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Mesh refinement in QuickPIC

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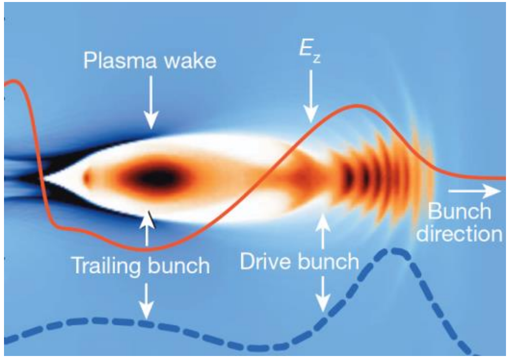
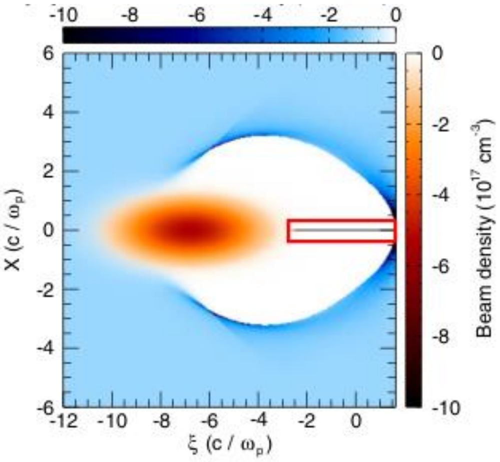
PWFA simulation for linear collider simulations is computationally expensive both in time and memory

- Plasma wakefield acceleration (PWFA) has made great progress with the help of particle-in-cell (PIC) simulation
- Standard electromagnetic code can be computationally expensive
- QuickPIC is an efficient quasi-static PIC code that can provide more than hundreds times of speed up compared to standard PIC codes for accurate PWFA simulation





- **PWFA-LC parameter for trailing bunch**
  - Normalized emittance in x, y direction ~ 2um, 0.005um
  - Matched spot size ~ 463.9 nm, 23.2 nm (Bubble radius ~ tens of μm **)**
- **Challenges**
  - Scales difference of bubble radius and trailing beam
  - Tightly focused trailing beam ($k_p\sigma_r \sim 10^{-3}$) causes ion motion
  - To fully resolve the trailing beam and ion motion, full QuickPIC need to set more than $10 \times 10^4 \times 10^4 \times 10^3$ 3D grids (tens of TB), takes more than 1,000,000,000 cpu hours
- **Speed-up method**
  - Mesh refinement (HiPACE ++, QuickPIC, QPAD)
  - Quasi-3d method (QPAD)
  - GPU (HiPACE++, QuickPIC/QPAD)

T. J. Mehrling, et. al. *IEEE AAC*, 2018

F. Li, et. al. Computer Physics Communications, 261:107784, 2021

S.Diederichs, et. al. Computer Physics Communications, 278: 108421, 2022

W. An, et. al., Physical Review Letters, 118:244801, 2017,

3D quasi-static PIC code QuickPIC

Quasi-static approximation (QSA)

Cartesian coordinates $(x, y, z; t)$

Co-moving coordinates

$(x, y, \xi = ct - z; s = z)$

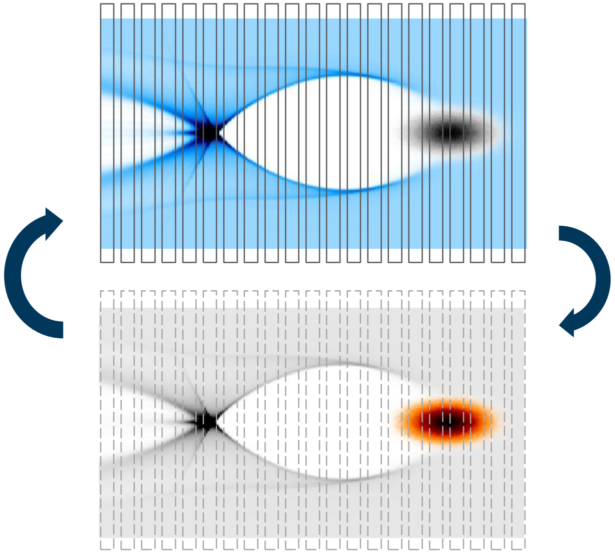
$\partial_s \ll \partial_\xi$

Plasma: $(x, y; \xi)$

Beam: $(x, y, \xi; s)$

Benefiting from QSA, the simulation time step is not limited by the numerical stability condition (CFL), which can achieve many orders of magnitude speedup compared to full explicit 3D PIC codes.

