Particle simulation of laser wakefield particle acceleration – M558
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LOASIS program, LBNL, http://loasis.lbl.gov
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C. Benedetti, M. Chen, E. Cormier-Michel, E. Esarey, C.B. Schroeder


Oxford
W. Andreas, S. Bajlekov, N. Bourgeois, T. Ibbotson, S.M. Hooker
Simulations support LOASIS experiments and BELLA design

Outline

- BELLA project + collaborators: High gradient laser – plasma accelerators
- Quantitative modeling of self-trapped low ΔE experiments\(^1\) using new numerics\(^2\)
- Physics of controlled trapping for low momentum spread bunches: downramp experiments\(^3\) & colliding pulse injection
- Design of efficient 10 GeV stages for BELLA and laser plasma collider concept & emittance control\(^4\)
- GeV stages - Thomson gamma sources for SNM detection\(^5\)
- Compute requirements & outlook

\(^1\) Geddes et al., SciDAC Review 2009 & Nature 2004; \(^2\) Cormier-Michel et al., PRE 2008; 
\(^3\) Geddes et al., PRL 2008; \(^4\) Cormier-Michel et al., ICAP 2009; \(^5\) Geddes et al., CAARI 2008
BELLA 40 J PW Laser – Components for a Laser Plasma Collider + Radiation

10 GeV stages

Energy spread & Emittance preservation

Injection + Staging

PW laser
40 J / 40 fs

Positron acceleration + PWFA expt.’s

Radiation sources

Will augment existing LOASIS experiments on two existing beam lines
LOASIS team – development of laser plasma accelerators

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M. Condon (0.5)
G. Rogers (0.1)

Collaborators include:
SciDAC team

Oxford: S. Hooker et al.
MPQ: F. Krausz, F. Gruener et al.
LOA: O. Albert, L. Canova
GSI: T. Stoehlker, D. Thorn
Simulation Collaborators

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        D. Ushizima, G. Weber
NERSC: M. Howison,...
DOE Scientific Discovery through Advanced Computing:
LBNL AMAC, CBP: R. Ryne, J.L. Vay, W. Fawley
UCLA: W.B. Mori, F.S. Tsung, C. Huang, M. Tzoufras, M. Zhou,
        W. Lu, S. Martins, M. Tzoufras, V. Dycek + collaborators at IST
USC/Duke: T. Katsouleas, X. Wang

Other collaborations include:
LWFA – Nebraska, B.A. Shadwick et al.;
Gas targets - STI Optronics, W. Kimura et al; LBNL APDEC, P. Collela et al
Alameda Applied Sciences – M. Krishnan et al
Simulation + theory required to model self consistent laser, wake, and bunch

Radiation pressure of intense laser excites space charge plasma wave which accelerates particles with high gradient

- Explicit particle in cell simulates required physics – resolves laser period
  - Mhours CPU for cm-scale GeV (VORPAL*)
  - Domain decomposition parallelization
  - present runs ~ 50cells^3/ processor

- Meter scale of 10 GeV stages – O[Ghours]
  explicit → scaling + new models

- Require improved accuracy & resolution (compute time) to model collider emittances

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Energy gain \( \sim n^{-1} \) (10 GeV at \( 10^{17}/cc \))
Length \( \sim n^{-3/2} \) (1m at \( 10^{17}/cc \))
Gradient \( \sim n^{1/2} \) (10 GV/m at \( 10^{17}/cc \))
Laser \( w_0,L \sim \lambda_p \) (100fs at \( 10^{17}/cc \))
Depletion \( \sim \) Dephasing for \( a_0 > 1 \)

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Simulations of past expt.’s: Geddes et al JPCS 2008; ScDAC Review 2009

Self trapped experiments: percent energy spread, physics, scaling

- Laser channeling: first low $\Delta E/E$ beams
  - 10 TW laser, 2mm plasma @ $2\times10^{19}$/cc
    - Accurately model bunch
    - VORPAL Simulation
    - Vis by O. Rübel
  - 3 mrad divergence, $\Delta E/E$ 4%, $E_{\text{peak}} \sim 170$ MeV
    - Geddes et al., Nature 2004*
    - Accurately model bunch

