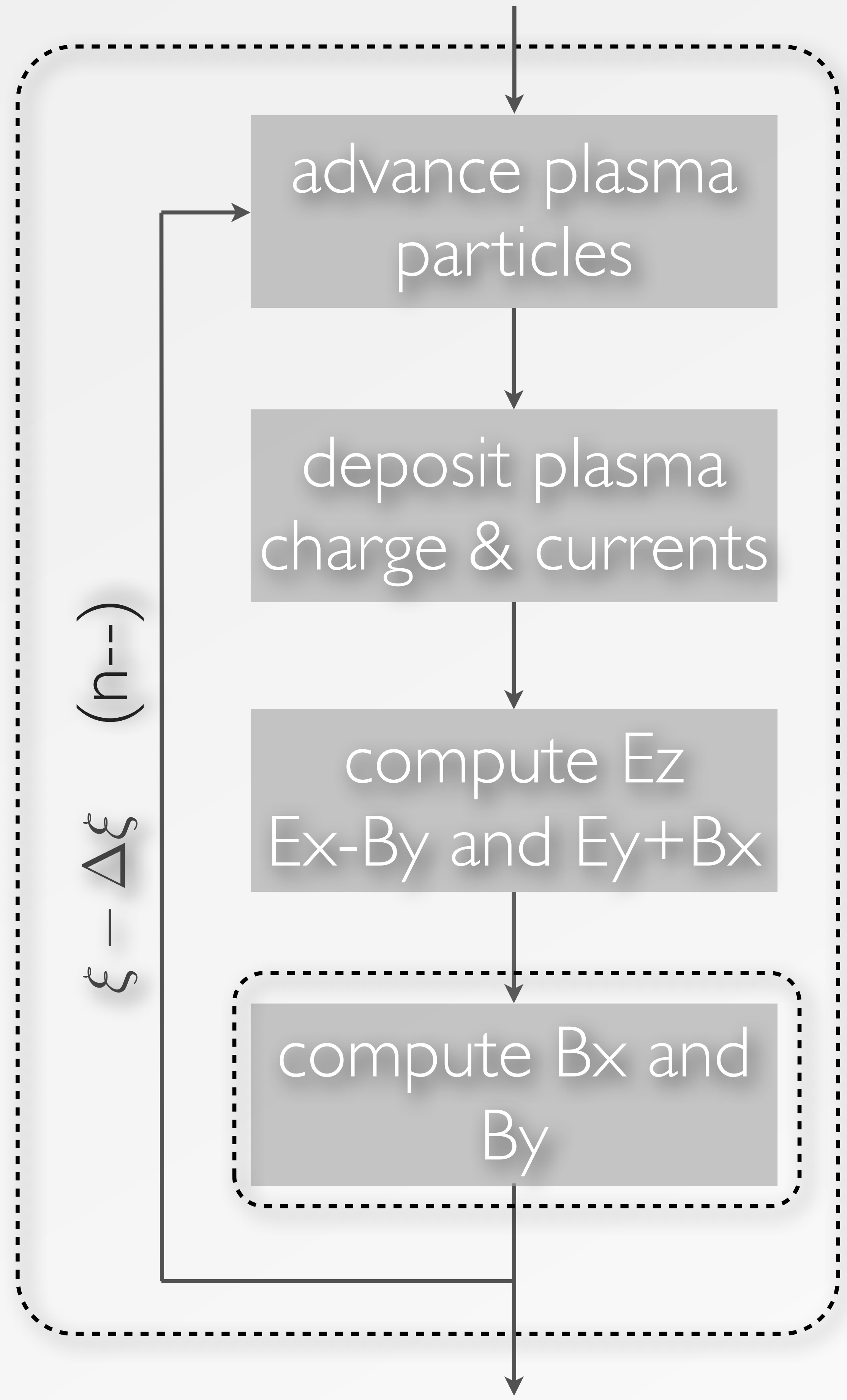
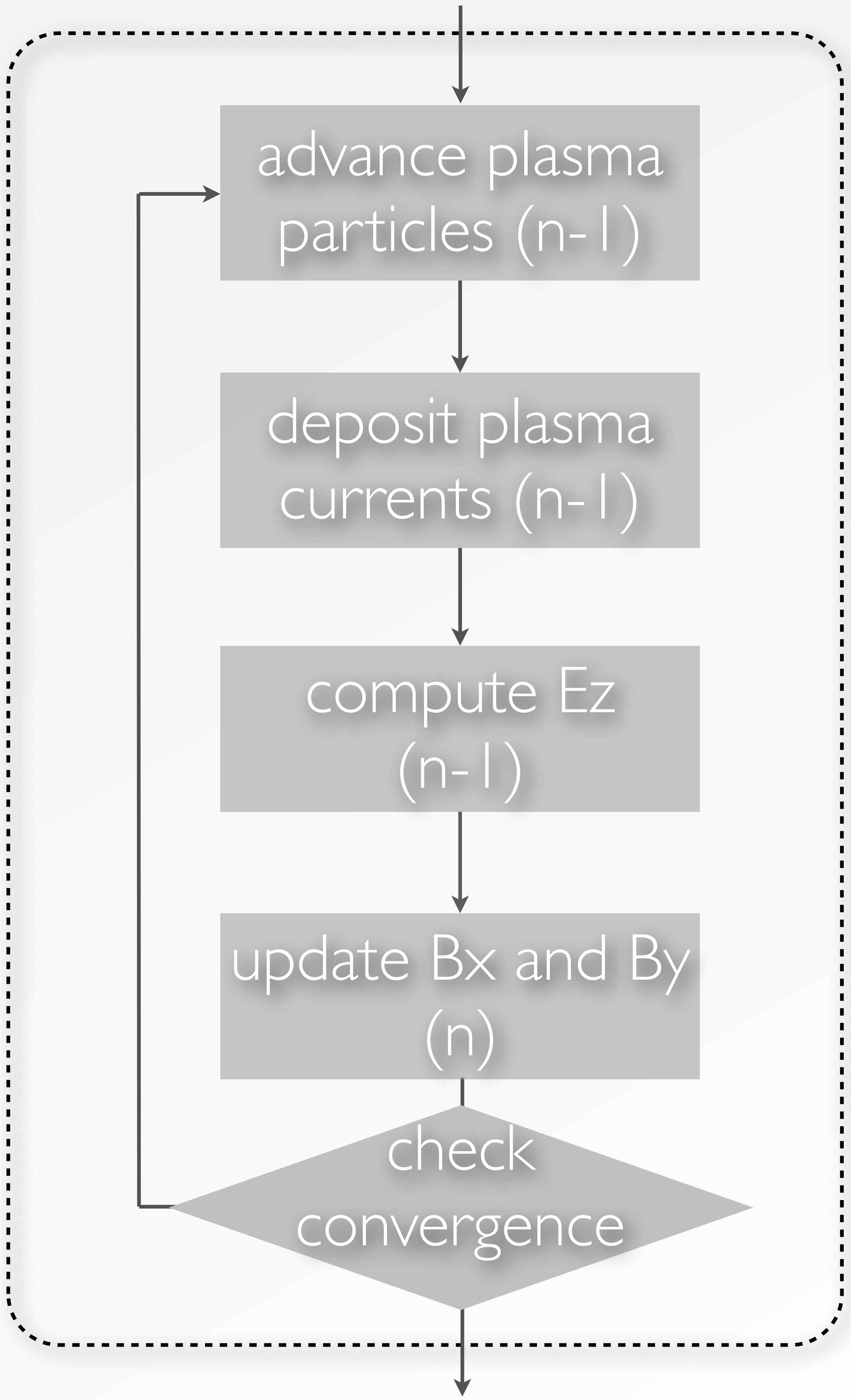
main loop



