Recent development on the quasi-static PIC codes QuickPIC and QPAD

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ICAP'24

QuickPIC/QPAD Collaboration

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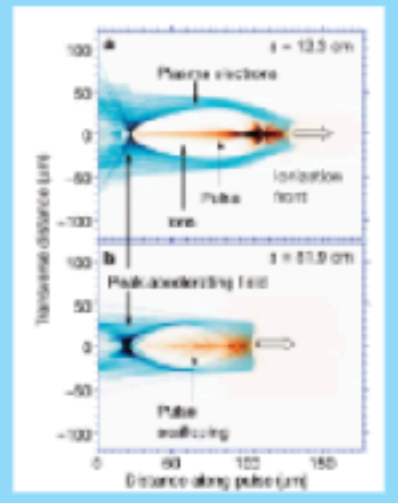
- Qianqian Su, Viktor Decyk, Lance Hildebrand, Yujian Zhao, Thamine Dalichaouch, Warren Mori
- Fei Li

A Brief History of QuickPIC

FACET & FACET II

M. Litos et. al.
Nature 2014

- QuickPIC
- 2006
  - Ionization
  - Laser
- 2013
  - Faster Algorithm
  - Ionization
- 2017
  - Open Source on Github
  - Object-Oriented
  - MPI+OpenMP Hybrid
- 2019
  - QPAD
- 2023
  - Laser in QPAD and Open Source
  - Particle Ionization
  - MPI+GPU
  - Betatron Radiation
  - Mesh Refinement



I. Blumenfeld et. al.,
Nature 445 741 (2007)

FFTB

AWAKE

CEPC

Plasma simulation has greatly impacted on PBA research.

The Quasi-Static PIC code

Embeds a 2D PIC code inside a 3D PIC code

Quasi-Static Approximation*

$(x, y, z; t)$

↓

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

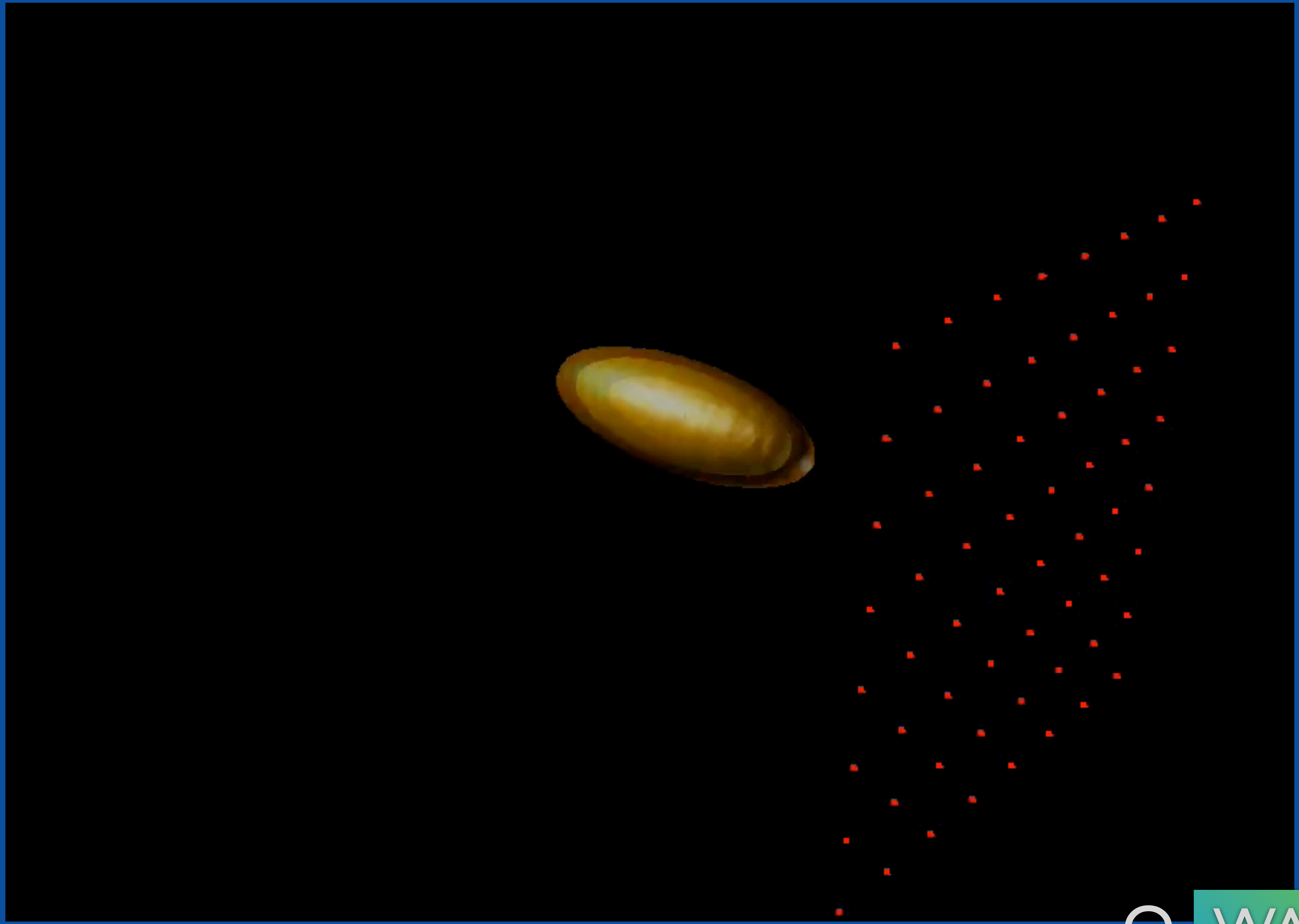
↓

$\partial_s << \partial_\xi$

↓

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

Beam: (x, y, ξ, s)



QuickPIC is a 3D parallel Quasi-Static PIC code, which is developed based on the framework UPIC.

https://gitee.com/bnu-plasma-astrophysics-sg/quick-pic-open-source

W. An et. al., JCP 250, 165 (2013)

Q S A

WAKE LCODE HIPACE

QPAD*: QuickPIC with Azimuthal Fourier Decomposition

- Azimuthal decomposition is a technique to speed up the simulation without much loss of accuracy. Some explicit PIC codes (e.g. Calder, quasi-3D OSIRIS, FBPIC, PLARES-PIC) have employed this algorithm to achieve 100x ~ 1000x speed-up.

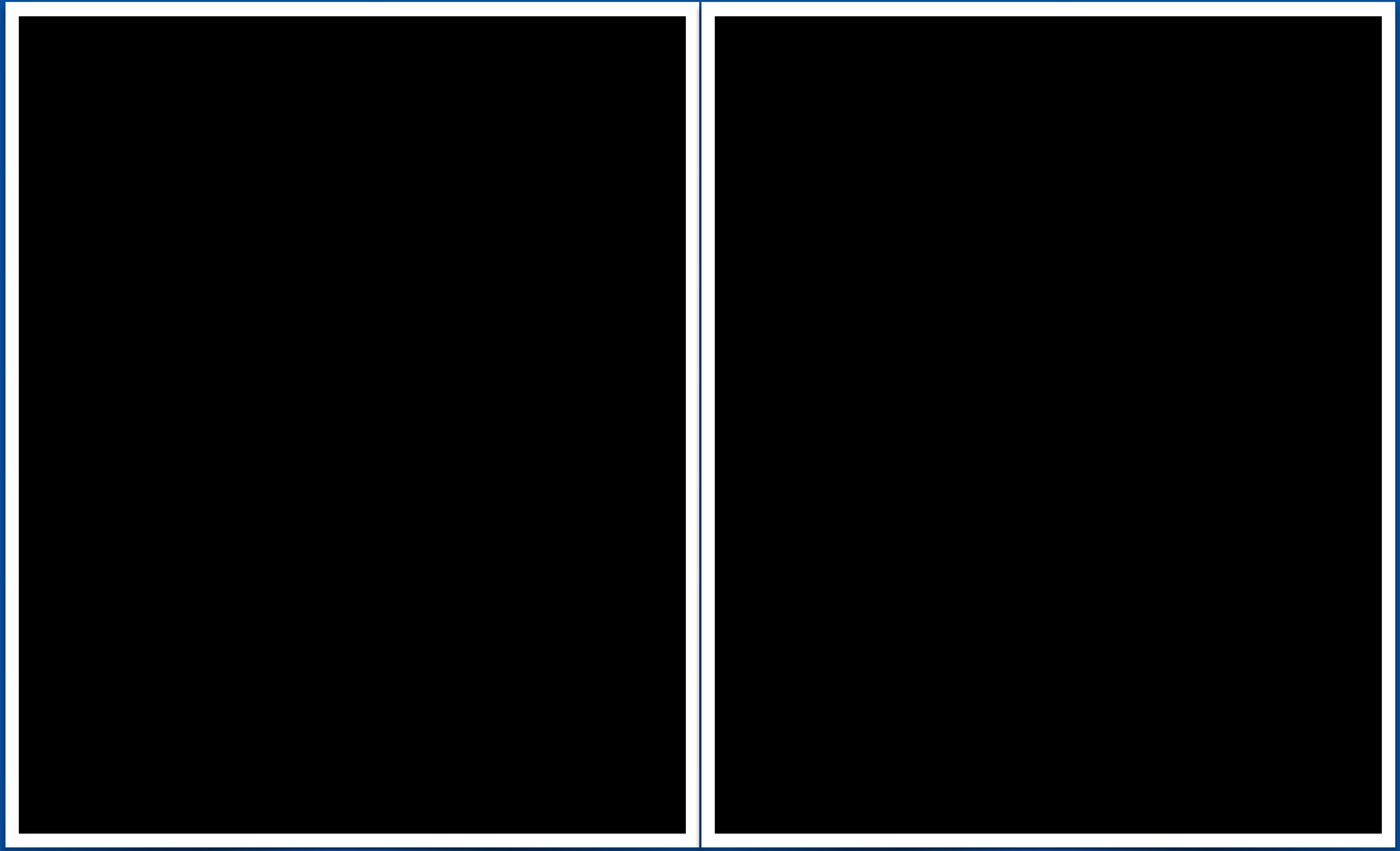
- None of current quasi-static PIC codes has this feature.

- QPAD is a newly developed code based on part of the frame work of open source QuickPIC.

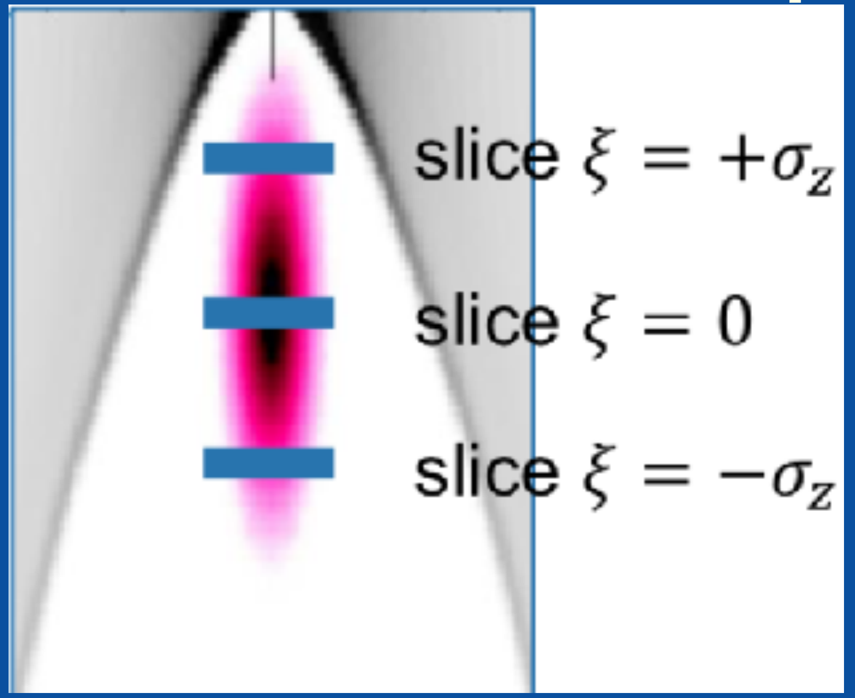
Fei Li, Weiming An*, Viktor K. Decyk, Xinlu Xu, Mark J. Hogan, Warren B. Mori, et. al., "A quasi-static particle-in-cell algorithm based on an azimuthal Fourier decomposition for highly efficient simulations of plasma-based acceleration: QPAD", Computer Physics Communications 261, 107784 (2021).

