Advances in simulation capability: A path towards modeling 10-100GeV plasma accelerator stages

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Collaborators:
And E-164x collaboration

http://exodus.physics.ucla.edu
Concepts For Plasma Based Accelerators

- Plasma Wake Field Accelerator (PWFA)
  A high energy electron bunch

- Laser Wake Field Accelerator (LWFA, SMLWFA, PBWA)
  A single short-pulse of photons

Need to model:
- Wake excitation: need to resolve $\omega_p, \lambda_p$
- Evolution of drive beam: evolves on $\beta$ and/or $x_R >> \sigma_z$ scales
- Evolution of trailing beam: need to run pump depletion distances

To model all of these necessitates particle-in-cell models
What Is a Fully Explicit Particle-in-cell Code?

Computational cycle
(at each step in time)

- Maxwell’s equations for field solver
- Lorentz force updates particle’s position and momentum

\[ \frac{d\vec{p}}{dt} = \vec{E} + \vec{v} \times \vec{B}/c \]

\[ \rho_{n,m}, \vec{J}_{n,m} \]

\[ \vec{E}_{n,m}, \vec{B}_{n,m} \]

Particle positions \( z_i, v_i \)

Typical simulation parameters:
- \( \sim 10^7-10^9 \) particles
- \( \sim 1-100 \) Gbytes
- \( \sim 10^5 \) time steps
- \( \sim 10^2-10^5 \) cpu hours
Computational challenges for modeling plasma-based acceleration (1 GeV Stage): 5000 hours/ GeV

<table>
<thead>
<tr>
<th>Beam-driven wake*</th>
<th>Fully Explicit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Δz</td>
<td>≤ .05 c/ωp</td>
</tr>
<tr>
<td>Δy, Δx</td>
<td>≤ .05 c/ωp</td>
</tr>
<tr>
<td>Δt</td>
<td>≤ .02 c/ωp</td>
</tr>
<tr>
<td># grids in z</td>
<td>≥ 350</td>
</tr>
<tr>
<td># grids in x, y</td>
<td>≥ 150</td>
</tr>
<tr>
<td># steps</td>
<td>≥ 2 x 10⁵</td>
</tr>
<tr>
<td>N_{particles}</td>
<td>~.25-1. x 10⁸ (3D)</td>
</tr>
<tr>
<td>Particles x steps</td>
<td>~.5 x 10¹³ (3D) - ≥ 5000 hrs</td>
</tr>
</tbody>
</table>

*Laser-driven GeV stage requires on the order of (ω_0/ω_p)^2=1000 x longer, however, the the resolution can usually be relaxed (~200,000 hours).*
Plasma Accelerators and the Livingston Curve

C. Joshi and T. Katsouleas, Physics Today, June 2003
One goal is to build a virtual accelerator:
A 100 GeV-on-100 GeV e⁻e⁺ Collider
Based on Plasma Afterburners
Motivation:

• Particle models are required but full PIC codes are too CPU intensive to model GeV LWFA stages and/or 100 GeV PWFA stages in three dimensions.
• Real time feedback between simulation and experiment is not possible

• What is the solution?

  • “Exploit” the physics: utilize the huge disparity in time scales.

  • In 1997 Whittum (PWFA) and Antonsen and Mora (LWFA) independently wrote particle-in-cell codes that made the frozen field or quasi-static approximation.

• We have used some of these ideas to construct a fully three dimensional, fully parallelized, quasi-static PIC code that can model PWFA/LWFA plus beam loading: QUICKPIC
QuickPIC:
quasi-static PIC + fully parallelized+ fully 3D

- Quasi-static approximation: driver evolves on a much longer distances than wake wavelength
  - Frozen wakefield over time scale of the bunch length

  • => $\beta$ and/or $x_R >> \sigma_z$ (very good approximation!)