plasma routine

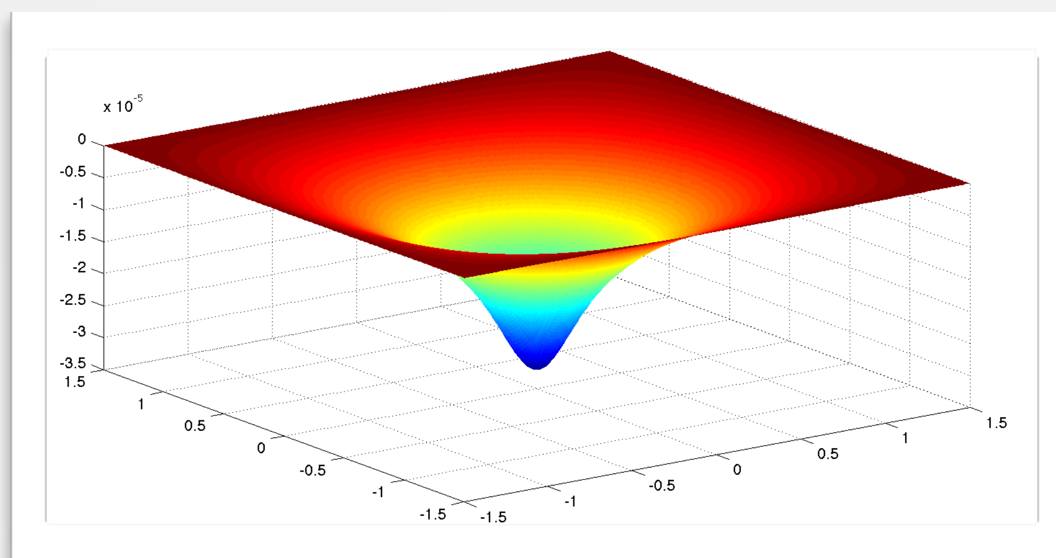


compute Bx and By

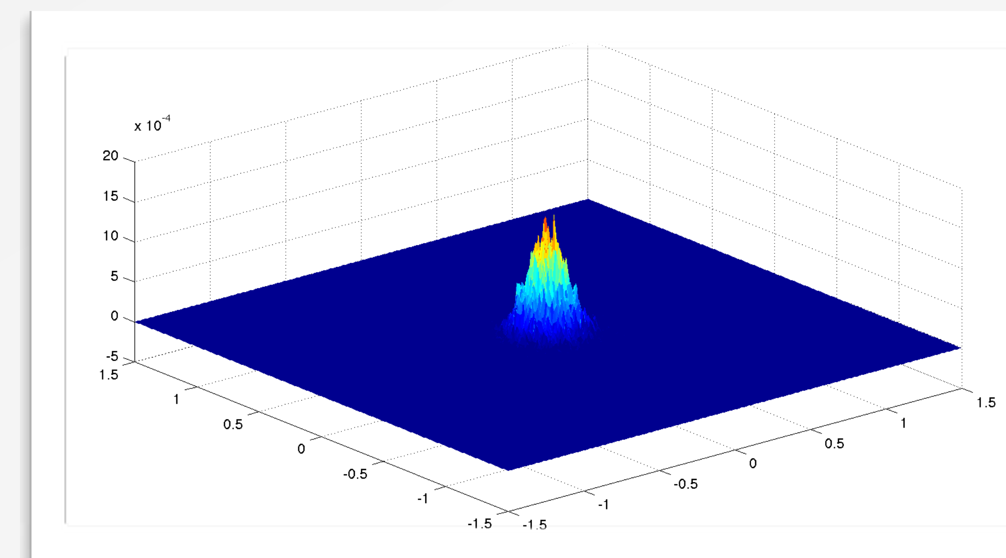


PLASMA ROUTINE

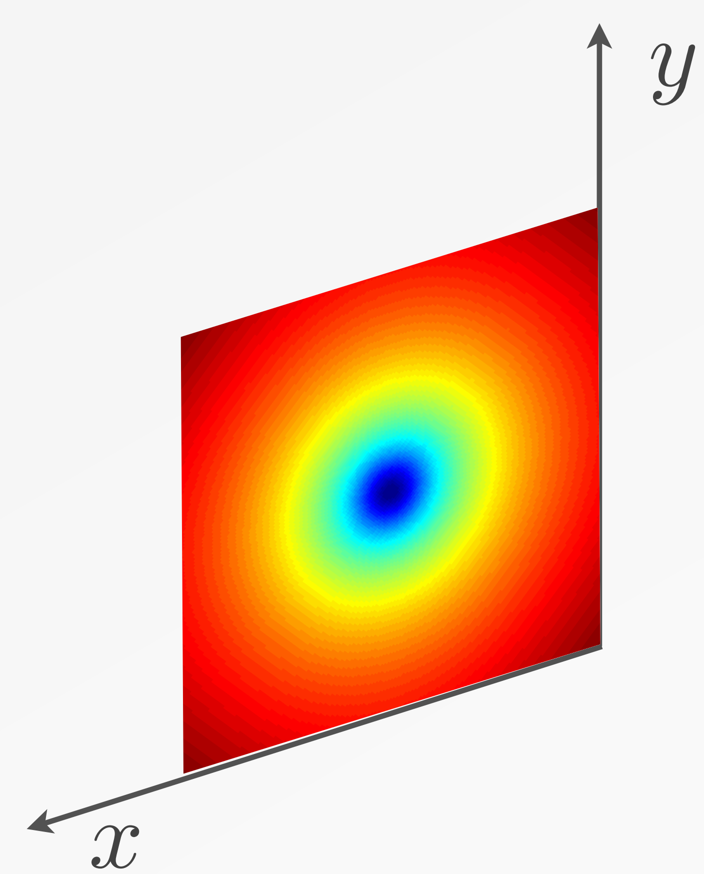
Plasma particle subroutine



Computing fields



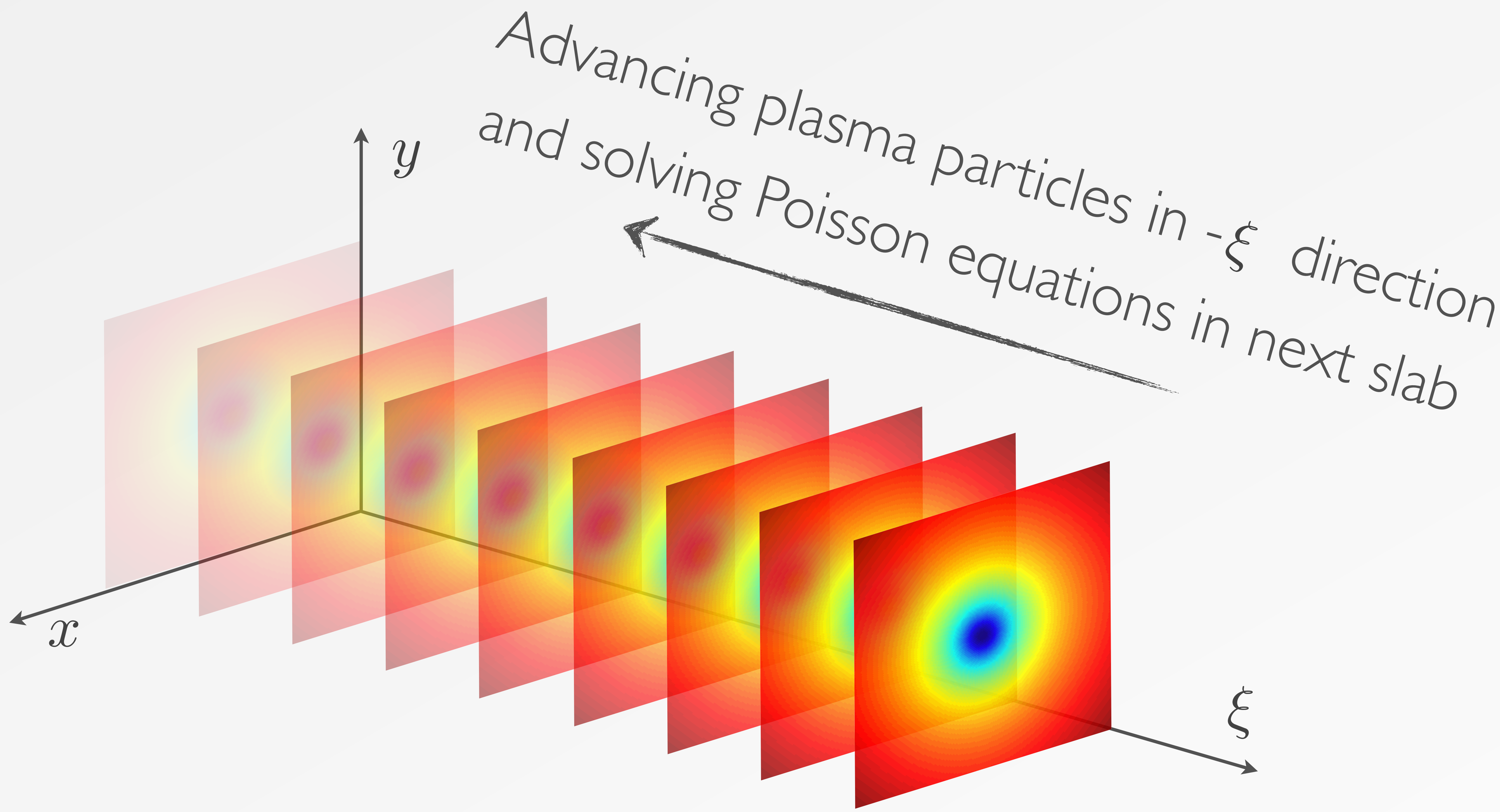
Pushing particles

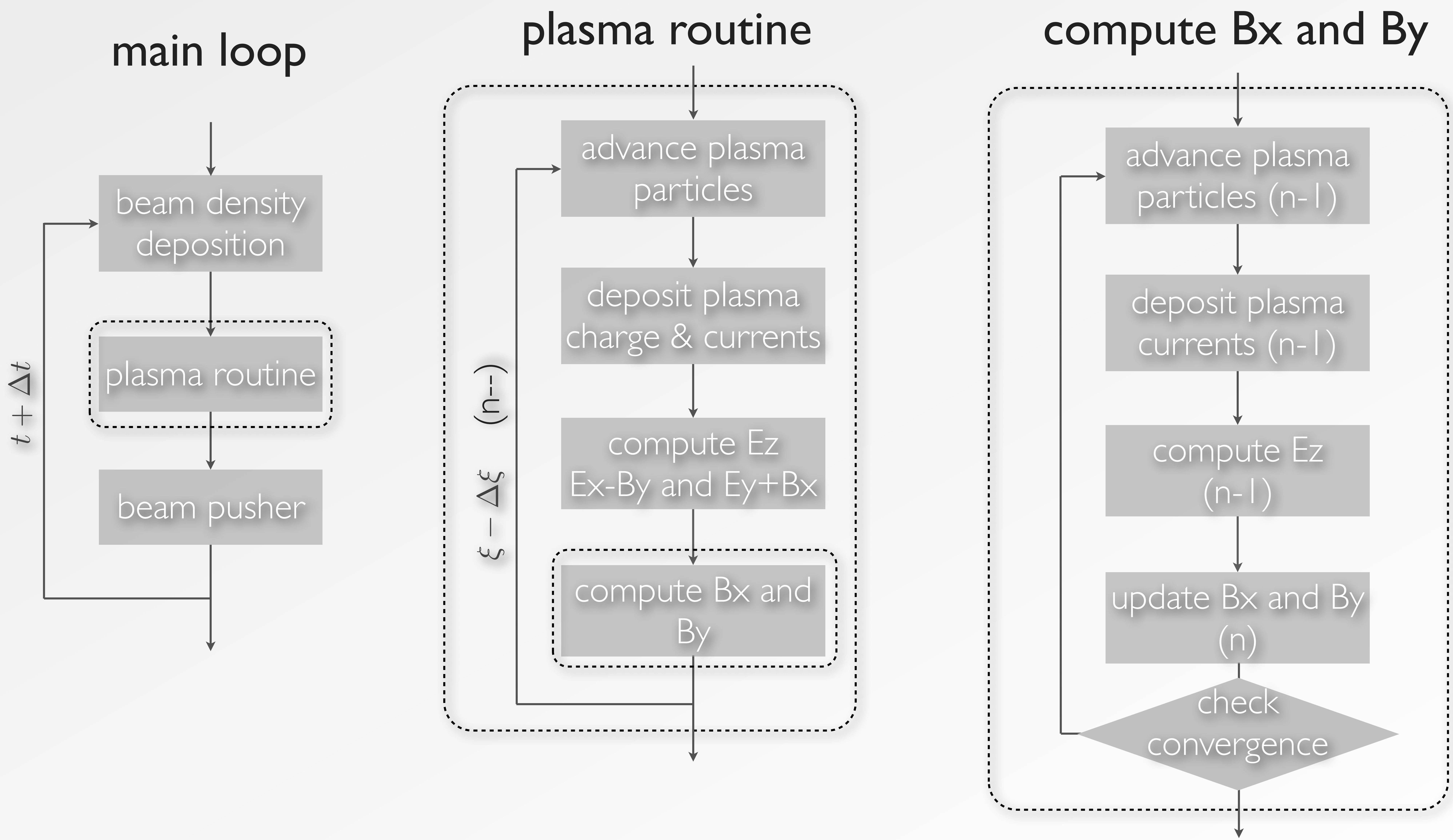


Current deposition

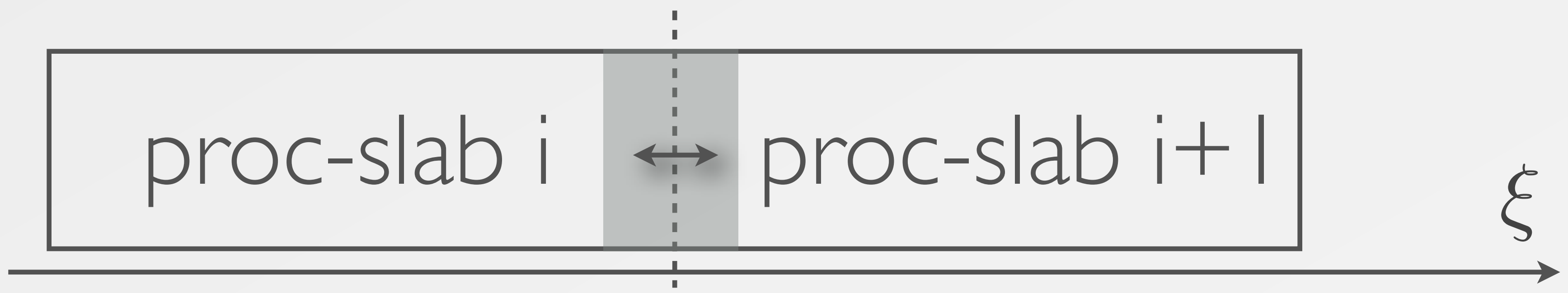
PLASMA ROUTINE

