Benefits of the Exascale ECP and CAMPA programs to the modeling of PWFA

Jean-Luc Vay

Lawrence Berkeley National Laboratory
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<td>Salman Habib (ANL)+LANL, LBNL</td>
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<td>Exascale Deep Learning and Simulation Enabled Precision Medicine for Cancer</td>
<td>Rick Stevens (ANL)+LANL, LLNL, ORNL, NIH/NCI</td>
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<td>Exascale Lattice Gauge Theory Opportunities and Requirements for Nuclear and High Energy Physics</td>
<td>Paul Mackenzie (FNAL)+BNL, TJNAF, Boston U., Columbia U., U. of Utah, Indiana U., UIUC, Stony Brook, College of William &amp; Mary</td>
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<td>Jean-Luc Vay (BNL)+LLNL, SLAC</td>
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<td>John Turner (ORNL)+LLNL, LANL, NIST</td>
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<td>NWChemEx: Tackling Chemical, Materials and Biomolecular Challenges in the Exascale Era</td>
<td>T. H. Dunning, Jr. (PNNL), +Ames, ANL, BNL, LBNL, ORNL, PNNL, Virginia Tech</td>
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<td>Amitava Bhattacharjee (PPPL)+ANL, ORNL, LLNL, Rutgers, UCLA, U. of Colorado</td>
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<td>Data Analytics at the Exascale for Free Electron Lasers</td>
<td>Amedeo Perazzo (SLAC)+LANL, LBNL, Stanford</td>
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<td>Transforming Combustion Science and Technology+Exascale Simulations</td>
<td>Jackie Chen (SNL)+LBNL, NREL, ORNL, U. of Connecticut</td>
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<td>Cloud-Resolving Climate Modeling of the Earth’s Water Cycle</td>
<td>Mark Taylor (SNL)+ANL, LANL, LLNL, ORNL, PNNL, UCI, CSU</td>
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**Exascale Modeling of Advanced Particle Accelerators**

**Goal (4 years):** Convergence study in 3-D of 10 consecutive multi-GeV stages in linear and bubble regime, for laser- & beam-driven plasma accelerators.

**How:** ➔ Combination of most advanced algorithms

➔ Coupling of Warp+BoxLib+PICSAR

➔ Port to emerging architectures (Xeon Phi, GPU)

**Who:** LBNL ATAP (accelerators) + LBNL CRD (computing science) + SLAC + LLNL

*Ultimate goal: enable modeling of 100 stages by 2025 for 1 TeV collider design!*
Plasma accelerators are challenging to model

Short driver/wake propagates through long plasma

**⇒** Many time steps.

For a 10 GeV LPA scale stage:

- ~1µm wavelength laser propagates into ~1m plasma
  **⇒** millions of time steps needed

**Non-linear regime:**

very small features

**⇒** small grid cells
20-100 stages need to be lined up for e⁻e⁺ linear collider

Simulations can currently take days for 1 stage (sometimes in RZ).
Need for ×100 stages ×100 ensemble ×1000 3D!
We will combine the most advanced algorithms

Lower # time steps:
• optimal Lorentz boosted frame
We will combine the most advanced algorithms

Lower # time steps:
• optimal Lorentz boosted frame

Higher accuracy:
• AMR
Boxlib will provide robust AMR capability

Warp

- User interface
- Vast collection of physics models & algorithms

BoxLib

- AMR
- Parallel I/O
- Load balancing

PICSAR

- Highly optimized elementary PIC operations

Hardware

Illustration

Warp’s refinement algorithm will be implemented in Boxlib


We will combine the most advanced algorithms

Lower # time steps:
- optimal Lorentz boosted frame

Higher accuracy:
- AMR
- Pseudo-spectral Analytical Maxwell solvers
Warp has arbitrary order EM solver in FDTD & PSTD (using leapfrog time integration)
Analytical pseudo-spectral solver offers exact solution + no Courant condition

Pseudo-Spectral Analytical Time-Domain \(^1\) (PSATD)
based on exact analytical integration in Fourier space

\[ B_{z}^{n+1} = \mathcal{F}^{-1} \left( C \mathcal{F} (B_{z}^{n}) \right) + \mathcal{F}^{-1} \left( iS k_{y} \mathcal{F} (E_{x}) \right) - \mathcal{F}^{-1} \left( iS k_{x} \mathcal{F} (E_{y}) \right) \]

with \[ C = \cos \left( kc \Delta t \right); \quad S = \sin \left( kc \Delta t \right); \quad k = \sqrt{k_{x}^{2} + k_{y}^{2}} \]

