U.S. NAVAL RESEARCH LABORATORY

Opportunities and Issues with the Unitary Particle Pusher

Daniel Gordon, Bahman Hafizi, Dan Younis

Advanced Accelerator Concepts Workshop, Hauppauge, NY
November 6-11, 2022

Quick Survey

<u>This work extends:</u>
D. Gordon et al., AIP Proc. **1812**, 050002 (2017)
D. Gordon et al., Comp. Phys. Comm. **258** 107628 (2021)

<u>Other literature on improving the particle advance</u>:
J.-L. Vay, Phys. Plasmas **15**, 056701 (2008)
A. Arefiev et al., Phys. Plasmas **22**, 013103 (2015)
A. Higuera and J. Cary, Phys. Plasmas **24**, 052104 (2017)
F. Li et al., J. Comp. Phys. **438**, 110367 (2021)

Issues with ultra-relativistic particle advances

In the ultra-relativistic region we have a new type of accuracy condition

$$\Delta s^3 \|\mathcal{F}^{(3)}\|_{\max} \ll 1$$

$$\mathcal{F}^{(3)} = \frac{e^3}{m^3 c^3} \left(\frac{[F_E, [F_E, F_B]]}{24} + \frac{[F_B, [F_E, F_B]]}{12} \right) . \qquad (F = F_E + F_B)$$

Because of the commutators, no scheme that factorizes electric and magnetic contributions to the Lorentz force can overcome this limit (e.g., Boris scheme).

Namely, something like this will never work well:

(new momentum) = (add impulse) (rotate about B) (add impulse) (old momentum)

Special Unitary Particle Pusher

NRL PPD

By making use of the spinor representation of a four-vector, an exact time translation in an arbitrary uniform field can be compactly written

$$\zeta = \begin{pmatrix} u^0 + u^3 & u^1 - iu^2 \\ u^1 + iu^2 & u^0 - u^3 \end{pmatrix}$$

spinor form of the four-momentum

$$\Lambda(\Delta s) = \cosh \Psi + \boldsymbol{\sigma} \cdot \frac{\boldsymbol{\Psi}}{\Psi} \sinh \Psi$$

time translation operator

$$\boldsymbol{\Psi} = \frac{\Delta s}{2} \frac{e}{mc} (\mathbf{E} + i\mathbf{B})$$

Minkowski-type angle

$$\zeta(s + \Delta s) = \Lambda(\Delta s) \zeta(s) \Lambda^{\dagger}(\Delta s)$$

Conservative Expansion Method

We would like to exactly conserve certain quantities

$$\Lambda = \lim_{n\to\infty} \left(1 + \boldsymbol{\sigma} \cdot \boldsymbol{\Psi}/n\right)^n$$

Since this is exact it respects all invariants; however truncation does not

$$\Lambda^{(n)} = \left(1 + \boldsymbol{\sigma} \cdot \boldsymbol{\Psi}/n\right)^{n/2} \left(1 - \boldsymbol{\sigma} \cdot \boldsymbol{\Psi}/n\right)^{-n/2}$$

This form ***does*** respect invariants to round-off

$$\frac{d}{ds} \det \zeta = 0.$$

Invariance of Minkowski norm

$$\frac{d}{ds} \mathrm{tr} \zeta = 0.$$

Invariance of energy *in static B-field*

$$\frac{d}{ds} \mathrm{tr} \left(1 - \boldsymbol{\sigma} \cdot \mathbf{e}_\parallel\right) \zeta = 0$$

Invariance of $\gamma - p_z$ *in a plane wave*

Specific Expansions

$$\Lambda^{(2)} = \frac{1 + \boldsymbol{\sigma} \cdot \boldsymbol{\Psi} + \boldsymbol{\Psi} \cdot \boldsymbol{\Psi}/4}{1 - \boldsymbol{\Psi} \cdot \boldsymbol{\Psi}/4}$$

Quadratic in time step, no special functions or roots, invariance properties accurate to round-off.
N.b. overall advance is quartic.