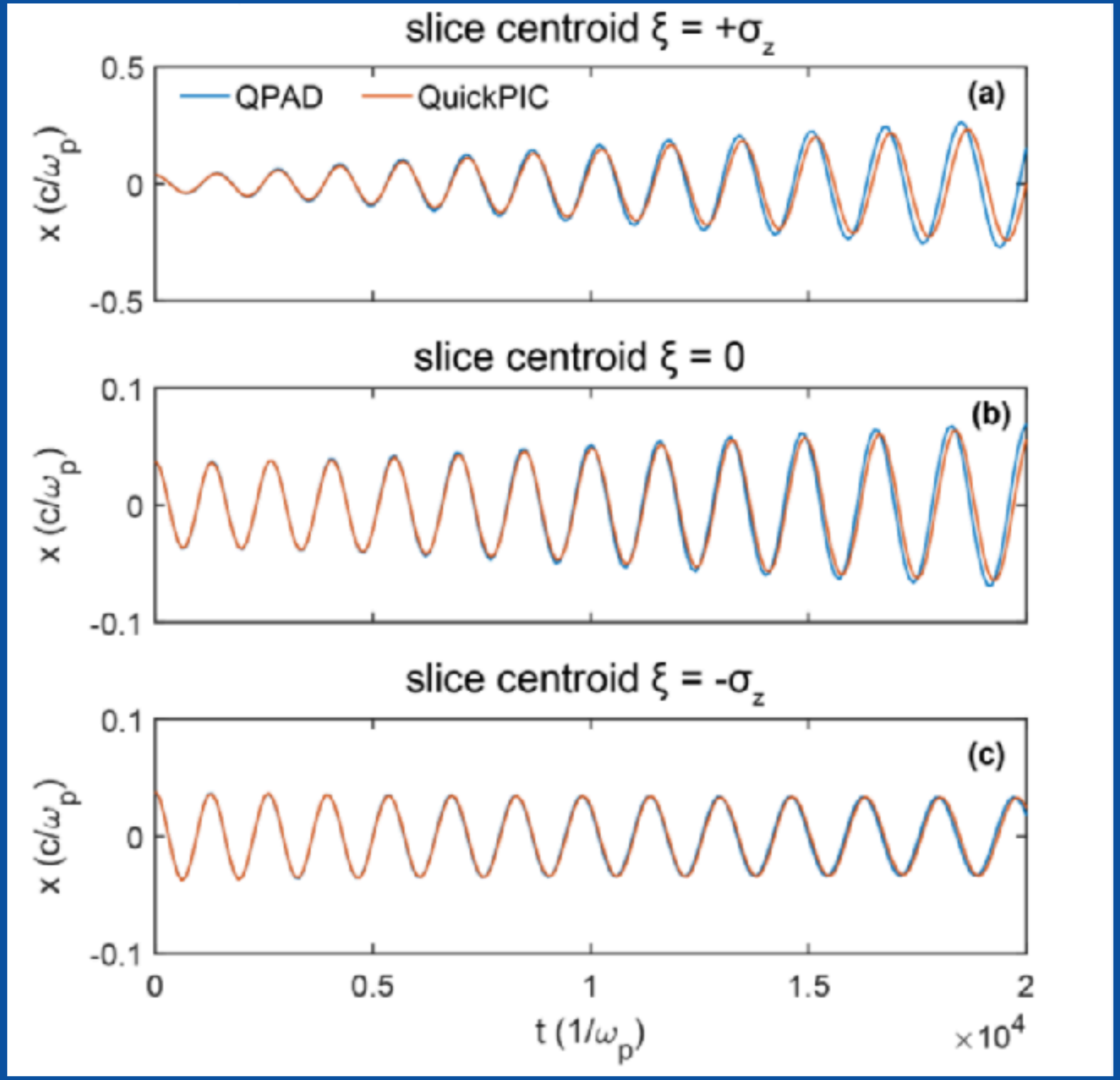
QPAD*: QuickPIC with Azimuthal Fourier Decomposition

QuickPIC　　　QPAD(4 modes)



drive beam: $k_p\sigma_r = 0.14, k_p\sigma_z = 0.48, \Lambda = 1.8, \gamma = 20000$
trailing beam: $k_p\sigma_r = 0.14, k_p\sigma_z = 0.24, \Lambda = 1.1\ \gamma = 20000, k_p\Delta_{\text{off}} = 0.0375$





Laser Module in QuickPIC

*Weiyu Meng et. al., in preparation.

Laser envelope equation：

$$2\frac{\partial}{\partial s}\left(-ik_0+\frac{\partial}{\partial\xi}\right)\hat{\mathbf{a}} - \nabla_\perp^2\hat{\mathbf{a}} = \chi\hat{\mathbf{a}}$$

Finite difference：

$$\left[-ik_0-\frac{1}{4}\Delta_s\left(\nabla_\perp^2+\chi^n\right)\right]a^{n+\frac{1}{2}}+\frac{\partial a^{n+\frac{1}{2}}}{\partial\xi}=\left[-ik_0+\frac{1}{4}\Delta_s\left(\nabla_\perp^2+\chi^n\right)\right]a^{n-\frac{1}{2}}+\frac{\partial a^{n-\frac{1}{2}}}{\partial\xi}.$$

$$\left(-\frac{1}{4}\Delta_s\nabla_\perp^2+\frac{3}{2\Delta_\xi}-\frac{1}{4}\Delta_s\chi_j\right)a_{\mathrm{R},j}+k_0a_{\mathrm{I},j}=\frac{1}{2\Delta_\xi}\left(4a_{\mathrm{R},j-1}-a_{\mathrm{R},j-2}\right)+S_{\mathrm{R},j},$$

$$\left(-\frac{1}{4}\Delta_s\nabla_\perp^2+\frac{3}{2\Delta_\xi}-\frac{1}{4}\Delta_s\chi_j\right)a_{\mathrm{I},j}-k_0a_{\mathrm{R},j}=\frac{1}{2\Delta_\xi}\left(4a_{\mathrm{I},j-1}-a_{\mathrm{I},j-2}\right)+S_{\mathrm{I},j}$$

where：

$$S_{\mathrm{R},j}=\frac{1}{4}\Delta_s\left(\nabla_\perp^2a_{\mathrm{R},j}+\chi_ja_{\mathrm{R},j}\right)+k_0a_{\mathrm{I},j}+D_\xi a_{\mathrm{R},j}$$

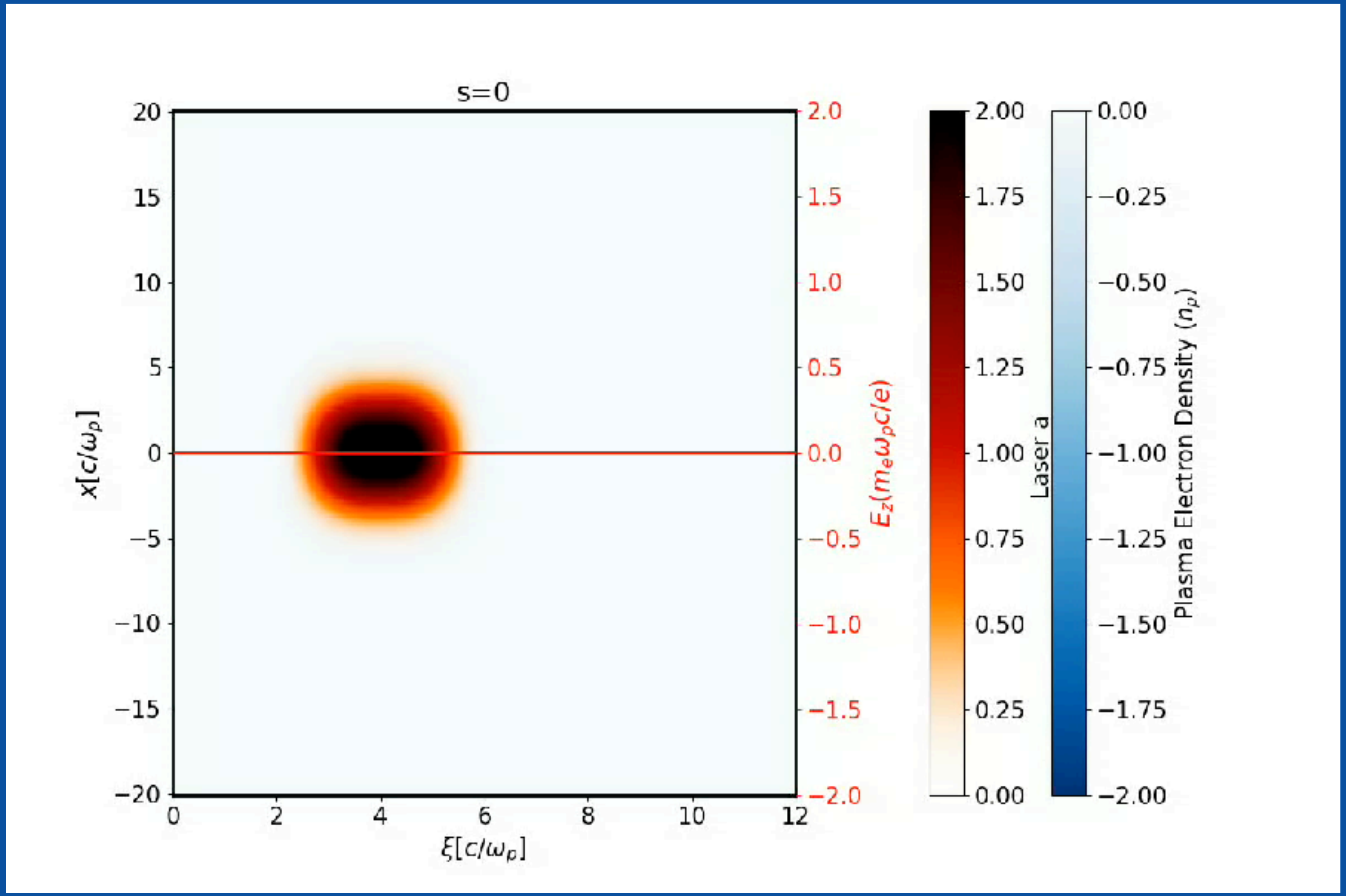
$$S_{\mathrm{I},j}=\frac{1}{4}\Delta_s\left(\nabla_\perp^2a_{\mathrm{I},j}+\chi_ja_{\mathrm{I},j}\right)-k_0a_{\mathrm{R},j}+D_\xi a_{\mathrm{I},j},$$

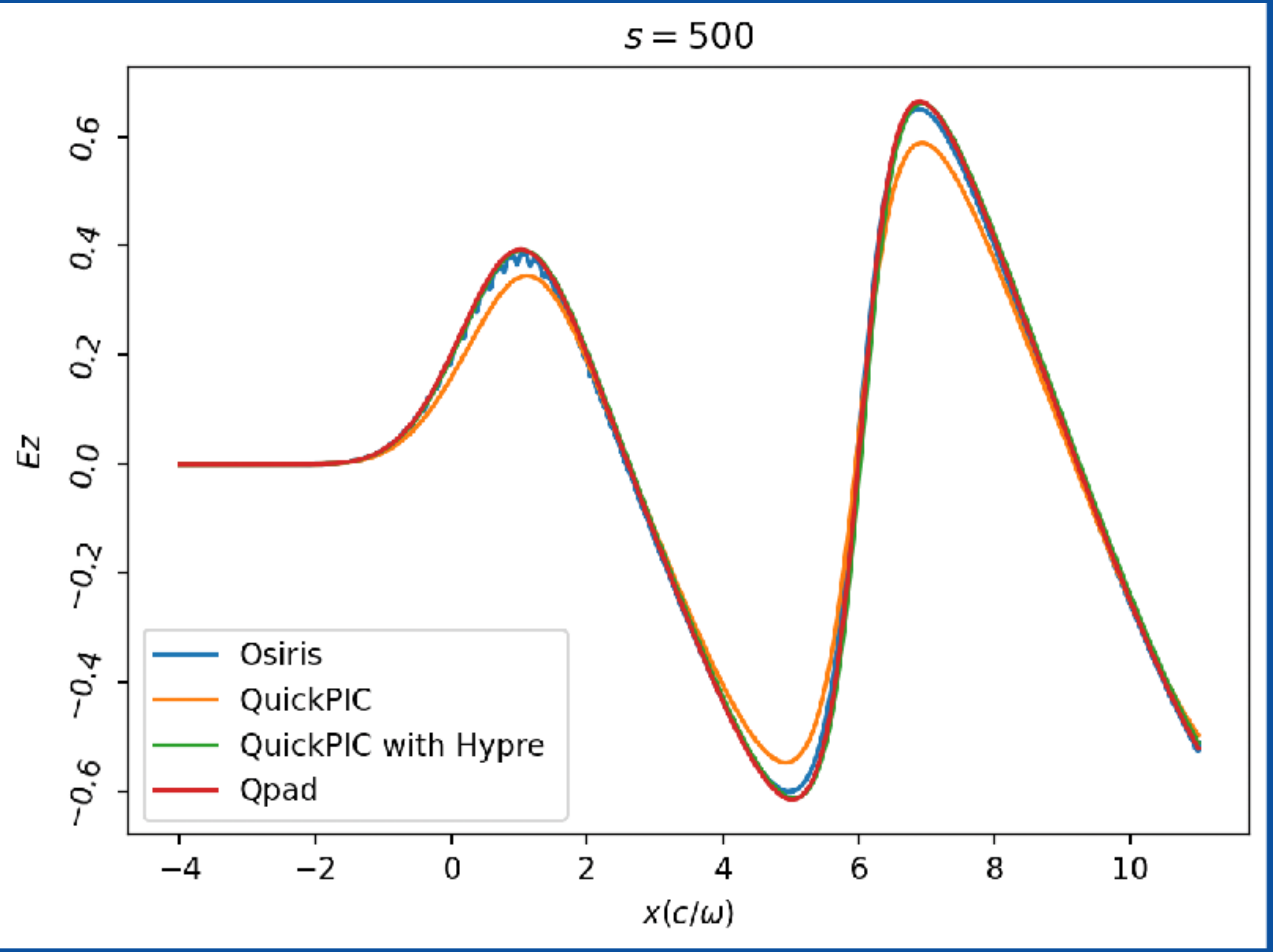
can be solved with Hypre*

*Falgout R D, Jones J E, Yang U M. Springer Berlin Heidelberg, 2006: 267-294.

Laser Module in QuickPIC

*Weiyu Meng et. al., in preparation.