  • Includes the best ideas from Antonsen and Mora with Whittum
Basic equations for approximate QuickPIC

• Quasi-static or frozen field approximation converts Maxwell’s equations into electrostatic equations
• Use ideas from Whittum 1997

Maxwell equations in Lorentz gauge

\[
\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right) A = \frac{4\pi}{c} j
\]

\[
\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right) \phi = 4\pi \rho
\]

\[\text{Quasi-static approx.}\]

\[\phi, A = \varphi, A(z - ct)\]

\[-\nabla^2 A = \frac{4\pi}{c}\]

\[-\nabla^2 \phi = 4\pi \rho\]

Local—\(\phi, A\) at any z-slice depend only on \(\rho, j\) at that slice!

\[\text{Forces:}\]

\[\text{plasma: } F_{e\perp} = -e\nabla \perp \phi\]

\[\text{beam: } F_{b\perp} = -e\nabla \perp \Psi\]

\[j = j_b + j_e \approx j_b = c \rho_b \hat{z}\]

\[(A = A_{\|} \hat{z})\]
Quasi-static PIC code

Beam evolves due to betatron oscillation determined by:

\[ k_\beta = \frac{k_p}{\sqrt{2\gamma_b}} \]

\( n\Delta s \) \hspace{1cm} \( (n+1)\Delta s \) \hspace{1cm} \( (n+2)\Delta s \)
Parallelization of QuickPIC
Full QuickPIC: PWFA or LWFA

- The axial motion of the plasma can be important! Need to include it.
- Use ideas from Antonsen and Mora 1997

Reduced Maxwell equations

\[-\nabla^2_A = \frac{4\pi}{c} \mathbf{j}\]
\[-\nabla^2 \phi = 4\pi \rho\]

\[\rho = \sum_{\text{particles}} \frac{q_i}{1 - v_{\parallel i}}\]
\[\vec{j} = \sum_{\text{particles}} \frac{q_i}{1 - v_{\parallel i}} \vec{v}\]

\[\bar{\gamma} - p_{\parallel} = 1 - q \psi\]
\[\bar{\gamma} = (1 + p^2 + a^2 / 2)^{1/2}\]
\[\psi = \phi - A_{\parallel}\]

For beam electrons:
\[\frac{\partial p_b}{\partial \xi} = -\frac{q_b}{c} \left[ \mathbf{E} + \frac{V_b}{c} \times \mathbf{B} \right] = -\frac{q_b}{c} \nabla \psi\]

For plasma electrons:
\[\frac{\partial p_{e\perp}}{\partial \xi} = \frac{q_e}{c - V_{e\parallel}} \left[ \mathbf{E}_{\perp} + \left( \frac{V_e}{c} \times \mathbf{B} \right)_{\perp} \right]\]

For laser beam
\[\left( 2i\omega \partial_{\tau} - 2\partial_{\tau \xi} - \nabla^2_{\perp} \right) a = \chi \ a\]
\[\chi = -\sum q \bar{\gamma} - p_{\parallel}\]
Assuming OSIRIS runs at a speed of 3\(\mu s\) per particle timestep (on SP3 processor), with 256 \(\times\) 256 \(\times\) 256 grids and 4 particles per cell, beam particles gain 1GeV in 0.1m (acceleration gradient is 10Gev/m).

For 50Gev energy gain, **250,000** node-hours is needed for the OSIRIS simulation.

<table>
<thead>
<tr>
<th>Simulation Codes</th>
<th>Feature</th>
<th>Grid size limit</th>
<th>Timestep limit</th>
<th>Total time of simulation per GeV stage (node-hour)</th>
</tr>
</thead>
<tbody>
<tr>
<td>OSIRIS</td>
<td>Full electromagnetic PIC code</td>
<td>(\approx 0.05c/\omega_p)</td>
<td>(\Delta t &lt; 0.05\omega_p^{-1})</td>
<td>5,234</td>
</tr>
<tr>
<td>QuickPIC</td>
<td>Quasi-static PIC code, beam, plasma evolution time scale separated</td>
<td>(\approx 0.05c/\omega_p)</td>
<td>(\Delta t &lt; 0.05\omega_{\beta}^{-1}) (= 0.05 \times \sqrt{2\gamma \omega_p^{-1}})</td>
<td>67</td>
</tr>
</tbody>
</table>

