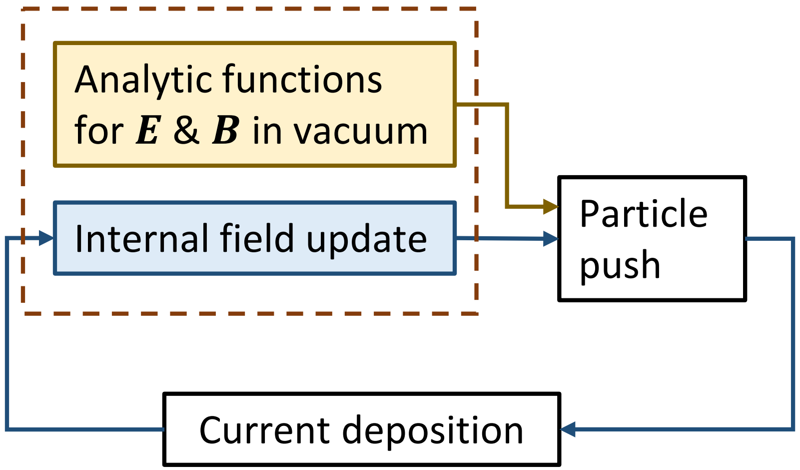
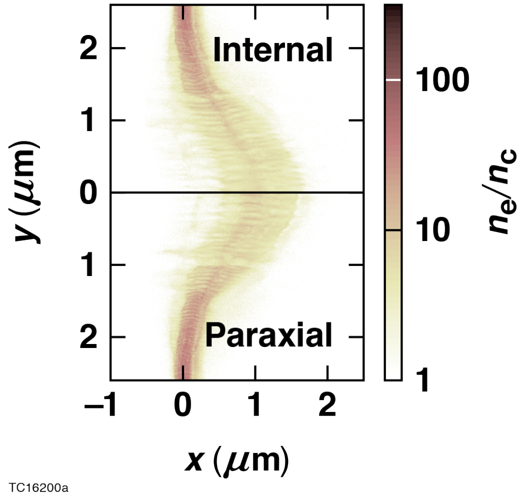
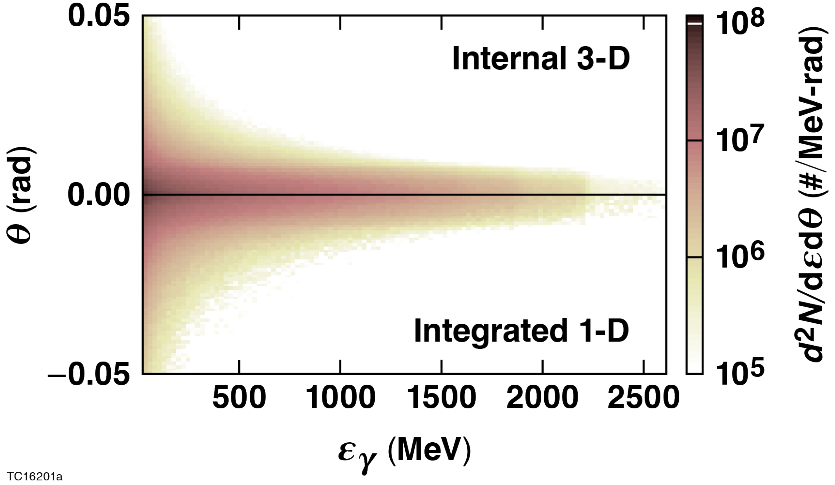
An Alternative Approach to Incorporating Laser Pulses in Particle-in-Cell Simulations



Approximate solutions to Maxwell's equations



Reduced dimensionality simulation



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64th Annual Meeting of the APS Division of Plasma Physics
17 – 21 October 2022

Incorporating laser pulses in particle-in-cell simulation using analytic functions offers a desirable, computationally efficient complement to traditional methods