Plasma particle subroutine

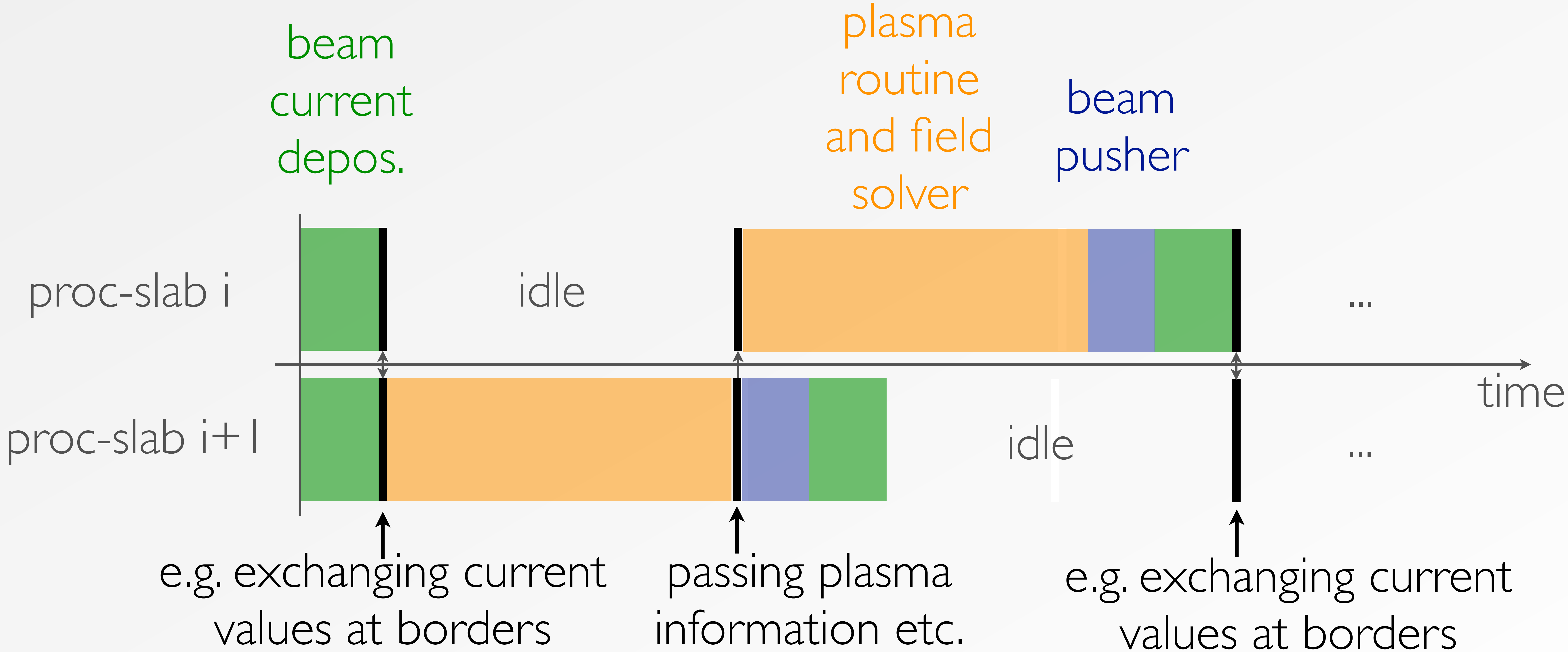



main loop
beam density deposition
plasma routine
beam pusher
$t + \Delta t$
plasma routine
advance plasma particles
deposit plasma charge & currents
compute Ez Ex-By and Ey+Bx
compute Bx and By
$\xi - \Delta\xi$ (n–)
compute Bx and By
advance plasma particles (n-1)
deposit plasma currents (n-1)
compute Ez (n-1)
update Bx and By (n)
check convergence

