Massively Parallel Particle-in-Cell Simulation of Advanced Particle Accelerator Concepts*

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Abstract – The quest to understand the fundamental nature of matter requires ever higher energy particle collisions, which in turn leads to ever larger and more expensive accelerator facilities. Advanced concepts for electron and positron acceleration are required to reduce the cost and increase the performance of next-generation accelerators. Plasma-based accelerators can sustain electron plasma waves with phase velocities close to the speed of light *c* and longitudinal electric fields on the order of the nonrelativistic wave breaking field, $E_0=cm_e\omega_p/e$, where $\omega_p=(4\pi n_e e^2/m_e)^{1/2}$ is the plasma frequency at an electron density n_e [1]. For $n_e\sim10^{18}$ cm^{-3}, $E_0\sim100$ GV/m. Massively parallel particle-in-cell (PIC) simulations are required to simulate both laser-driven (LWFA) [2] and beam-driven (PWFA) [3] concepts, in order to support on-going experiments and to explore new ideas. We summarize recent successes in the use of parallel PIC codes VORPAL [4], OSIRIS [5] and QuickPIC [6] to validate computations with experimental data, to benchmark codes with independent implementations and to benchmark reduced PIC algorithms. Code performance and representative algorithms are discussed in the context of past work and future challenges.

Code Validation & Benchmarking

- VORPAL simulations of LWFA are validated against experimental data from LBNL [7]:

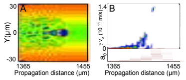


Fig. 1. VORPAL sim.'s show high-quality e- beams in agreement with experiment [7,8] –
a) e- density contours;
b) particle momenta & (lower) laser pulse envelope.

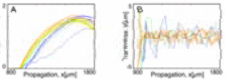


Fig. 2. Accelerated e- trajectories from VORPAL simulations of LWFA [8] –
a) deceleration begins after laser pulse reaches dephasing length;
b) transverse focussing of accelerated e-'s is seen.

VORPAL makes "dream beam" cover

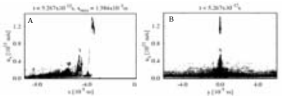


Fig. 3. Simulated VORPAL particles for LBNL experiments – a) long. phase space, x-u_x (=γv_x); b) transverse position, y-u_x; shows low energy e-'s blown out transversely & high energy e-'s are transversely focussed.

- 3D OSIRIS simulations of LWFA are validated against experimental data from RAL [9]:

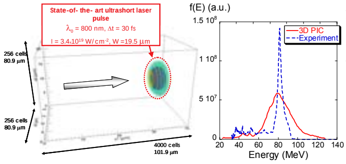


Fig. 4. 3D OSIRIS simulations of Rutherford Appleton Lab's (RAL) experiments – left: schematic with typical param's; right: comparison of charge & energy spread –
experiment shows ~ 1.4×10^8 e-'s
OSIRIS predicts ~ 0.9×10^8 e-'s

These results were included in Nature's "Dream beam" issue.

- Simulations of tunneling ionization validated against experimental data from LBNL [10]:

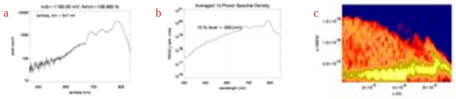


Fig. 5. a) spectrum of 800 nm laser pulse (LBNL data), blue-shifted after tunnel-ionizing He gas over many Raleigh lengths; b) FFT spectrum from 2D PIC simulation, using ADK model; c) spatially-resolved FFT from simulation shows most blue-shifting occurs at front of pulse.

- PWFA simulations show tunneling ionization can self-generate the necessary plasma [11]:

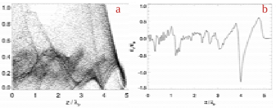


Fig. 6. a) tunnel-ionized e-'s from a 50 GeV afterburner (neutral Li); b) the resulting wake is just as strong as for a pre-ionized plasma.

Results in Fig. 5 & 6 were originally generated with OOPIC Pro – the same ADK algorithm has been implemented in VORPAL.