- Conventional approaches to modeling laser pulses are subject to limitations imposed by the usual electromagnetic field update.
- Splitting the field update to incorporate analytically-defined laser pulses preserves the same total fields when numerical dispersion is matched.
- The modified field update is cost-effective at scale.
- Analytically-defined laser pulses enable new areas of investigation, including
  - Evaluating approximate solutions to Maxwell’s equations
  - Reduced-dimensionality simulation
  - Spatio-temporally shaped (e.g., flying focus) pulses

Collaborators

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XSEDE Extreme Science and Engineering Discovery Environment

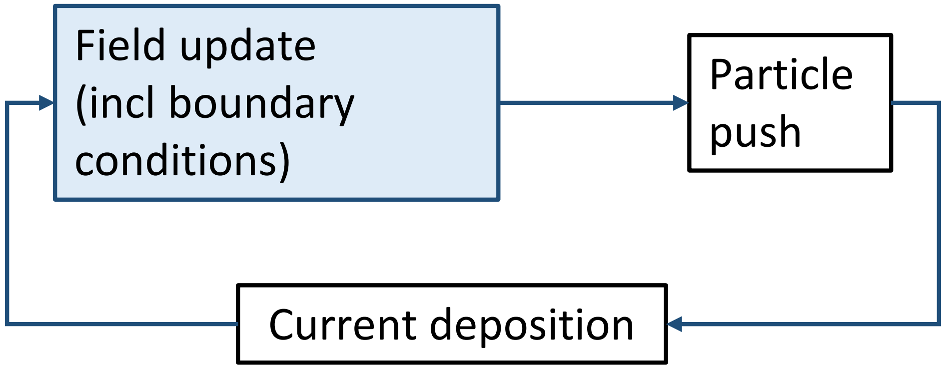
TACC TEXAS ADVANCED COMPUTING CENTER

EPOCH

U.S. DEPARTMENT OF ENERGY Office of Science

The usual electromagnetic field update in particle-in-cell (PIC) simulation requires laser pulses be fully self-consistent, which can have undesirable consequences

”Internal” field update



- **Laser pulses must be full solutions to Maxwell’s equations**
  - **Theory usually involves approximations (e.g., Laguerre-Gaussian beams)**
- **Capturing the effect of focusing on intensity requires 3D simulation**
  - **Expensive when plasma is otherwise 1D-like**
- **Focusing dynamics must be properly captured in the domain/boundary conditions**
  - **Prohibitively expensive and/or complex for pulses with moving focal spots (e.g., spatiotemporally shaped flying focus pulses)**

These limitations can be bypassed by modifying the field update

The linearity of Maxwell's equations allows splitting the electromagnetic field update into two pieces

Separate algorithms for vacuum, plasma response

$$\frac{1}{c}\frac{\partial \boldsymbol{B}_1}{\partial t} = -\nabla \times \boldsymbol{E}_1 \qquad \frac{1}{c}\frac{\partial \boldsymbol{E}_1}{\partial t} = \nabla \times \boldsymbol{B}_1$$