Parallelization



schematic parallel main loop flow



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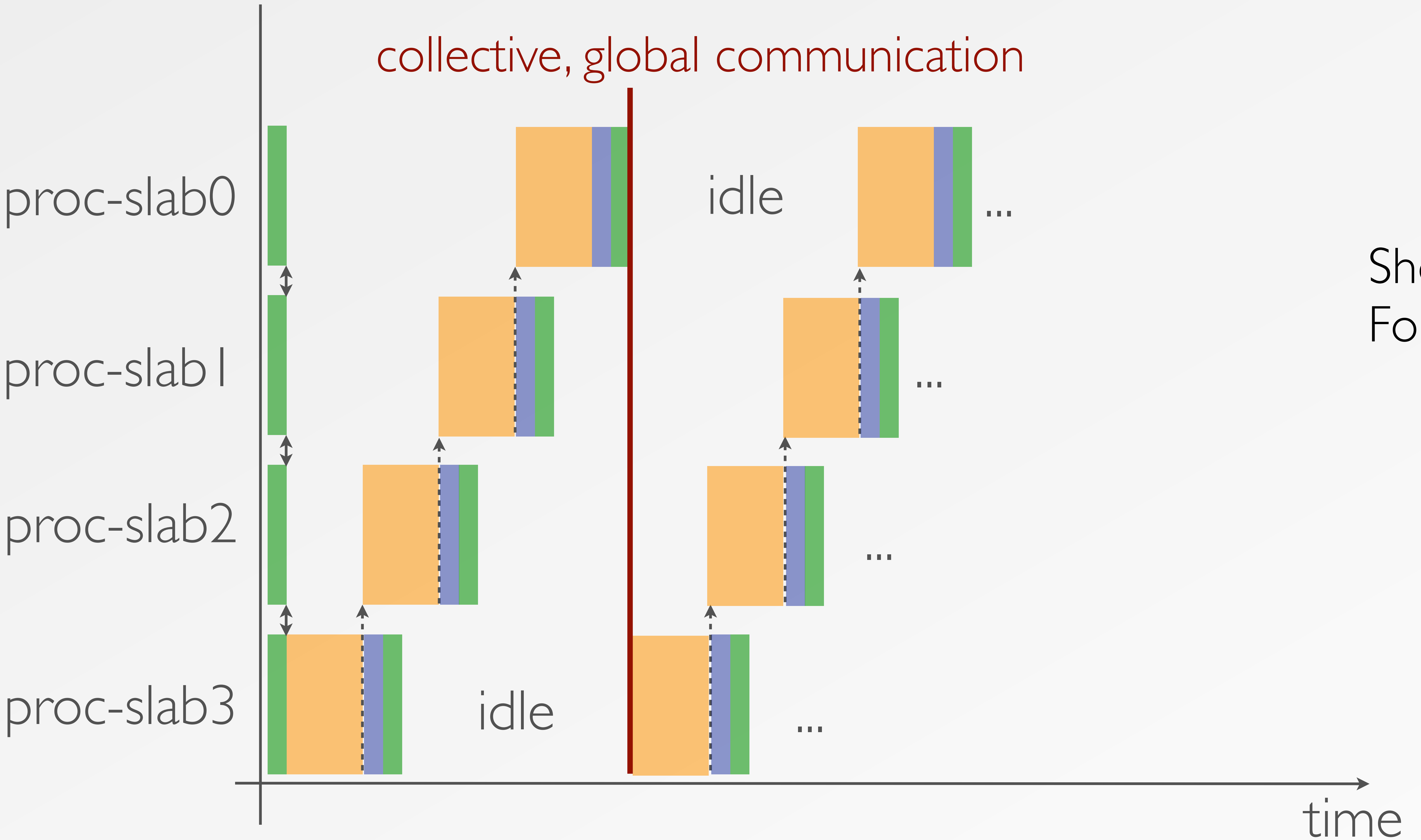
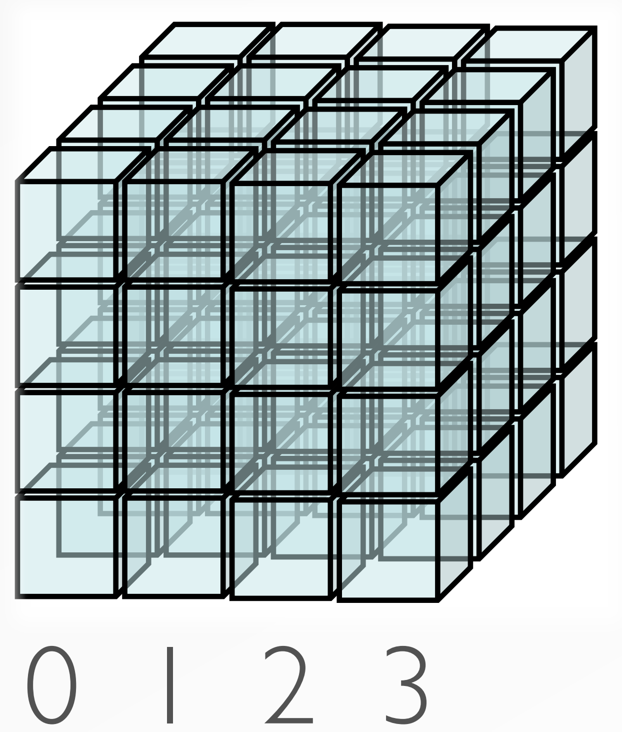


Showcase domain decomposition:
Four processes in propagation-direction



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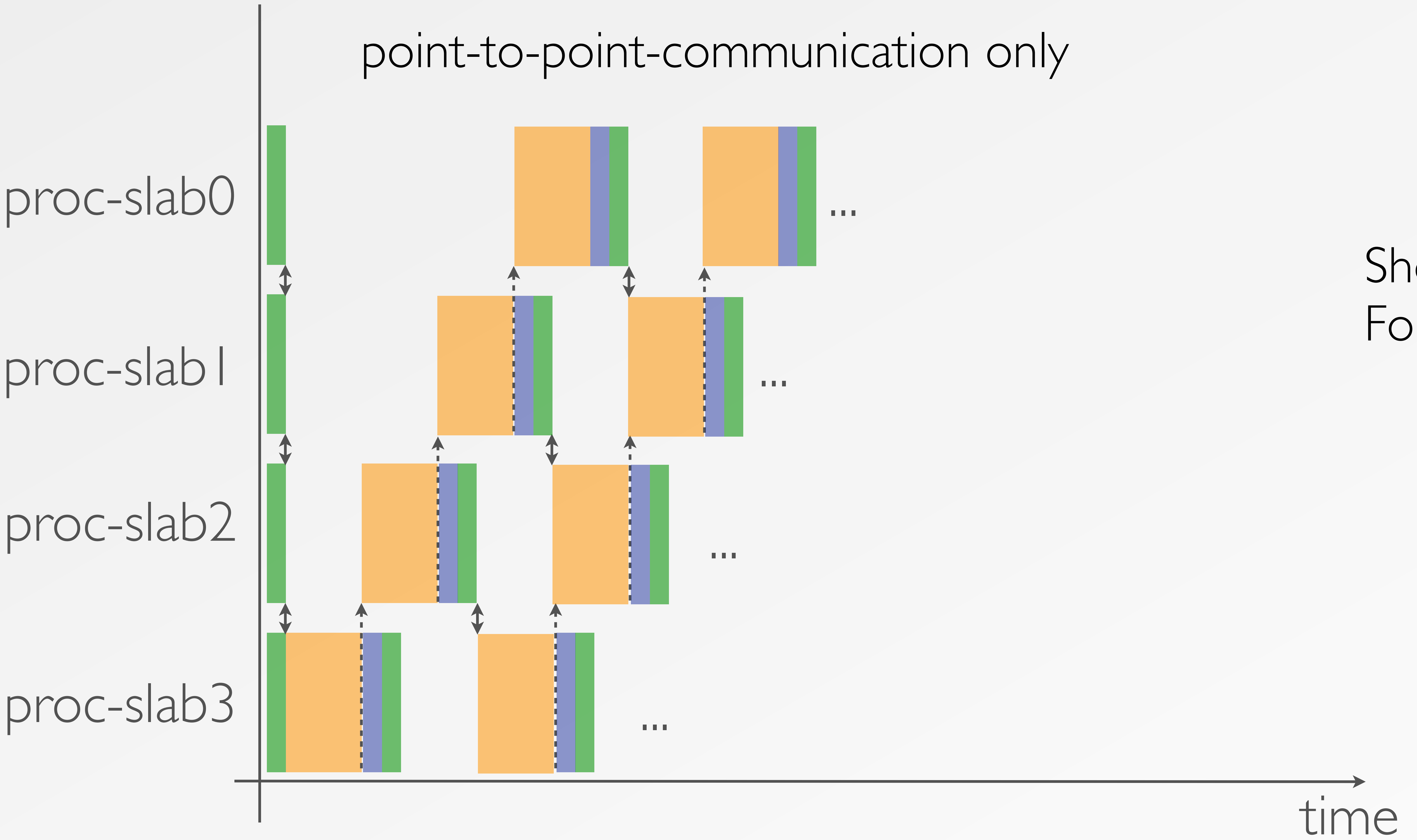

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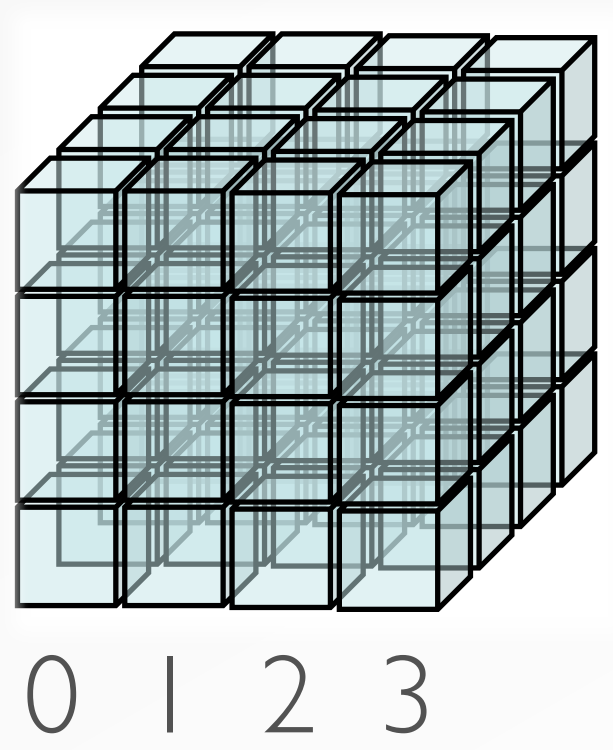

