Warp-X: a new exascale computing platform for Beam-Plasma Simulations

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Outline

• Context & overview of the project
• Code structure
• Advanced algorithms
• Progress
• Next steps
Recent reports from US/Europe present roadmaps for plasma-based collider with design by 2035-2040
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 $\times 100$ stages $\times 100$ ensemble $\times 1000$ 3D!
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
ECP Project WarpX: 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+AMReX+PICSAR
  - Port to emerging architectures (Intel KNL, GPU, ...)

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

**Ultimate goal:** enable modeling of 100 stages by 2025 for 1 TeV collider design!
### DOE Exascale Computing Project Applications (1ST ROUND)

| Title                                                                 | Team                                                                 |
|----------------------------------------------------------------------|----------------------------------------------------------------------|
| Computing the Sky at Extreme Scales                                   | Salman Habib (ANL)+LANL,LBNL                                          |
| Exascale Deep Learning and Simulation Enabled Precision Medicine for  | Rick Stevens (ANL)+LANL, LLNL, ORNL, NIH/NCI                          |
| Cancer                                                               |                                                                      |
| Exascale Lattice Gauge Theory Opportunities and Requirements for      | Paul Mackenzie (FNAL)+BNL,TJNAF,Boston U.,Columbia U., U. of Utah,    |
| Nuclear and High Energy Physics                                      | Indiana U., UIUC,Stony Brook,College of William & Mary               |
| Molecular Dynamics at the Exascale: Spanning the Accuracy, Length     | Arthur Voter (LANL)+SNL, U. of Tennessee                              |
| and Time Scales for Critical Problems in Materials Science           |                                                                      |
| Exascale Modeling of Advanced Particle Accelerators                   | Jean-Luc Vay (BNL)+LLNL, SLAC                                        |
| An Exascale Subsurface Simulator of Coupled Flow,Transport,Reactions  | Carl Steefel (BNL)+LLNL, NETL                                        |
| and Mechanics                                                        |                                                                      |
| Exascale Predictive Wind Plant Flow Physics Modeling                  | Steve Hammond (NREL)+SNL,ORNL, U. of Texas Austin                     |
| QMCPACK: A Framework for Predictive and Systematically Improvable     | Paul Kent (ORNL)+ANL,LLNL,SNL,Stone Ridge Technology, Intel, Nvidia   |
| Quantum-Mechanics Based Simulations of Materials                      |                                                                      |
| Coupled Monte Carlo Neutronics and Fluid Flow Simulation of Small     | Thomas Evans (ORNL,PI)+ANL, INL, MIT                                  |
| Modular Reactors                                                     |                                                                      |
| Transforming Additive Manufacturing through Exascale Simulation       | John Turner (ORNL)+LLNL, LANL, NIST                                   |
| (TrAMEx)                                                             |                                                                      |
| NWChemEx: Tackling Chemical,Materials and Biomolecular Challenges in  | T. H. Dunning,Jr. (PNNL),+Ames, ANL, BNL, LBNL, ORNL, PNNL, Virginia |
| the Exascale Era                                                      | Tech                                                                |
| High-Fidelity Whole Device Modeling of Magnetically Confined Fusion  | Amitava Bhattacharjee (PPPL)+ANL,ORNL, LLNL, Rutgers, UCLA, U. of    |
| Plasma                                                               | Colorado                                                             |
| Data Analytics at the Exascale for Free Electron Lasers              | Amedeo Perazzo (SLAC)+LANL, LBNL, Stanford                            |
| Transforming Combustion Science and Technology+Exascale Simulations   | Jackie Chen (SNL)+LBNL, NREL, ORNL, U. of Connecticut                |
| Cloud-Resolving Climate Modeling of the Earth’s Water Cycle          | Mark Taylor (SNL)+ANL, LANL, LLNL, ORNL, PNNL, UCI, CSU              |
U.S. DOE Exascale Computing Project (ECP)

• ECP’s work encompasses
  – applications,
  – system software,
  – hardware technologies and architectures, and
  – workforce development to meet scientific and national security mission needs.

• As part of the National Strategic Computing initiative, ECP was established to accelerate delivery of a capable exascale computing system that integrates hardware and software capability to deliver approximately 50 times more performance than today’s 20-petaflops machines on mission critical applications.
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• Advanced algorithms

• Progress

• Next steps
UML Diagram of WarpX details code structure

- WarpX: loop control, data structure, ...
- PICSAR: low-level optimized PIC loop
- AMReX: AMR & parallelism
- Warp: problem setup, extra physics, ...