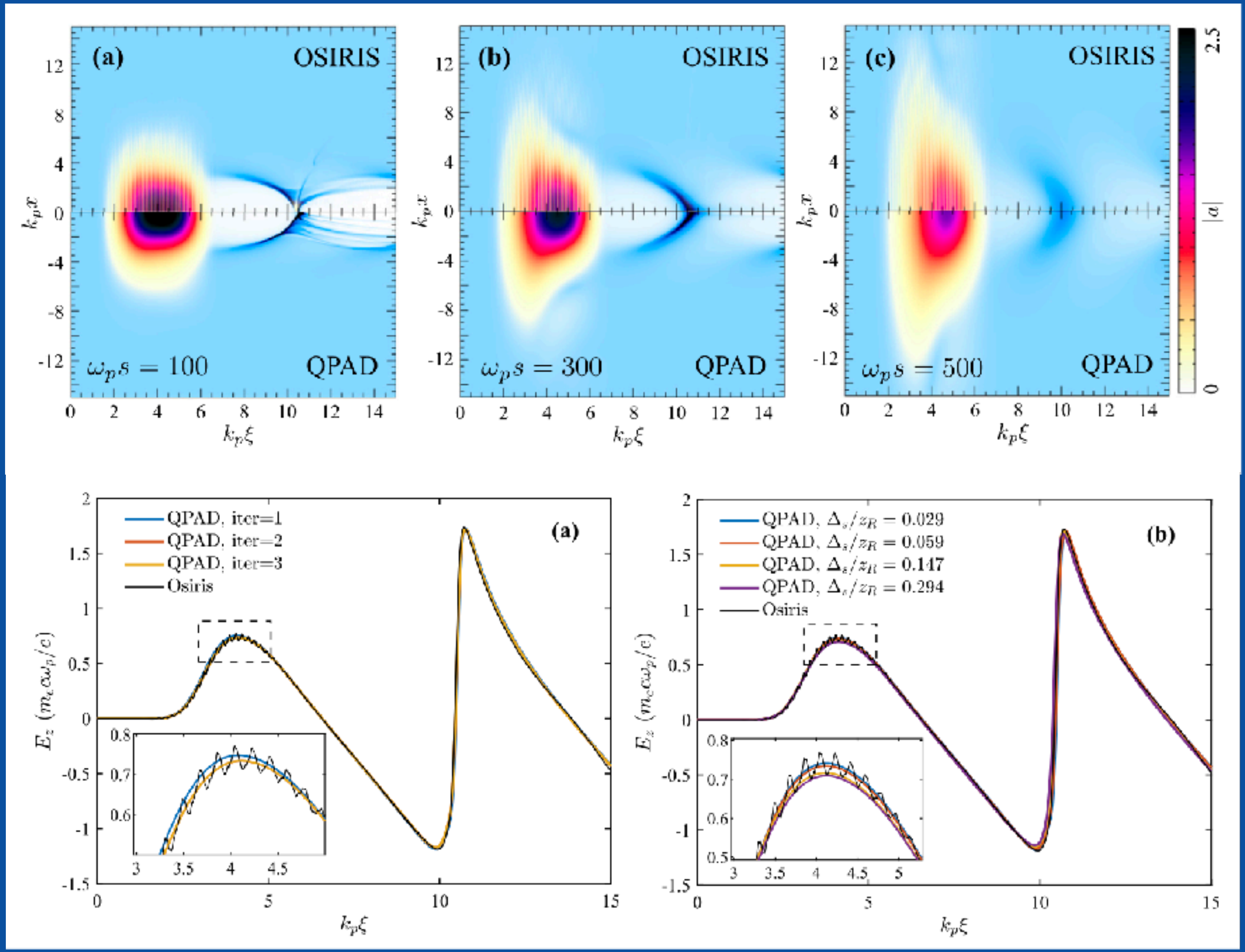


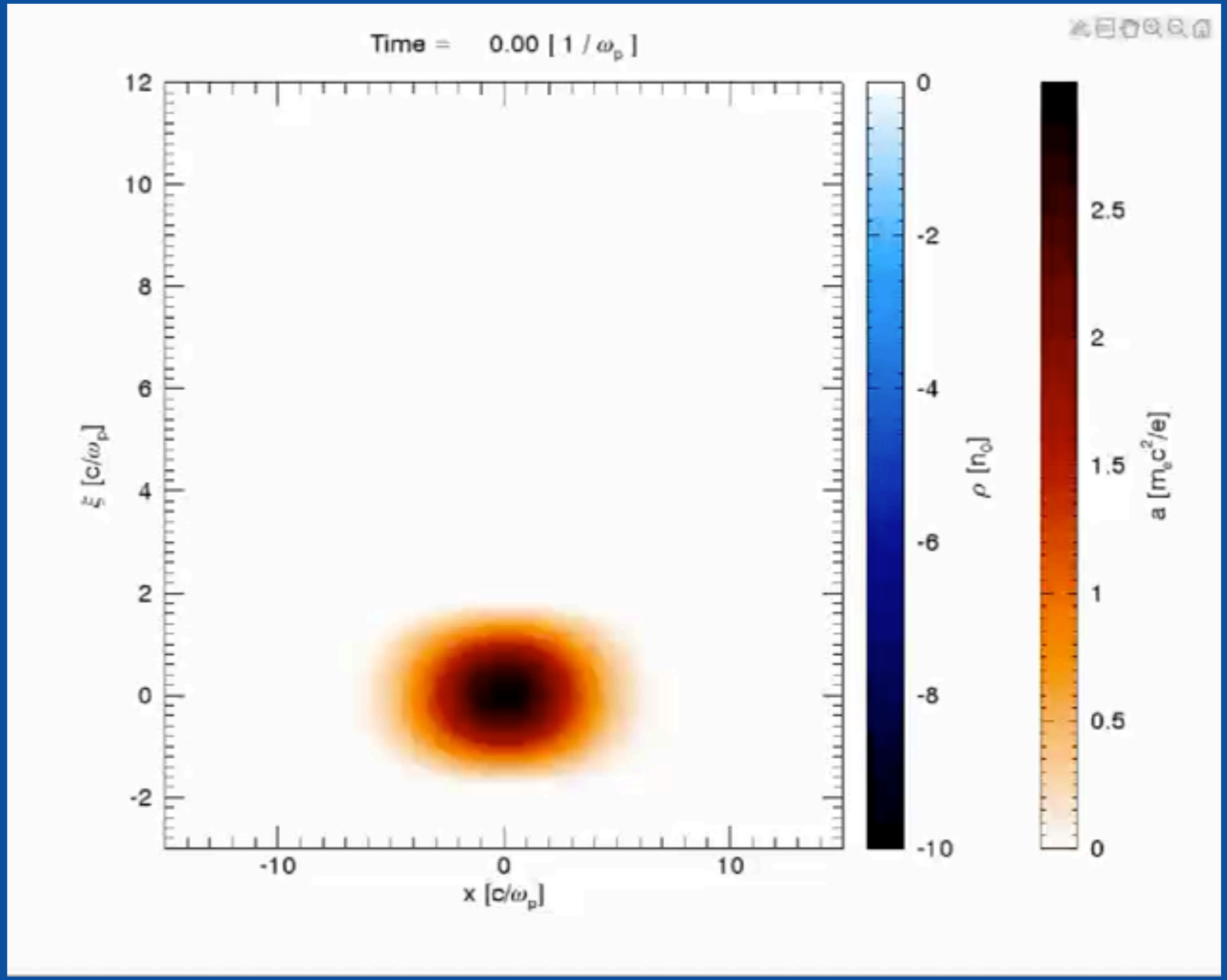


QuickPIC vs Osiris vs Qpad

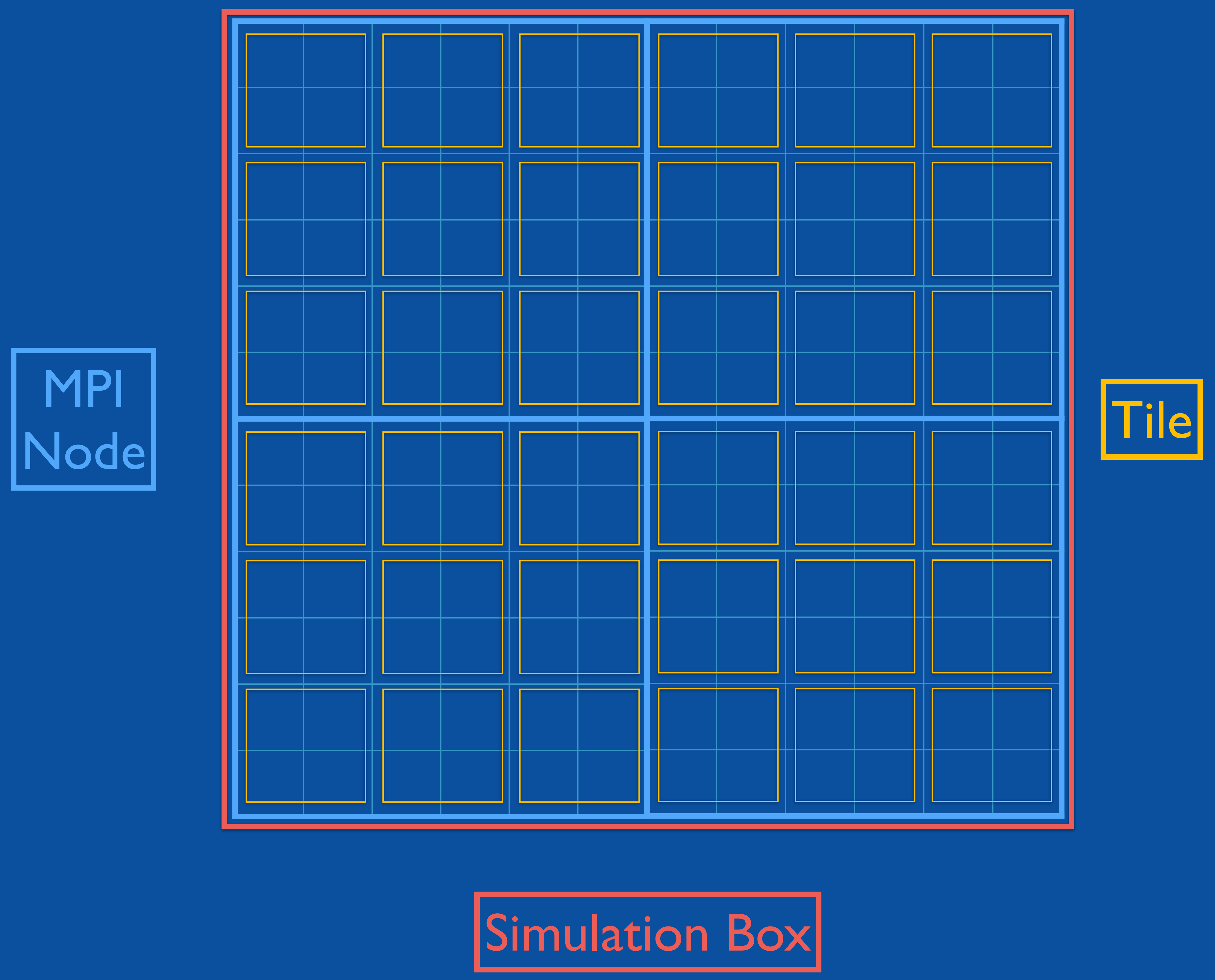
Laser Module in QPAD

*Fei Li, Weiming An, Frank S. Tsung, Viktor K. Decyk, Warren B. Mori, JCP 470 111599 (2022).





QuickPIC on GPU (GPU+MPI)



MPI + OpenMP

MPI + GPU

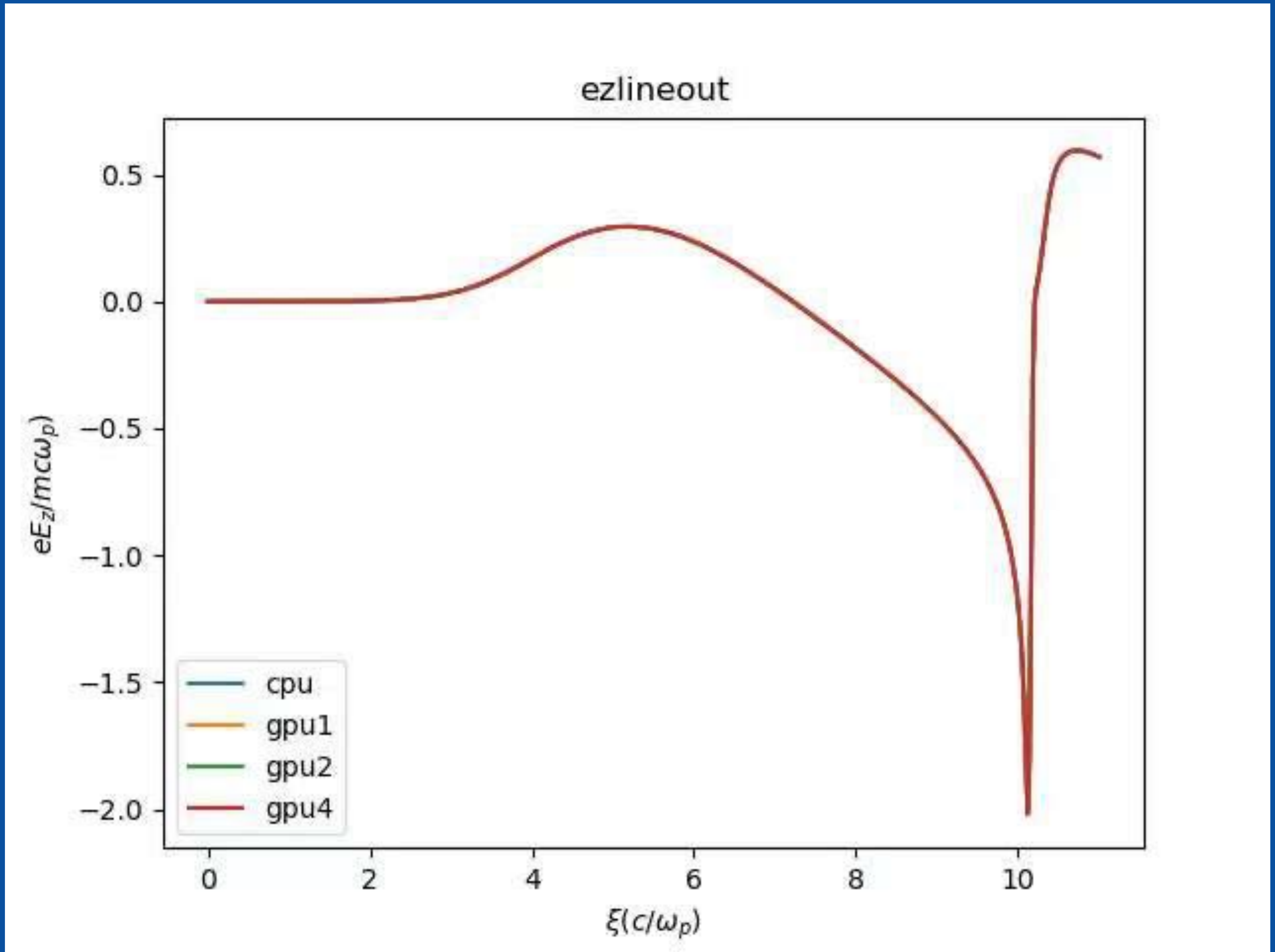
Particle Manager

FFT

*Victor K. Decyk et al, Particle-in-Cell algorithms for emerging computer architectures, Computer Physics Communications 185 (2014) 708-719.