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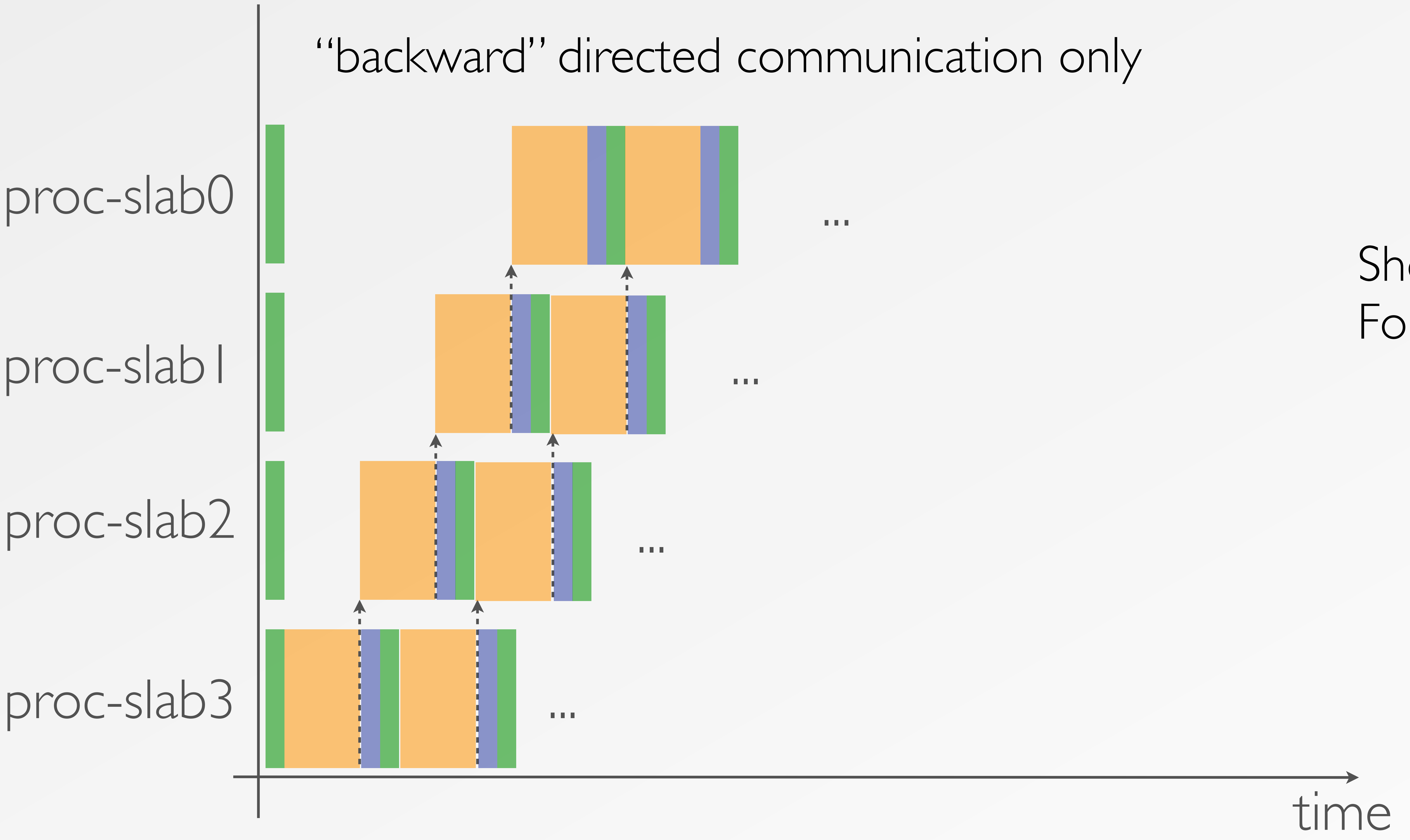

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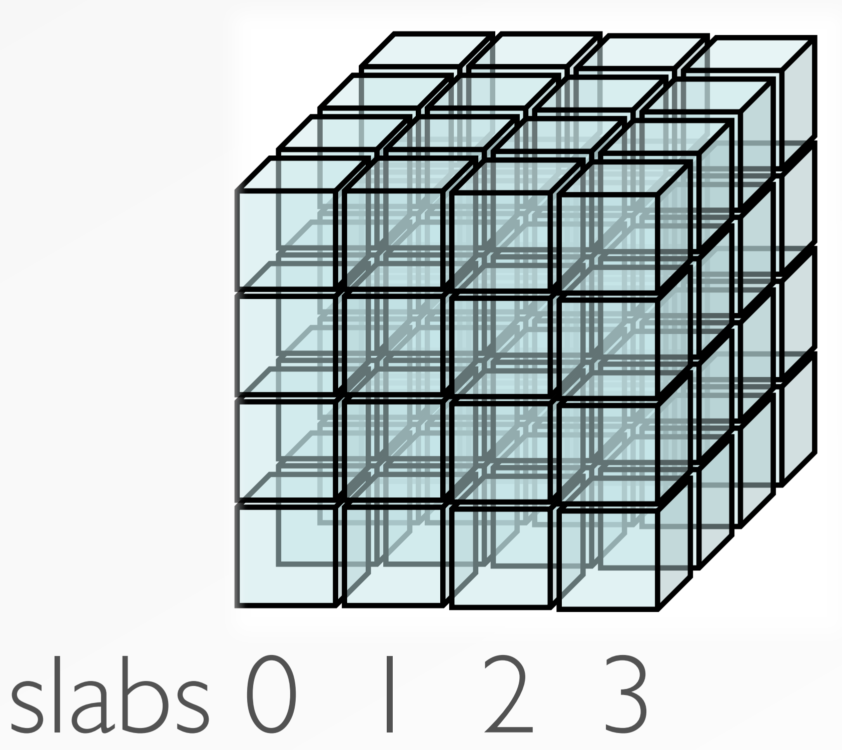
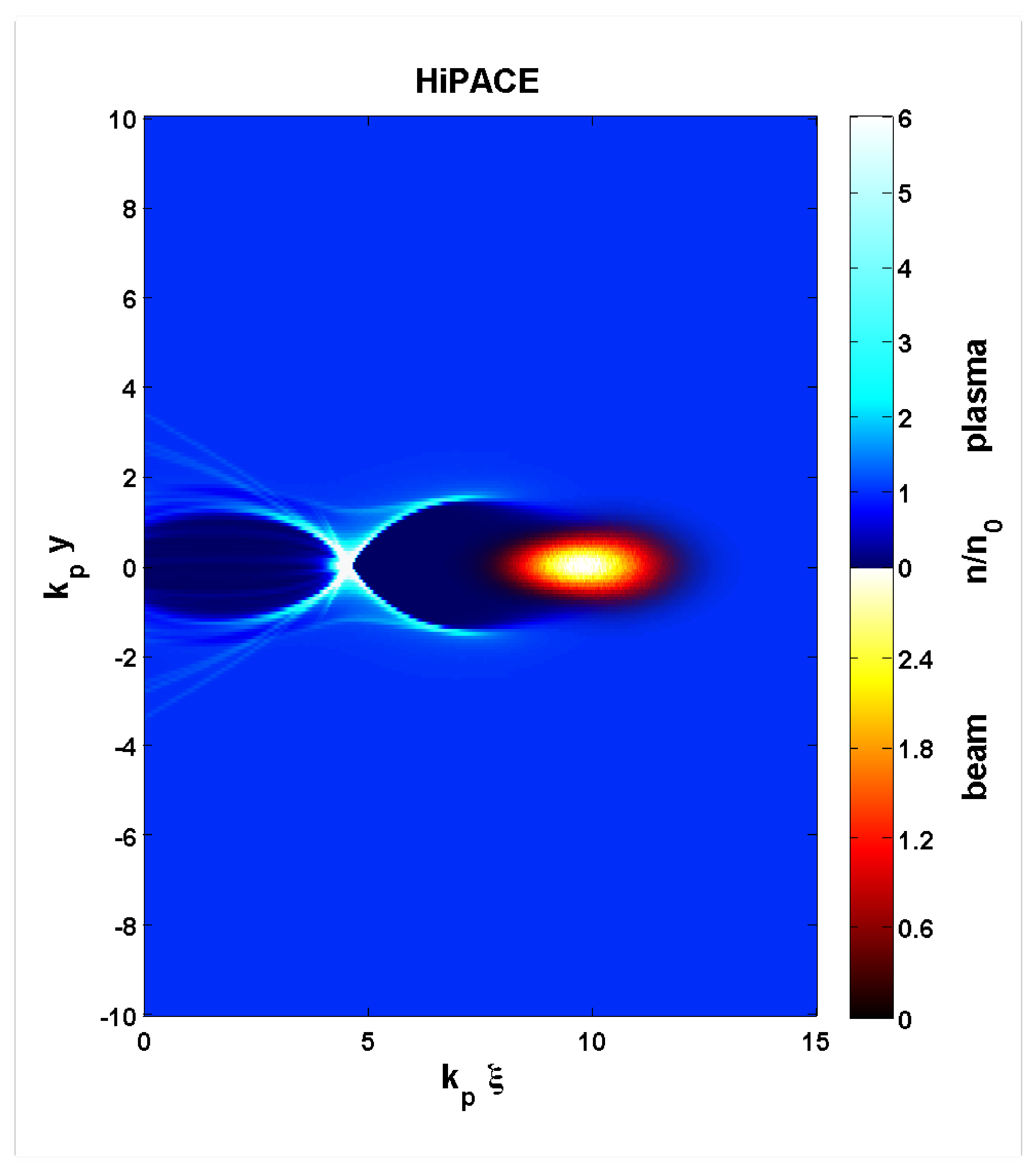
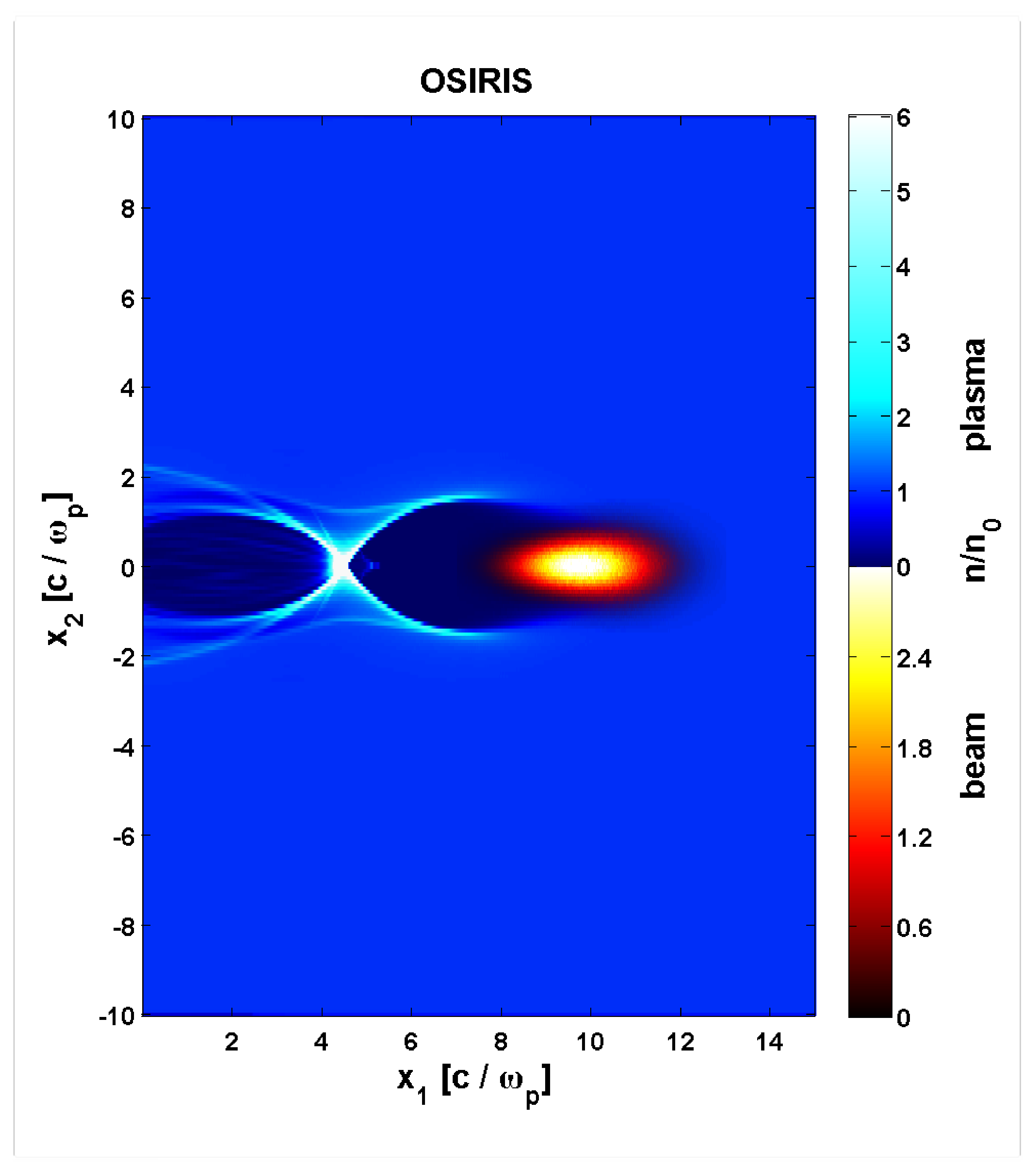