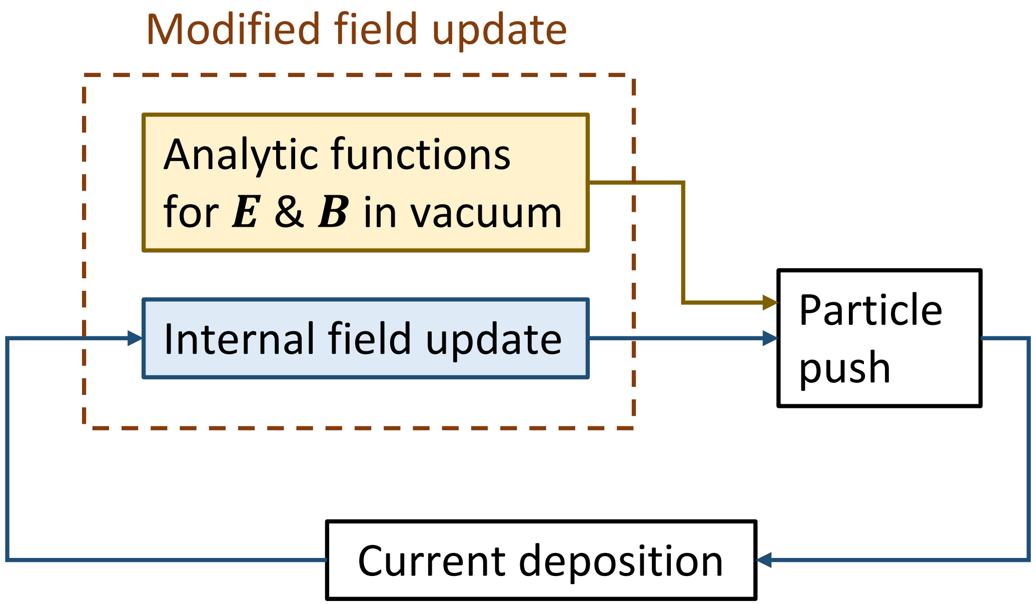
Analytic function

$$\frac{1}{c}\frac{\partial \boldsymbol{B}_2}{\partial t} = -\nabla \times \boldsymbol{E}_2 \qquad \frac{1}{c}\frac{\partial \boldsymbol{E}_2}{\partial t} = \nabla \times \boldsymbol{B}_2 + \frac{4\pi}{c}\boldsymbol{J}$$

Usual internal update

Particle push uses the total fields

$$\frac{d\boldsymbol{p}}{dt} = \boldsymbol{f}(\boldsymbol{E}_1 + \boldsymbol{E}_2, \boldsymbol{B}_1 + \boldsymbol{B}_2)$$



The particle dynamics is unchanged provided the analytic laser pulse is consistent with the numerical implementation of Maxwell's equations used for the plasma response

Analytic laser pulses implemented in the EPOCH PIC code demonstrate good agreement with a fully-internal 2nd order Yee solver

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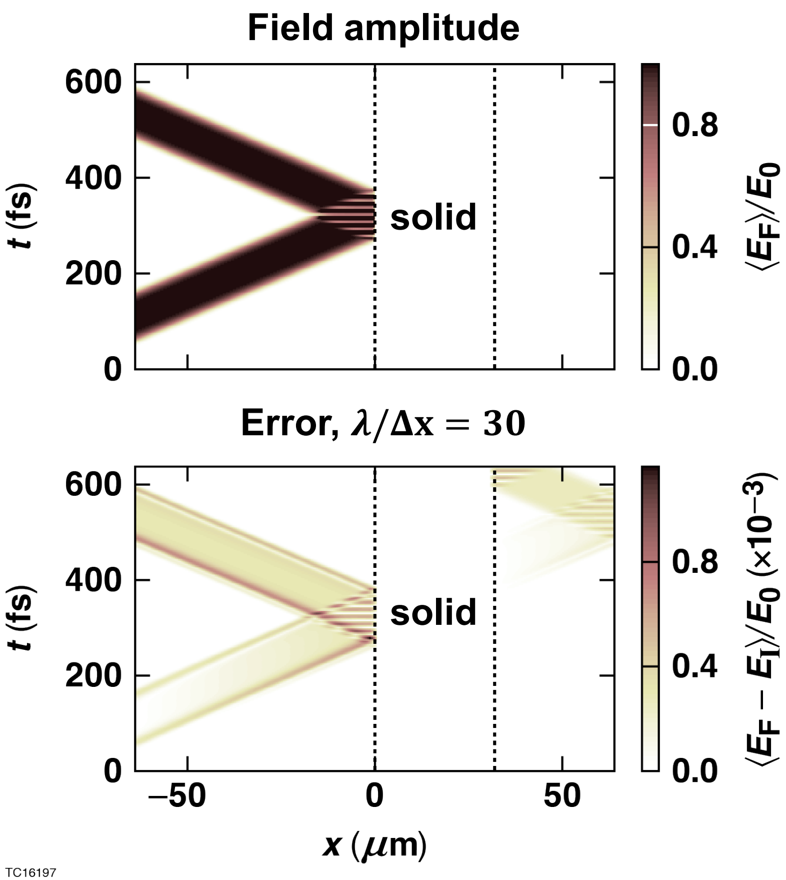
Reflection of low-intensity plane wave from solid