Quasi-static loop: beam is frozen while plasma and field is evolved



3D loop: field and plasma particles are frozen while beam is advanced.

C. Huang et. al. Journal of Computational Physics, 217(2):658–679, 2006,
W. An, et. al. Journal of Computational Physics, 250:165–177, 2013.

Mesh refinement algorithmic flow in QuickPIC

ξ loop

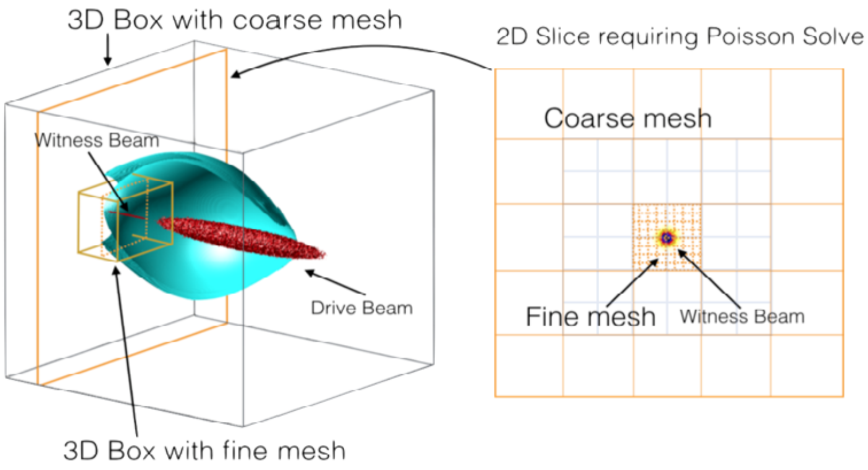
s loop

Solve 2D slice Poisson like equations and push plasma particles

Push beam particles

Deposit beam particles

Deposit plasma charge and current density, operations of density



All the operations done for both fine mesh and coarse mesh

$$\nabla_\perp^2 \phi_l = q_l, \nabla_\perp^2 \phi_l - \phi_l = q_l$$

where q_l is the source at grid l

Interpolate field on coarse grid ϕ_l onto the boundary of ϕ_{l+1}

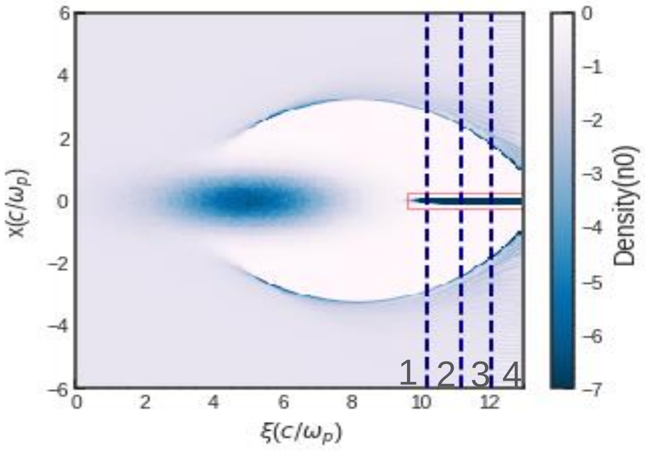
Use FFT solver to solve ϕ_1, multigrid algorithm to solve $\phi_{l>1}$

