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Optimization of transformer ratio and beam loading in plasma wakefield accelerator with a structure-exploiting algorithm

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Optimization tools to improve beam quality

For the linear collider application of PWFA, we aim for a stable and efficient acceleration of the trailing bunch with good qualities.

Beam distribution $f\left(x, y, z, p_x, p_y, p_z, t\right)$

- Minimize relative energy spread

$$\frac{\sigma_p}{\overline{p}}, \sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$$

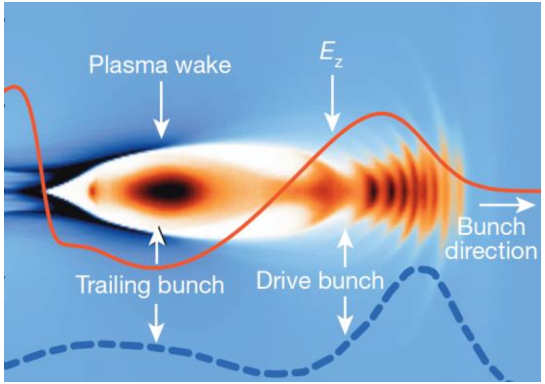
- Maximize energy transfer efficiency and transformer ratio

$$\eta = \frac{\Delta W_{tr}}{\Delta W_{dr}}, \Delta W = \int d\vec{x} E_z(\vec{x})\rho_b(\vec{x}) \qquad T = \frac{\max|E_z||_{\text{Trailing}}}{\max|E_z||_{\text{Drive}}}$$

- Minimize normalized emittance

$$\epsilon_{nx} = \sqrt{\langle x^2\rangle \langle {p_x}^2\rangle - \langle xp_x\rangle^2} \qquad \epsilon_{ny} = \sqrt{\langle y^2\rangle \langle {p_y}^2\rangle - \langle yp_y\rangle^2}$$

- Mitigate instability (Hosing)



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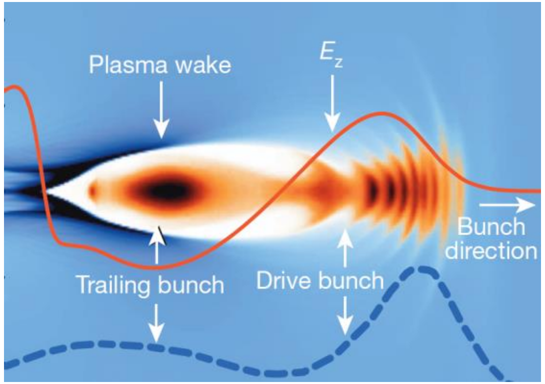
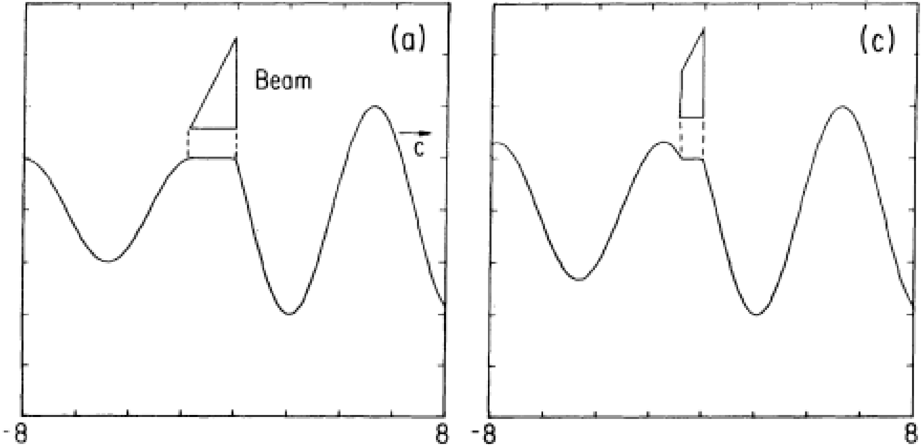


Wakefield in linear regime is fully predictable

In linear regime, the wakefield is predictable by a convolution of the field of each particles