TC16197

Numerical dispersion

$$\frac{v_\phi}{c} \approx 1 - \frac{1}{24}\left[1 - \left(\frac{c\Delta t}{\Delta x}\right)^2\right]\left[\frac{\omega\Delta x}{c}\right]^2 \qquad \frac{v_g}{c} \approx 1 - \frac{1}{8}\left[1 - \left(\frac{c\Delta t}{\Delta x}\right)^2\right]\left[\frac{\omega\Delta x}{c}\right]^2 \qquad \frac{B_0}{E_0} \approx 1 - \frac{1}{2}(\omega\Delta t)^2$$

Monochromatic plane-wave-like approximation

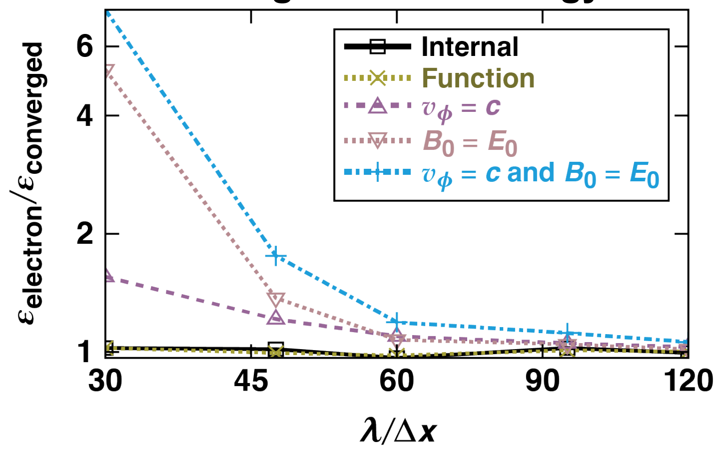
$$E \approx E_0(t - x/v_g)\cos(\omega t - \omega x/v_\phi)$$
$$B \approx B_0(t - x/v_g)\cos(\omega t - \omega x/v_\phi)$$

Analytic laser pulses cannot bypass numerical dispersion

- Unphysical heating at low resolution (e.g., numerical Cerenkov)
- Slow convergence

Test case:
1 mm linear ramp to $n_e = 0.01 n_c$
1 ps FWHM with $a_0 = |e|E_0/mc\omega = 1$