We will combine the most advanced algorithms

**Lower # time steps:**
- optimal Lorentz boosted frame

**Higher accuracy:**
- AMR
- Pseudo-spectral Analytical Maxwell solvers

**Higher stability**
- Galilean T. to suppress Numerical Cherenkov Instability
PSATD also enables integration in Galilean frame

Use Galilean coordinates that follow the relativistic plasma.

\[
\begin{align*}
\frac{\partial B}{\partial t} &= -\nabla \times E \\
\frac{1}{c^2} \frac{\partial E}{\partial t} &= \nabla \times B - \mu_0 j
\end{align*}
\]

+ integrate analytically, assuming \( j(x, t) \) is constant over one timestep.

Original idea by Manuel Kirchen (PhD student at U. Hamburg)
Derivation of the algorithm: Lehe et al., arxiv (2016)
Galilean PSATD is stable for uniform relativistic flow

Uniform plasma streaming in 2D periodic box

**Analysis**

Instability growth rate

**Simulation**

Lehe et al., arxiv (2016)
Galilean PSATD stability is geometry independent

Laser plasma acceleration simulation with FBPI*C
(uses azimuthal Fourier decomposition with 2 modes)


FBPIC is Open source: \url{https://github.com/fbpic/fbpic}.
We will combine the most advanced algorithms

**Lower # time steps:**
- optimal Lorentz boosted frame

**Higher accuracy:**
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**Higher stability**
- Galilean T. to suppress Numerical Cherenkov Instability

**Higher scalability**
- FFT Maxwell solvers+domain decomposition
Spectral solvers involve global operations:

- harder to scale to large # of cores

**Spectral**

- global “costly” communications

**Finite Difference (FDTD)**

- local “cheap” communications

**Finite speed of light ➔ local FFTs ➔ spectral accuracy + FDTD scaling!**

PIC+PSATD scales very well to ~1M cores

strong parallel scaling for uniform warm plasma up-to >800,000 cores (Mira – ANL)

(Courtesy: H. Vincenti)
We will combine the most advanced algorithms

Lower # time steps:
- optimal Lorentz boosted frame

Higher accuracy:
- AMR
- Pseudo-spectral Analytical Maxwell solvers

Higher stability
- Galilean T. to suppress Numerical Cherenkov Instability

Higher scalability
- FFT Maxwell solvers+domain decomposition

Lower dimensionality
- FFT+Hankel Transform Maxwell solver for quasi-RZ geom

....and porting to fastest hardware.
We were already preparing for Exascale with NERSC Exascale Applications Program (NESAP)

NESAP Codes

- Advanced Scientific Computing Research
  - Almgren (LBNL) - BoxLib
  - AMR Framework
  - Trebotich (LBNL) - Chombo-crunch

- High Energy Physics
  - Vay (LBNL) - WARP & IMPACT
  - Toussaint (Arizona) - MILC
  - Habib (ANL) - HACC

- Nuclear Physics
  - Maris (Iowa)
  - Joo (JLAB)
  - Christ/Kars (Columbia)

Warp kernel ➔ Particle-In-Cell Scalable Architecture Resources (PICSAR)

Optimized MPI + OpenMP + vec. + tiling/sorting

- Brian Friesen
  - Ex-NESAP postdoc (now at NERSC)

- Mathieu Lobet
  - NESAP postdoc

- Collaboration with
  Henri Vincenti
  Marie Curie postdoc fellowship (CEA, Saclay, France)

Set of milestones provides progressive path toward end of award period deliverable