1D linear thoery $$E_z = -4\pi \int_x^\zeta d\zeta' \rho_b(\zeta') \cos k_p (\zeta - \zeta')$$



Optimal trailing beam profile:

$$\rho_b(\zeta) = -\frac{k_p E_0}{4\pi} \left[(k_p \cos k_p \xi_0)\, \xi + (\sin k_p \xi_0 - k_p \zeta_0 \cos k_p \zeta_0) \right]$$

Optimal drive beam profile:

$$\rho(\zeta) = -\frac{E_0}{4\pi\alpha} \left[\left(\alpha^2 + k_p^2\right) e^{-\alpha\zeta} + k_p^2(\alpha\zeta - 1) \right], \alpha \to \infty$$

P. Chen, et. al.. Physical Review Letters, 56:1252–1255, 1986.
T. Katsouleas et. al, Particle Accelerators, 22:81–99, 1987

The multi-sheath model predict an accurate wakefield at rear of the bubble in the nonlinear blowout regime for symmetric beams

In the 3D blowout (nonlinear) regime, the wakefield is predicted by a modeling of the bubble sheath

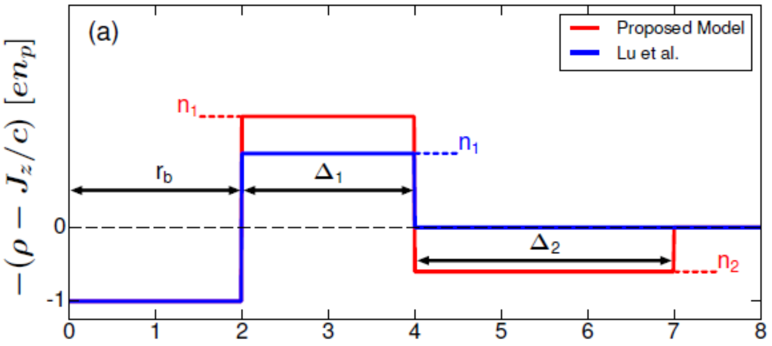
Multisheath model

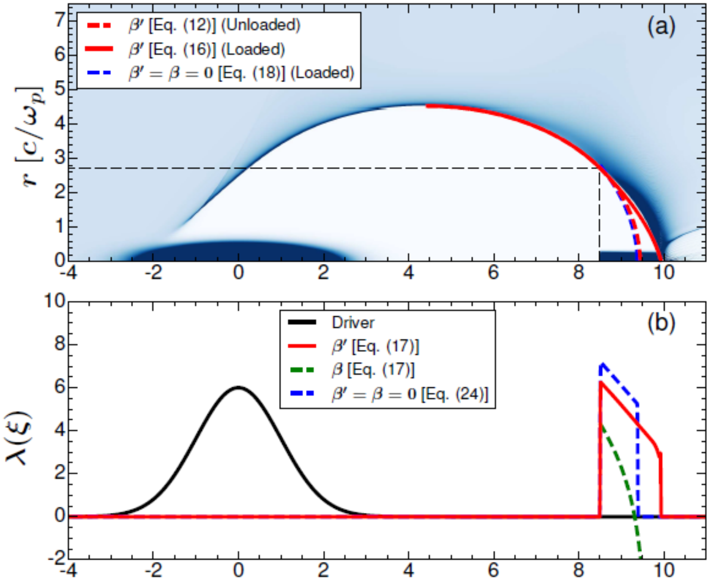
$$A'(r_b)\frac{d^2 r_b}{d\xi^2} + B'(r_b) r_b \left(\frac{dr_b}{d\xi}\right)^2 + C'(r_b) r_b = \frac{\lambda(\xi)}{r_b}.$$

$$E_z(\xi) = \frac{d}{d\xi}\psi_0(\xi) = D'(r_b) r_b \frac{dr_b}{d\xi},$$

$$\psi(r,\xi) = \psi_0(\xi) - \frac{r^2}{4}$$
$$= \frac{r_b^2(\xi)}{4}(1+\beta') - \frac{r^2}{4}$$