- 3D QuickPIC w/ tunneling ionization is validated against E-164x PWFA experiments [12,13]:

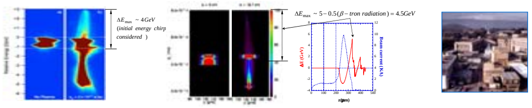


Fig. 7. QuickPIC can accurately model these E-164x experiments at SLAC in 3D, with tunneling ionization physics, and 100x speed-up over explicit PIC.

Note: the ADK algorithm first implemented in OOPIC Pro (and now VORPAL) was benchmarked against the alternate implementation in OSIRIS; QuickPIC was then benchmarked against OSIRIS.

Parallel Algorithms & Reduced Models

- Quasi-static model in QuickPIC works with beam (PWFA) & laser (LWFA) drivers:

Maxwell equations in Lorentz gauge

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

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

quasi - static : $\partial_s\approx0$

Reduced Maxwell equations

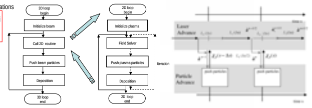
$$-\nabla_\perp^2\mathbf{A}=\frac{4\pi}{c}\mathbf{j}$$

$$-\nabla_\perp^2\phi=4\pi\rho$$

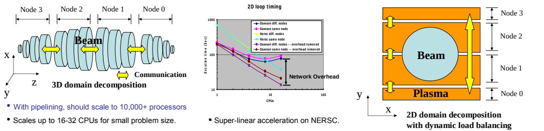
Laser envelope equation: $2\frac{\partial}{\partial s}\left(-ik_0+\frac{\partial}{\partial\xi}\right)a-\nabla_\perp^2a=k_s^2\chi_p a=-k_0^2\left\langle\frac{\omega_p^2}{\omega_0^2\gamma_p}\right\rangle a$

For beam electrons: $\frac{d\mathbf{P}_b}{ds}=-\frac{q_b}{c}\left[\mathbf{E}+\frac{\mathbf{V}_b}{c}\times\mathbf{B}\right]$

For plasma electrons: $\frac{d\mathbf{P}_{e\perp}}{d\xi}=\frac{q_e}{c-V_{e//}}\left[\mathbf{E}_\perp+\left(\frac{\mathbf{V}_e}{c}\times\mathbf{B}\right)_\perp\right]$

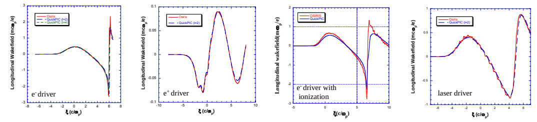


- Parallelization of QuickPIC will enable use of ~10^4 processors in the future:



- With pipelining, should scale to 10,000+ processors
- Scales up to 16-32 CPUs for small problem size.
- Network overhead dominates on Dawson cluster (GigE).
- Super-linear acceleration on NERSC.
- 4 times performance boost with infiniband hardware.

- Benchmarking QuickPIC against OSIRIS shows excellent agreement and 100x speed-up:



- Ponderomotive guiding center (i.e. envelope) model [14] of laser pulse is a powerful technique:

$$(\Delta+\partial_{tt})(A+\tilde a)=-J-j+\nabla\partial_t\phi\qquad\left(\Delta_\perp+i\omega\frac{2}{c^2}\partial_\tau+\frac{2}{c^2}\partial_{\tau\xi}\right)a=\chi a\qquad(c\partial_x+\partial_t)a=\frac{c^2}{2i\omega}\left(1+\frac{c}{i\omega}\partial_x\right)(\chi+\Delta_\perp)a$$

$$j=-\tilde a\sum_i\frac{q_i\rho_i}{m_i}\qquad\tilde a=\tfrac{1}{2}a(x,y,t)e^{i\psi}+cc\qquad\xi=x-ct,\tau=t\qquad\chi=-\mu_0\sum\frac{q_i\rho_i}{m_i}$$

1) the fast time scale is averaged away, so the laser wavelength/frequency need not be resolved
2) the particles respond to the ponderomotive force & carry an internal "wiggle" momentum
3) other electromagnetic fields interact with the particles via standard, explicit PIC
4) speed-up is $O(\omega_{laser}/\omega_{plasma})^2$, which can be orders of magnitude – less efficient than quasi-static, but can treat accelerated particles
5) both QuickPIC and VORPAL have implemented ponderomotive guiding center (envelope) models for LWFA simulations.