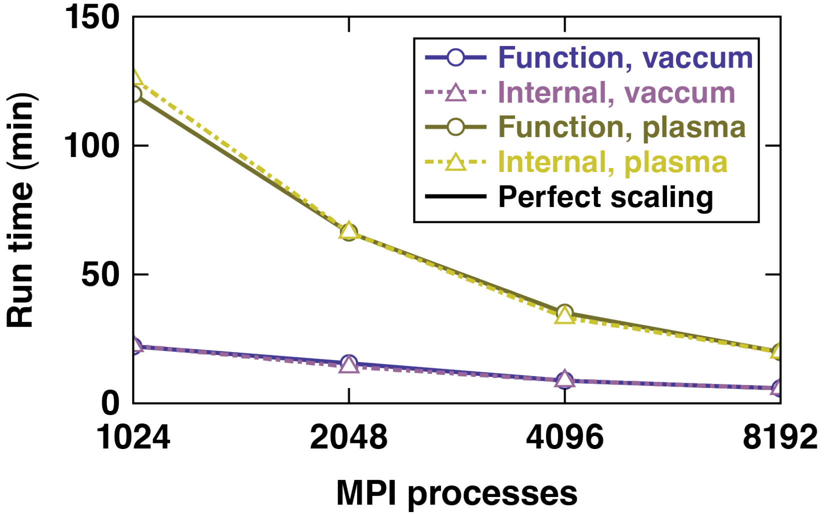
Average electron energy

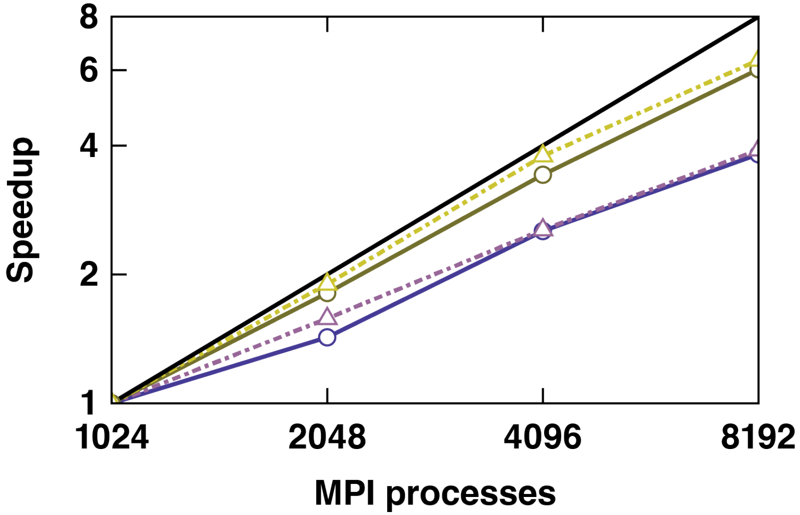


TC16199

The modified field update exhibits similar scaling and performance to the internal field update alone

Strong scaling results (KNL nodes on TACC Stampede2)





TC16198

3D plane wave $100\ fs$ FWHM propagating through box $64\ \mu m \times 8\ \mu m \times 8\ \mu m$ Vacuum or low density $(10^{-6} n_c)$ plasma with 4 ppc

Analytic functions do not significantly affect run time for simulations including a reasonable amount of particles*

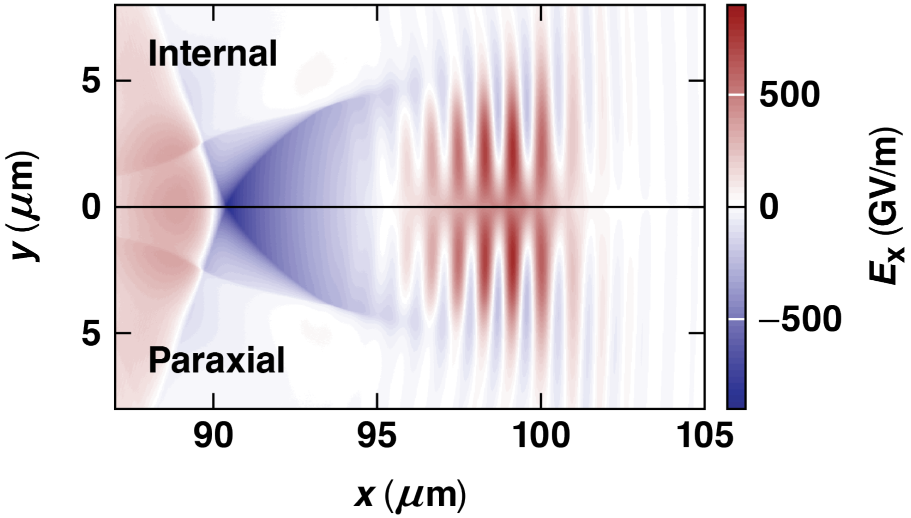
*Provided functions are hard-coded and not overly complex