$\beta' \rightarrow \beta$ if $n_2 \rightarrow 0$
single sheath model





W. Lu, et. al. Physics of Plasmas, 13(5):056709, 2006
M. Tzoufras, et. al. Physics of Plasmas, 16(5):056705, 2009.
T. N. Dalichaouch et al., Physics of Plasmas, 28, 063103, (2021)

Optimization from simulation is required and faces great challenges

At present no theory describes all degrees of nonlinearity for a wide range of plasma and beam parameters

One simulation can be computationally expensive

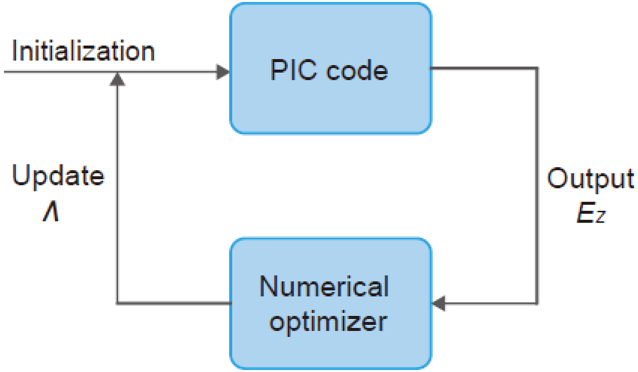
Some parameters might be coupled, multivariate optimization needs more runs of PIC code

Constraint optimization

- **Goals**
  - The algorithm needs to be efficient
  - Fast PIC code (or surrogate models)

Platform for Optimization of Particle Accelerators (POPAS)

- **Platform for Optimization of Particle Accelerators at Scale (POPAS)**
  - Integrated platform for coordinating the evaluation and numerical optimization of accelerator simulations on super computers.
- **PIC code : QuickPIC , QPAD, OSIRIS**
- **Method**
  - Randomly select initial parameters, or initialize with theoretical model, then optimize with model-exploiting second-order trust-region algorithm
  - Get great acceleration if objective is a known function of some output variable



$$\min_{x} \quad f(F(x))$$
$$\text{s.t.} \quad lb \leq x \leq ub$$

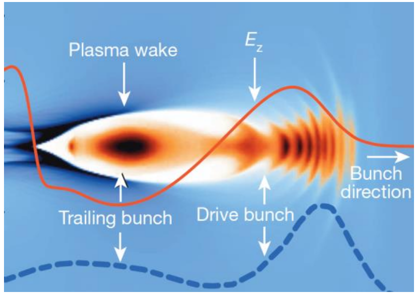
$$F_i(x) = c_i + g_i^T (x - x_0) + \frac{1}{2} (x - x_0)^T H_i (x - x_0)$$

f is known, F use quadratic function to approximate

Optimize transformer ratio by flattening Ez field

$$\eta = \frac{\Delta W_{tr}}{\Delta W_{dr}}, \Delta W = \int d\vec{x} E_z(\vec{x}) \rho_b(\vec{x})$$

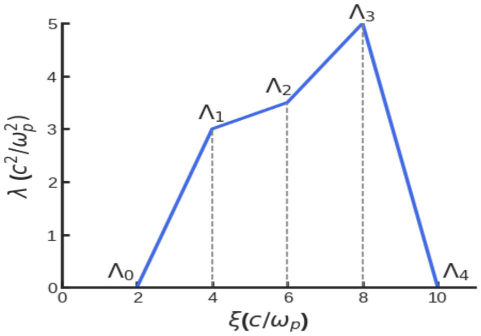
$$T = \frac{\max |E_z||_{\text{Trailing}}}{\max |E_z||_{\text{Drive}}} \qquad \frac{\sigma_p}{\overline{p}}, \sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$



Initialize longitudinally piecewise-linear beam
Output Ez lineout at the center
Two constraints : bound or fixing the total charge

$$\underset{\Lambda_1,\ldots,\Lambda_p}{\text{minimize}} \quad f(\boldsymbol{\Lambda}) = \sum_{k=1}^{q} \left([\boldsymbol{E}_z]_k (\boldsymbol{\Lambda}) - \overline{\boldsymbol{E}}_z(\boldsymbol{\Lambda}) \right)^2$$

$$\text{subject to:} \quad \sum_{i=1}^{p-1} 0.5 * (\Lambda_{i+1} + \Lambda_i) \Delta\xi_i = Q, \quad \boldsymbol{\Lambda}_l \leq \boldsymbol{\Lambda} \leq \boldsymbol{\Lambda}_u$$