- VORPAL's envelope model [15] agrees with PIC for a_0~1, showing ~200x speed-up:

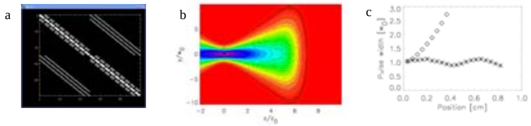


Fig. 8. a) sparsity pattern of the discretized envelope evolution equation; b) contours of laser pulse envelope in vacuum; c) envelope width in vacuum (diamonds) and in a plasma channel (stars).

VORPAL can now simulate LBNL's 3 cm capillary discharge channel in a few processor-hours.

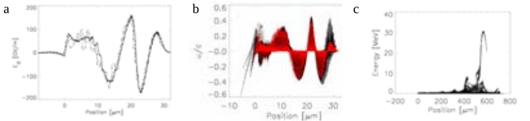


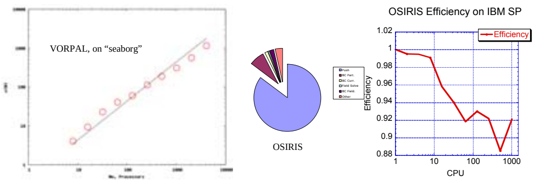
Fig. 9. VORPAL results: a) accelerating wake fields for PIC (solid) & envelope; b) normalized e-velocities for envelope (red) & PIC; c) background e-'s can be trapped for a_0=2.5

- Perfectly Matched Layer (PML) absorbing BC's [16] have been implemented in VORPAL:

1) these efficiently absorb a wide range of electromagnetic wavelengths, regardless of propagation angle
2) a 10-20 cell buffer region is required around the simulation domain (must be thicker than the longest relevant wavelength)
3) a modest number of PIC macro-particles entering the PML region does not appear to cause problems
4) in some cases, significant speed-up for LWFA simulations is obtained by greatly reducing the transverse size of the domain
5) for long LWFA simulations with a moving window, reflected waves are a concern; PML's directly address this issue

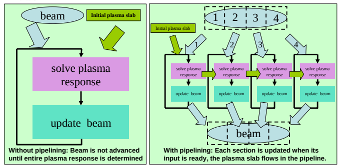
Code Performance & Future Concepts

- VORPAL and OSIRIS scale efficiently to >1,000 processors on "seaborg" IBM SP at NERSC:



VORPAL and OSIRIS are expected to scale to >10^4 processors for sufficiently large problem sizes (e.g. longer Ti-Saphire laser pulses for lower-density LWFA).

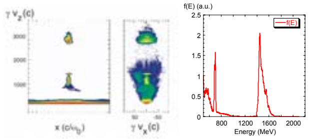
QuickPIC will require some code development to reach this scale of parallel computing – use of pipelining for long, 3D drivers:



Without pipelining: Beam is not advanced until entire plasma response is determined

With pipelining: Each section is updated when its input is ready, the plasma slab flows in the pipeline.

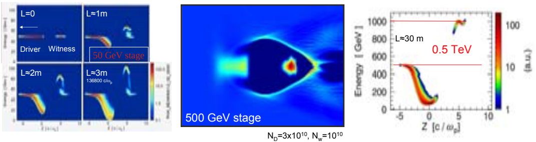
- 3D OSIRIS simulation of 1.5 GeV LWFA stage (interesting "light source" candidate as well):



Full-scale 3D modeling of a 1.5 GeV LWFA stage: 4000 x 256 x 256 mesh; 5×10^8 particles; 300,000 timesteps.

OSIRIS predicts a mono-energetic e-beam with ~1 nC of charge!