Comparison between the full PIC code OSIRIS and HiPACE: 1 GeV gaussian electron beam, nb/n0 = 2.0





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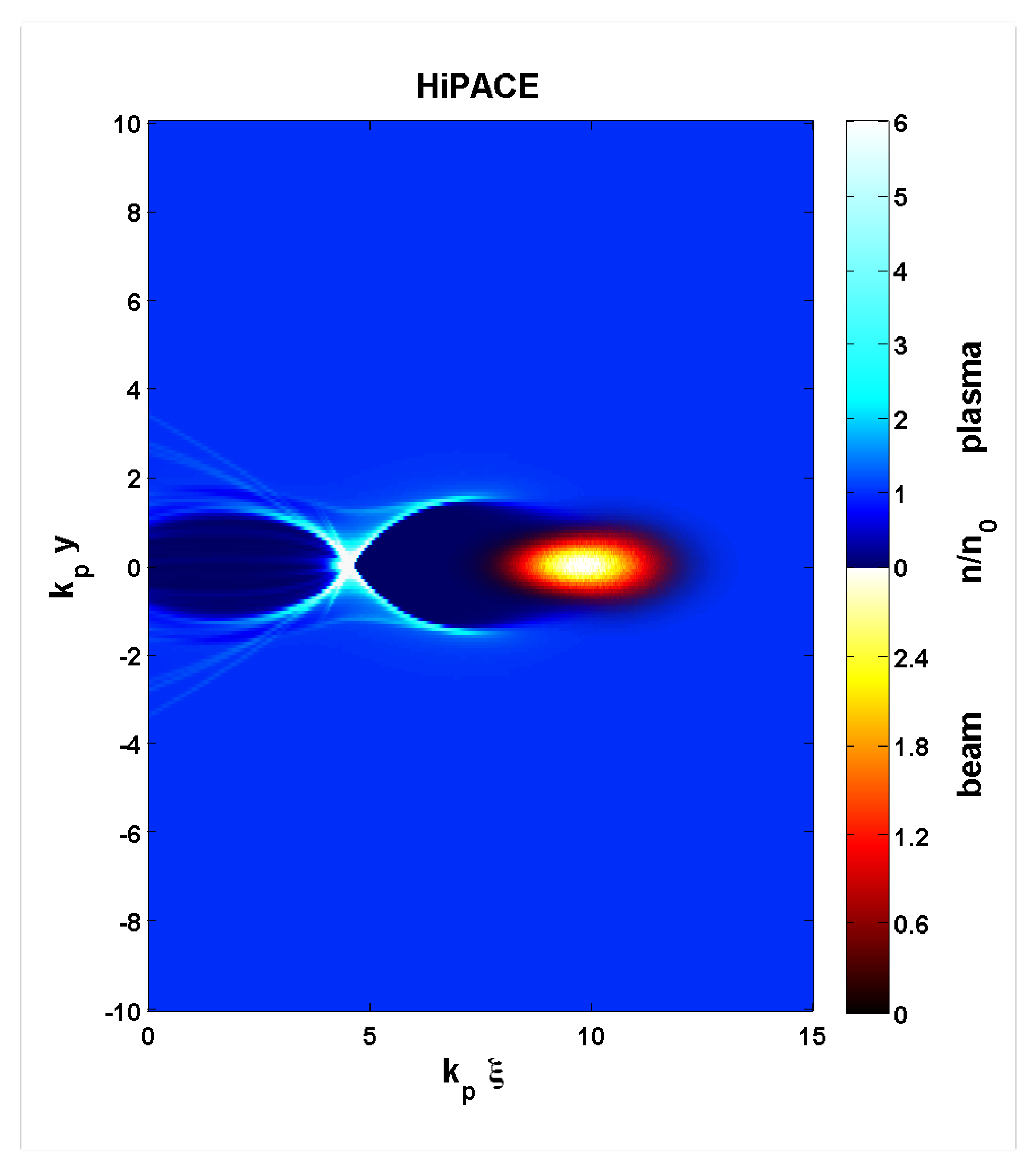