Applications

The modified field update allows otherwise self-consistent consideration of approximations to Maxwell's equations, e.g., Laguerre-Gaussian pulses

Wakefield acceleration
Good agreement

$8\ \mu m$ FWHM

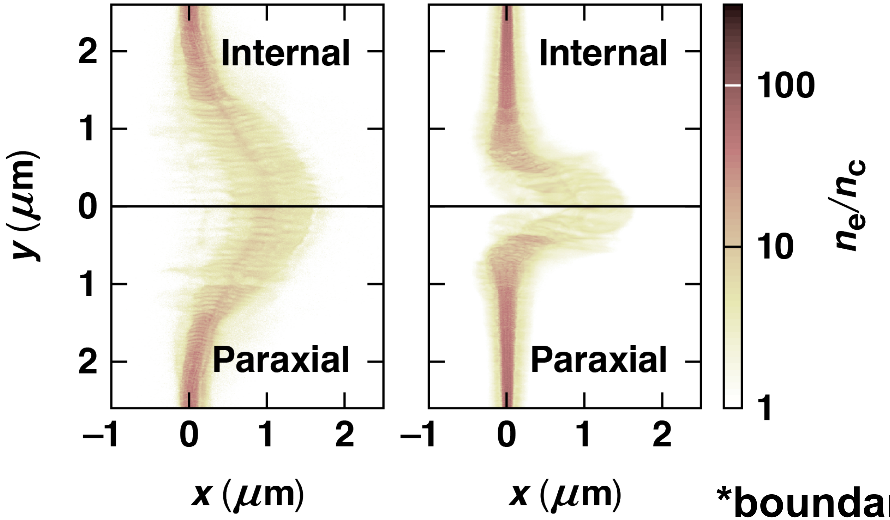


TC16200

$n_e = 0.01 n_c$
$a_0 = |e|E_0/mc\omega = 3$, $15\ fs$ FWHM

Radiation pressure acceleration
Agreement depends on spot size

$3\ \mu m$ FWHM $1\ \mu m$ FWHM*



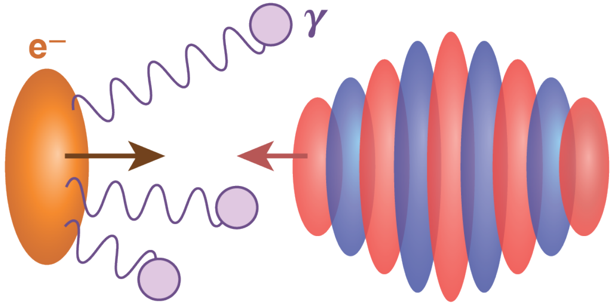
$50\ nm$ thick plastic ($n_e = 180\ n_c$)
$a_0 = |e|E_0/mc\omega = 20$, $15\ fs$ FWHM

*boundary conditions used to launch pulse break down

Incorporation of analytic laser pulses allows direct evaluation of approximations employed in theoretical models

The modified field update allows 1D simulations to capture effects of 3D intensity profile