These are merely 2x2 matrix operations, easy to program

Interesting note: in a plane wave $\Psi \cdot \Psi = 0$, and the lowest order truncation is actually exact!

$$\Lambda^{(1)} = 1 + \sigma \cdot \mathbf{\Psi}$$

Lowest order - exact in a plane wave

Position Update

Spinor representation of spacetime coordinate:

$$\theta = \begin{pmatrix} x^0 + x^3 & x^1 - ix^2 \\ x^1 + ix^2 & x^0 - x^3 \end{pmatrix}$$

Exact solution:

$$\lambda[\theta(s) - \theta(0)] + [\theta(s) - \theta(0)]\lambda^\dagger = \zeta(s) - \zeta(0)$$

$$\lambda = \frac{1}{2}\sigma \cdot (\mathbf{E} + i\mathbf{B})$$

Compare with vector form (cf. Schwinger 1951 eq. 3.3):

$$F[x(s) - x(0)] = u(s) - u(0)$$

(Li et al. use a Taylor expansion of this)

There are some pathologies in the exact expressions, best to use expansion

Possible Issues

$$\zeta = \begin{pmatrix} u^0 + u^3 & u^1 - iu^2 \\ u^1 + iu^2 & u^0 - u^3 \end{pmatrix}$$

Notice round-off can affect diagonal. So far no noticeable issues.

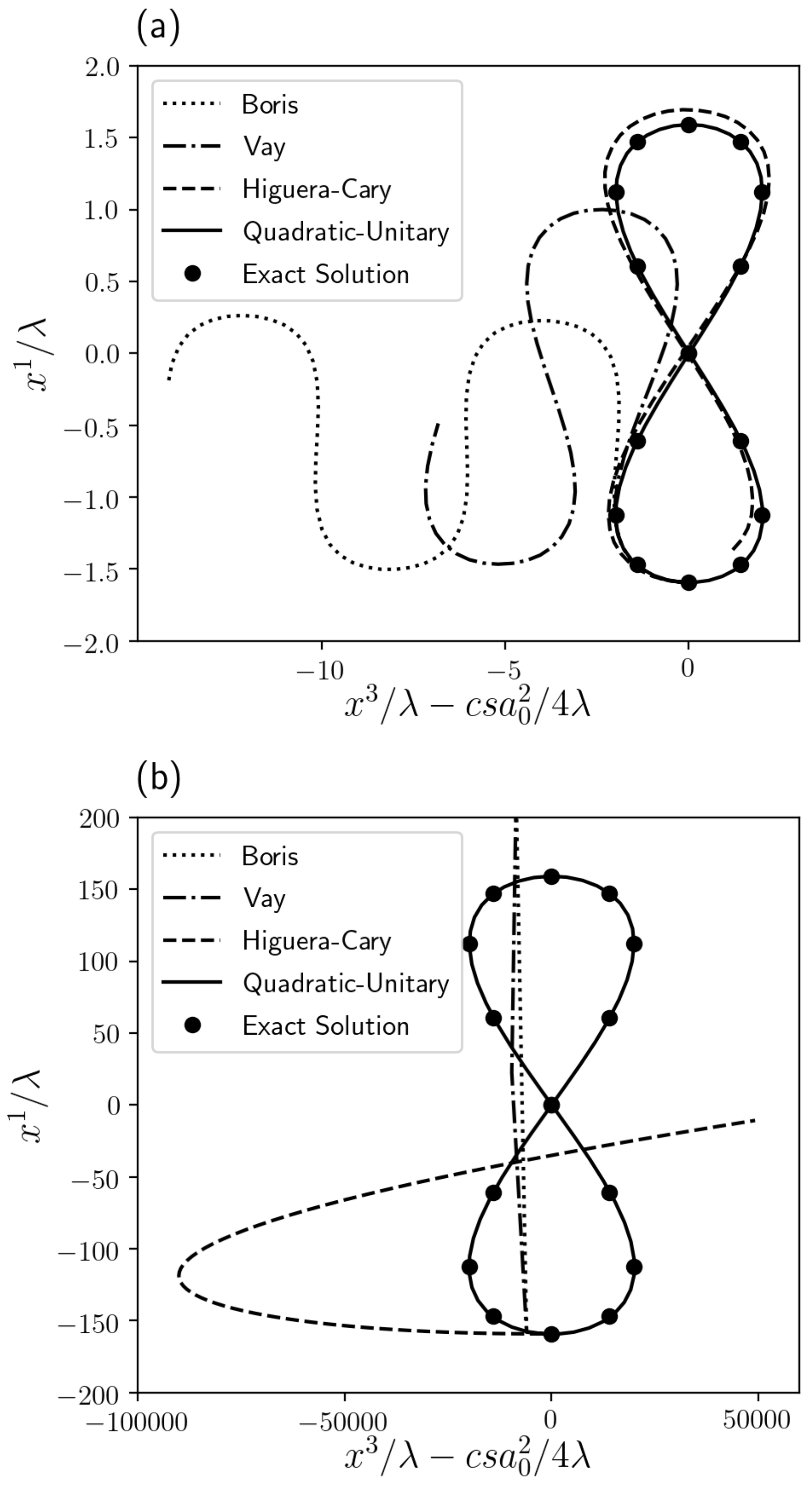
Kinetic energy can come out negative since energy and momentum are updated independently, or put another way, $\gamma \geq 1$ only holds to within a round-off error. So far no noticeable issues.