Change piecewise-linear density in bins $\Rightarrow$ $\Lambda_i = \left(n_{b0} * \sigma_r^2 / n_p \right) f_{z_i}$

POUNDER Algorithm estimates a more accurate gradient and Hessian from the expression of optimization objective

$$-\nabla f(\boldsymbol{\Lambda}) = -2\sum_k \left[\left([\boldsymbol{E}_z]_k(\boldsymbol{\Lambda}) - \frac{1}{q}\sum_j [\boldsymbol{E}_z]_j(\boldsymbol{\Lambda})\right)\left(\nabla[\boldsymbol{E}_z]_k(\boldsymbol{\Lambda}) - \frac{1}{q}\sum_j \nabla[\boldsymbol{E}_z]_j(\boldsymbol{\Lambda})\right)\right]$$

$$\begin{aligned}\nabla^2 f(\boldsymbol{\Lambda}) =& 2\sum_i \Bigg[\left([\boldsymbol{E}_z]_i(\boldsymbol{\Lambda}) - \frac{1}{q}\sum_j [\boldsymbol{E}_z]_j(\boldsymbol{\Lambda})\right)\left(\nabla^2[\boldsymbol{E}_z]_i(\boldsymbol{\Lambda}) - \frac{1}{q}\sum_j \nabla^2[\boldsymbol{E}_z]_j(\boldsymbol{\Lambda})\right) \\ &+ \left([\boldsymbol{E}_z]_i(\boldsymbol{\Lambda}) - \frac{1}{q}\sum_j [\boldsymbol{E}_z]_j(\boldsymbol{\Lambda})\right)\left(\nabla[\boldsymbol{E}_z]_i(\boldsymbol{\Lambda}) - \frac{1}{q}\sum_j \nabla[\boldsymbol{E}_z]_j(\boldsymbol{\Lambda})\right)^T\Bigg]\end{aligned}$$

Model each $[\boldsymbol{E}_z]_k$ via a quadratic $q_i(\Lambda) = c_i + g_i^T(\Lambda - \Lambda_0) + \frac{1}{2}(\Lambda - \Lambda_0)^T H_i(\Lambda - \Lambda_0)$.
We can get $\nabla[\boldsymbol{E}_z]_k$ and $\nabla^2[\boldsymbol{E}_z]_k$ by evaluating the neighborhood of Λ_0.

The result can also be improved by causality

S. M. Wild, *Advances and trends in optimization with engineering applications*, p529-539, (2017)

The algorithm find a profile agrees with multi-sheath model with small improvement for the trailing beam

Multisheath model

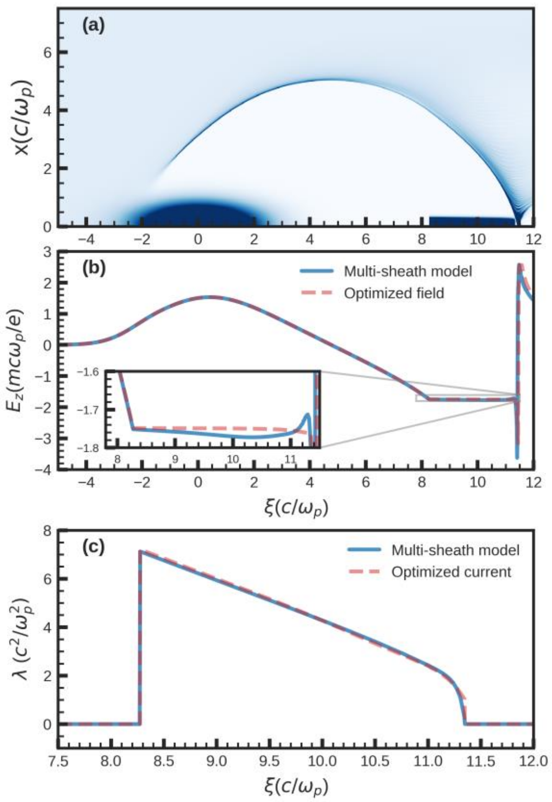
$$A'(r_b)\frac{d^2 r_b}{d\xi^2} + B'(r_b)\, r_b \left(\frac{dr_b}{d\xi}\right)^2 + C'(r_b)\, r_b = \frac{\lambda(\xi)}{r_b}.$$