- Maxwell
  - Field solve
    - Newton-Lorentz
    - Push particles
    - Deposit charge/current
    - Gather forces
  - Smoothing

- Particle push
- Particle
- Data Iterator
- Communication
- Load Balance
- Field gather
- Current deposition
- Maxwell solver
- Smoothing

- Warp: Problem Setup
- Loop Control
- Extra Physics
- Data Analysis
- Visualization

- WarpX:
  - Loop control
  - Plasma particles
  - Moving window
  - Laser injection
  - Plasma injection
  - Moving window

- Python
  - C++

- BoxLib/AMReX
  - Adaptive Mesh
  - Particle
  - Data Iterator
  - Communication
  - Load Balance

ECP Exascale Computing Project
Python layer and connection to Warp are optional

WarpX can be run in 3 modes:

1. Compiled languages only: main in C++.

2. Compiled languages + Python: main in Python
   a. Standalone.
   b. With Warp.
PICSAR created as part of NERSC Exascale Applications Program (NESAP)

Warp EM-PIC kernel extracted
⇒ Particle-In-Cell Scalable Architecture Resources (PICSAR) library + miniapp

Optimized with new vectorization algo.* + tiling/sorting + OpenMP + MPI

PICSAR is now open source: [https://picsar.net](https://picsar.net)
Used in Warp, WarpX & SMILEI.

*H. Vincenti, R. Lehe, R. Sasanka and J.-L. Vay, Compt. Phys. Comm. 210, 145-154 (2017).
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We are combining advanced algorithms

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

![Diagram showing Lorentz Transform and speedup calculation.]

\[ \lambda' = \lambda \gamma (1 + \beta) \]

\[ L' = L / \gamma \]

# time steps \( \propto L / \lambda \)

# time steps \( \propto L' / \lambda' \)

\[ \text{Speedup } \sim \gamma^2 (1 + \beta) \]
We are combining advanced algorithms

Lower # time steps:
• optimal Lorentz boosted frame

Higher accuracy:
• AMR provided by BoxLib/AMReX library
Implementation of mesh refinement based on Warp algorithm

- Need to avoid spurious:
  1. self-forces
  2. wave reflections
  3. `ghost stuck' particles

  - 1. buffer regions
  - 2. PMLs around patches
  - 3. Extended Maxwell with divergence cleaning

Substitution:

\[ F^{n+1}(a) = I[F^n(a) - F^{n+1}(c)] + F^{n+1}(r) \]

1. J.-L. Vay, P Colella, P Mccorquodale, B Van Straalen, A Friedman, and D. P. Grote. Laser & Particle Beams 20, 569–575, (2002).
2. J.-L. Vay, J.-C. Adam, A. Héron, Computer Physics Comm. 164, 171-177 (2004).
3. J.-L. Vay, D. P. Grote, R. H. Cohen, & A. Friedman, Computational Science & Discovery 5, 014019 (2012).
We are combining advanced algorithms

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

**Higher accuracy:**
- AMR
- Arbitrary order & pseudo-spectral Analytical Maxwell solvers
Arbitrary-order Maxwell solver offers flexibility in accuracy (on centered or staggered grids)

Finite-difference
\[ c\Delta t/\Delta x \approx 0.45 \]

Higher order
\[ c\Delta t/\Delta x \approx 0.045 \]

Smaller time steps

Kronecker \(\delta\) pulse

Accurate but expensive (with leapfrog integrator)

\[ N \rightarrow \infty = \text{Pseudo-spectral (FFT)} \]
Analytical integration in Fourier space offers infinite order

Pseudo-Spectral Analytical Time-Domain\(^1\) (PSATD)

\[
B_{z}^{n+1} = \mathcal{F}^{-1} \left( C \mathcal{F} \left( B_{z}^{n} \right) \right) + \mathcal{F}^{-1} \left( iS k_y \mathcal{F} \left( E_x \right) \right) - \mathcal{F}^{-1} \left( iS k_x \mathcal{F} \left( E_y \right) \right)
\]

with \( C = \cos \left( k c \Delta t \right) \); \( S = \sin \left( k c \Delta t \right) \); \( k = \sqrt{k_x^2 + k_y^2} \)

Easy to implement arbitrary-order \( n \) with PSATD \((k = k^\infty \rightarrow k^n)\).

Both arbitrary order FDTD and PSATD to be implemented in WarpX.

\(^1\)I. Haber, R. Lee, H. Klein & J. Boris, *Proc. Sixth Conf. on Num. Sim. Plasma*, Berkeley, CA, 46-48 (1973)
We are combining 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.