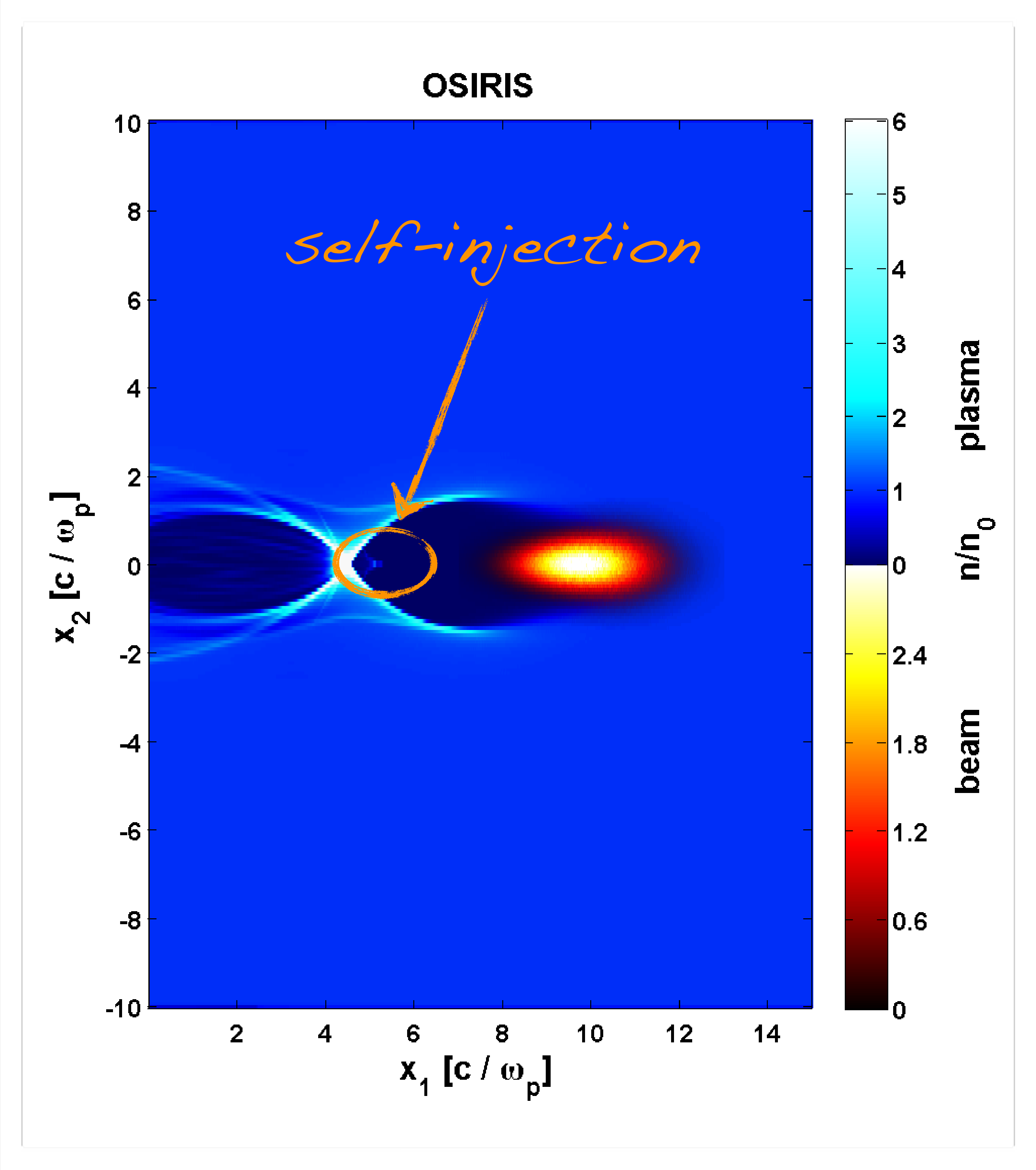
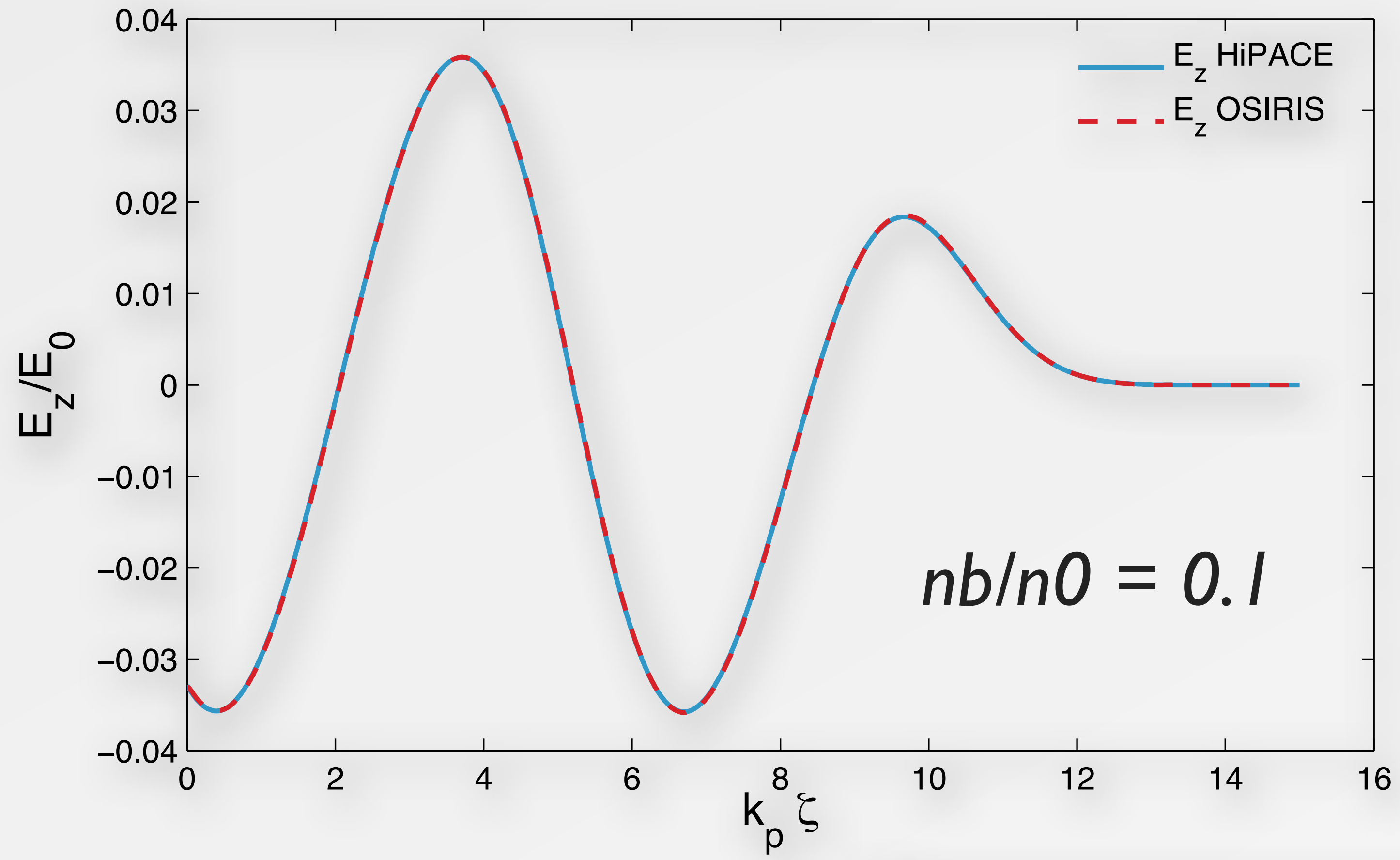
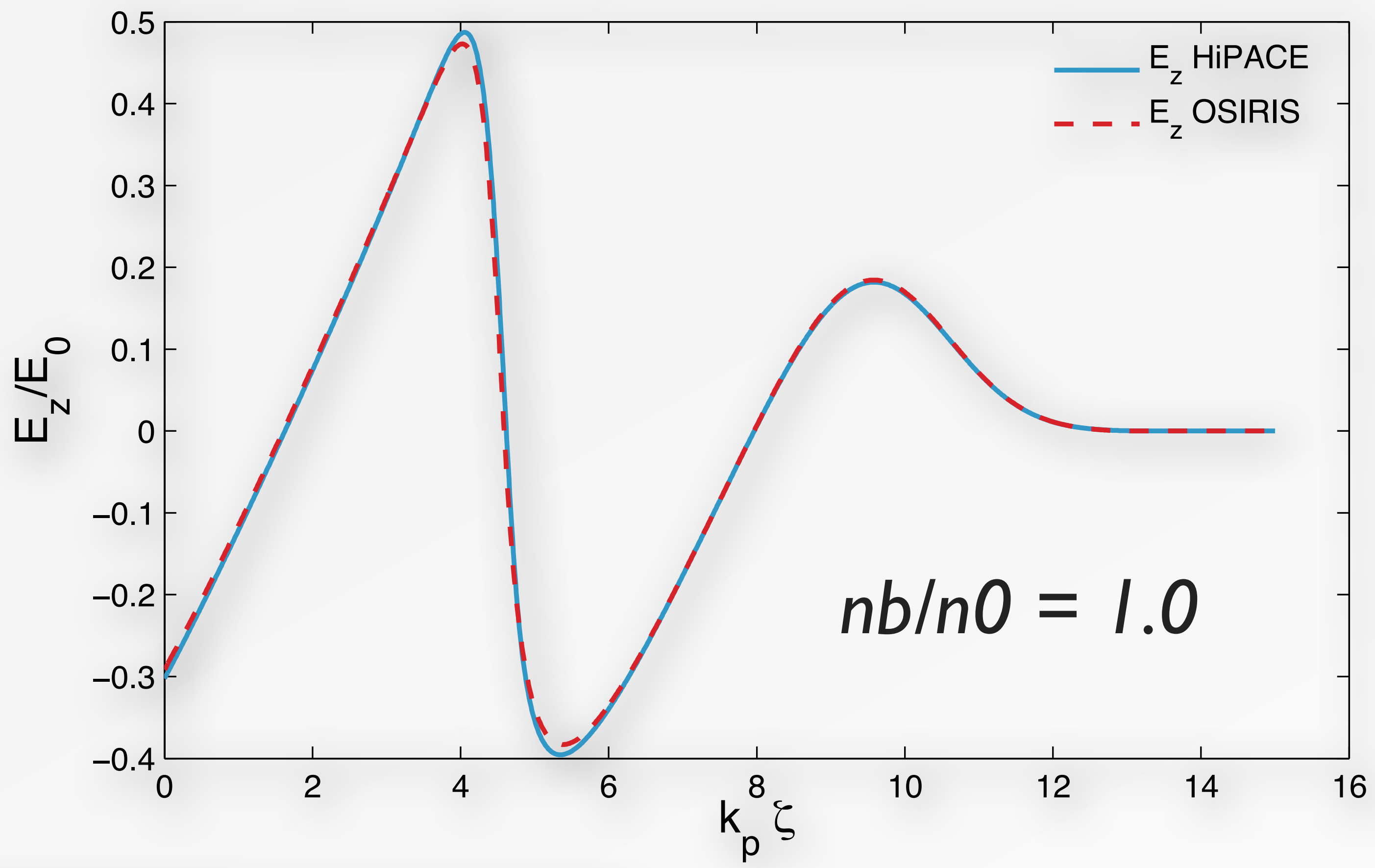
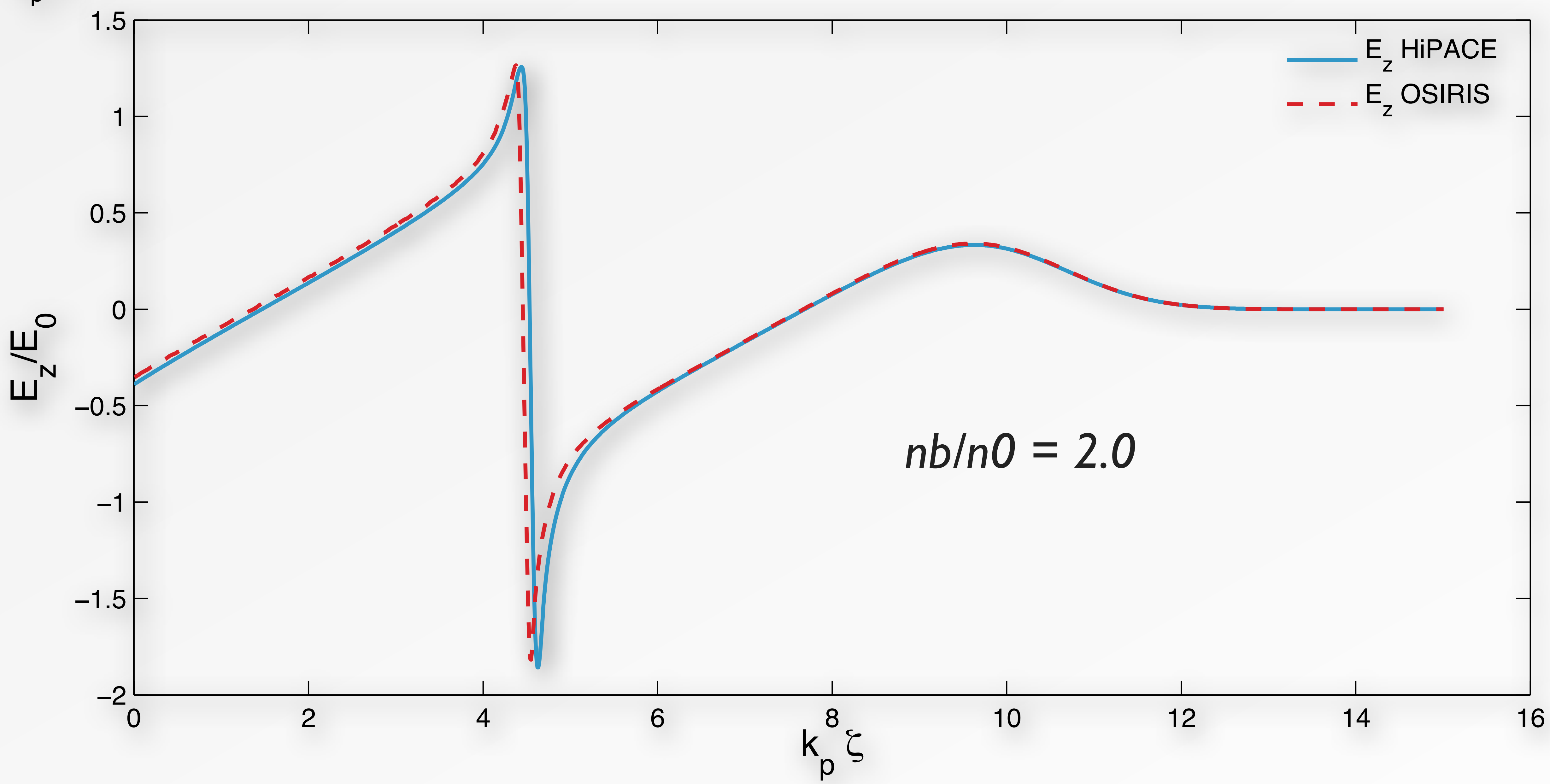




