

Next Generation Computational Tools for the Modeling and Design of Particle Accelerators at Exascale



Axel Huebl

Lawrence Berkeley National Laboratory

Invited Oral - TUYE2
*Computing and Data Science
for Accelerator Systems*

North American Particle
Accelerator Conference (NAPAC22)

location: Albuquerque, NM, USA
August 9th, 2022

On behalf of the BLAST team (lead: Jean-Luc Vay @ LBNL)
LBNL, LLNL, SLAC, CEA, DESY, Modern Electron, CERN

CAMPA

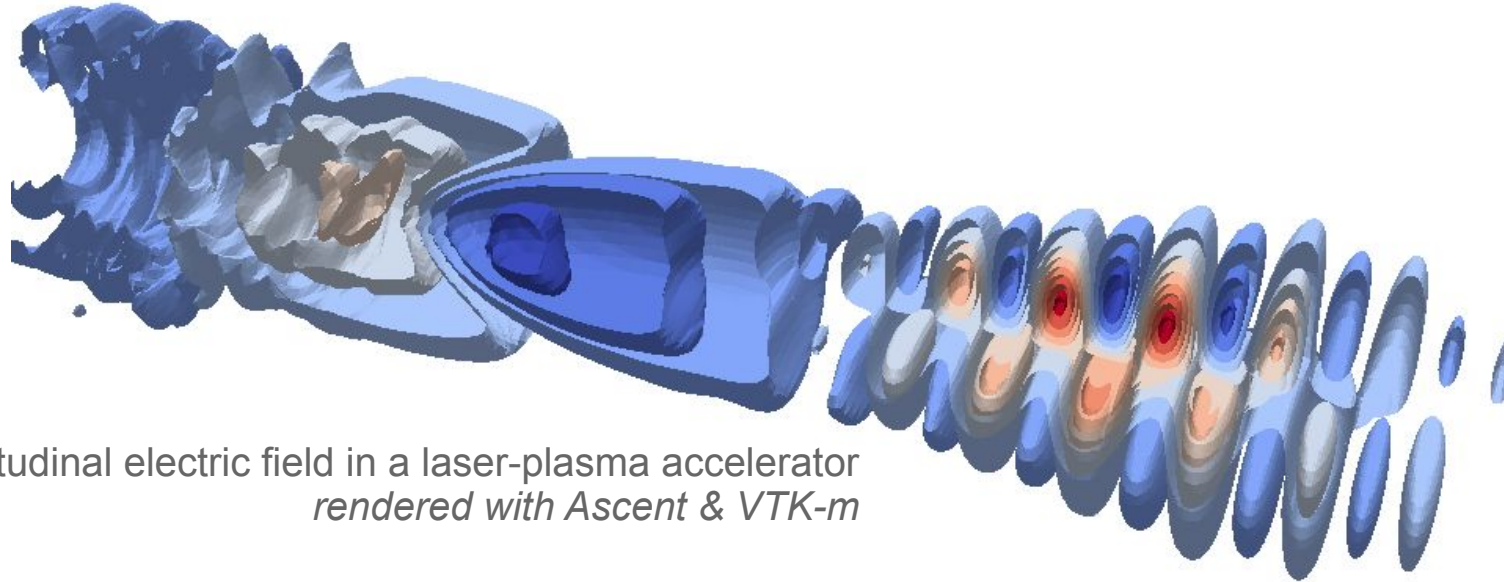
Consortium for Advanced Modeling
of Particle Accelerators



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Funding Support



WarpX: longitudinal electric field in a laser-plasma accelerator
rendered with Ascent & VTK-m

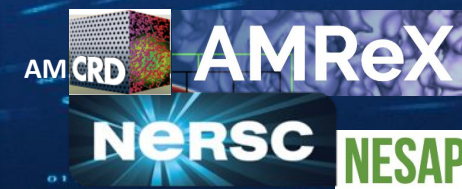


This research was supported by the **Exascale Computing Project** (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation's exascale computing imperative. This work was supported by the **Laboratory Directed Research and Development Program** of Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC02-05CH11231. This research used resources of the **Oak Ridge Leadership Computing Facility**, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725, the **National Energy Research Scientific Computing Center** (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231 using NERSC award ASCR-ERCAP0022112. This work used computational resources of the supercomputer Fugaku provided by **RIKEN** through the HPCI System Research Project (Project ID: ra010013)

- BLAST: Beam pLasma Accelerator Simulation Toolkit
- IO, Standardization & Open Development
- HPC: The Exascale Computing Project and Beyond



Multidisciplinary, Multi-Institutional Contributor Team



Jean-Luc Vay
(ECP PI)



Ann Almgren
(ECP coPI)



David Grote
(ECP coPI)



Marc Hogan
(ECP coPI)



Marco Garten



John Bell



Lixin Ge



Axel Huebl
(LDRD PI)



Kevin Gott



(NESAP)

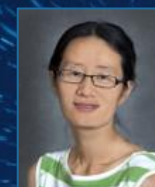
Cho Ng



Rémi Lehe



Junmin Gu



Chad Mitchell



Revathi Jambunathan



Henri Vincenti



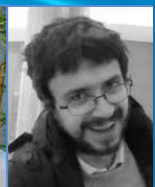
Ji Qiang



Hannah Klion



Luca Fedeli



Ryan Sandberg



Prabhat Kumar



Antonin Sainte-Marie



Olga Shapoval



Andrew Myers



Neil Zaim



Yinjian Zhao



Weiqun Zhang



Maxence Thévenet



Severin Diederichs



Alexander Sinn



+ a growing list of contributors



CEA Saclay (France)



CERN (Switzerland)



Lorenzo Giacomel



DESY (Germany)