QuickPIC on GPU (GPU+MPI)

- 2D particle and field solver functions completely on GPU
- using CUDA-aware MPI, GPU+MPI parallel simulation



The explicit solver in QuickPIC/QPAD

	ξ-1/2$\Delta\xi$	ξ	ξ+1/2$\Delta\xi$	$\xi+\Delta\xi$	ξ+3/2$\Delta\xi$
Known quantities	$\psi, \vec{J}, \vec{B}, \vec{E},$	$\vec{p}, \gamma$	$\vec{x}_\perp$		
Quantities calculated before the iteration			$\rho - J_z$		
			ψ		
			$\nabla_\perp \psi$		
			E_z, B_z		
Quantities predicted or corrected				$\vec{p}_\perp$	
			$\vec{p}_\perp, \vec{J}, p_z, \frac{\partial \vec{p}_\perp}{\partial \xi}, \frac{\partial \vec{J}_\perp}{\partial \xi}, \gamma$		
			$\vec{B}_\perp$		
			E_z, B_z		
Quantities known after the iteration			$\vec{E}_\perp$		
				$\vec{p}, \gamma$	$\vec{x}_\perp$

Iterative Solution

$$\nabla_\perp^2 \vec{B}_\perp^{\text{new}} - \vec{B}_\perp^{\text{new}} = \hat{z} \times \left(\frac{\partial}{\partial \xi} \vec{J}_\perp + \nabla_\perp J_z \right) - \vec{B}_\perp^{\text{old}}$$

Explicit Solution*

$$\nabla_\perp^2 \vec{B}_{plasma,\perp} - \frac{q_e(\rho - J_z)_e}{m_e(1 - \frac{q_e}{m_e}\psi_e)} \vec{B}_{e,\perp} S(\vec{x}_\perp - \vec{x}_{i\perp}) - \frac{q_i(\rho - J_z)_i}{m_i(1 - \frac{q_i}{m_i}\psi_i)} \vec{B}_{i,\perp} S(\vec{x}_\perp - \vec{x}_{i\perp})$$

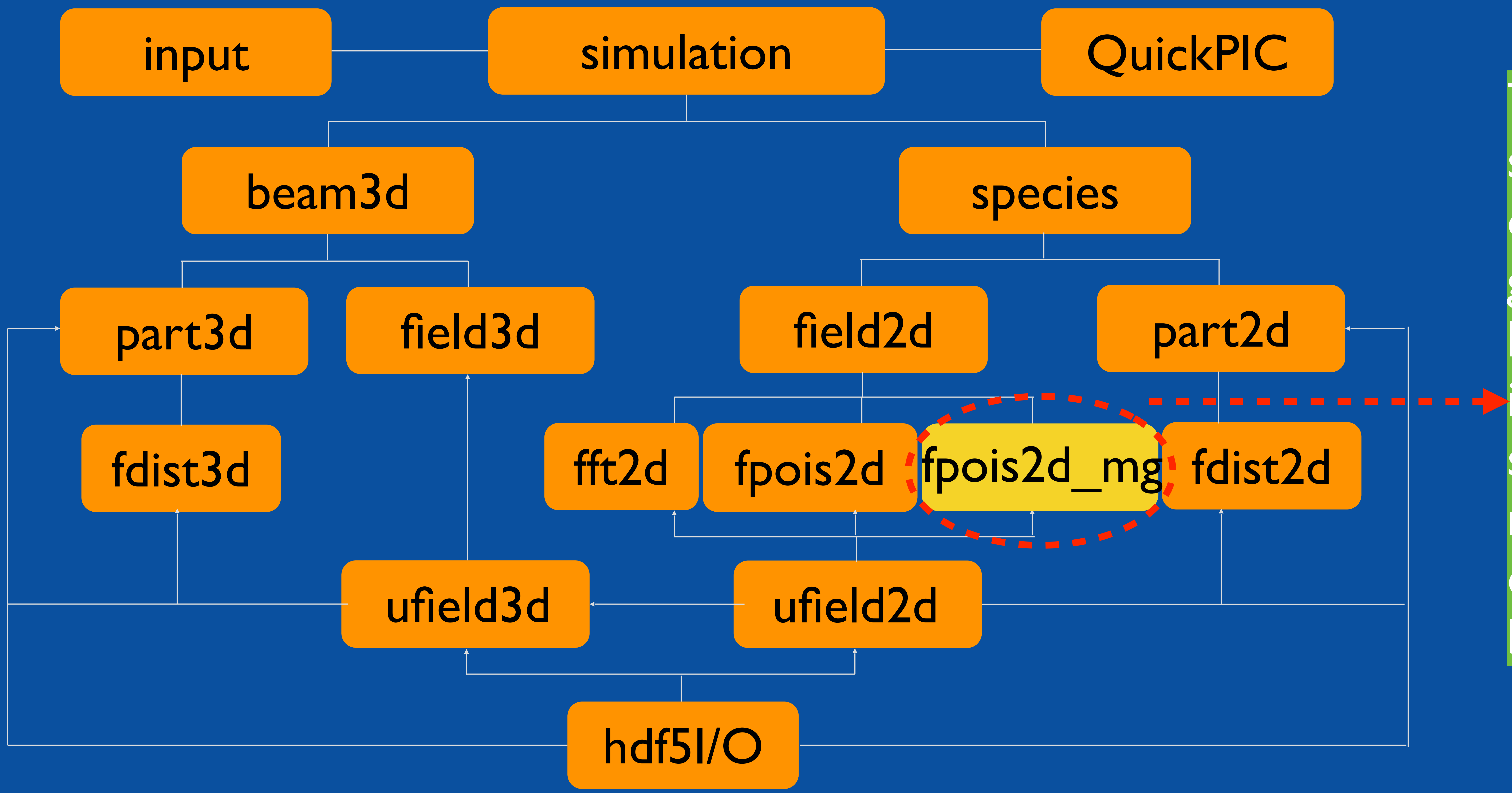
$$= \hat{z} \times \left\{ \frac{q}{\text{Volume}} \sum_s \frac{q_s}{m(1 - \frac{q_s}{m_s}\psi_s)} \left(\frac{-\gamma_s \nabla_\perp \psi_s}{1 - \frac{q_s}{m_s}\psi_s} - \hat{z} \times \vec{B}_{beam,\perp} + \frac{\vec{p}_{s\perp} \times B_{sz}\hat{z}}{1 - \frac{q_s}{m_s}\psi_s} + \frac{\vec{p}_{s\perp}(E_{sz} + \nabla_\perp \psi_s \cdot \frac{\vec{p}_{s\perp}}{1 - \frac{q_s}{m_s}\psi_s})}{1 - \frac{q_s}{m_s}\psi_s} \right) S\left(\vec{x}_\perp - \vec{x}_{s\perp}\right) \right\}$$

$$-\hat{z} \times \left[\frac{q}{\text{Volume}} \nabla_\perp \cdot \sum_s \frac{\vec{p}_{s\perp}\vec{p}_{s\perp}}{\left(1 - \frac{q_s}{m_s}\psi_s\right)^2} S\left(\vec{x}_\perp - \vec{x}_{s\perp}\right) \right] + \hat{z} \times \nabla_\perp J_z$$

solved with finite difference method

*Wang, Tianhong, et al. , Physical Review Accelerators and Beams 25.10 (2022): 104603.

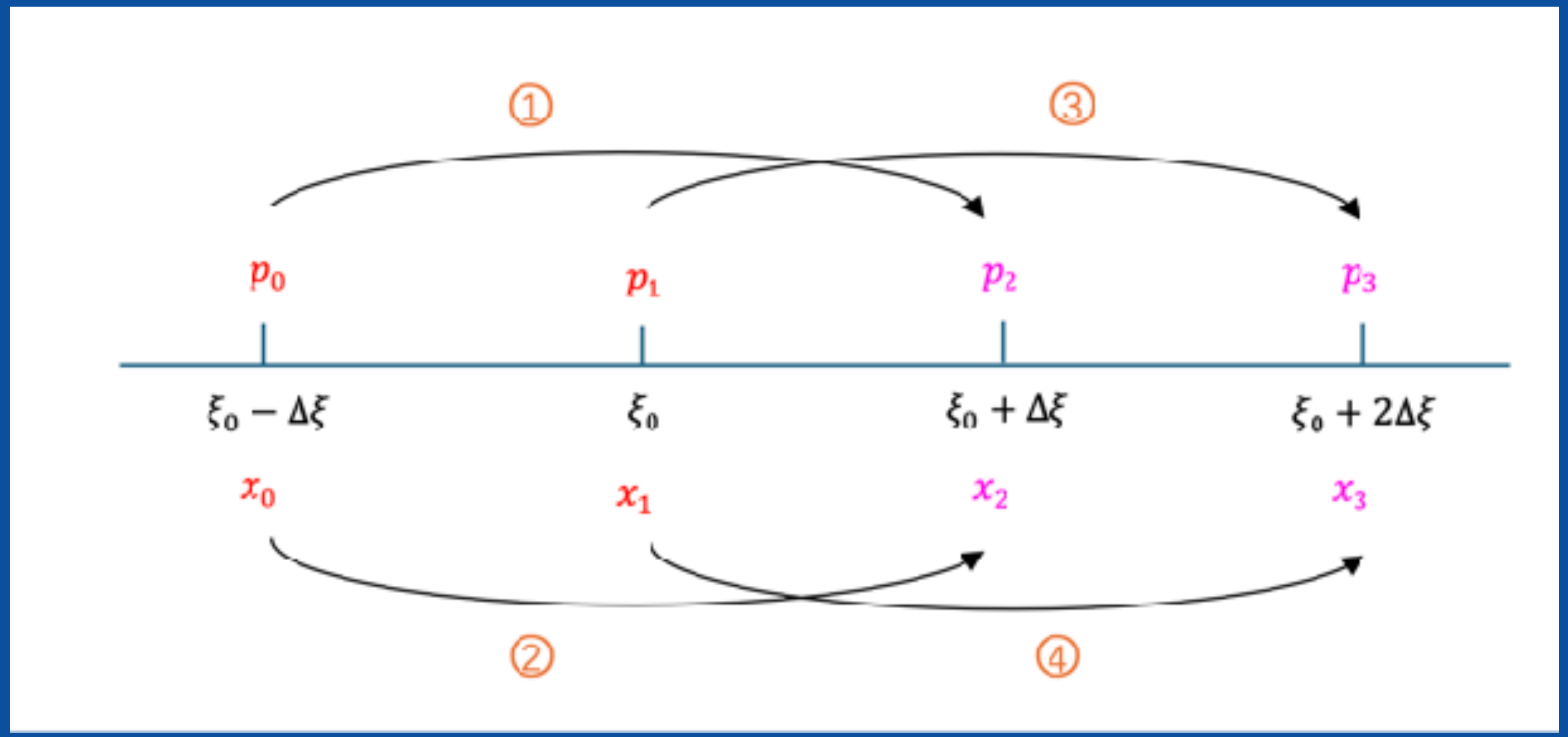
The explicit solver in QuickPIC/QPAD



This module is used to solve Poisson equations on a two-dimensional grid. With the HYPRE library, it provides a set of interfaces for setting and solving Poisson or modified Helmholtz equations with different boundary conditions.

The explicit solver in QuickPIC/QPAD

algorithm design



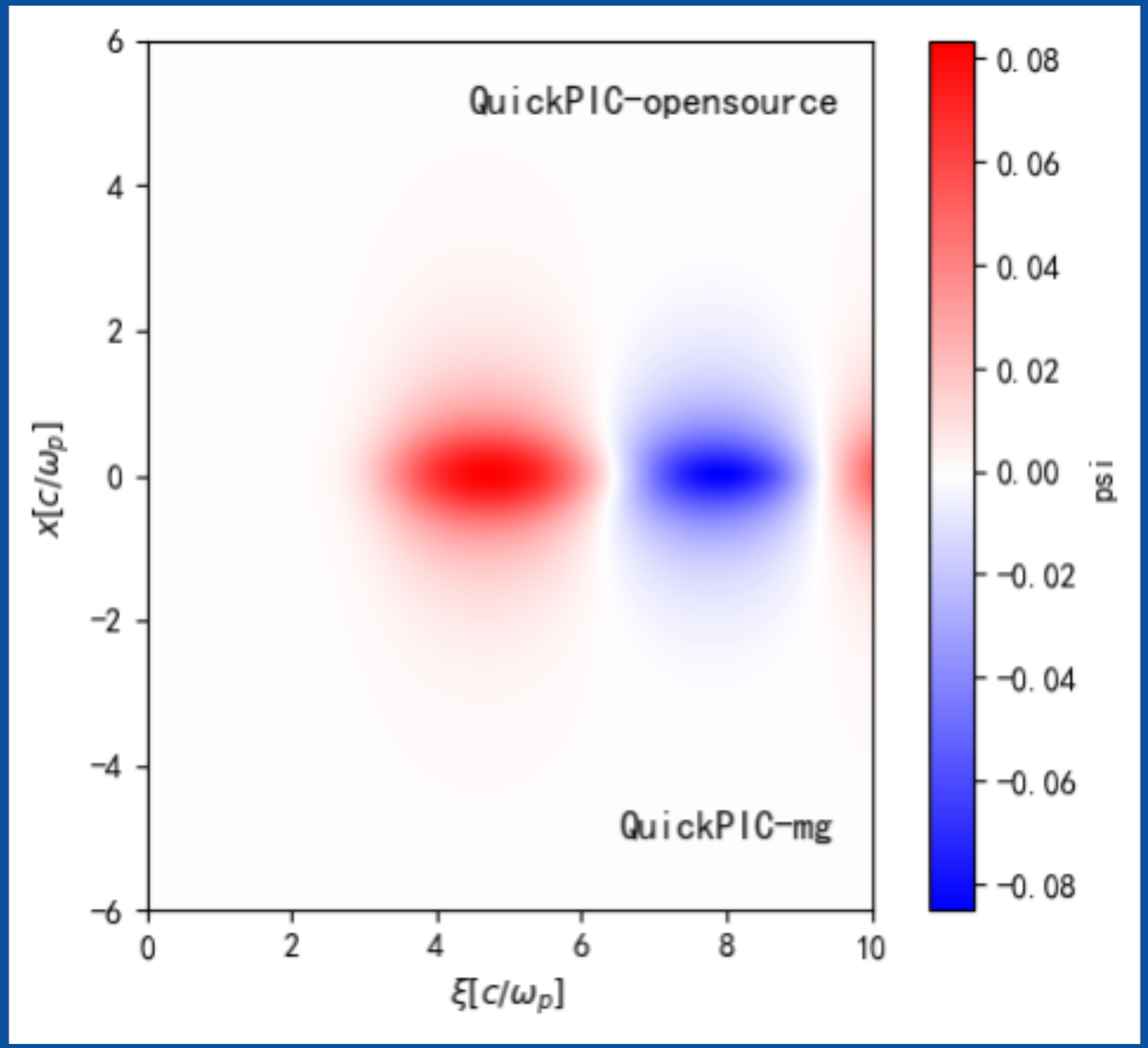
$$\vec{x}_0 \longrightarrow \vec{x}_2, \quad \vec{p}_1 \longrightarrow \vec{p}_3$$