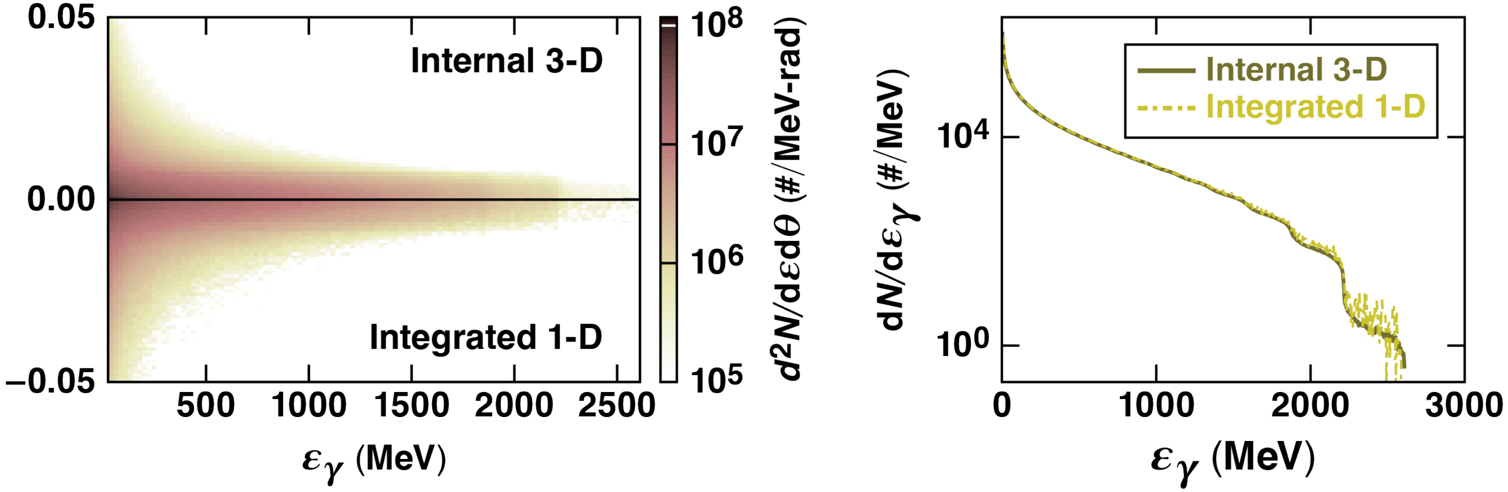
Inverse Compton scattering can be approximately modeled using 1D intensity slices when the electron energy is high



TC16201

$\gamma_e = 5000$, $a_0 = |e|E_0/mc\omega = 50$,
$15\ fs$ and $3\ \mu m$ FWHM

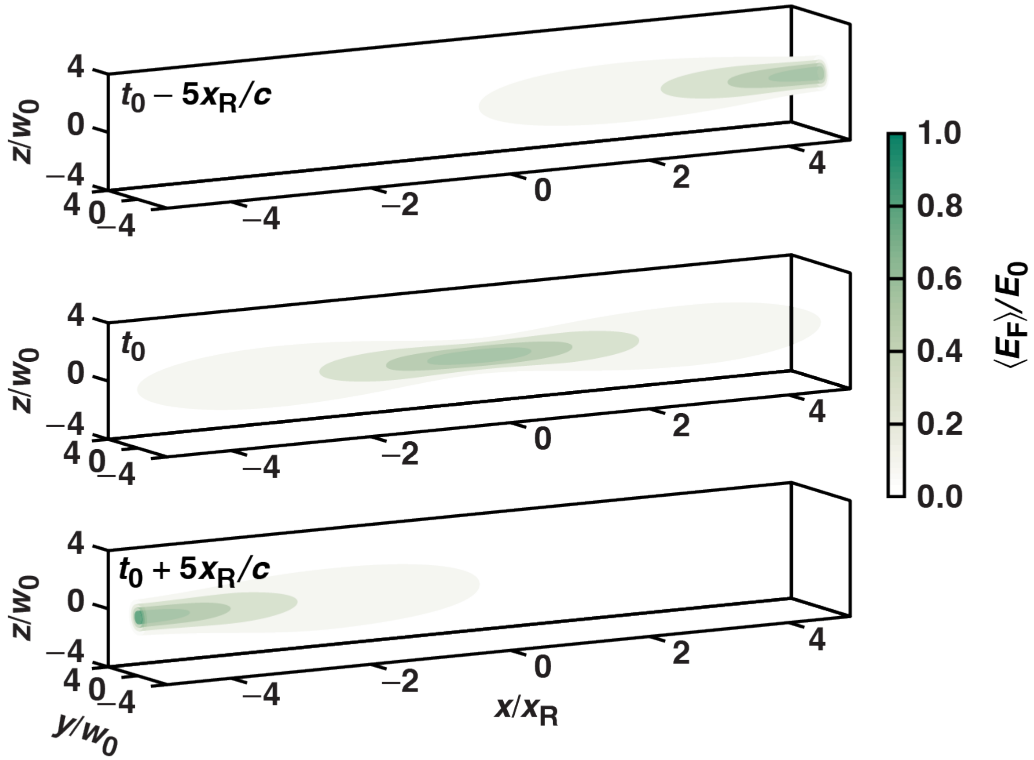
Photon spectra, with 30 radial slices in 1D