**Potential savings for PWFA**
Benchmark result of longitudinal wakefield between QuickPIC and 2D OSIRIS for both

**a)** electron drive beam \( \frac{n_b}{n_p} = 25.9 \) and **b)** positron drive beam \( \frac{n_b}{n_p} = 15.2 \)
# Full 3D Simulation parameters

<table>
<thead>
<tr>
<th>Beam shape</th>
<th>E164X</th>
<th>Afterburner</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plasma Density</td>
<td>$n=1.6\times10^{17}\text{cm}^{-3}$</td>
<td>$n=5.66\times10^{16}\text{cm}^{-3}$</td>
</tr>
<tr>
<td>Beam charge</td>
<td>$N=1.8\times10^{10}$</td>
<td>$N_{\text{drive}}=3\times10^{10}$, $N_{\text{trailing}}=1\times10^{10}$</td>
</tr>
<tr>
<td>Longitudinal:</td>
<td>Drive beam : wedge shape, $L=145\mu\text{m}=6.5c/\omega_p$</td>
<td>Trailing beam : Gaussian profile, $\sigma_z=10\mu\text{m}=0.45c/\omega_p$</td>
</tr>
<tr>
<td>Transverse: Gaussian profile, $\sigma_r=12\mu\text{m}=0.9c/\omega_p$</td>
<td>Transverse: Gaussian profile, $\sigma_r=15\mu\text{m}=0.67c/\omega_p$</td>
<td></td>
</tr>
</tbody>
</table>
Even in Blowout regime, bunch shaping can lead to higher transformer ratios.

Bi-Gaussian shape, $\sigma_z = 1.2 \ c/\omega_p$, $n_b/n_p = 26$

Wedge shape, beam length = $18 \ c/\omega_p$, $n_b/n_p = 3$

Wedge shape, beam length = $6 \ c/\omega_p$, $n_b/n_p = 8.4$
Ideal beam loading scenarios can be found

Trailing beam spot size and charge

$N_{\text{drive}} = 3 \times 10^{10}$, $N_{\text{trailing}} = 1 \times 10^{10}$

$N_{\text{drive}} = 3 \times 10^{10}$, $N_{\text{trailing}} = 0.5 \times 10^{10}$
Afterburner simulation
Minimal hosing!

1) Matched wedge shape drive beam with trailing bi-Gaussian beam.

2) Background plasma density.
50 Gev energy gain in 3 meters!

Accelerating field
24GeV/m at the load
QuickPIC provides the proper LWFA wakes

Laser wakefield in a near-1D QuickPIC benchmark run

Benchmarked against Theory and OSIRIS
Axial Electric Field

\[ \xi = ct - z \]

Laser Pulse

1.8 nC electron bunch
25 MeV injection energy

Reduced amplitude due to effects of beam loading
Full-PIC is still needed!

1. When self-trapping is important
2. For benchmarking
3. For moderate energy beams

OSIRIS, VORPAL, TurboWAVE ....
Simulation Parameters

- Laser:
  - $a_0 = 3$
  - $W_0 = 9.25 \lambda = 7.4 \, \mu m$
  - $\omega_l/\omega_p = 22.5$

- Particles
  - 1x2x2 particles/cell
  - 240 million total

- Channel length
  - $L = 0.828 \, \text{cm}$
  - 300,000 timesteps

The parameters are similar to those at LOA and LBNL.
Evolution of laser leads to self-injection

(b) y
-28μm

(ê) z

28μm

.24cm

.43cm

.64cm

x (k)

Density (n_e)

0

5.0

Phasespace p1x1
Time - 964.80 [1/ω_p]