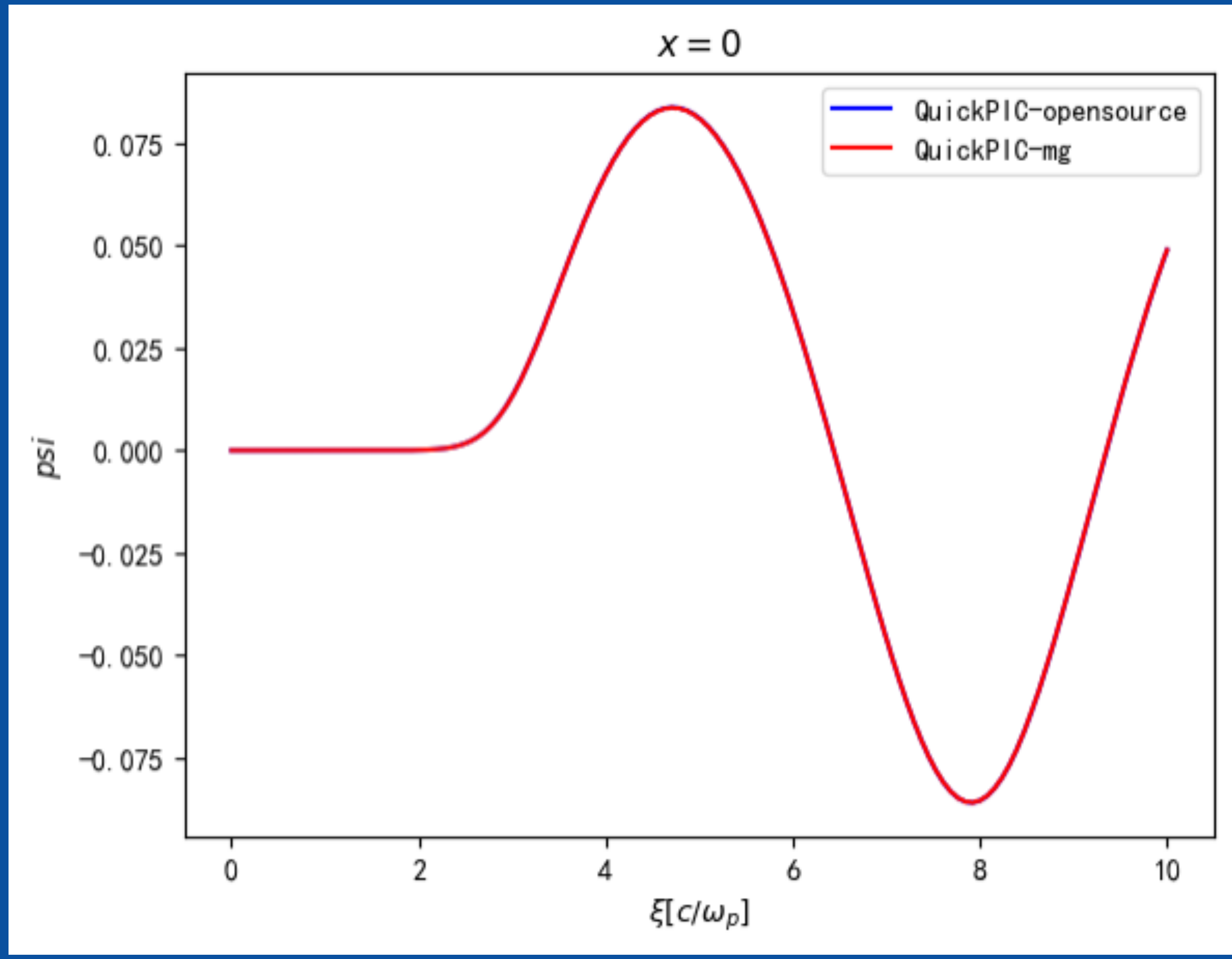
$$\vec{x}_1 \longrightarrow \vec{x}_3, \quad \vec{p}_2 \longrightarrow \vec{p}_4$$

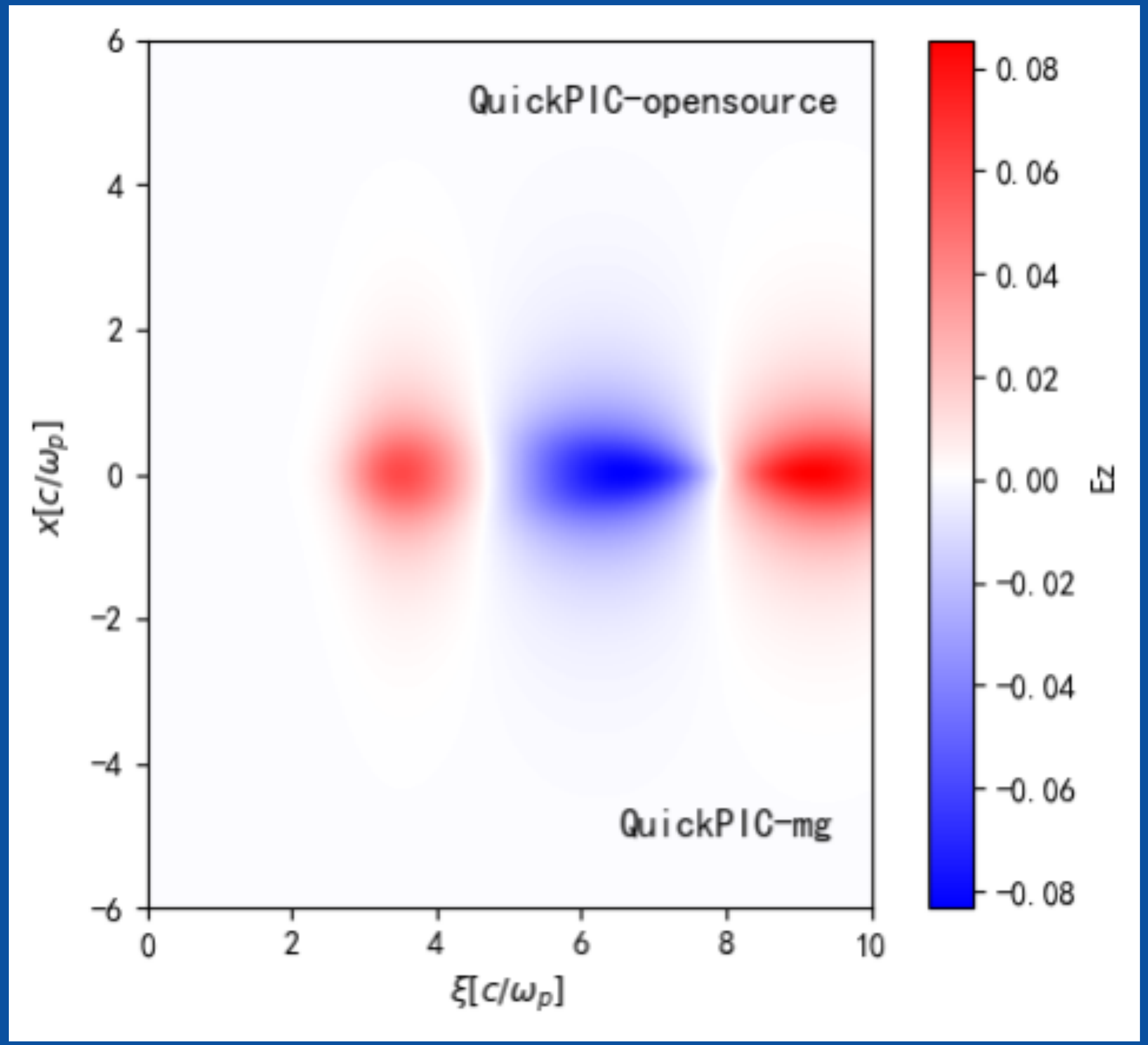
……

	ξ-Δξ	ξ	ξ+Δξ	ξ+2Δξ
Known quantities	$\vec{p}, \vec{x}$	$\vec{p}, \vec{x}$		
Quantities calculated		$\rho - J_z$		
		ψ		
		$\nabla_\perp \psi$		
		$\vec{J}, B_z, E_z$		
		$\vec{B}_\perp, \vec{E}_\perp$		
			$\vec{p}, \vec{x}$	
			$\rho - J_z$	
			ψ	
			$\nabla_\perp \psi$	
			$\vec{J}, B_z, E_z$	
			$\vec{B}_\perp, \vec{E}_\perp$	
				$\vec{p}, \vec{x}$

The explicit solver in QuickPIC/QPAD







The explicit solver in QuickPIC/QPAD

- In QPAD, we need to perform a Fourier expansion of the field quantities.

$$\frac{\frac{q}{m}(\rho - J_z)}{1-\frac{q}{m}\psi}B_\perp = \frac{\sum_{n1=-\infty}^{+\infty} a_{n1}e^{-in_1\phi}}{1+\sum_{n_2=-\infty}^{+\infty} b_{n_2}e^{-in_2\phi}}B_\perp = \sum_{n_3=-\infty}^{+\infty} u_{n_3}e^{-in_3\phi}\sum_{n_4=-\infty}^{+\infty} B_{\perp,n_4}e^{-in_4\phi} = \sum_{n_5=-\infty}^{+\infty} X_{\perp,n_5}e^{-in_5\phi}$$

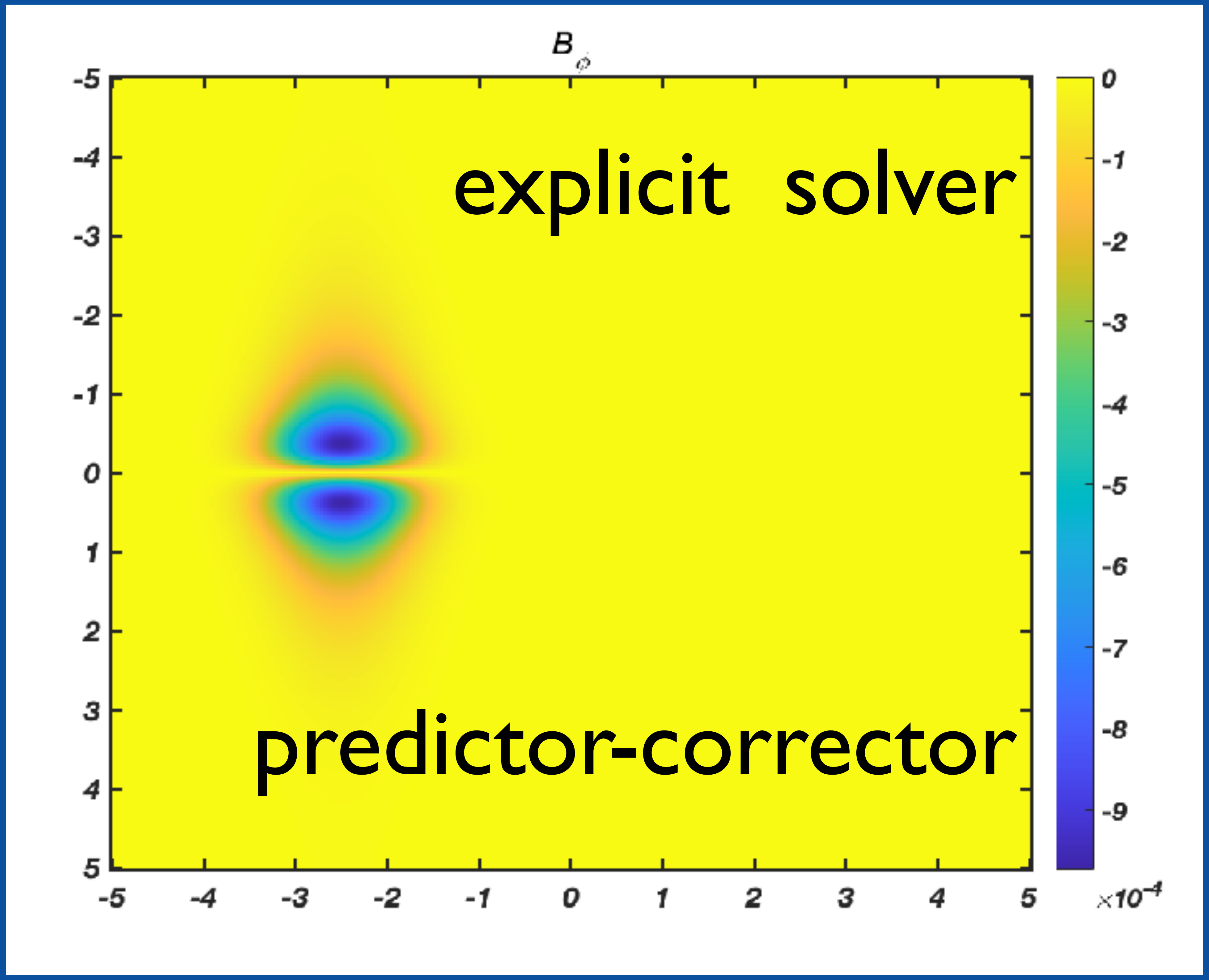
- The transverse magnetic field equation for each mode :