3D intensity profile can be captured in 1D simulations, enabling significant cost savings
Results shown: ~40,000x savings

The modified field update enables significant savings and/or reduced complexity for pulses with moving focal position

- Simulations must ordinarily capture beam size at domain boundary, or require non-standard boundary conditions
- For spatiotemporally shaped flying focus pulses, boundary can be many Rayleigh ranges from focus, leading to prohibitive cost and/or complexity



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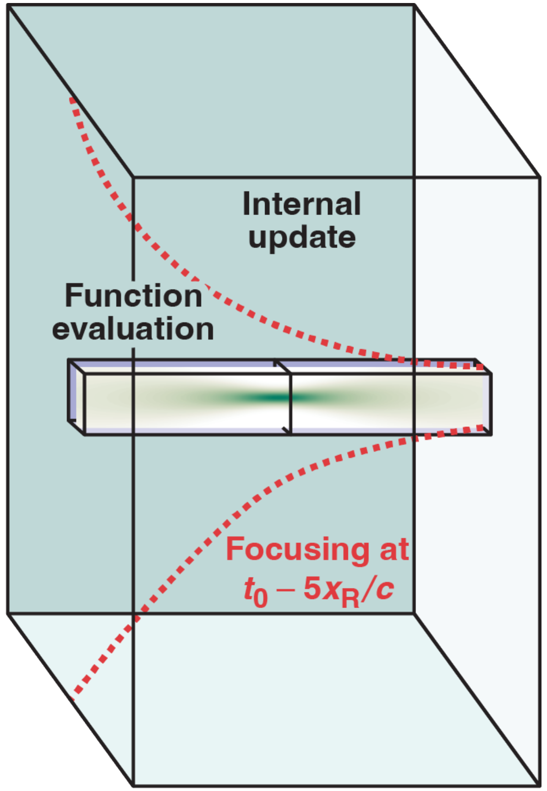

Using analytic laser pulses eliminates the need for multi-boundary antennas and allows simulation box to cover only the high-intensity region

The split field update can be extended to include analytic current (ongoing work)

Analytic functions

$$\frac{1}{c}\frac{\partial \boldsymbol{B}_1}{\partial t} = -\nabla \times \boldsymbol{E}_1 \qquad \frac{1}{c}\frac{\partial \boldsymbol{E}_1}{\partial t} = \nabla \times \boldsymbol{B}_1 + \frac{4\pi}{c}\boldsymbol{J}_1$$

Internal update

$$\frac{1}{c}\frac{\partial \boldsymbol{B}_2}{\partial t} = -\nabla \times \boldsymbol{E}_2 \qquad \frac{1}{c}\frac{\partial \boldsymbol{E}_2}{\partial t} = \nabla \times \boldsymbol{B}_2 + \frac{4\pi}{c}\left(\boldsymbol{J}_{particles} - \boldsymbol{J}_1\right)$$

$J_1 \approx J_{particles}$ may facilitate the modeling of laser pulses when plasma touches the domain boundary

Incorporating analytic laser pulses in particle-in-cell simulation offers a desirable, computationally efficient alternative to traditional injection methods

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