- QuickPIC can simulate a TeV PWFA afterburner in 3D with only 5,000 node hours [17]:



$N_D=3\times10^{10}$, $N_W=10^{10}$
$\varepsilon_{Nx}=\varepsilon_{Ny}=2230\times10^{-6}$ m-rad, $\sigma_x=\sigma_y=15$ μm, (beam matched to plasma)
$\sigma_{zD}=145$ μm, $\sigma_{zW}=10$ μm, Δz=100 μm; $N_e=5.66\times10^{16}$ cm^{-3}, L_p=30 (or 3) m

Doubling the energy of a 500 (or 50) GeV bunch in only 30 (or 3) m!

- VORPAL will have 2nd-order accurate conformal BC's (work in progress):

- Direct coupling between a plasma accelerator stage (e.g. an injector) and a conventional *rf* structure is important for future work
- A Cartesian FDTD code can accurately model complex EM structures [18, 19]; and also do relativistic PIC for intense beams!
- Adding to VORPAL via DoD SBIR funding.
- Other contributors: D. Barnes, J. Hesthaven, E. Kashdan, P. Schoessow and P. Stoltz

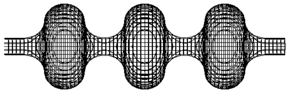


Fig. 10. 3D conformal mesh representing elliptical *rf* cavities, generated by VORPAL; development of 2nd-order electromagnetic field advance is still in progress.

- Some agenda items for future work include:
  - Simulation tools must continue moving from qualitative physics to quantitative prediction.
  - In particular, we must simulate in detail the e- beam emerging from the plasma -- including emittance, energy spread, bunch length & total charge.
  - Investigate mesh refinement, fluid & Vlasov models, high-order field & particle algorithms
  - Push our codes to ~10^4 processors; continue improving serial performance
  - Model upcoming 1 GeV LWFA (LBNL, RAL, LOA) and 10 GeV PWFA (SLAC) exp'ts
  - Push our reduced PIC models to the 100 GeV - 1 TeV range; get scaling laws correct
  - Model e-cloud physics (LHC, ILC damping ring); add circular/elliptical pipes to QuickPIC

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[1] E. Esarey *et al.*, IEEE Trans. on Plasma Sci. 24, 252 (1996).
[2] T. Tajima & J. Dawson, Phys. Rev. Lett. 43, 267 (1979).
[3] C. Joshi *et al.*, Nature 311, 525 (1984).
[4] C. Nieter & J. Cary, J. Comp. Phys. 196, 448 (2004).
[5] R. Hemker, Ph.D thesis, UCLA (2000);
R. Fonseca *et al.*, Lect. Notes Comput. Sci. **2331**, 342 (2002).
[6] C. Huang *et al.*, J. Comp. Phys. (submitted).
[7] C.G.R. Geddes *et al.*, Nature **431**, 538 (2004).
[8] C.G.R. Geddes *et al.*, Proc. Part. Accel. Conf. (2005), in press.
[9] S.P.D. Mangles *et al.*, Nature **431**, 535 (2004).
[10] D. Dimitrov *et al.*, Proc. Advanced Accel. Workshop, AIP **647**, 192 (2002).
[11] D. Bruhwiler *et al.*, Phys. Plasmas **10**, 2022 (2003). *(Invited)*
[12] M. Zhou *et al.*, Proc. Part. Accel. Conf. (2005), in press.
[13] M. Hogan *et al.*, Phys. Rev. Lett. (2005), accepted.
[14] D. Gordon *et al.*, IEEE Trans. Plasma Science **28**, 1135 (2000).
[15] P. Messmer *et al.*, Proc. Part. Accel. Conf. (2005), in press.
[16] S. Gedney, IEEE Trans. Anten. & Prop. **44**, 1630 (1996).
[17] C. Huang *et al.*, Proc. Part. Accel. Conf. (2005), in press.
[18] S. Dey & R. Mittra, IEEE Micro. Guided Wave Lett. **7**, 273 (1997).
[19] I. Zagorodnov *et al.*, Int. J. Num. Model. **16**, 127 (2003).