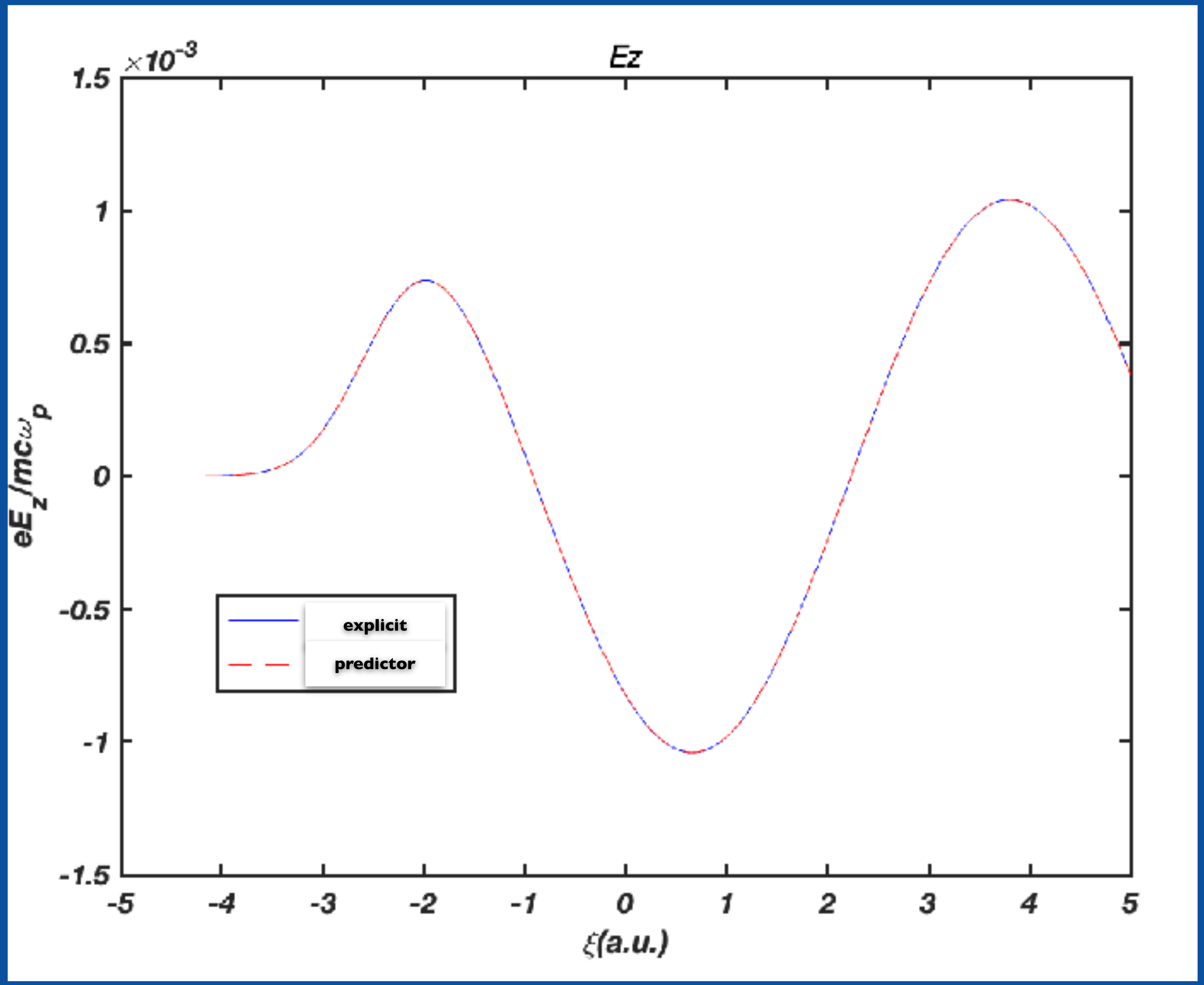
$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{(k \pm 1)^2}{r^2}\right)B_{\pm,k} + X_k = S_{\pm,k}, \quad k = [-m, m], \quad X_k = \sum_{n=k-m} B_n U_{k-n}$$

We use Hypre[1,2] to solve these linear equations.

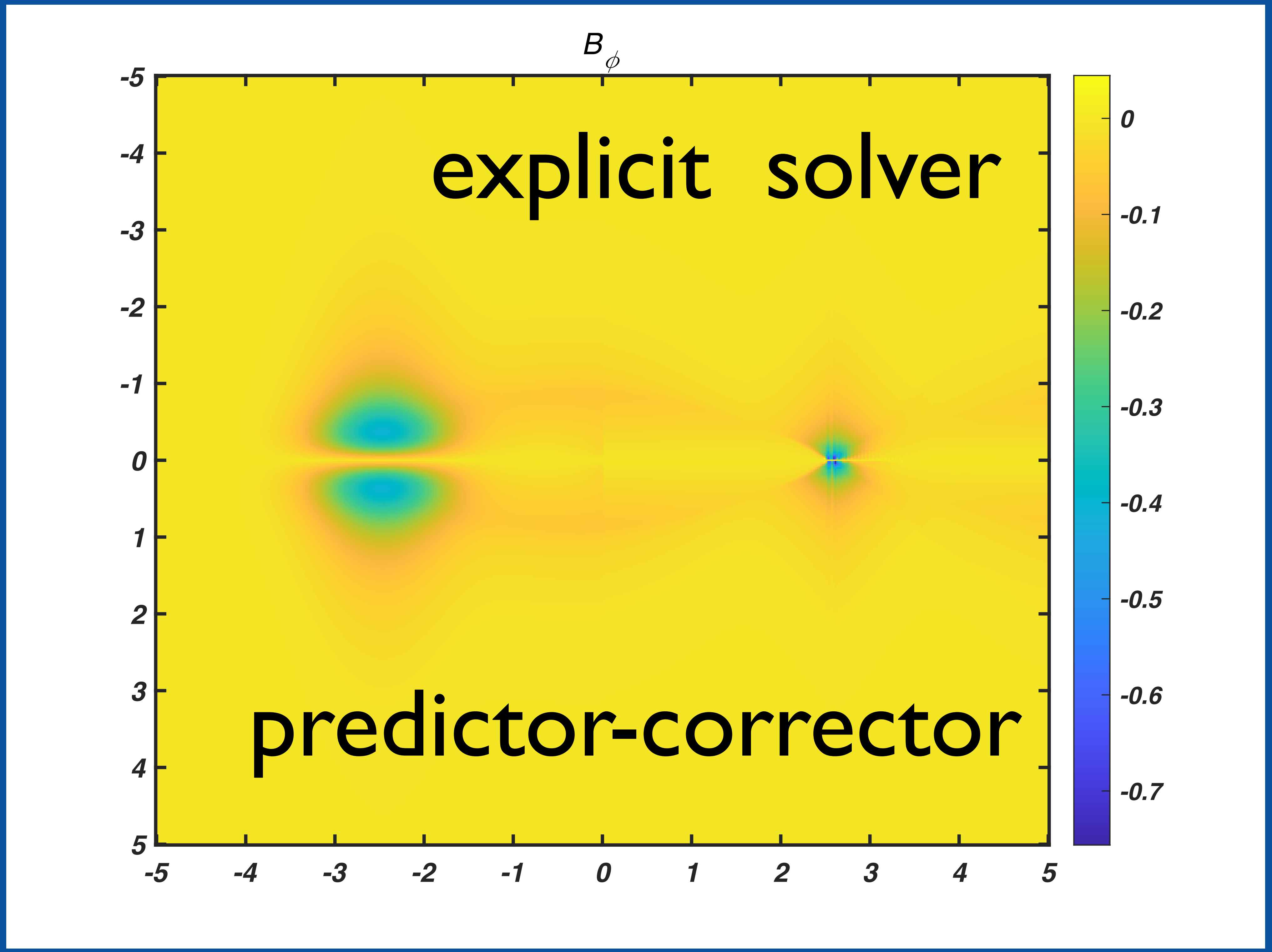
[1] https://github.com/hypre-space/hypre/tags
[2] Falgout R D, Jones J E, Yang U M. Springer Berlin Heidelberg, 2006: 267-294.