Is there a directional bias? Since the whole formulation is Lorentz invariant, any directional bias can only be due to round-off error.

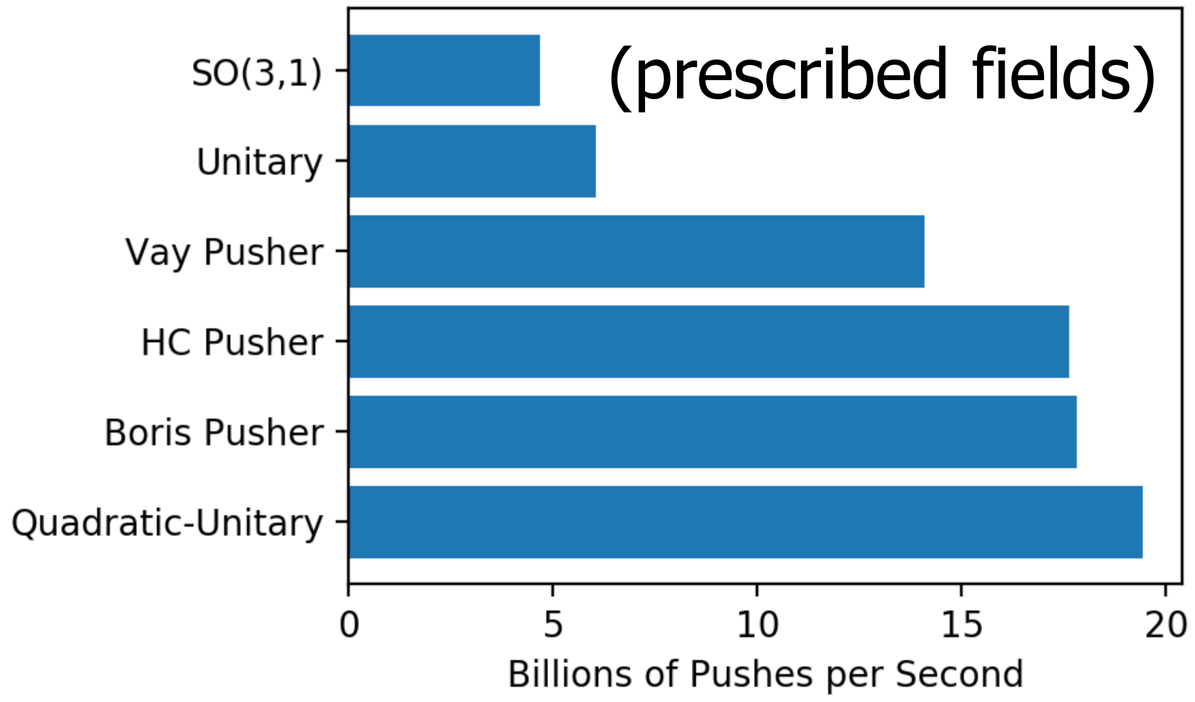
Comparison of Various Methods

a=10

a=1000

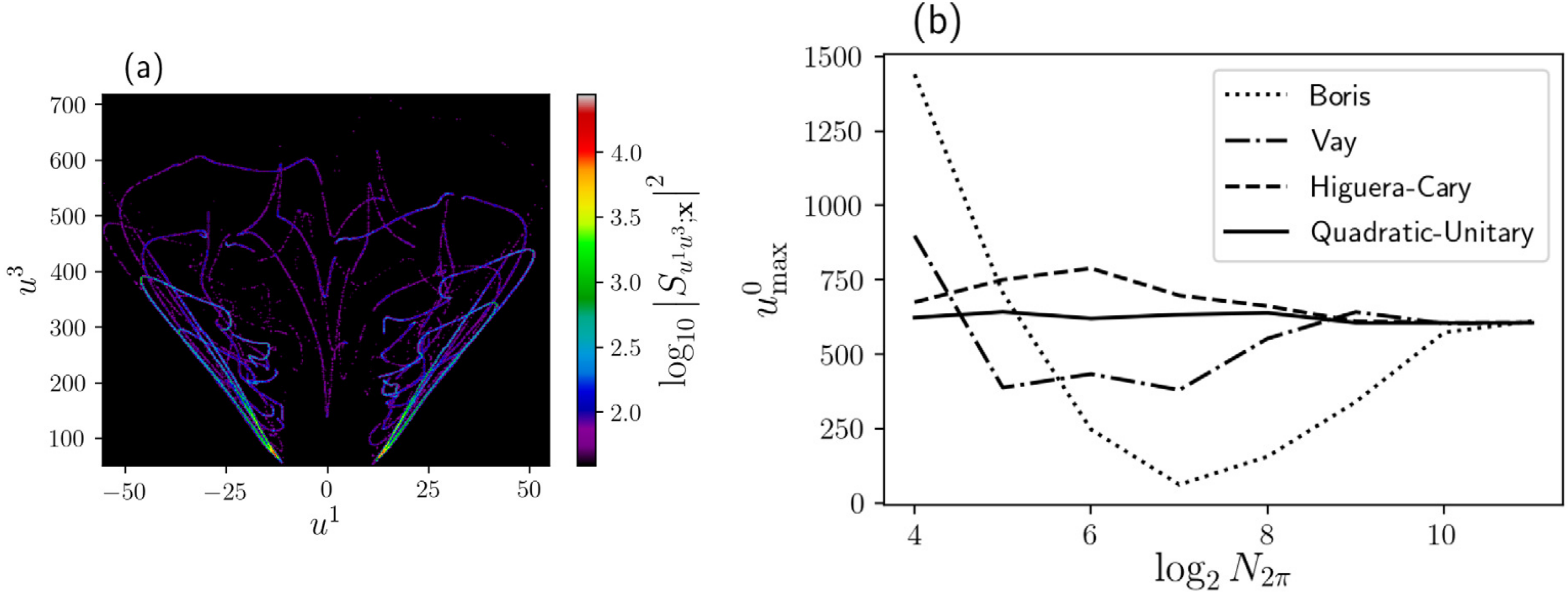


Performance on Titan V



63 steps per period in the particle's frame

Test case for tunneling ionization of H-like argon



Steps to go through 360 deg of phase

Synchronizing particles for PIC applications

NRL PPD

- Require a **time dilation estimate** for each particle

In the spinor view we have $\frac{dt}{ds} = u^0 = \frac{1}{2}\mathrm{tr}\left[\Lambda(s)\zeta(0)\Lambda^\dagger(s)\right]$