$$\begin{aligned}\psi(r,\xi) &= \psi_0(\xi) - \frac{r^2}{4} \\ &= \frac{r_b^2(\xi)}{4}(1+\beta') - \frac{r^2}{4}\end{aligned}$$

$$E_z(\xi) = \frac{d}{d\xi}\psi_0(\xi) = D'(r_b)\, r_b \frac{dr_b}{d\xi},$$

The current profile can be reverse engineered by

$$\lambda(\xi) = C'\tilde{r}_b^2 + \left(\frac{B'}{D'^2} - \frac{A'F'}{D'^3\tilde{r}_b^2}\right) f(\xi)^2 + \left(\frac{A'}{D'}\right)\frac{df(\xi)}{d\xi}$$



3-10n bins to converge

T. N. Dalichaouch et al., Phys. Plasmas, 28, 063103, (2021)

The optimized beam current shows a precursor at front of the drive beam which cannot be predicted by nonlinear theory

In linear regime, the optimal longitudinal profile is a delta function followed by a linear ramp

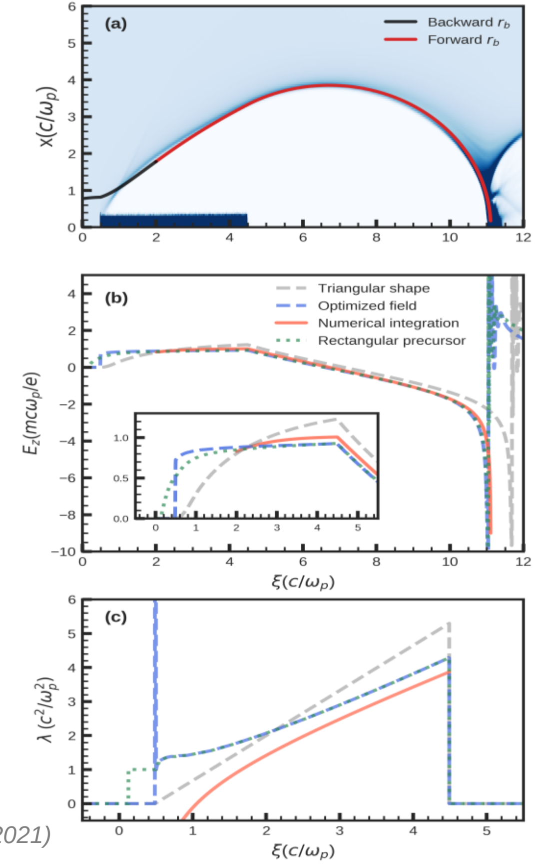
$$\rho(\zeta) = -\frac{E_0}{4\pi\alpha}\left[\left(\alpha^2 + k_p^2\right)e^{-\alpha\zeta} + k_p^2(\alpha\zeta - 1)\right], \alpha \to \infty$$

In nonlinear regime, Lu et. al. proposed a linear ramp by assuming an adiabatic response $\frac{d^2 r_b}{d\xi^2} \ll 1, \frac{dr_b}{d\xi} \ll 1$

$$r_b \frac{d^2 r_b}{d\xi^2} + 2\left(\frac{dr_b}{d\xi}\right)^2 + 1 = \frac{4\lambda(\xi)}{r_b^2}$$

$$\psi(0,\xi) \approx \frac{r_b^2(\xi)}{4},\ \Lambda(\xi) = \frac{\xi}{L_0}\Lambda_0,\ \psi(0,\xi) \approx \frac{\xi}{L_0}\Lambda_0$$