Standard PSATD PIC

Galilean PSATD PIC

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

\[
(x', t) = (x - v_{gal} t, t)
\]

+ integrate analytically, assuming \( j(x, t) \) and \( j(x', t) \) is constant over one timestep.

Original idea by Manuel Kirchen (PhD student at U. Hamburg)
Concept and applications: *Kirchen et al., Phys. Plasmas 23, 100704 (2016)*
Derivation of the algorithm: *Lehe et al., Phys. Rev. E 94, 053305 (2016)*
Galilean PSATD is stable for uniform relativistic flow

Uniform plasma streaming in 2D periodic box

**Analysis**

Instability growth rate

**Simulation**

Lehe et al., Phys. Rev. E 94, 053305 (2016)
We are combining 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 on local domains + domain decomposition
Spectral solvers involve global operations ➔ harder to scale to large # of cores

**Spectral**
- global “costly” communications

**Finite Difference (FDTD)**
- local “cheap” communications

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Harder to scale

Easier to scale

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

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J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260 (2013)
H. Vincenti, J.-L. Vay, *Comput. Phys. Comm.* **200**, 147 (2016)
Finite-order stencil offers scalable ultra-high order solver

Truncation error analysis ➔ ultra-high order possible with much improved stability

Enabled demonstration of novel spectral solver with local FFTs scaling to ~1M cores

Truncation error $|\zeta|$ vs. number of guard cells $N_{\text{guards}}$ for different spectral orders $p$.

- $p=10$, $p=20$, $p=40$, $p=1000$, $p=\infty$

H. Vincenti et al., *Comput. Phys. Comm.* 200, 147 (2016).

Applied successfully to modeling of LPAs at DESY\(^1\) and plasma mirrors at CEA Saclay\(^2,3\) in cases where standard second-order FDTD solvers fail.

[1] S. Jalas, I. Dornmair, R. Lehe, H. Vincenti, J.-L. Vay, M. Kirchen, A. R. Maier, *Phys. Plasmas* 24, 033115 (2017).
[2] G. Blaclard, H. Vincenti, R. Lehe, J. L. Vay, Phys. Rev. E 96, 033305 (2017)
[3] A. Leblanc, S. Monchoce, H. Vincenti, S. Kahaly, J.-L. Vay, F. Quere, Phys. Rev. Lett. (in press)
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First simulations of plasma-based accelerators with WarpX (03/17)

Laser driven
Longitudinal electric field (GV/m)

Particle beam driven
Longitudinal electric field (GV/m)

WarpX successfully benchmarked against Warp.
Electromagnetic MR was implemented and tested (06/17)

Single particle orbiting around an external magnetic field, emitting synchrotron radiation

MR improves result with negligible spurious effects (self-force, waves reflection, ghost particles).

Note: buffer region not implemented yet; expected to improve results once implemented.
Validation on many particles `beam breathing’ test

Electron Gaussian distribution with inward initial radial velocity on top of static proton dist.

Electron beam contraction/expansion depends on resolution.

MR enables higher accuracy, covering fraction of box.
Laser injection with mesh refinement was validated

Laser generated with antenna.
First simulations of plasma accelerators with MR patch (09/17)

Laser driven

Particle beam driven

Simulations with small MR patch recover results using finer grid over the entire box.
Simulations with small MR patch recover results using finer grid over the entire box.
WarpX visualization tools are being developed

3D rendering of WarpX plasma accelerator simulation with yt

- 2D/3D visualization with matplotlib, yt, VisIt
  - Supports AMReX & OpenPMD data structures
- Interface using Python, Jupyter notebooks or GUI.
Examples of movies using Yt

Movies by Maxence Thevenet

NERSC

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7-year plan for Exascale project WarpX
From initial code coupling to ensemble of 100 GeV-scale stages

- 2016: Initial coupling of Warp+Boxlib+PICSAR
- 2017: Modeling of single plasma accelerator stage with static mesh refinement
- 2018: Modeling a single GeV-scale plasma accelerator stage
- 2019: Modeling of 3 consecutive GeV-scale plasma accelerator stages
- 2020: Modeling of 10 consecutive GeV-scale plasma accelerator stages
- 2021: Modeling of 30 consecutive GeV-scale plasma accelerator stages
- 2022: Modeling of 100 consecutive GeV-scale plasma accelerator stages
- 2023: Modeling of ensembles of 100 consecutive GeV-scale plasma accelerator stages

End current ECP project

Aurora – 1 ExaFlops

Now

Code to be released open source to community.

2nd ECP ExaFlop system
Thank you!

Questions?