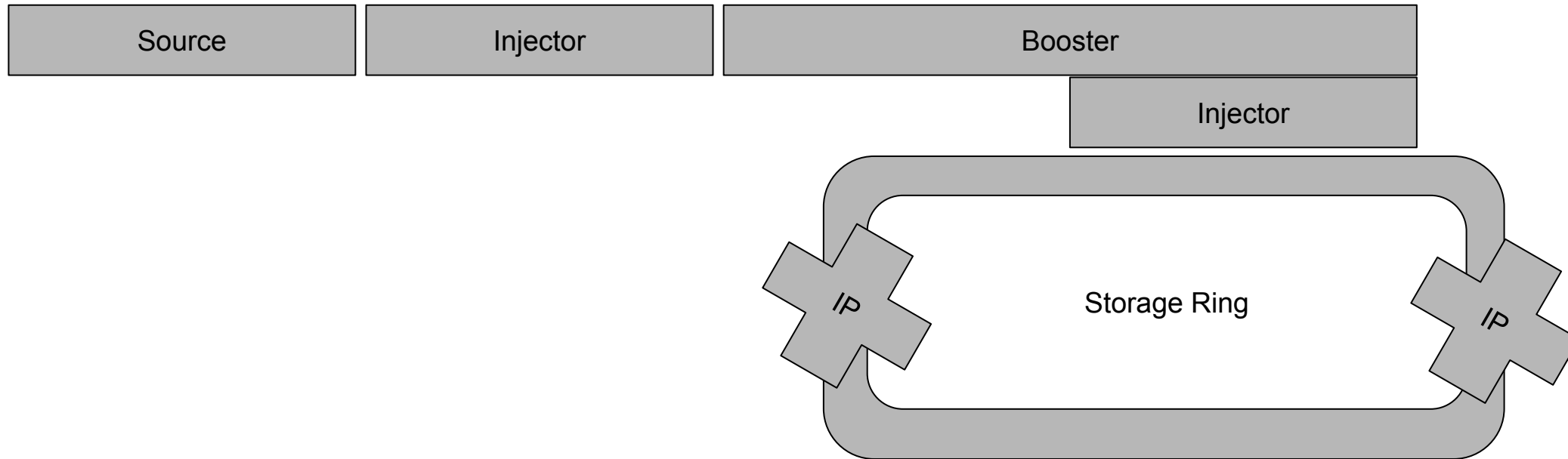
Peter Scherpelz,
Michael Kiebertz,
Kevin Zhu, Roelof
E. Groenewald



Phil Miller

Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.

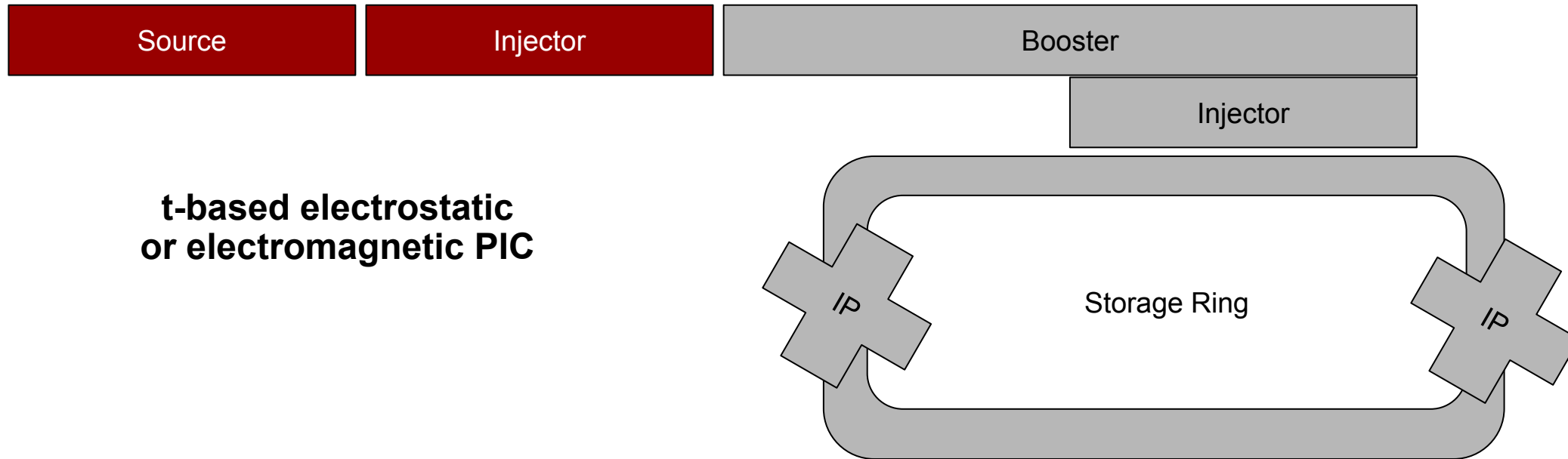


Goal
Start-to-end modeling in an open software ecosystem.



Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.



Goal
Start-to-end modeling in an open software ecosystem.

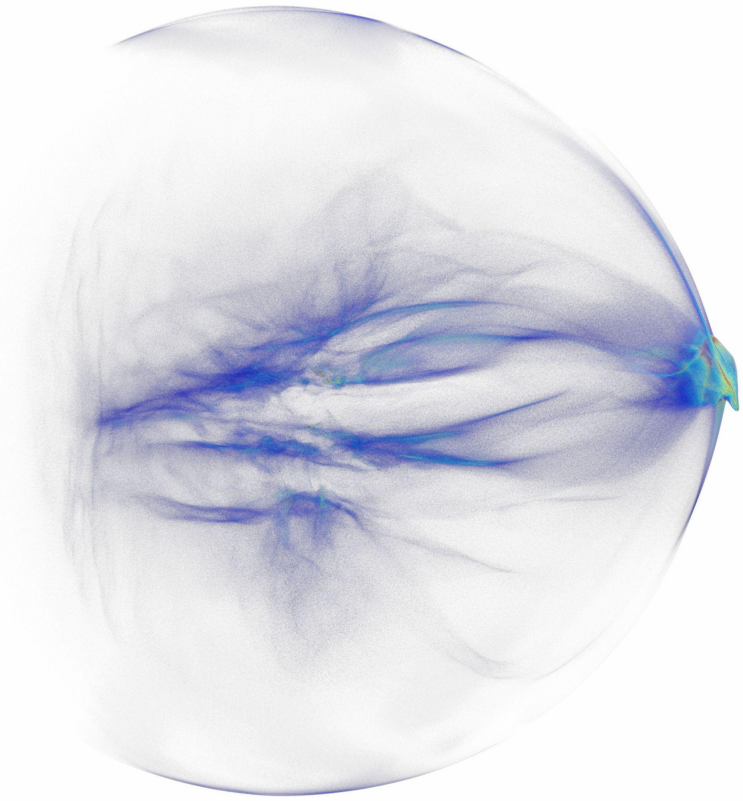


Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.