$$E_z(\xi) = \frac{d\psi}{d\xi} \approx \frac{\Lambda_0}{L_0}$$



P. Chen, et al. Phys. Rev. Lett., 56, 12, 1986
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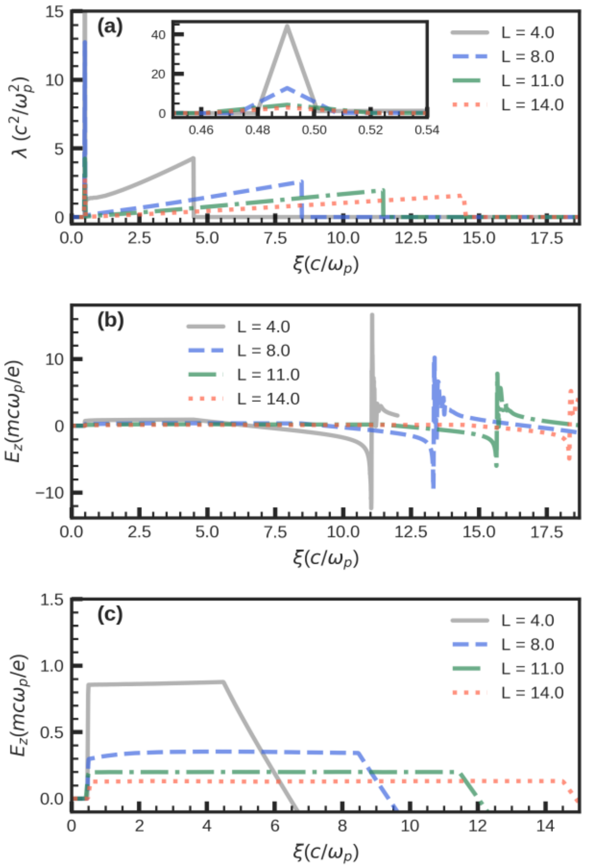
Optimized beam profile fixing the total charge



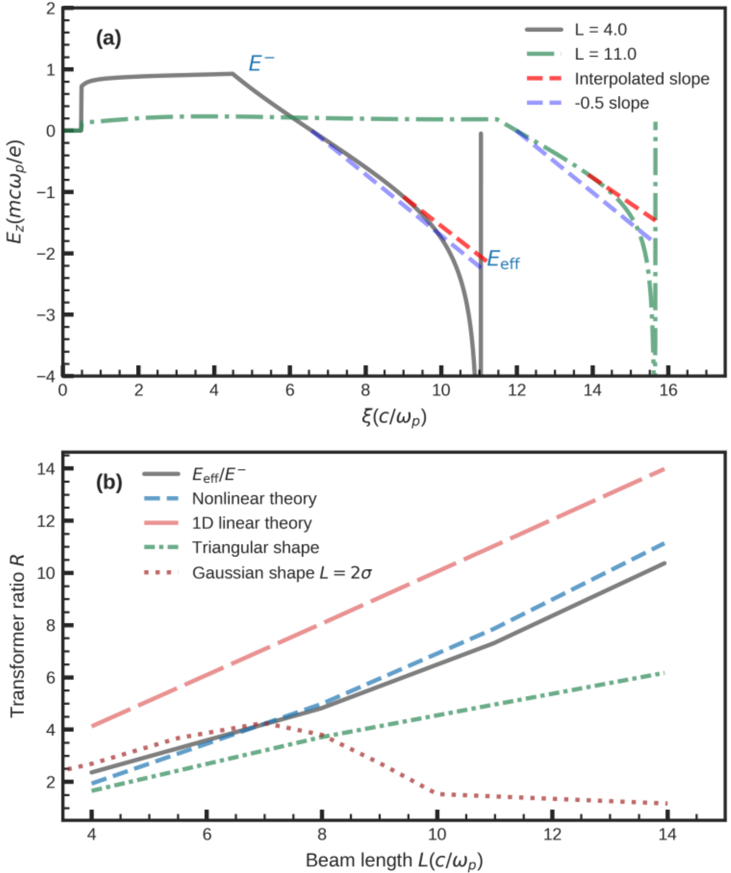
Charge is fixed as $Q = 5nC$

$$E_+ \approx \frac{1}{2} r_m \approx \sqrt{\Lambda_0} \qquad E_+/E_- \approx \sqrt{\Lambda_0}/\left(\frac{\Lambda_0}{L_0}\right) = \frac{L_0}{\sqrt{\Lambda_0}}$$