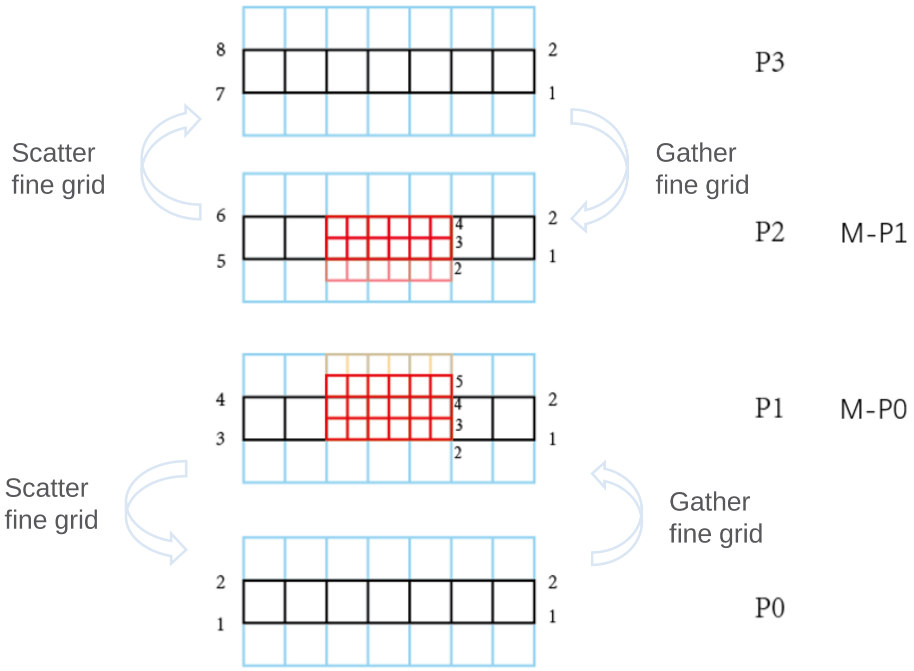
Option to correct coarse grid solution by iteration between meshes

Option to use square cells and rectangular box for refined mesh

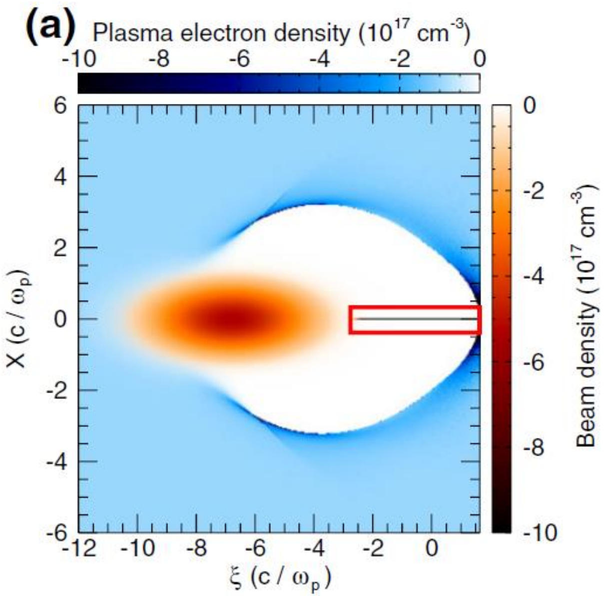
Load balance is important so that solving fine-mesh field does not dominate simulation

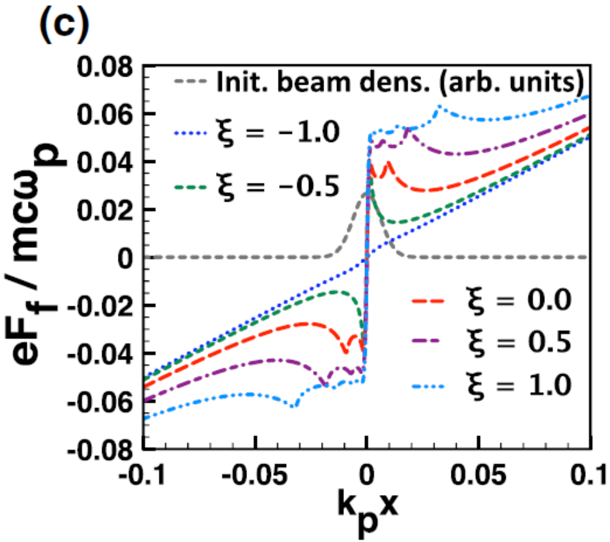
- **Fast fine mesh solver**
  - Parallelized with MPI + OpenMP
  - Scatter fine grid to other mpi ranks
- **Load balanced pipelining parallelization**