- 1 GeV beams, stable beams at 0.5 GeV
  - Leemans et al., Nature Phys 2006

- Capillary channels + low $n_e = \text{GeV}$ in 3 cm
  - 40 TW laser, 3cm plasma @ $4-5\times10^{18}$/cc
  - 1/4 of ‘04 density

- Simulations show physics of self trapping production of narrow $\Delta E$:
  - Accurate modeling of phase space with interpolation & smoothing developed**
  - 100 MeV 3D production runs at 11kprocessor/36 hr, 2D 256 processor/1 hr

3-5 year outlook: routine 3D modeling at GeV & beyond; parameter scans & auto-analysis


VORPAL: Nieter et al., JCP 2004
Developing low emittance injectors: plasma downramp & colliding pulse

**Process:** ramp control of trapping reduces emittance

**Validate:** VORPAL simulations vs. multiple diagnostics

**Shows:** Bunches ~ 30fs long at formation -> injector

- Narrow energy spread, emittance preserved

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**Process:** beat between two lasers injects particles

**Separate:** wake excitation, injection

- repeatability
- tunable energy
- reduce emittance by controlling injection

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3-5 year outlook: extend resolution and use many runs to design low emittance injector
Develop efficient 10 GeV 40 J, collider-relevant BELLA Stages

- Use and verify linear theory predictions
  - Field $\sim 1/\lambda_p$ @ const. $a_0, k_p L_{\text{laser}}, k_p w_0$

- Starting to predict 10 GeV performance
  - $\sim 1$ m at $10^{17}$/cc $\rightarrow$ Ghours (explicit)
  - Laser spot size, length, effect of beam loading
  - Lorentz & envelope sim.s $\rightarrow$ emittance
  - Outlook: loaded emittance, $\Delta E$, shaping

Wake scales with density
Scaled simulations at $a=1$

Field $\sim 1/\lambda_p$

$10^{19}$ cm$^{-3} = 120$ GV/m
$10^{18}$ cm$^{-3} = 40$ GV/m

**Antonsen and Mora 1996

Leemans & Esarey, Phys. Today 2009; Schroeder et al AAC 08;
Cormier-Michel et al, Proc. AAC 200; Geddes et al PAC & SciDAC review 2009;
Cowan AAC 08; Vay PRL 07
New models - full scale 10 GeV simulation

Increased capacity needed for accuracy

Boosted computational frame* reduces scale disparity - allows 10 GeV stage simulations

*J.L. Vay et al. PRL 2007

Envelope model - reduced resolution requirement - allows 10 GeV stage simulations

Laser modeled as envelope + phase reduces required resolution

VORPAL – Cowan AAC 08; also in turboWAVE, & at NRL; WAKE, QuickPIC+quasistatic

3-5 year outlook: fast codes + new comp. capacity to accurately model collider stages for e-/e+ including very low emittance, radiation, scattering contributions, and staging
Compact plasma accelerators – BELLA PW laser and towards conceptual future LPLC & sources

Collider concept
Leemans & Esarey, Phys. Today 2009

~10 GeV stages
Current HPC Requirements

• Architectures: Cray XT

• Compute/memory load
  • 3.5 Mhours in 2009
  • production simulations up to 11k-processors – typical 4k (scheduling convenience)
  • 24 hours/run
  • Memory 100GB (<1GB/core)
  • processors communicate edge cells each time step to neighbors – order 30k-cells
  • Run startup often requires python scripts for set up
  • Analysis most efficient on fewer nodes with large memory – 4GB

• Data read/written
  • 2TB written per run – sets disk requirements
  • 50 Gb/checkpoint (approx every 30 minutes)
  • restart involves read of one checkpoint
  • 5 TB/year moved out of NERSC
  • Off line storage 20 TB
Current HPC Requirements

- Codes: VORPAL (WARP, other finite difference time domain)
  - Fields and fluids are represented on a structured Cartesian mesh
  - Plasma usually represented by particles by using 2nd-order leap-frog algorithm via PIC (particle-in-cell), or fluid
  - Laser and EM fields:
    - Explicit FDTD advance in lab or boosted frame OR
    - Envelope representation of laser field with Trilinos library suite (Aztec)
  - WARP and VORPAL also used for RF accelerators – relevant to staging

- Necessary software, services or infrastructure
  - HDF5 and assistance in tuning and working with it for large jobs
  - Tuning assistance – particularly file system
  - VisIt, IDL, perl, python
  - Visualization work and assistance in visualizing and analyzing large datasets, and in extracting physics data from them.