**t-based electrostatic
or electromagnetic PIC**



Goal
Start-to-end modeling in an open software ecosystem.



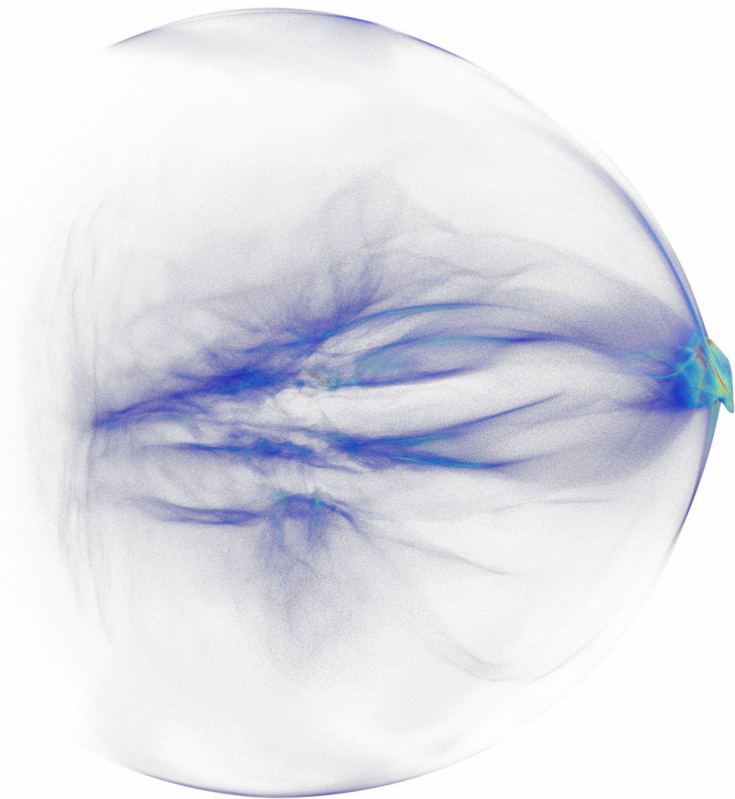
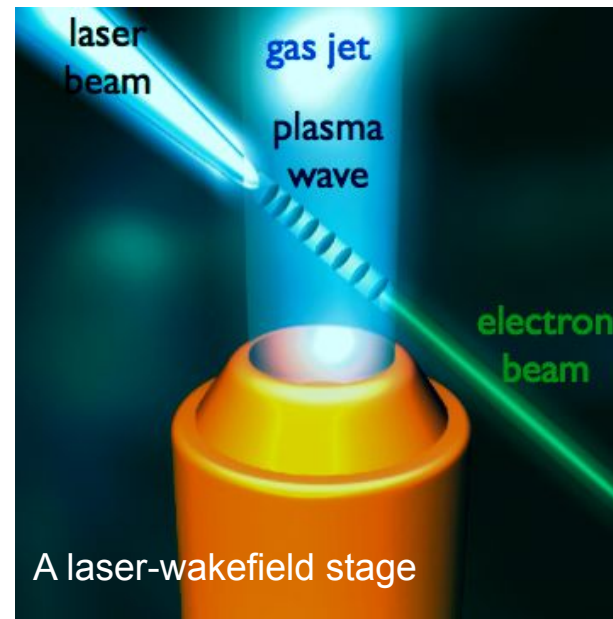
Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.



t-based electrostatic or electromagnetic PIC

Quasistatic PIC
separates the timescale for plasma wakefield and beam evolution



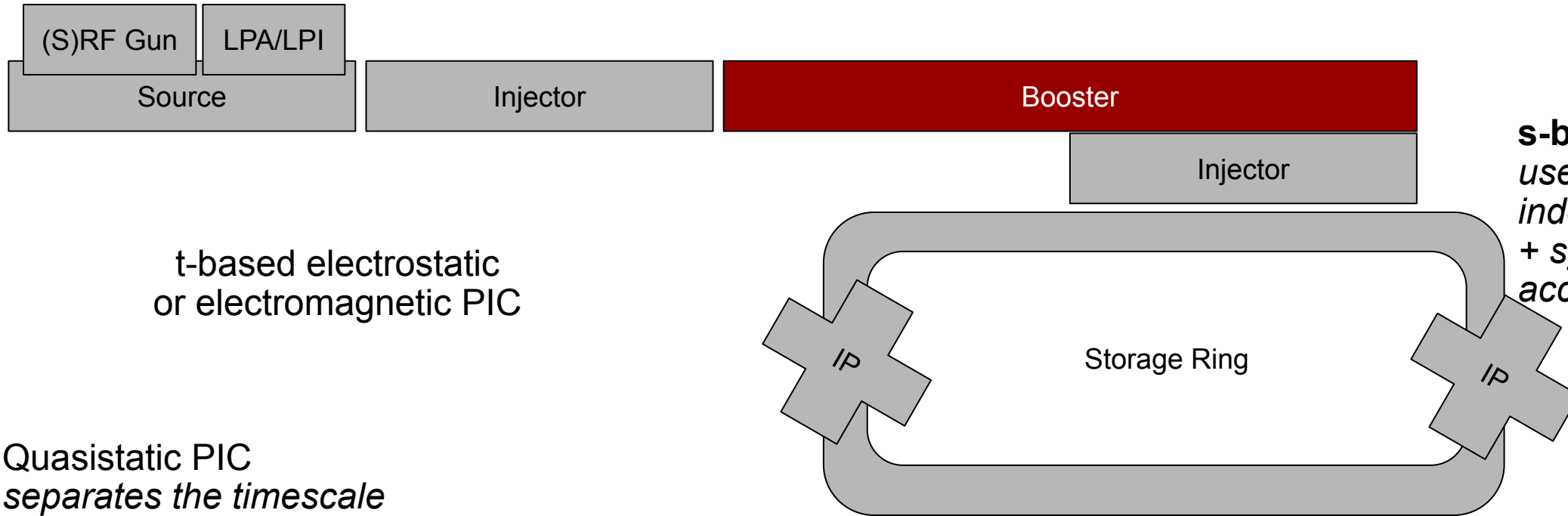
3D visualization of the plasma proton density during the acceleration process of a few-fs, 1.15nC beam
Hilz, Ostermayr, Huebl et al.; Nat. Comm. **9**.432, 2018

Goal
Start-to-end modeling in an open software ecosystem.



Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.



t-based electrostatic
or electromagnetic PIC

Quasistatic PIC
*separates the timescale
for plasma wakefield
and beam evolution*

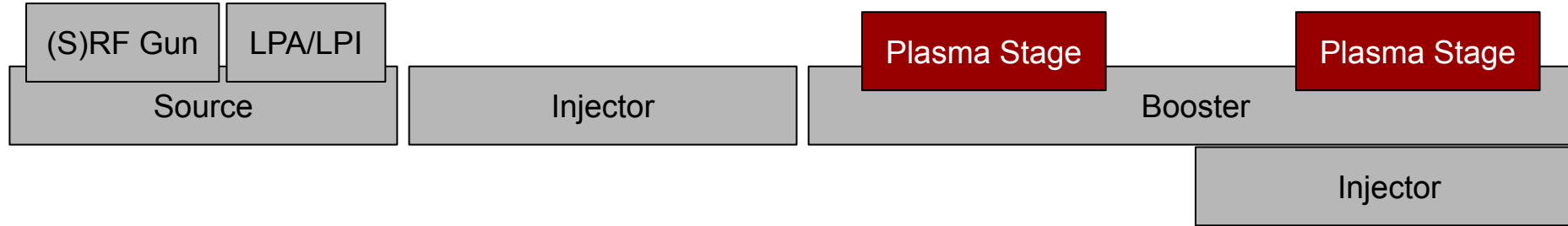
s-based PIC
*uses s instead of t as
independent variable
+ symplectic maps for
accelerator elements*

Goal
Start-to-end model-
ing in an open
software ecosystem.



Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

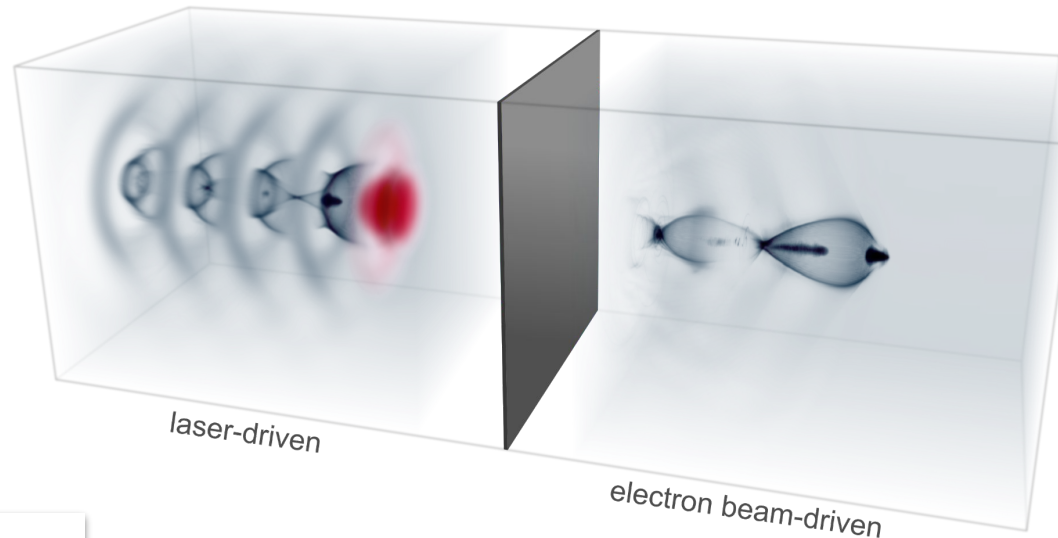
Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.



**t-based electrostatic
or electromagnetic PIC**

Quasistatic PIC
*separates the timescale
for plasma wakefield
and beam evolution*

Goal
Start-to-end model-
ing in an open
software ecosystem.

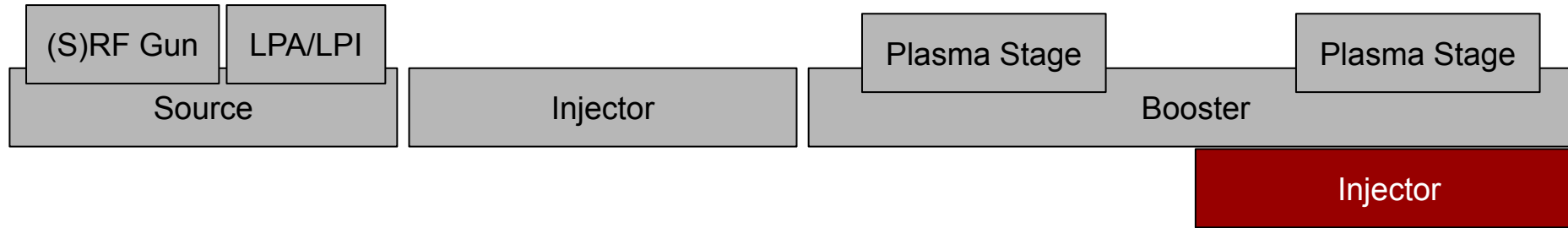


s-based PIC
*uses s instead of t as
independent variable
+ symplectic maps for
accelerator elements*

Left: Laser-driven wakefield accelerator (LWFA) stage with the drive laser propagating to the right shown in red; right: plasma wakefield accelerator (PWFA) driven by the electron beam from the LWFA stage (figure credits: Thomas Heinemann/Strathclyde and Alberto Martinez de la Ossa/DESY).
T. Kurz, T. Heinemann, et al. Nat. Comm. **12**.2895 (2021)

Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

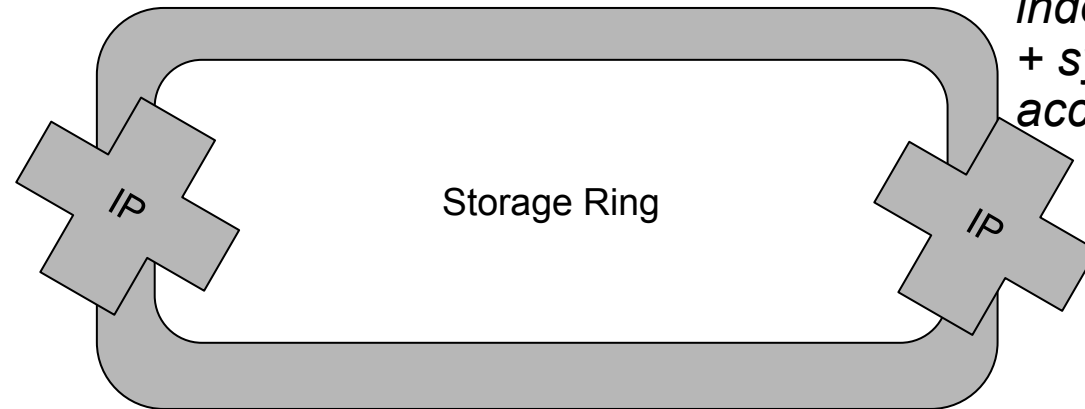
Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.



t-based electrostatic or electromagnetic PIC

Quasistatic PIC separates the timescale for plasma wakefield and beam evolution

s-based PIC uses s instead of t as independent variable + symplectic maps for accelerator elements

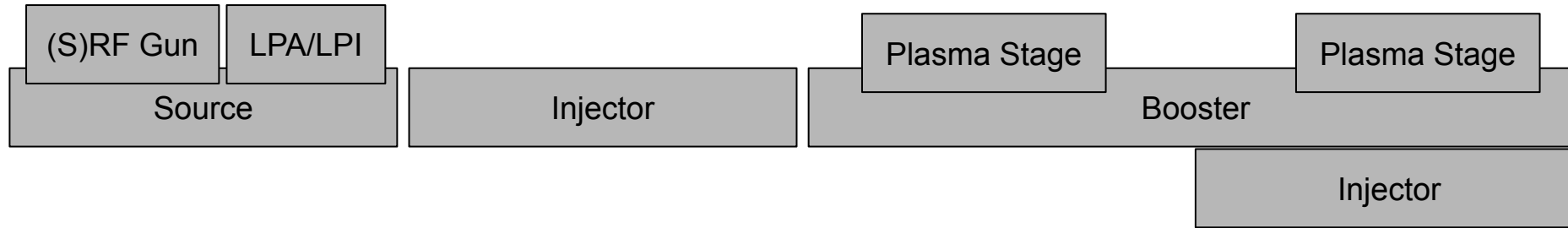


Goal
Start-to-end modeling in an open software ecosystem.



Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.



t-based electrostatic
or electromagnetic PIC

Quasistatic PIC
*separates the timescale
for plasma wakefield
and beam evolution*

s-based PIC
*uses s instead of t as
independent variable
+ symplectic maps for
accelerator elements*



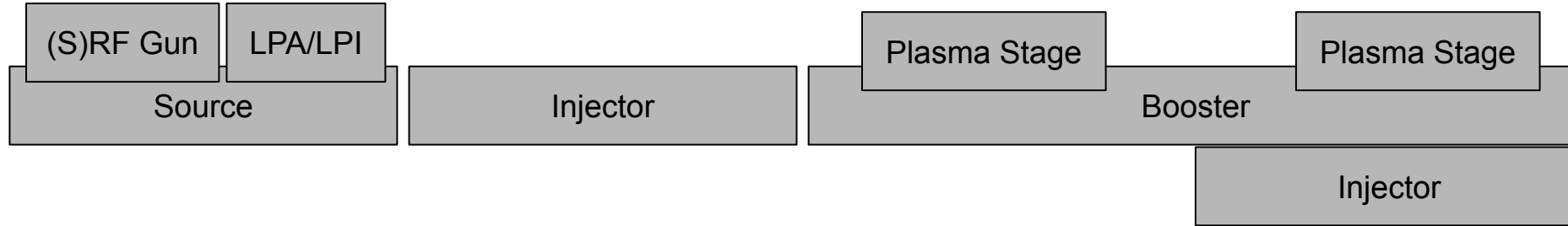
*buildup of electron clouds,
secondary electron yield*

Goal
Start-to-end model-
ing in an open
software ecosystem.



Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

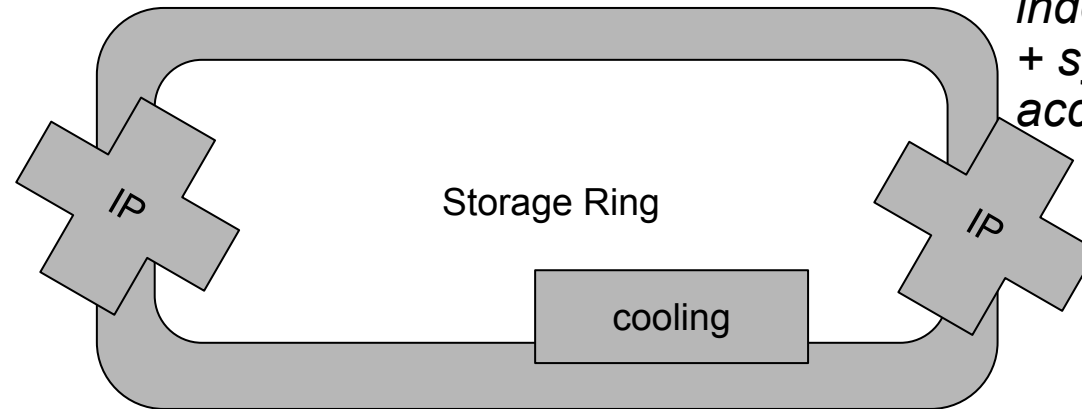
Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.