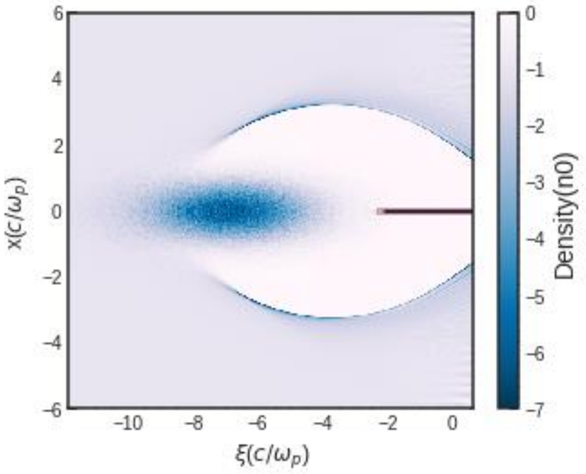
Focusing force and emittance growth from ion motion was modeled by isolating small region with fine resolution



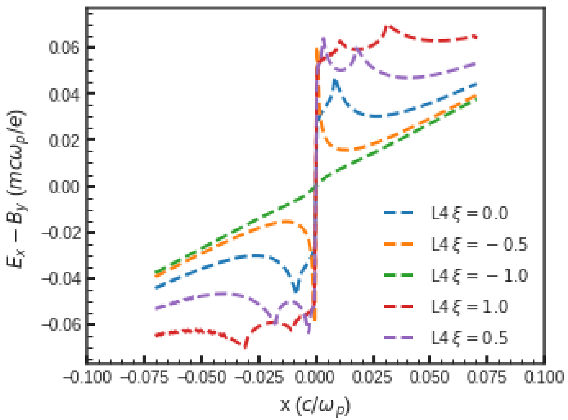


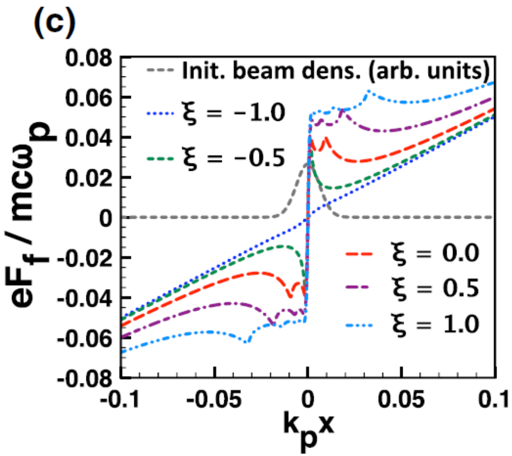
1 step simulation with 8192 × 8192 × 1024 grids
Trailing-beam-only simulation with smaller domain (red box) and higher resolution of 6.1 × 6.1 × 115.23 nm.

Fully self-consistent mesh refinement simulation shows good agreement for the focusing force



Mesh refinement





W. An, et. al., Physical Review Letters, 118:244801, 2017

Trailing beam parameter $k_p\sigma_r = 0.00595$, $k_p\sigma_z = 0.595$

3 refinement levels, each increase 4x resolution
Coarse grid has 1024 × 1024 × 1024 grids

The finest grid has resolution of 6.1 × 6.1 × 115.23 nm

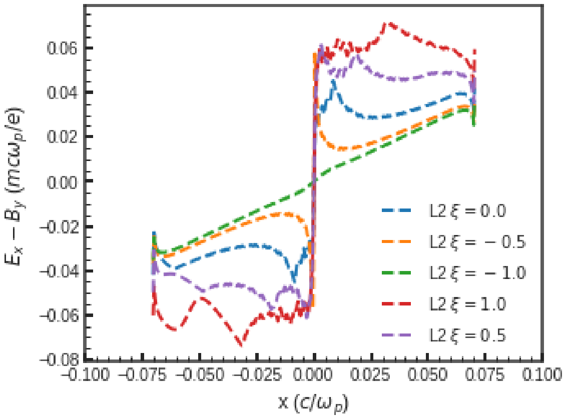
Need multiple refinement levels for accurate fields at the boundaries