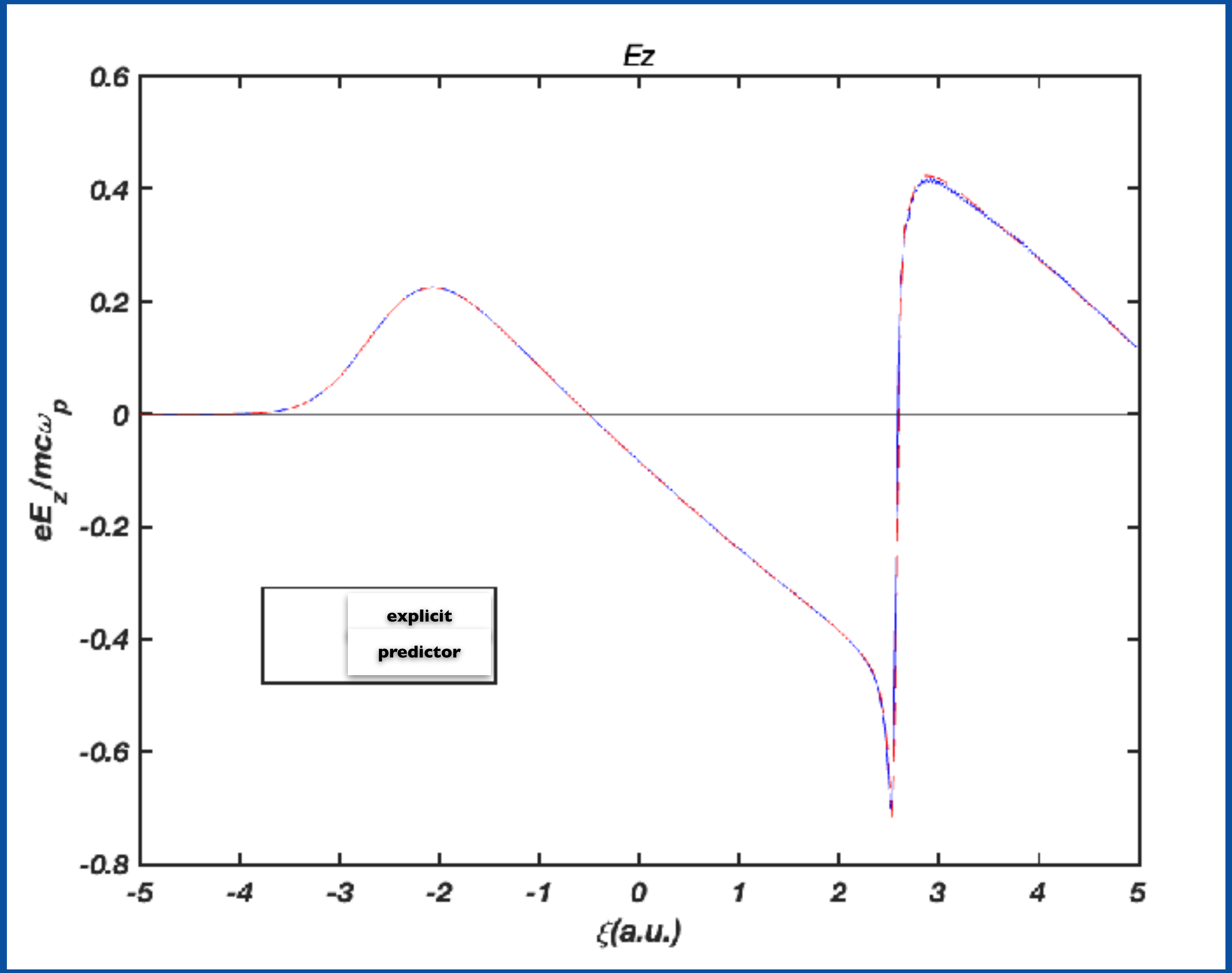
The explicit solver in QuickPIC/QPAD





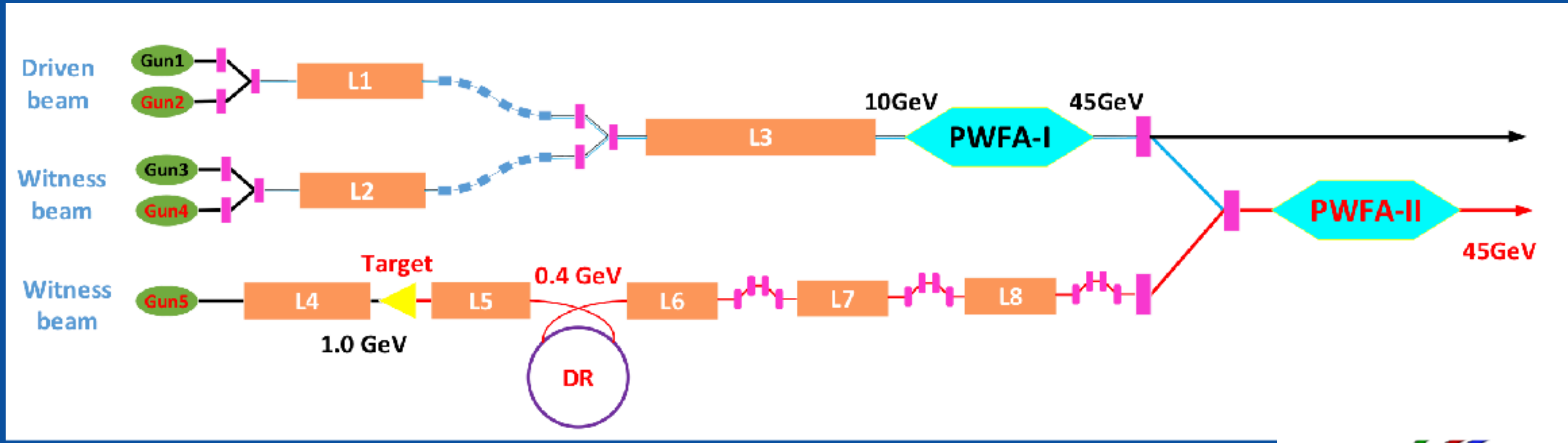
The explicit solver in QuickPIC/QPAD





QuickPIC/QPAD @ CEPC

Design CEPC Plasma Injector



IHEP

THU

BNU

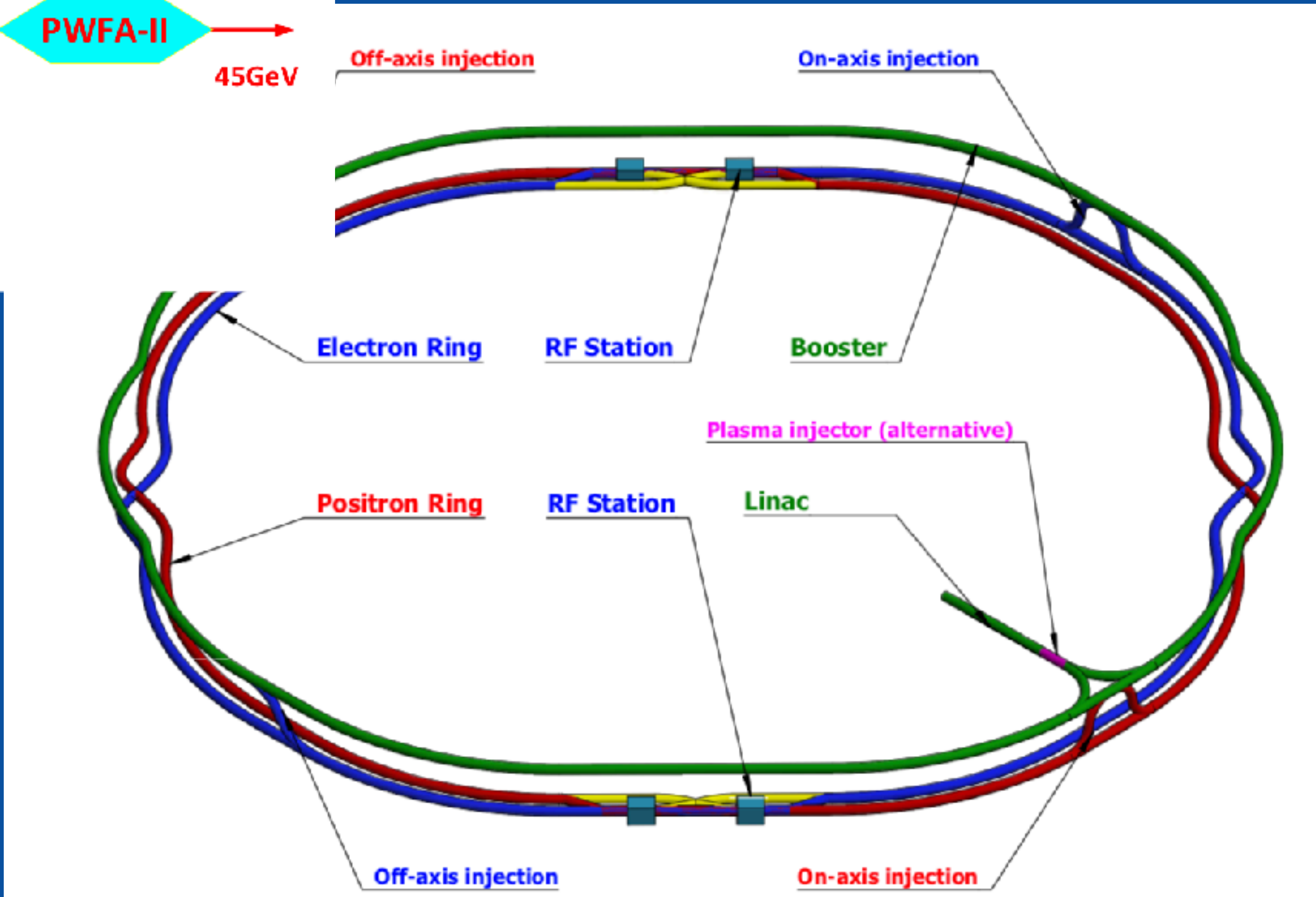
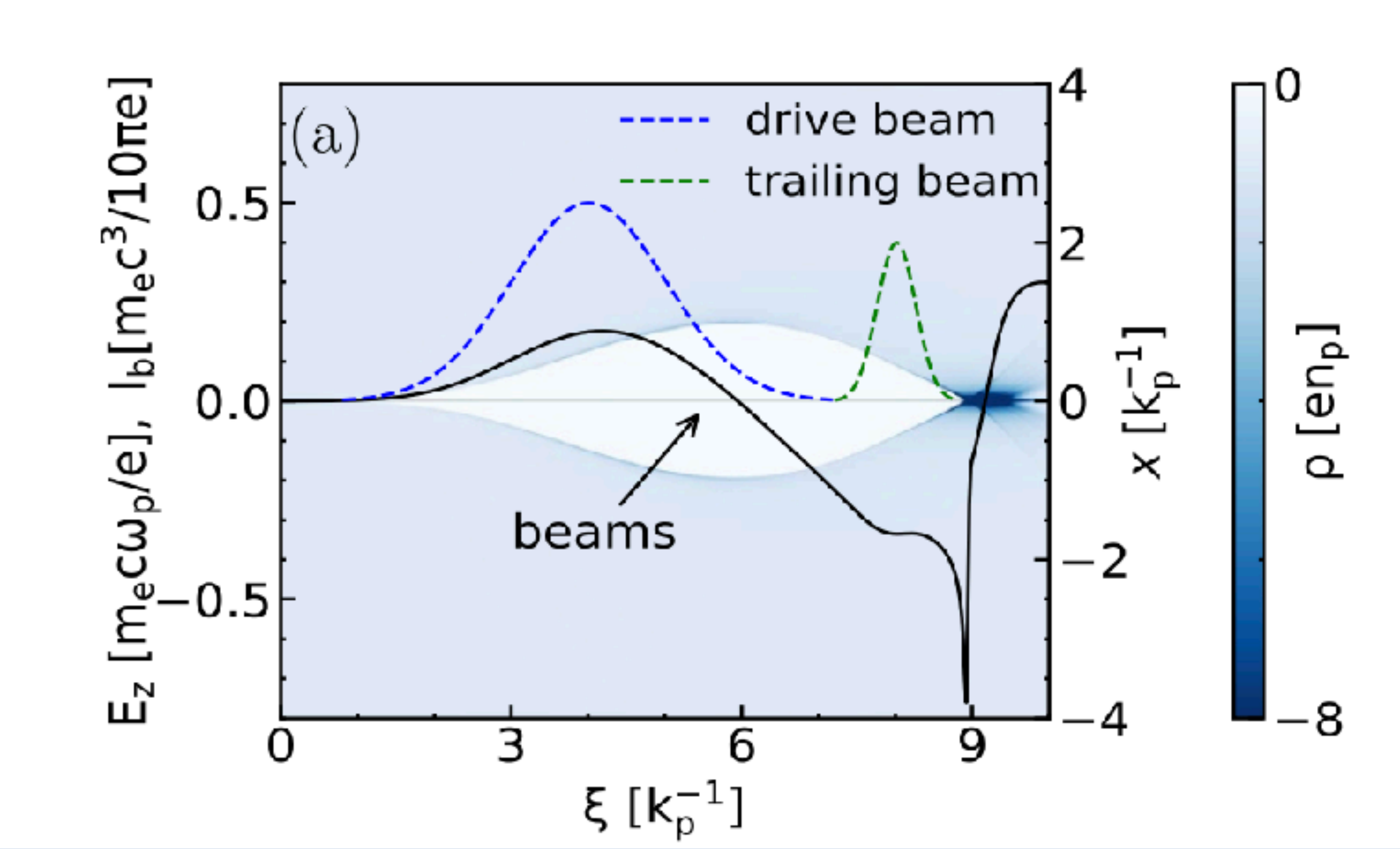


Fig. 1. CEPC layout. The blue one corresponds to the electron ring and the red one corresponds to the positron ring. There are two interaction regions, two RF regions and four injection regions in the collider.[1]

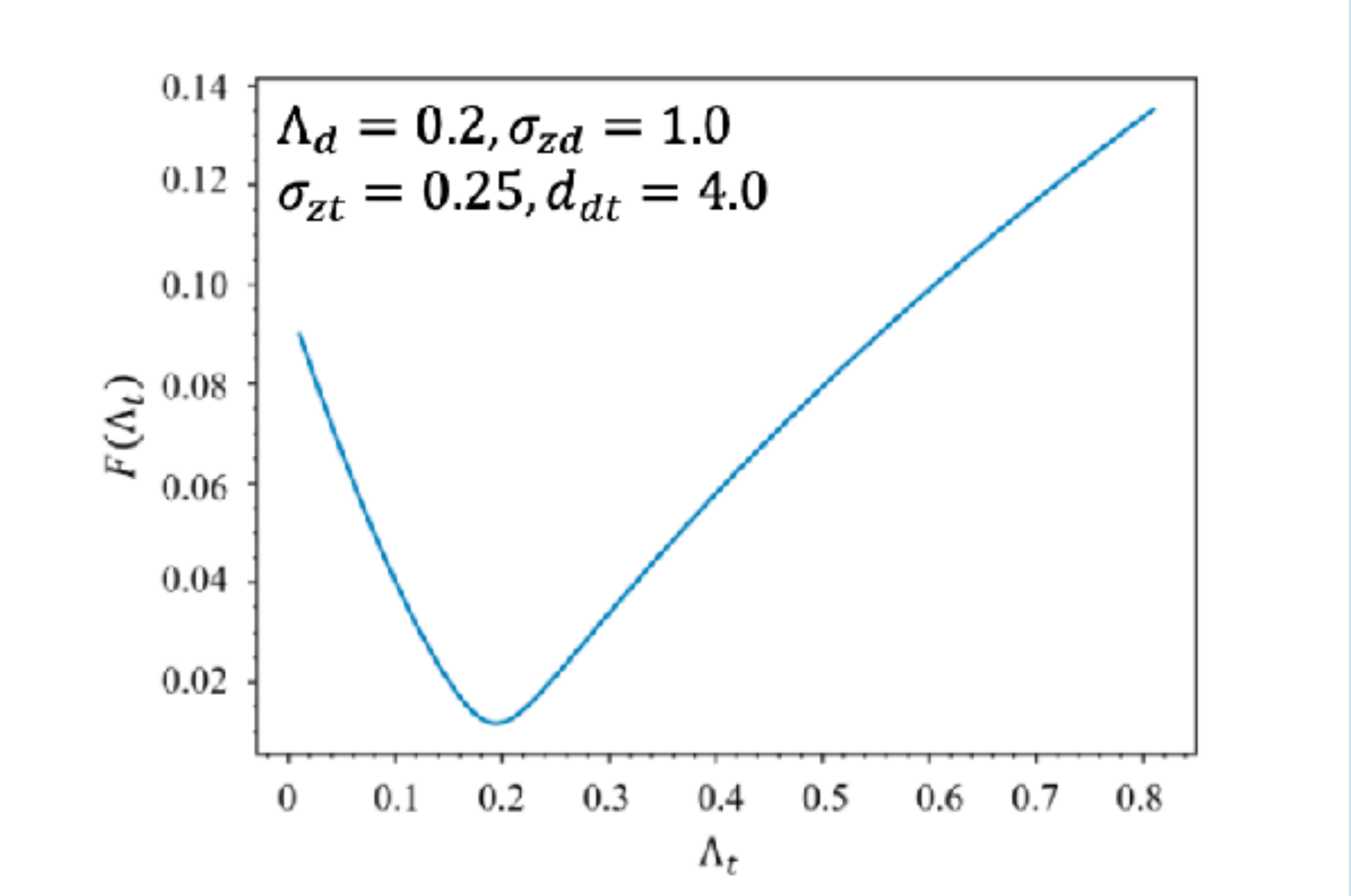
Find the Optimal Beam Loading

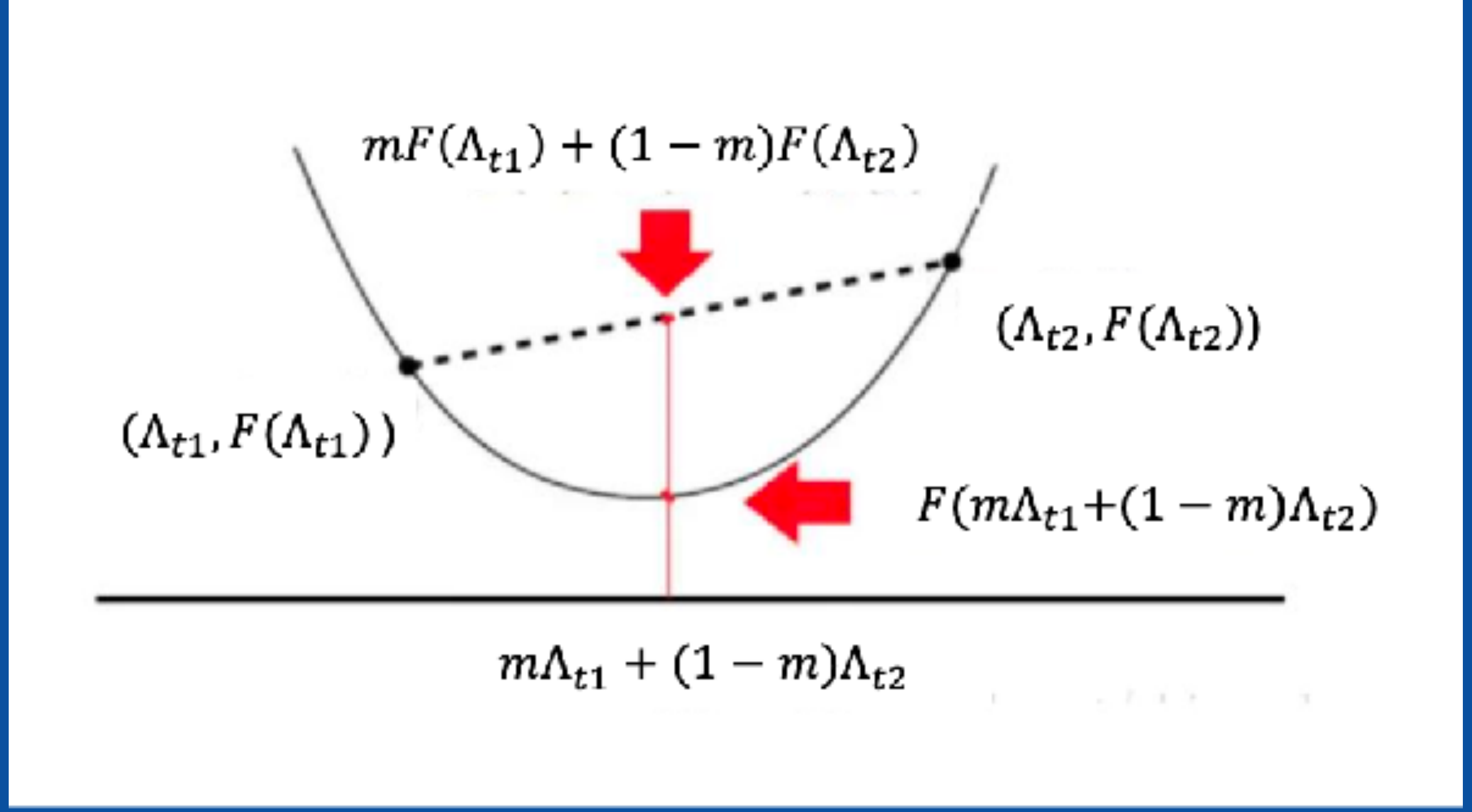
*Xiaoning Wang, et. al., Plasma Phys. Control. Fusion 64, 065007 (2022).