t-based electrostatic
or electromagnetic PIC

Quasistatic PIC
*separates the timescale
for plasma wakefield
and beam evolution*

s-based PIC
*uses s instead of t as
independent variable
+ symplectic maps for
accelerator elements*



*buildup of electron clouds,
secondary electron yield*

*modeling of radiative &
space-charge effects*

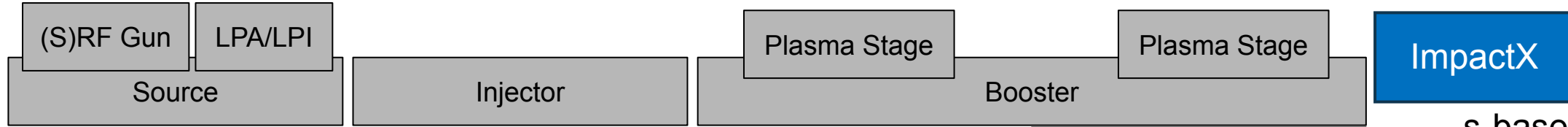


Goal
Start-to-end model-
ing in an open
software ecosystem.



Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

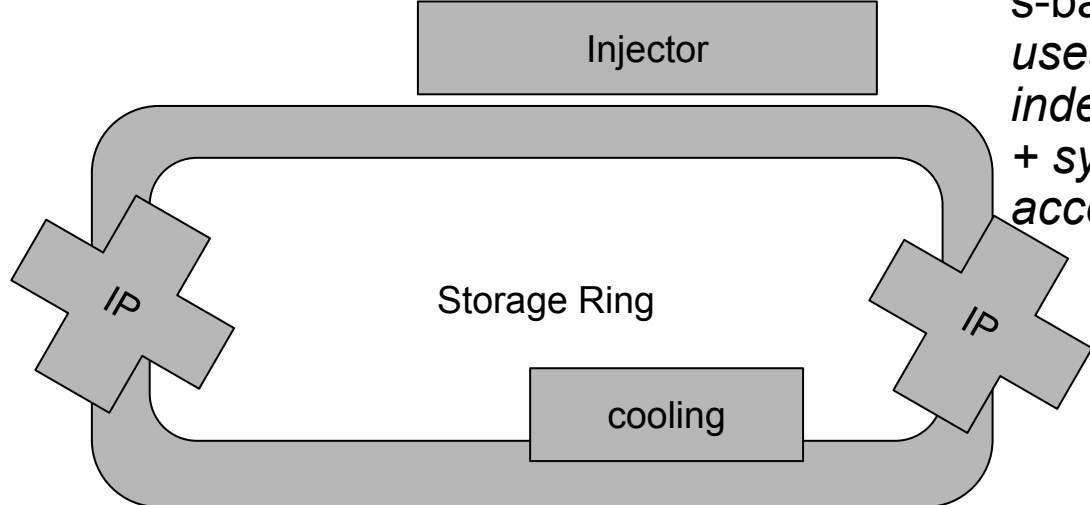
Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.



WarpX
t-based electrostatic or electromagnetic PIC

HiPACE++

Quasistatic PIC separates the timescale for plasma wakefield and beam evolution



s-based PIC uses s instead of t as independent variable + symplectic maps for accelerator elements