$$\nabla_\perp^2 \psi = -(\rho - J_z)$$

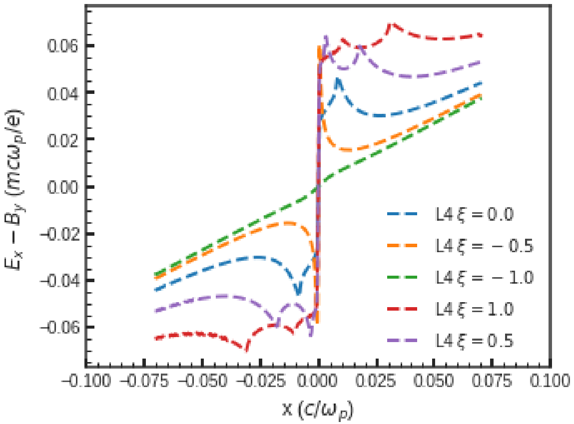
The error induced when calculating focusing force by $\boldsymbol{E}_\perp + e_z \times \boldsymbol{B}_\perp = -\nabla_\perp \psi$

Match the Dirichlet boundary from linear interpolation, but derivative not continuous between different levels

1 refinement level
64x higher resolution

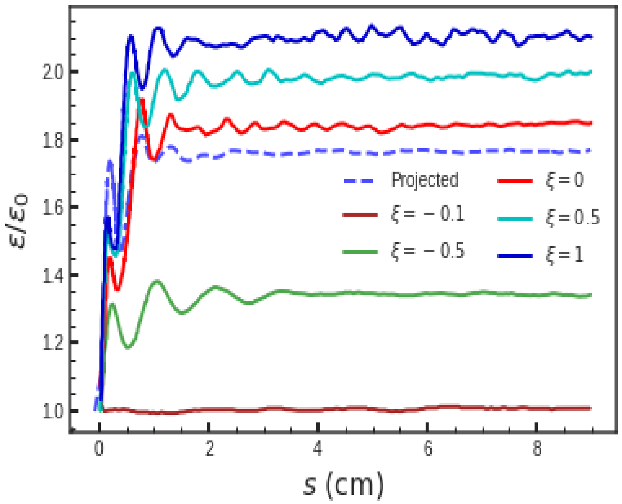


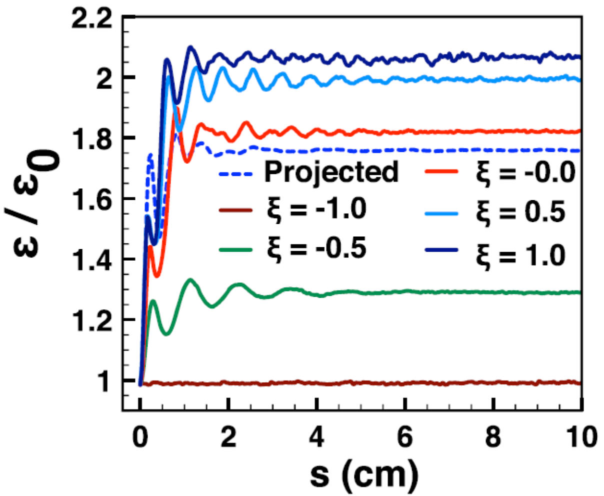
3 refinement levels
each 4x higher resolution



Long range acceleration with mesh refinement shows agreement with previous results