- Known limitations/obstacles/bottlenecks
  - Operators are all local, which enables local communication via MPI
  - Production simulations up to 11k-processors – limited by capacity/allocation
  - Scaling of parallel I/O (e.g. H5) needed especially for non-constant domain sizes
  - For production parameter exploration, tools for batch executing, checking and relaunching, and automated analysis
HPC Usage and Methods Next 3-5 Years

- Upcoming changes to codes/methods/approaches
  - Computational approach anticipated to scale to >100k-core
  - Radiation and scattering models will become increasingly important
  - GPU development in progress – VORPAL, OSIRIS, others
  - PIC codes (e.g. VPIC) also perform well on cell

- Changes to Compute/memory load
  - 50x scaling in resources anticipated to accurately design collider scale stages
  - New models in conjunction with new computers: laser envelope, Lorentz
  - This will be used to:
    - Simulate 10 GeV stages at high resolution to model collider/light source emittances
    - Simulate staging of multiple modules for high energies
    - Run multiple 3D simulations to explore parameter space to improve beam quality
      - important to allow simulations to predictively explore parameter space to guide experiments
      - Simulate particle injector at high resolution to determine combination of techniques to produce the required beam quality
  - 150Mhours/year
  - 500kcores @ 12-24hours for large runs + many at 5-50kcores
  - 100 TB memory (< 1 Gb/core)
HPC Usage and Methods Next 3-5 Years

- Anticipated limitations/obstacles/bottlenecks on 10K-1000K PE system.
  - Parallel file I/O such as H5 must be scaled to 10's - 100's of thousands of processors, and must be made robust to varying mesh sizes on different processors.
  - Communication of the edge information from each processor to processors handling neighboring domains is required each step- may need to be multi-layered on many-core or GPU systems

- Strategy for dealing with multi-core/many-core architectures
  - Algorithm scales to 100’s of k-cores at this time
  - Different communication can be used between cores and nodes
HPC Usage and Methods Next 3-5 Years

• Changes to Data read/written
  • 50+ TB for large runs – determines on line storage
  • 1 TB/dump (assumes some data subsetting developed – else ~ 50TB)
  • Off line storage 200TB

• Changes to necessary software, services or infrastructure
  • Parallel file I/O such as H5 must be scaled to 10's - 100's of thousands of processors, and be made robust to varying mesh sizes on different processors.
  • Data subsetting must be developed in line to reduce dump file size
  • Error checking and job-relaunch services that detect if a job has terminated partway through and automatically restart
  • Scans of parameter space are needed requiring automation to generate and run sequentially large numbers of jobs, and to extract the data from them.
  • Parallel visualization and analytics tools must be further developed, to provide similar functionality to well-known serial tools
Summary

- NERSC architecture, configuration and service requirements:
  - Parallel I/O scalability + access to data for analytics
  - Failure detection and ability to restart jobs

- With access to ~50X NERSC resources:
  - Design of collider relevant laser plasma accelerator stages & emittance
  - Many 3D simulations allowing exploration of parameter space to predictively design experiments
  - Simulate controlled injection and beam conditioning with high fidelity

- “Expanded HPC resources” important for project:
  - availability of 500+ kcores for large runs
  - batch execution of many runs at the 5-50kcore level
  - job error detection and restart services

- Any other special needs or NERSC wish lists?
  - Parallel analytics tools matching functionality of serial solutions
  - Development of H5 and other parallel file architectures & flexible domains
end
Simulation challenges

- Accurate kinetics and bunch emittance
  - Improve accuracy in momentum advance
  - EM dispersion (cerenkov and particle noise)
  - Mesh refinement at particle bunch
  - Noise control – fluids
  - Incorporate radiation & scattering

- Meter scale structures
  - Accurate reduced models
  - EM dispersion (laser propagation)
  - Error accumulation
  - Scaling

Others:
- Automation & data mining
- Detailed validation
Developed visualization and analysis
Two student projects + VACET

FastBit indexing and query, parallel coordinates*

VisIt 3D visualization

Interactive exploration of TB datasets

Fuzzy clustering in 6D phase space+peak detection**

* O. Rubel et al., accepted SC08
** D. Ushizima et al., sub ICMLA08