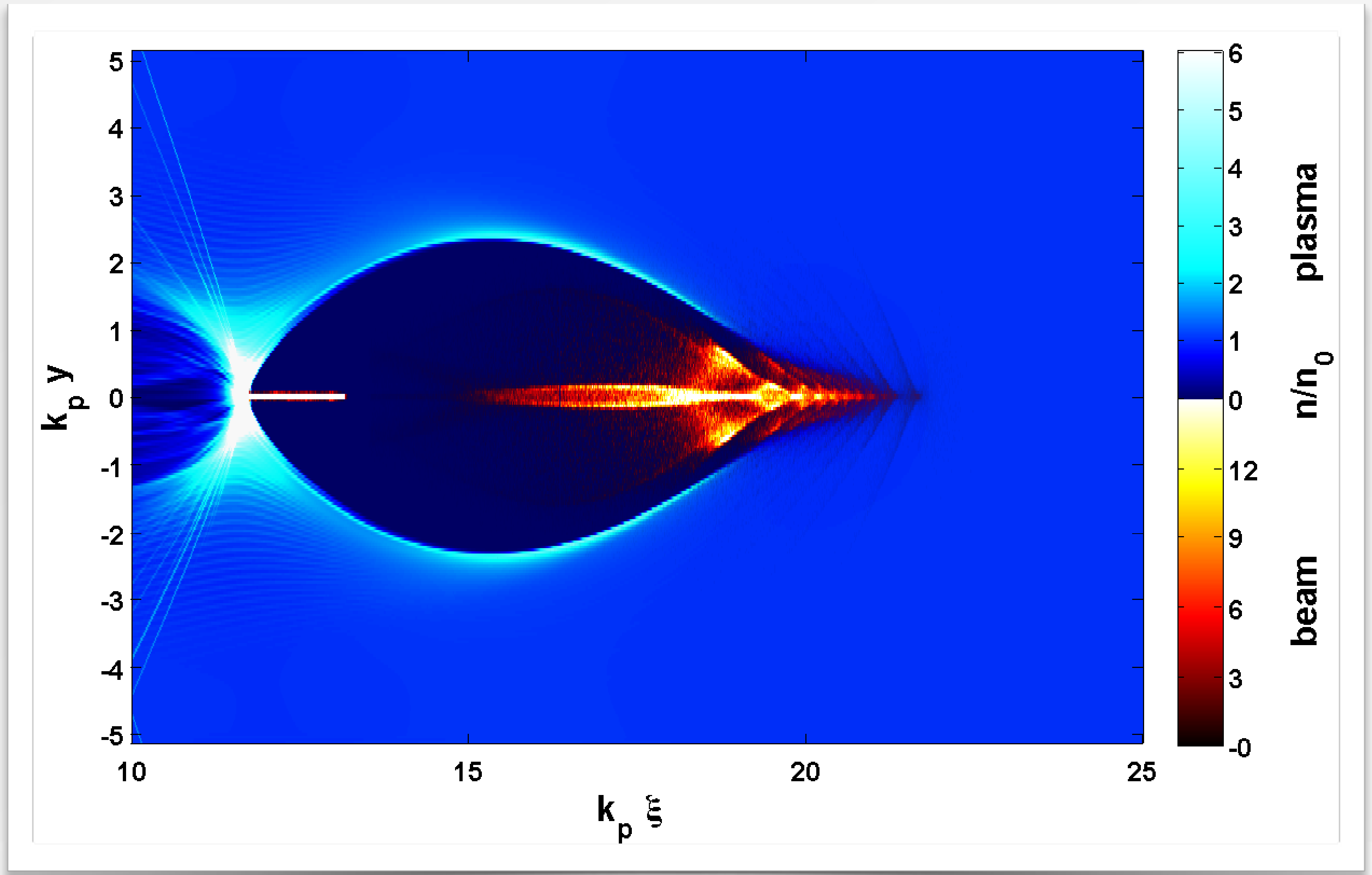
Comparison of long. field: HiPACE and OSIRIS







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

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- Code is currently improved in speed, functionality and stability
  - Implementation of plasma fluid routine

Summary and Outlook

Thanks for listening!