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<tr>
<th>Year/Quarter</th>
<th>Milestone</th>
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<td>Year 1/Q1</td>
<td>Initial coupling of Boxlib and Warp/PICSAR.</td>
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<td>Year 1/Q2</td>
<td>Modeling of single plasma-based accelerator stage with WarpX on single grid.</td>
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<tr>
<td>Year 1/Q3</td>
<td>Add MR to coupling of Boxlib and PICSAR</td>
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<tr>
<td>Year 1/Q4</td>
<td>Modeling of single plasma-based accelerator stage with WarpX with static MR.</td>
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<tr>
<td>Year 2/Q1</td>
<td>Assess performance of python parallel startup, dump/restart, I/O, Lorentz back transformation diagnostic, in-situ and post-processing capabilities on hundreds of thousands to a million of cores.</td>
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<tr>
<td>Year 2/Q2</td>
<td>Optimized simulations of a uniform plasma on hundreds of thousands to millions of cores, without MR; assess strong scaling.</td>
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<tr>
<td>Year 2/Q3</td>
<td>Convergence study in 3-D of one multi-GeV plasma-based accelerator stage in linear &amp; bubble regime, without MR.</td>
</tr>
<tr>
<td>Year 2/Q4</td>
<td>Convergence study in 3-D of one multi-GeV plasma-based accelerator stage in linear &amp; bubble regime, with MR.</td>
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<tr>
<td>Year 3/Q1</td>
<td>Assess performance of python parallel startup, dump/restart, I/O, Lorentz back transformation diagnostic, in-situ and post-processing capabilities on up-to 5 millions of cores.</td>
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<tr>
<td>Year 3/Q2</td>
<td>Conduct simulations of a uniform plasma on 5-to-10 millions of cores, without MR, and assess strong scaling.</td>
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<tr>
<td>Year 3/Q3</td>
<td>Convergence study in 3-D of three multi-GeV stages in linear &amp; bubble regime, without MR.</td>
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<tr>
<td>Year 3/Q4</td>
<td>Convergence study in 3-D of three multi-GeV stages in linear &amp; bubble regime, with MR. Release of software.</td>
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<tr>
<td>Year 4/Q1</td>
<td>Assess performance of python parallel startup, dump/restart, I/O, Lorentz back transformation diagnostic, in-situ and post-processing capabilities on up-to 10 Millions of cores.</td>
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<tr>
<td>Year 4/Q2</td>
<td>Conduct simulations of a uniform plasma on up-to 10 Millions of cores, without MR, and assess strong scaling.</td>
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<tr>
<td>Year 4/Q3</td>
<td>Convergence study in 3-D of ten consecutive multi-GeV stages in linear &amp; bubble regime, without MR.</td>
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<tr>
<td>Year 4/Q4</td>
<td>Convergence study in 3-D of ten consecutive multi-GeV stages in linear &amp; bubble regime, with MR. Release of software.</td>
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Emerging national consortium for accelerator modeling provides the foundations for community connections

**Consortium for Advanced Modeling of Particle Accelerators**

**Points of contact:**
- **LBNL:** J.-L. Vay
- **SLAC:** C.-K. Ng
- **FNAL:** J. Amundson
- **UCLA:** W. Mori

**Activities:**
- High Performance Computing (beyond SciDAC),
- coordination/integration of codes/modules, user interfaces, data formats, ...
- dissemination, support & training.

**CAMPA**

- **BLAST** (Warp, IMPACT, BeamBeam3D, PICSAR, Posinst)

**SLAC**

- **ACE3P** (Omega3P, S3P, Track3P, T3P, PIC3P, TEM3P)

**Fermilab**

- **SYNERGIA** (space-charge, wakes, e-cloud, beam-beam…)

**UCLA**

- **PICKSC** (Osiris, QuickPIC, UPIC, UPIC-EMMA, Oshun)
FY17: focus on developing common data formats & interfaces

- Example of cross-cutting data format:
  - a common I/O standard for simulations with particles and meshes
  - standardized layout of data in file (using hdf5, netcdf, ADIOS, ..)
  - for easy comparisons between codes, common visualization tools
  - implemented in various PIC codes: Warp, PIConGPU, FBPIX.
  - OpenPMD Viewer based on IPython+Matplotlib available
  - VisIt/Paraview reader in development

FY17: focus on developing common data formats & interfaces

• Currently, each code has own input script & output format
  ➔ user needs 1 input script/code & different data reader or software

Bridge codes to enable:
  • unified input/output interface
  • separation of description/resolution/analysis

• Define standard for common input
  ➔ translate to individual code “language”

• Usage of common data format enables common output & data analysis/visualization software
Summary

• New “Exascale Modeling of Advanced Particle Accelerators” to develop advanced PIC code with AMR for exascale computing
  ➔ enable fast converged simulations of chains of stages (LPA & PWFA)

• CAMPA to provide collaboration with other efforts

• We are looking forward to helping the PWFA research at FACET-II
Thank you for your attention!

Questions?