Phasespace p1x1
Time - 1507.80 [1/ω_p]
Nanocoulombs of charge is accelerated

First Bunch
- Total Charge: 0.519 nC
- Beam well-confined within the channel

Second Bunch
- Total Charge: 0.663 nC
- Emittance: 18.81 µm (along b) 40.89 µm (along e)

\[
\left[ \varepsilon_N \right]_i = \frac{\pi}{c} \left[ \left( \frac{\Delta u_i^2}{\Delta x_i^2} \right) - \left( \frac{\Delta x_i \Delta u_i}{\Delta x_i^2} \right)^2 \right]^{1/2}
\]
Wakes can be produced in field ionized produced plasma by either Laser or Particle beam drivers: OSIRIS

LWFA

PWFA
Summary and future work:

- **quasi-static PIC (QuickPIC)**
  - It works! Can reproduce full PIC results at .01 the cost.
  - 50 GeV stages can be modeled in ~1000 node hours
  - E-164x can be modeled in ~500 node hours
  - Laser field solve is now working and simulations are beginning
  - Also being used to model the e-cloud problem for circular accelerators
- Full PIC is alive and well: OSIRIS, VORPAL, TurboWAVE .....  
  - 3D with ionization
  - GeV LWFA acceleration in a plasma channel

**Future work for QuickPIC:**
- Dynamic load balancing (a first pass should be completed in 1 month)
- Ionization (work will begin over the summer)
- Mesh refinement to handle tightly focused matched beams
- A recipe for handling self-trapped particles
QuickPIC is being applied to “mainstream” accelerator problems:
  e-cloud

For high current circular accelerators the limiting issue is E-cloud.

The e-cloud is seeded by the beam halos or synchrotron radiation hitting the walls.

The proton/positron electron cloud mechanism is very similar to beam plasma interactions.
Study of the Long Term Beam Dynamics

3 snapshots of beam over CERN-SPS ring. a) At $t_0=0.4\text{ms}$ (18 turns). b) At $t_1=t_0+T_B/4$ c) At $t_2=t_0+ T_B/2$, where $T_B$ is the nominal betatron period ($0.9\mu\text{s}$). The beam is initially off centered 1mm from the axis of the pipe.

Initially Off-Centered Beam

Initially Tilted Beam

These figures show that no matter how the beam is initially perturbed, the beam ends up having a similar long term dynamics.
Hosing

Beam centroid vs. propagation distance

Full QuickPIC shows less hosing than what theory and basic QuickPIC predict for afterburner.

E.S. Dodd PRL 88(12), 2002
Other issue: Plasma lens

10 cm wide plasma slab

50GeV electron beam

compressed beam
To meet our ever increasing computational needs we are building a 512 processor cluster: DAWSON

The “Dawson” cluster under construction at UCLA: NSF MRI
QuickPIC loop (based on UPIC): 2-D plasma slab

1. initialize beam
2. solve $\nabla^2 \varphi = \rho, \nabla^2 \psi = \rho_e \Rightarrow F_p, \psi$
3. push plasma, store $\psi$
4. step slab and repeat 2.
5. use $\psi$ to giant step beam
Adding the laser field into quickPIC
(A Maryland and UCLA collaboration)

Use ponderomotive guiding center approach of Antonsen and Mora

\[
\frac{d\vec{P}}{dt} = q(\vec{E} + \vec{v} \times \vec{B}) - \frac{1}{4} q \nabla |a|^2 \quad \text{where} \quad \gamma = \sqrt{1 + \frac{P^2}{\gamma} + \frac{|a|^2}{2}}
\]

A parallelized laser envelope solver has been added into the code by J. Cooley and T. Antonsen’s

\[
\left(2i \omega \partial_{\tau} - 2 \partial_{\xi} \tau - \nabla^2 \right) a = \chi a
\]

\[
\chi = -\sum \frac{q}{\gamma}
\]