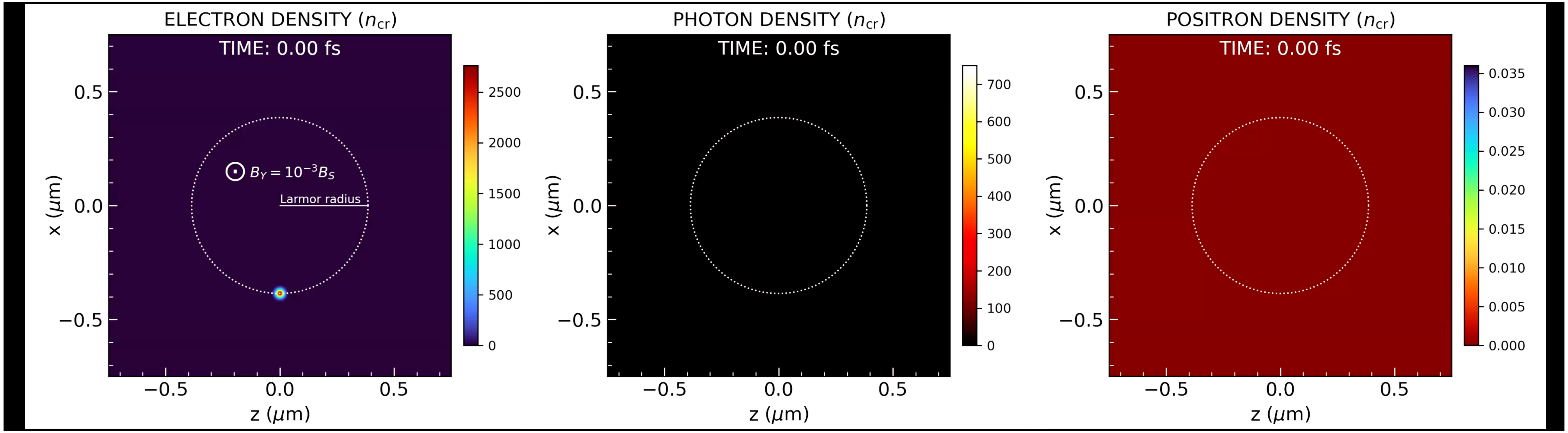
In general this leads to a root-finding problem. A simple estimate is

$$\Delta s = \frac{\Delta t}{u^0} - \frac{e\mathbf{E}\cdot\boldsymbol{u}}{2(u^0)^3 mc}\Delta t^2 + O(\Delta t^3)$$

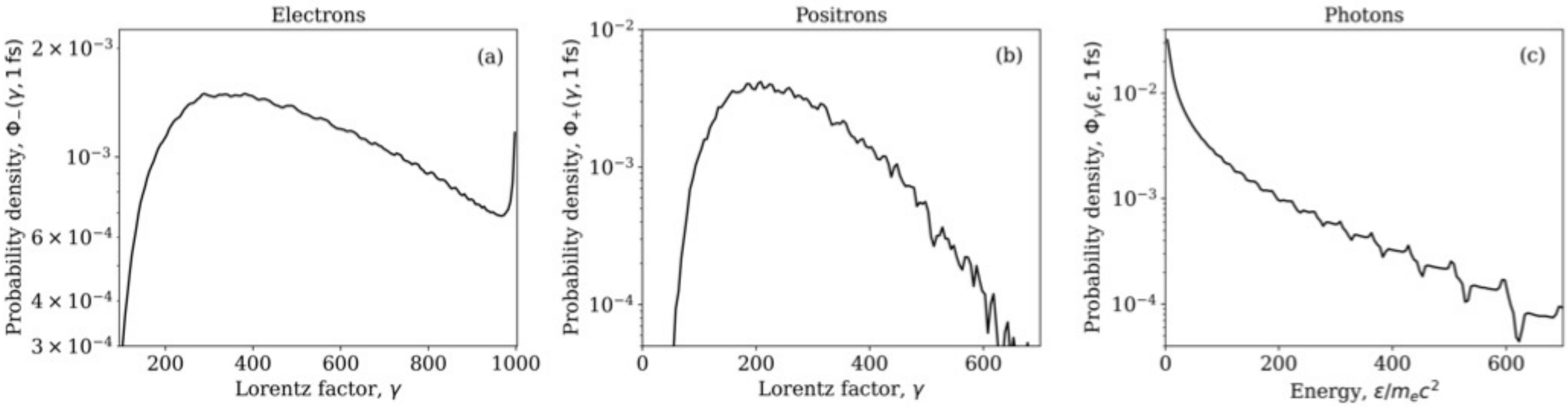
This is used in all that follows, but a more accurate estimate is being put in