The Object Function

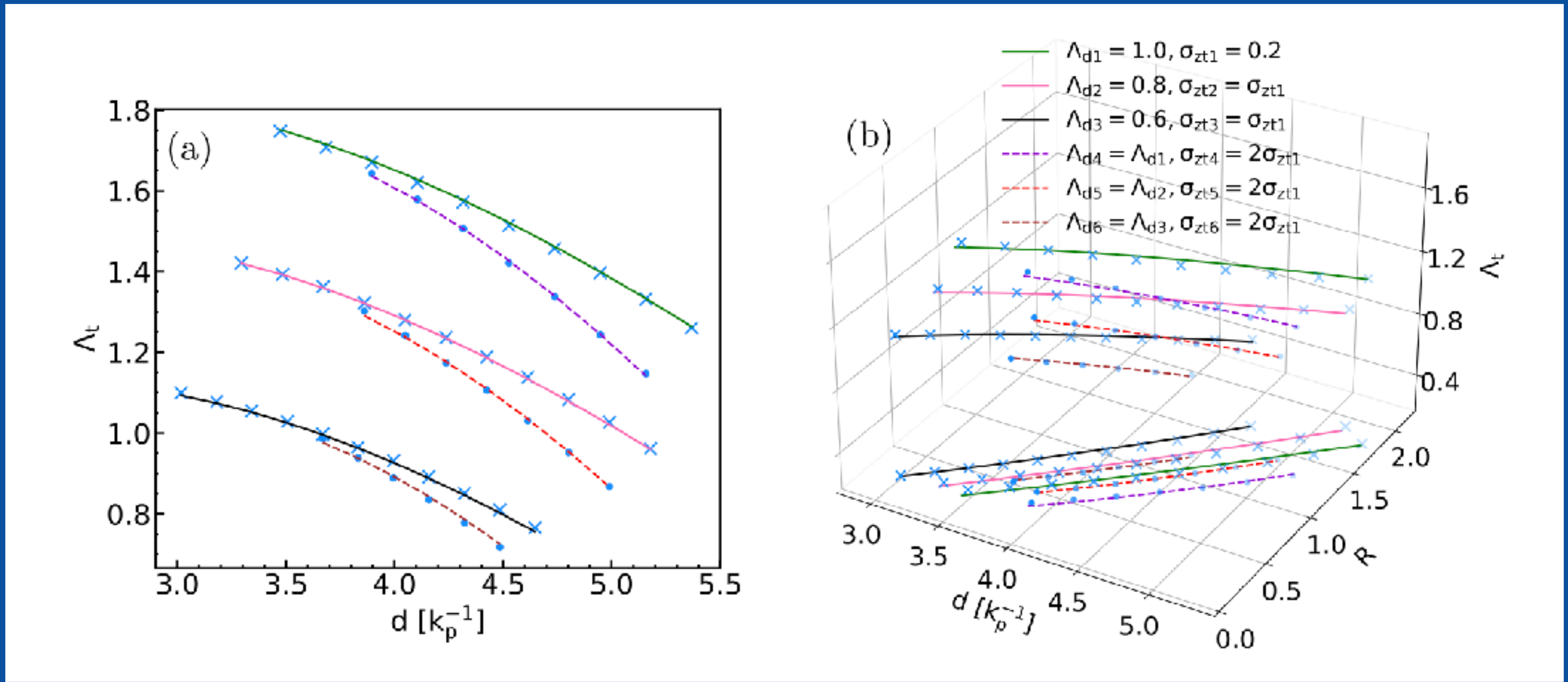
$$F(\Lambda_t) = \sqrt{\frac{\int_{\xi_s}^{\xi_e} (E_z(\xi))^2 \lambda_{bt}(\xi) d\xi}{\int_{\xi_s}^{\xi_e} \lambda_{bt}(\xi) d\xi} - \left(\frac{\int_{\xi_s}^{\xi_e} E_z(\xi) \lambda_{bt}(\xi) d\xi}{\int_{\xi_s}^{\xi_e} \lambda_{bt}(\xi) d\xi}\right)^2}$$





BFGS Method

Polynomial Fitting for Λ_t

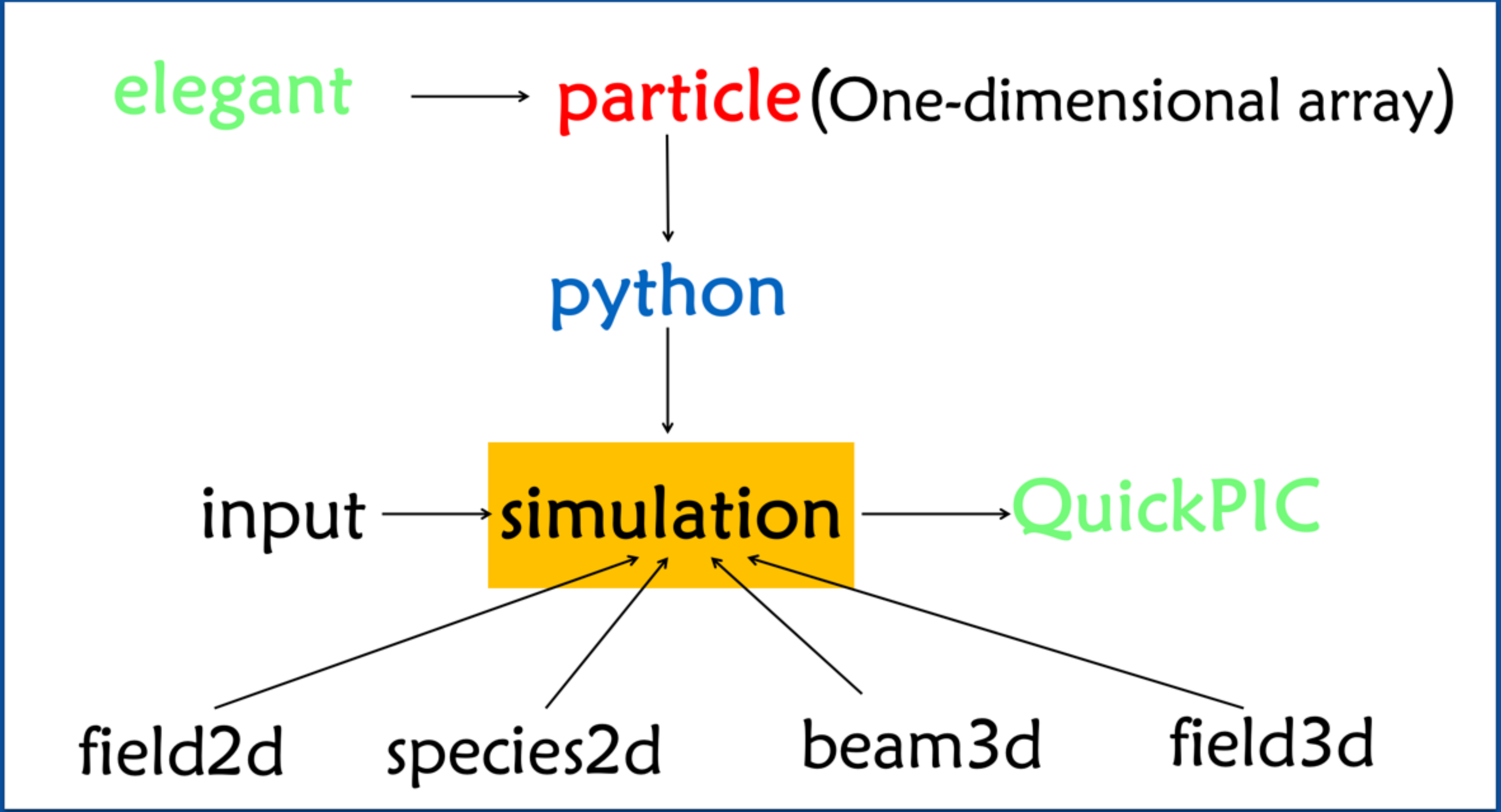


$\Lambda_t = \mathrm{f}(\Lambda_d, \sigma_{zd}, \sigma_{zt}, d_{dt})$: r^2=0.999 at degree=3

$$
\begin{aligned}
\Lambda_t = {} & h_0 + h_1\Lambda_d + h_2\sigma_{zd} + h_3\sigma_{zt} + h_4 d + h_5\Lambda_d^2 + h_6\Lambda_d\sigma_{zd} \\
& + h_7\Lambda_d\sigma_{zt} + h_8\Lambda_d d + h_9\sigma_{zd}^2 + + h_{10}\sigma_{zd}\sigma_{zt} + h_{11}\sigma_{zd} d \\
& + h_{12}\sigma_{zt}^2 + h_{13}\sigma_{zt} d + h_{14} d^2 + h_{15}\Lambda_d^3 + h_{16}\Lambda_d^2\sigma_{zd} \\
& + h_{17}\Lambda_d^2\sigma_{zt} + h_{18}\Lambda_d^2 d + h_{19}\Lambda_d\sigma_{zd}^2 + h_{20}\Lambda_d\sigma_{zd}\sigma_{zt} \\
& + h_{21}\Lambda_d\sigma_{zd} d + h_{22}\Lambda_d\sigma_{zt}^2 + h_{23}\Lambda_d\sigma_{zt} d + h_{24}\Lambda_d d^2 \\
& + h_{25}\sigma_{zd}^3 + h_{26}\sigma_{zd}^2\sigma_{zt} + h_{27}\sigma_{zd}^2 d + h_{28}\sigma_{zd}\sigma_{zt}^2 + h_{29}\sigma_{zd}\sigma_{zt} d \\
& + h_{30}\sigma_{zd} d^2 + h_{31}\sigma_{zt}^3 + h_{32}\sigma_{zt}^2 d + h_{33}\sigma_{zt} d^2 + h_{34} d^3, \qquad (2)
\end{aligned}
$$

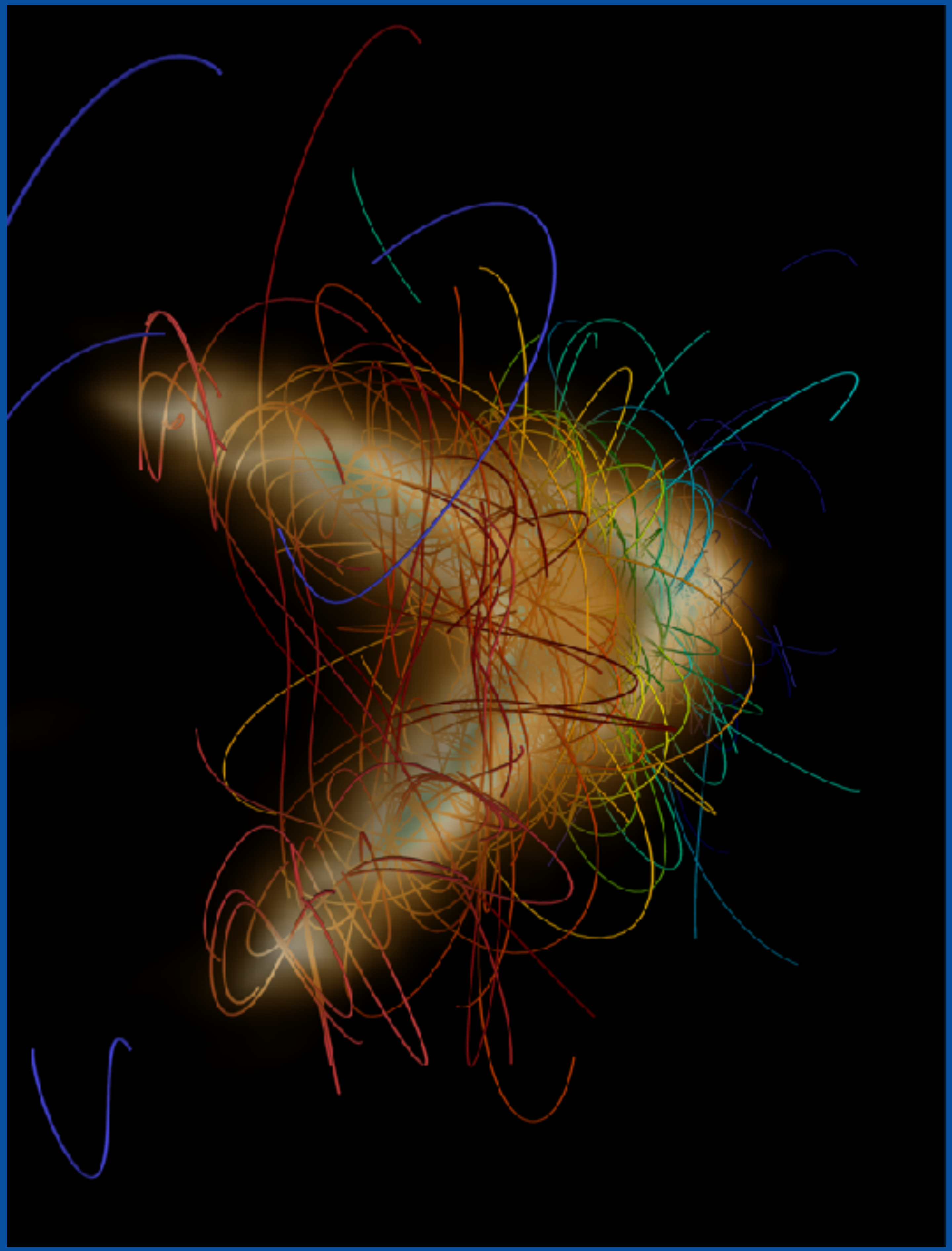
$\mathrm{R} = \mathrm{f}(\Lambda_d, \sigma_{zd}, \sigma_{zt}, d_{dt}, \Lambda_t)$: r^2=0.99 at degree=2

Plasma-based Accelerator Optimization Framework



CTYPES

Thanks!



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