Mesh refinement





W. An, et. al., Physical Review Letters, 118:244801, 2017

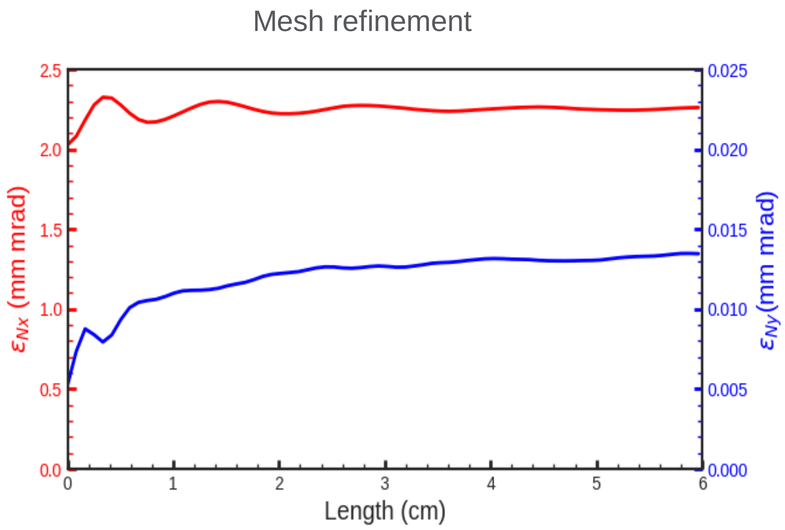
18.8 cpu hour (on cori 4 nodes) per 3D step with highest resolution 6.1 × 6.1 × 115.23 nm

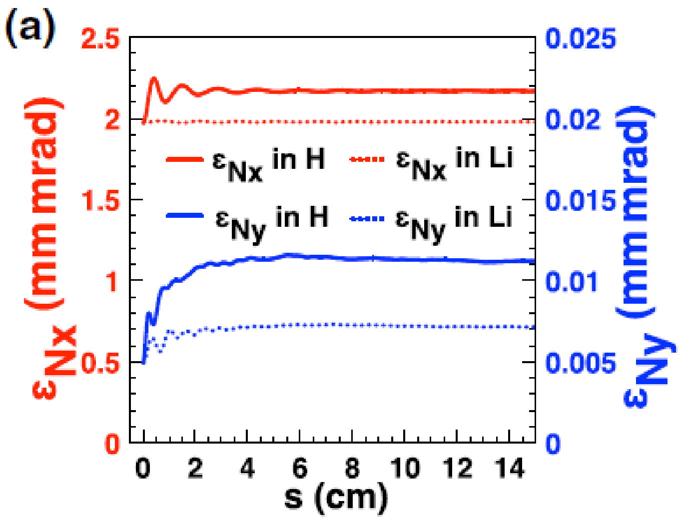
56.5 cpu hour (on cori 4 nodes) per 3D step with (6.1 × 32) × (6.1 ×32) × 115.23 nm resolution for the whole simulation box

Estimation of roughly a thousand times speed-up compared to full QuickPIC with fine resolution everywhere