turboWAVE QED Module Example: uniform QED-scale magnetic field

Load Gaussian electron bunch with γ=1000 into $B = B_S/1000$



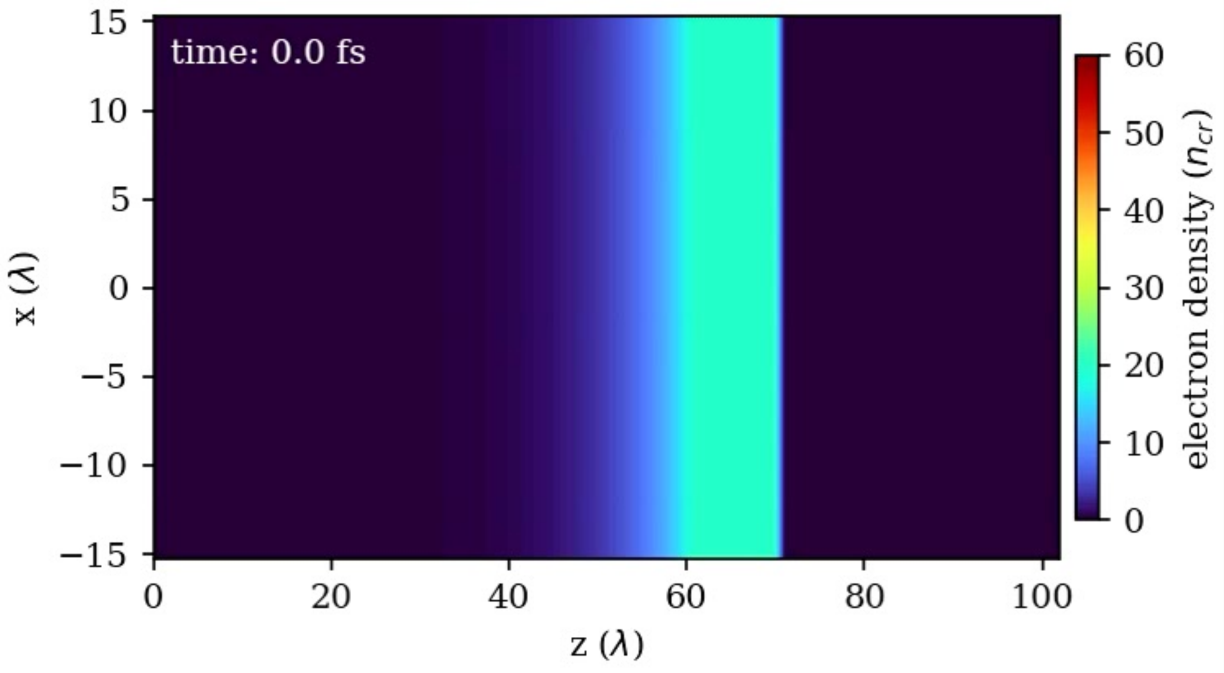
turboWAVE QED Module Benchmarking

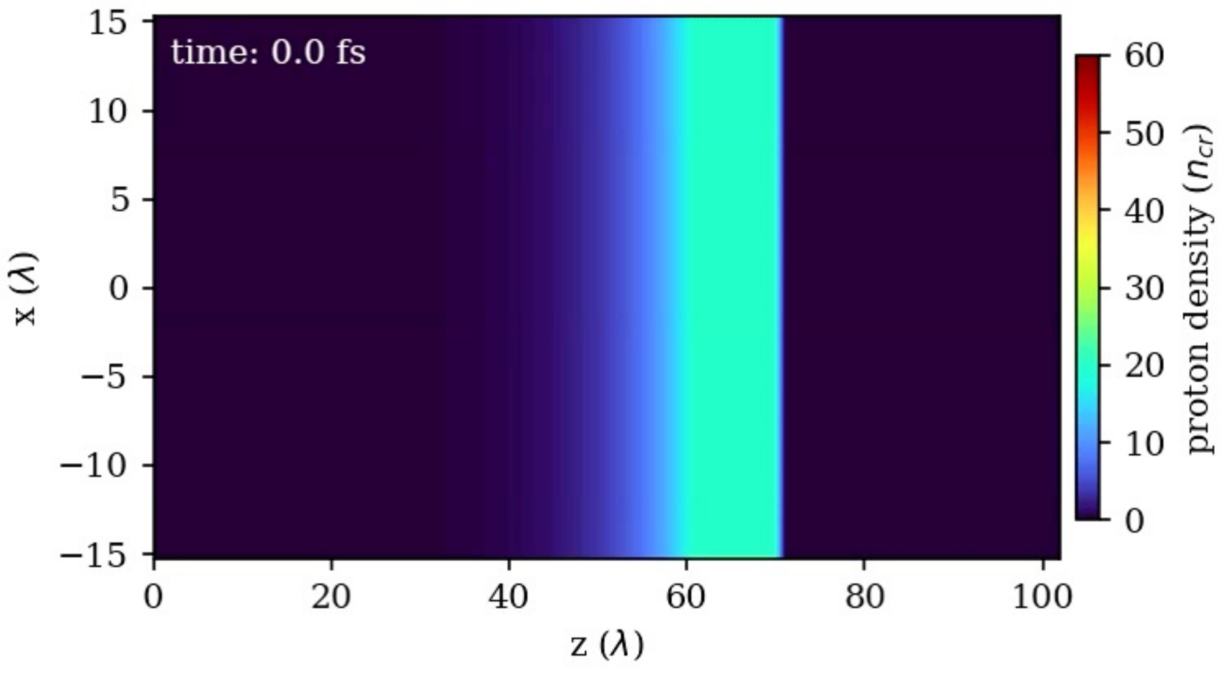


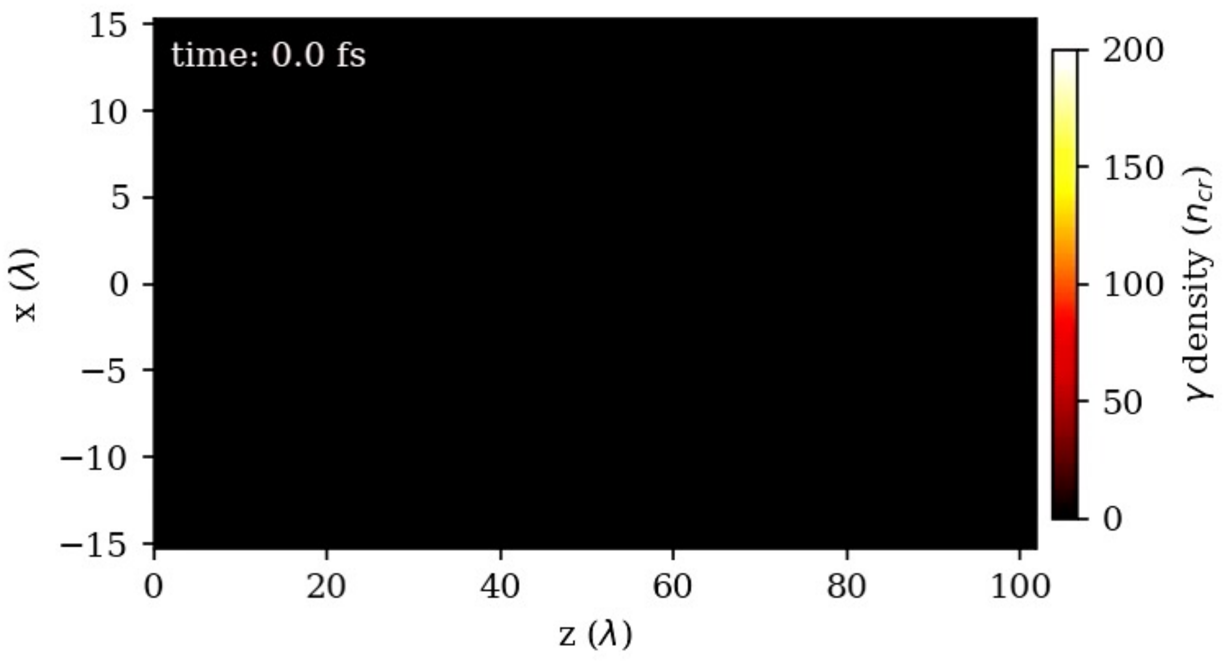
Cf. similar figure in J. Comp. Phys. **260**, 273 (2014)

QED-PIC example with unitary pusher

Example showing gamma generation with multi-PW pulse and thin target







<u>Laser parameters</u>

a = 380, I = 2e23 w/cm^2

λ = 1 um, τ = 30 fs, r = 5 um

<u>Plasma parameters</u>

Pre-plasma = 40 um

Slab = 10 um

n = 20n_{crit}

Summary

- Unitary Pusher has been developed and implemented in turboWAVE
- This respects important invariance properties even when truncated
- Pusher is fast
- QED-PIC simulations are a natural application
- So far everything working satisfactorily
- Time dilation estimate is being improved