buildup of electron clouds, secondary electron yield

modeling of radiative & space-charge effects

FEL

Legend

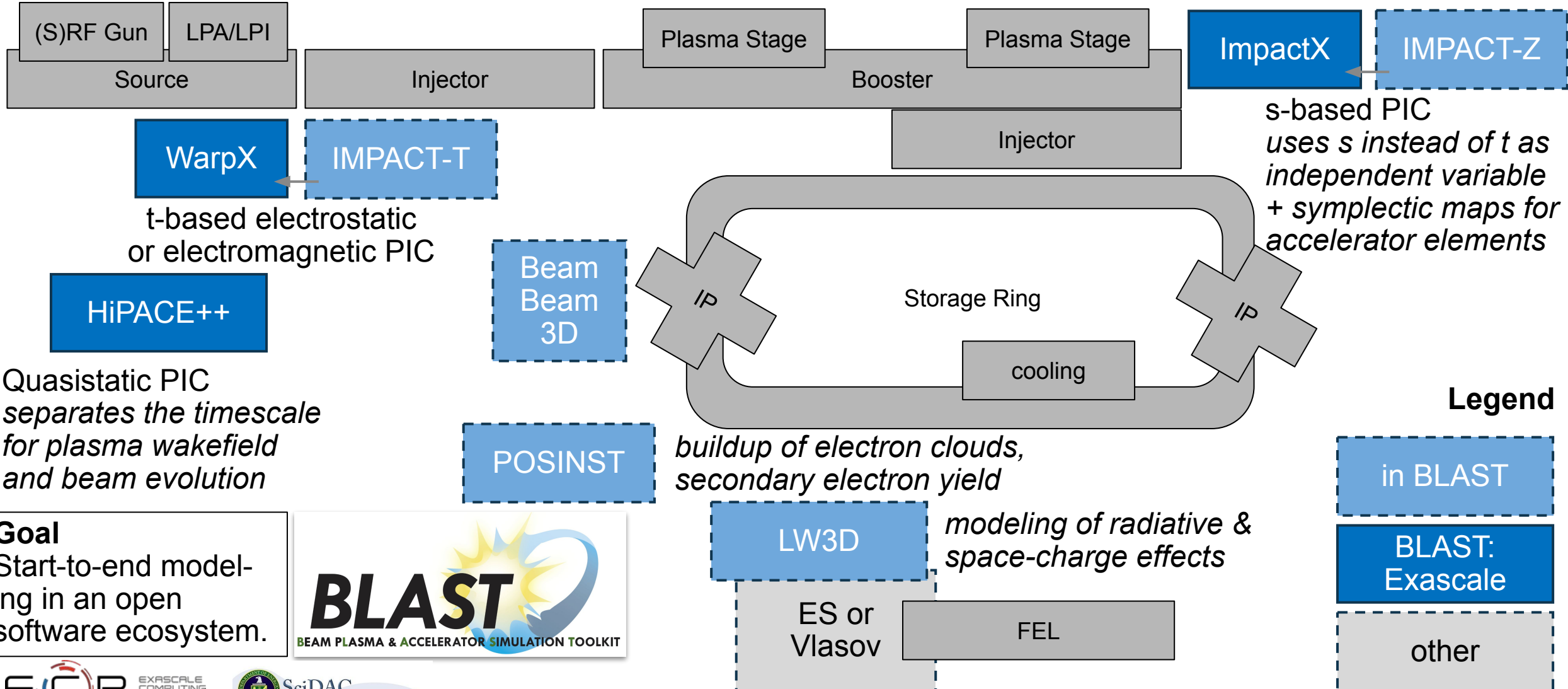
BLAST: Exascale

Goal
Start-to-end modeling in an open software ecosystem.



Simulation of Beam Sources & Dynamics Requires Different Types of PIC Codes

Imagine a future, **hybrid particle accelerator**, e.g., with conventional and plasma elements.

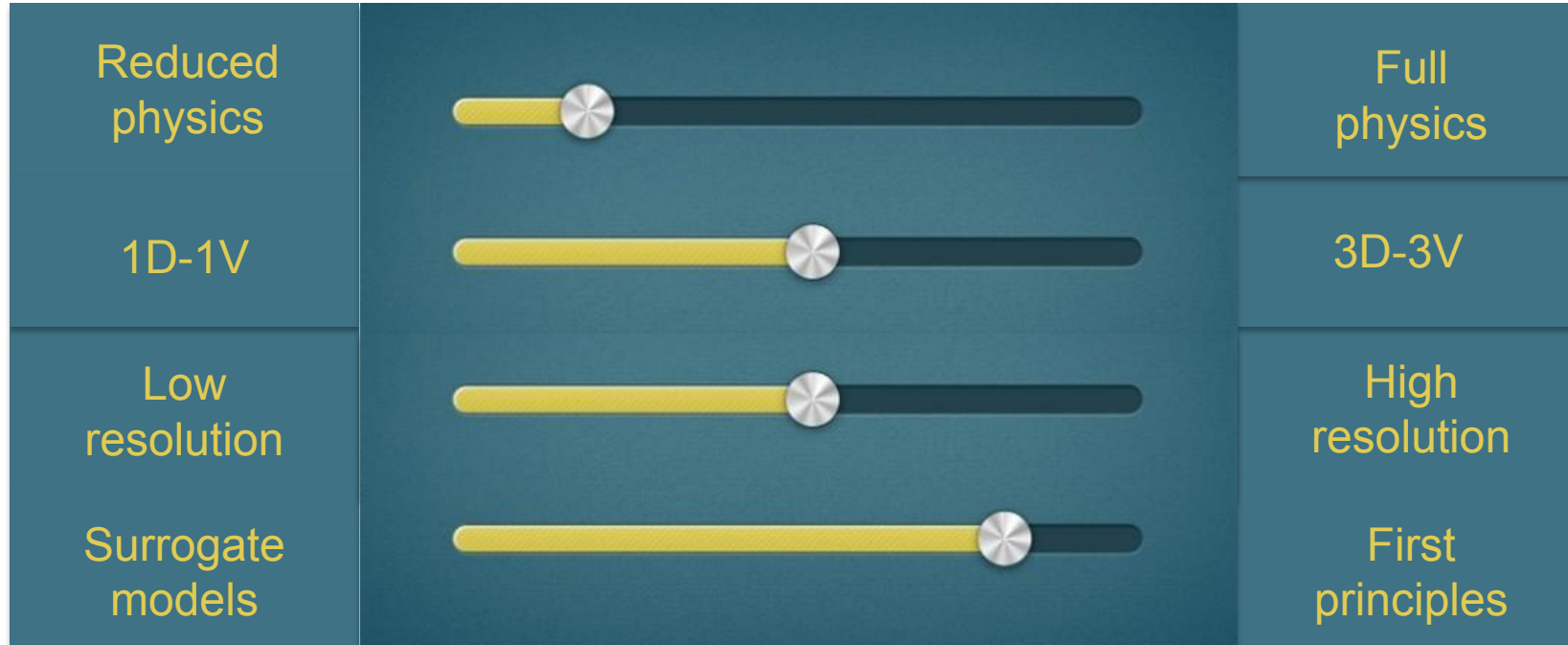


Goal
Start-to-end modeling in an open software ecosystem.



Ultimate goal: offer on-the-fly tunability of physics & numerics complexity to users

Great for ensemble runs for design studies



Great for detailed runs for physics studies

Goal

Start-to-end modeling in an open software ecosystem.



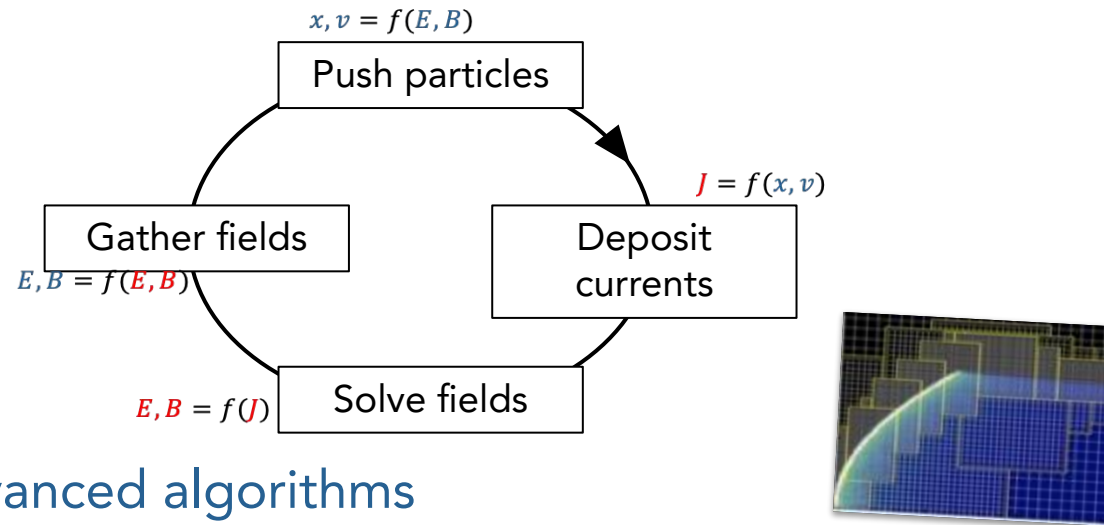
Start-to-End Modeling R&D

- advanced models: numerics, AI/ML surrogates
- speed & scalability: team science with computer sci.
- flexibility & reliability: modern software ecosystem