Use non-uniform bins to resolve the beam profile

Get “perfectly” flattened Ez field under current simulation resolution with objective down to 10^{-5}

The optimized profile has a higher transformer ratio compared with triangular and Gaussian shape

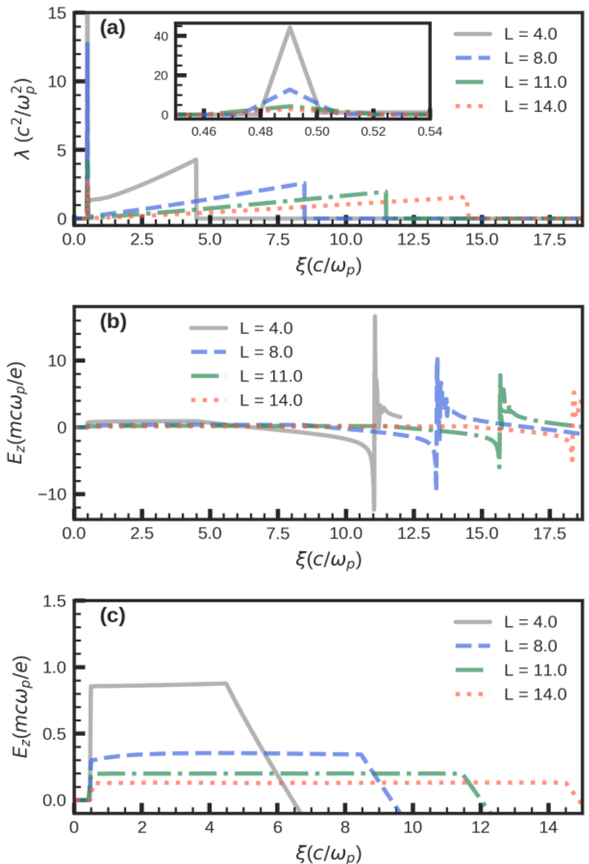


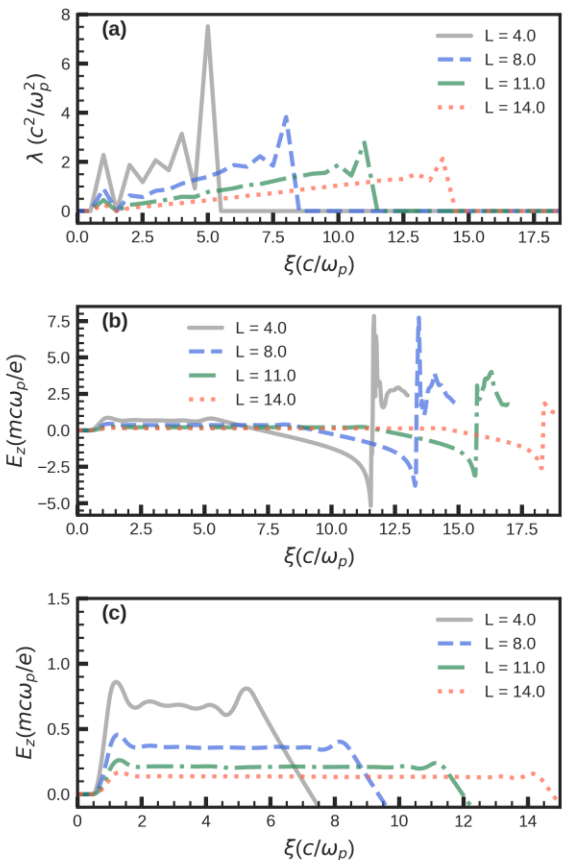
$$Q = 5nC$$

Transformer ratio $R = E_{\mathrm{eff}} / E^-$

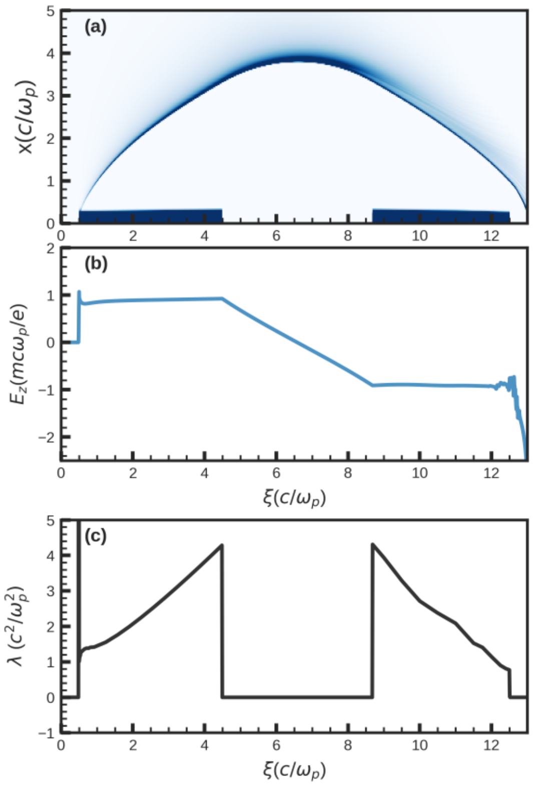
$$E_+ \approx \frac{1}{2} r_m \approx \sqrt{\Lambda_0} \qquad E_+/E_- \approx \sqrt{\Lambda_0} / \left(\frac{\Lambda_0}{L_0}\right) = \frac{L_0}{\sqrt{\Lambda_0}}$$

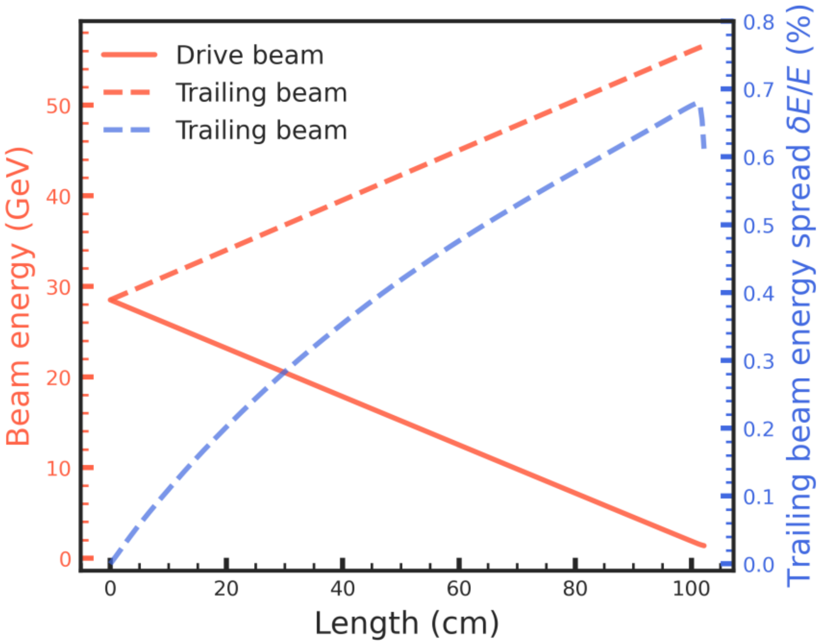
A finite bin size of current profile will give a precursor and oscillation at front and end of the beam





Long range simulation with QPAD shows high efficiency and low energy spread growth





84% efficiency from drive beam to the trailing beam
With an energy spread growth from 0% to less than 0.7%

Summary

- We utilize an optimization tool developed at ANL, to efficiently find optimized drive beam profile and witness beam profile in PWFA

- The algorithm converges quickly, and find witness beams shapes similar to those calculated by a recent multi-sheath model for the nonlinear wakefield

- It can also obtain optimized drive beam profiles that give high transformer ratios with constraint of fixing the total charge

- Some thoughts
  - Modeling of sheath at front of the beam
  - Long range acceleration optimization (surrogate models)

Thanks for your attention!