Opportunities and Issues with the Unitary Particle Pusher

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Distribution A. Approved for public release.
This work extends:
D. Gordon et al., Comp. Phys. Comm. 258 107628 (2021)

Other literature on improving the particle advance:
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

\[ \Delta s^3 \| F^{(3)} \|_{\text{max}} \ll 1 \]

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

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:

\[ \text{(new momentum)} = \text{(add impulse)} \text{(rotate about } B) \text{(add impulse)} \text{(old momentum)} \]
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

\[
\Lambda(\Delta s) = \cosh \Psi + \sigma \cdot \frac{\Psi}{\Psi} \sinh \Psi
\]
time translation operator

\[
\Psi = \frac{\Delta s}{2} \frac{e}{mc} (E + iB)
\]
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

\[ \Lambda = \lim_{n \to \infty} (1 + \sigma \cdot \Psi / n)^n \]

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

\[ \Lambda^{(n)} = (1 + \sigma \cdot \Psi / n)^{n/2} (1 - \sigma \cdot \Psi / n)^{-n/2} \]

This form \textbf{does} respect invariants to round-off

\[ \frac{d}{ds} \det \zeta = 0. \quad \text{Invariance of Minkowski norm} \]

\[ \frac{d}{ds} \text{tr} \zeta = 0. \quad \text{Invariance of energy in static B-field} \]

\[ \frac{d}{ds} \text{tr} (1 - \sigma \cdot e_\parallel) \zeta = 0 \quad \text{Invariance of } \gamma - p_z \text{ in a plane wave} \]
Specific Expansions

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

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!

\[ \Lambda^{(1)} = 1 + \sigma \cdot \Psi \]

Lowest order - exact in a plane wave.
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:

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

$$\lambda = \frac{1}{2} \sigma \cdot (E + iB)$$

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
Special Unitary Time Translation

This section derives the unitary form of the exact time translation operator of the four-momentum in a constant, uniform, electromagnetic field, with arbitrary polarization. Ordinarily one has a four-velocity $u^\mu$, satisfying the equation of motion

$$m \frac{du^\mu}{ds} = eF^\mu\nu \nu, \text{ where } s \text{ is the proper time.}$$

For constant, uniform fields, the exact solution is furnished by taking the matrix exponential. The expression for the matrix exponential is tractable, but somewhat onerous, even after employing a rotation to simplify it [5]. The particle pusher obtained this way is exactly Lorentz invariant. Preservation of the Euclidean norm of the velocity in a magnetic field is merely a special case.

In order to obtain an equivalent pusher that can be expressed more easily, we employ the relationship between four-vectors and second rank spinors [11].

Let $\gamma$ be the $2 \times 2$ matrix representing the spinor that represents momentum. Then

$$u^\mu = \frac{1}{2} \text{tr}(\gamma^\mu) \quad (3)$$

Here $\mu$ are the Pauli matrices if $\mu = [1, 2, 3]$ and the identity if $\mu = 0$. The inverse operation gives the matrix

$$\gamma = u_0 + u_3 u_1 + iu_2 u_0$$

The steps used in [11] to derive the boost and rotation operators are a useful guide in deriving the operator of time translation. Let the time translation operator be denoted $\gamma(s)$, where $s$ is any interval in proper time. The spinor is transformed as

$$\gamma(s + s') = \gamma(s') \gamma(s) \gamma(s')^\dagger \quad (5)$$

It is useful to define the generator $\gamma$ by

$$\gamma(ds) = 1 + ds \gamma.$$ The equation of motion for $\gamma$ is then

$$\frac{d\gamma}{ds} = \gamma + \gamma^\dagger. \quad (6)$$

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

$a=10$

$a=1000$

63 steps per period in the particle’s frame
Test case for tunneling ionization of H-like argon

![Diagram](image_url)

Steps to go through 360 deg of phase

Interagency Agreement 89243018SSC000006.
Synchronizing particles for PIC applications

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

In the spinor view we have

$$\frac{dt}{ds} = u^0 = \frac{1}{2} \text{tr}\left[\Lambda(s)\zeta(0)\Lambda^+(s)\right]$$

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

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

This is used in all that follows, but a more accurate estimate is being put in
Load Gaussian electron bunch with $\gamma=1000$ into $B=B_S/1000$
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

**Laser parameters**
\[ a = 380, \quad I = 2 \times 10^{23} \text{ w/cm}^2 \]
\[ \lambda = 1 \text{ um}, \quad \tau = 30 \text{ fs}, \quad r = 5 \text{ um} \]

**Plasma parameters**
\[ \text{Pre-plasma} = 40 \text{ um} \]
\[ \text{Slab} = 10 \text{ um} \]
\[ n = 20n_{\text{crit}} \]

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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