Can be run on 4 cori nodes or less with 512 GB memory

Mesh refinement also works for asymmetric beam with rectangular fine region

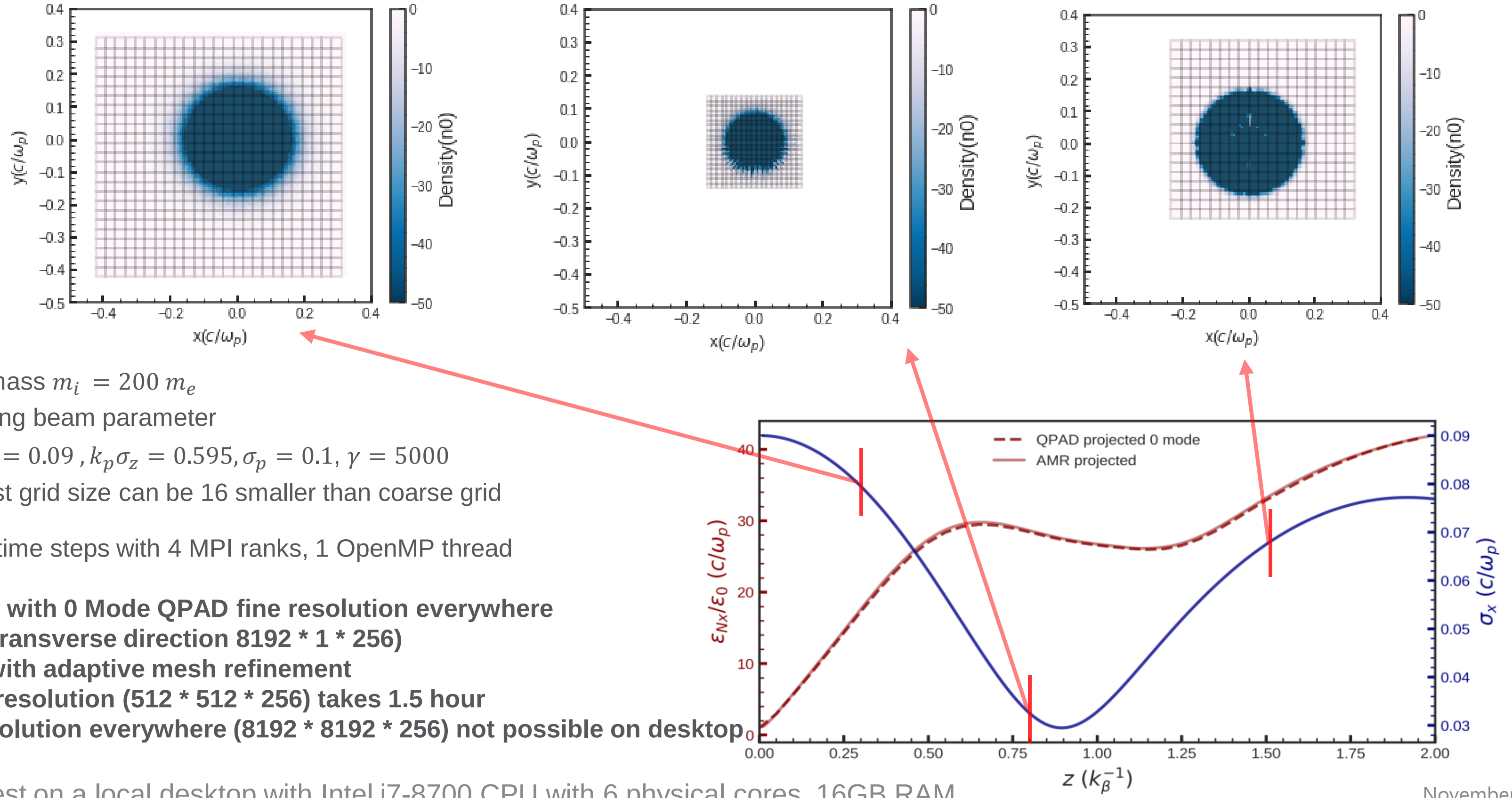




Matched trailing beam parameter $k_p\sigma_x = 0.0273, k_p\sigma_y = 0.0014,\ k_p\sigma_z = 0.595$

Weiming An et al., Phys. Rev. Lett. 2017,

Adaptive mesh grid setting for evolving beams



Ion mass $m_i = 200\, m_e$

Trailing beam parameter

$k_p\sigma_r = 0.09\,, k_p\sigma_z = 0.595, \sigma_p = 0.1,\ \gamma = 5000$

Finest grid size can be 16 smaller than coarse grid

For 200 time steps with 4 MPI ranks, 1 OpenMP thread

1.5 hour with 0 Mode QPAD fine resolution everywhere
(1 d in transverse direction 8192 * 1 * 256)
4 hour with adaptive mesh refinement
Coarse resolution (512 * 512 * 256) takes 1.5 hour
Fine resolution everywhere (8192 * 8192 * 256) not possible on desktop

Both test on a local desktop with Intel i7-8700 CPU with 6 physical cores, 16GB RAM

Summary

- **We have developed a MPI + OpenMP parallelized mesh refinement code based on QuickPIC, it enables simulations using witness beams with spot sizes several orders of magnitude small than the accelerator structure.**

- **The scalability of the code has been improved by using pipelining, several strategies has been used to improve the load balancing of both field solver and pipelines.**

- **We also developed an adaptive mesh refinement option for an evolving beam.**

- **Several benchmark cases have been tested and get consistent result as previously published papers and a Quasi-3d QS PIC code QPAD.**

- **Future work on QuickPIC and QPAD**
  - Adaptive 2d step
  - Improve load balance of AMR and particle routines
  - GPU support
  - Mesh refinement in quasi-3d code

Thanks for your attention!