Overview of the Particle-In-Cell code WarpX

Available Particle-in-Cell Loops

- electrostatic & electromagnetic (fully kinetic)



Advanced algorithms

boosted frame, spectral solvers, Galilean frame, embedded boundaries + CAD, MR, ...

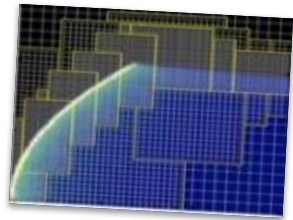
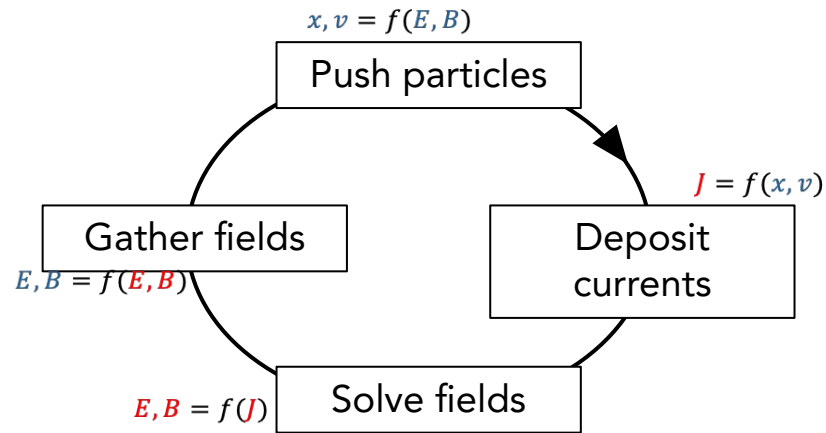
Multi-Physics Modules

field ionization of atomic levels, Coulomb collisions, QED processes (e.g. pair creation), macroscopic materials

Overview of the Particle-In-Cell code WarpX

Available Particle-in-Cell Loops

- electrostatic & electromagnetic (fully kinetic)



Advanced algorithms

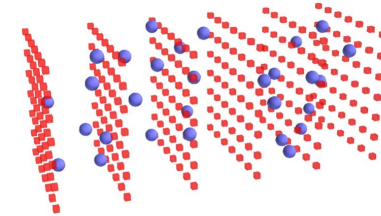
boosted frame, spectral solvers, Galilean frame, embedded boundaries + CAD, MR, ...

Multi-Physics Modules

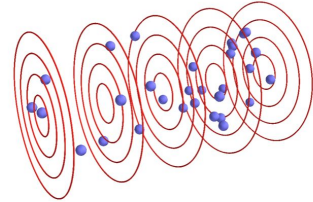
field ionization of atomic levels, Coulomb collisions, QED processes (e.g. pair creation), macroscopic materials

Geometries

- 1D3V, 2D3V, 3D3V and RZ (spectral cylindrical)



3D Cartesian grid



Cylindrical grid (schematic)

Multi-Node parallelization

- MPI: 3D domain decomposition
- dynamic load balancing



On-Node Parallelization

- GPU: CUDA, HIP and SYCL
- CPU: OpenMP

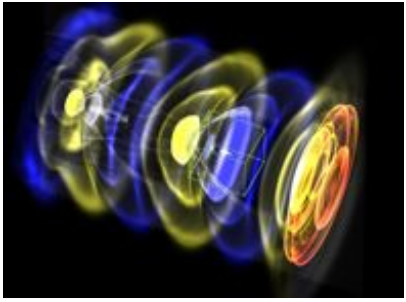


Scalable, Parallel I/O

- AMReX plotfile and openPMD (HDF5 or ADIOS)
- in situ diagnostics

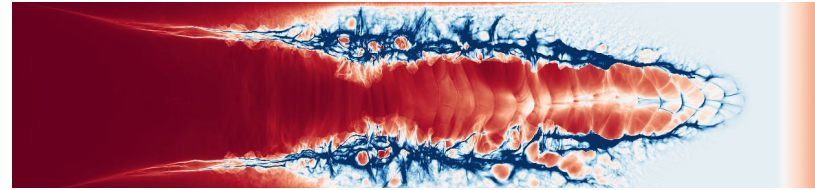


WarpX supports a growing number of applications

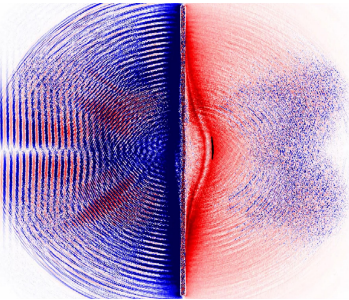
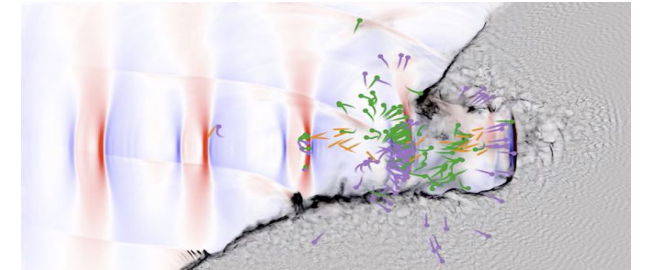


Plasma accelerators (LBNL, DESY, SLAC)

Laser-ion acceleration - advanced mechanisms (LBNL)

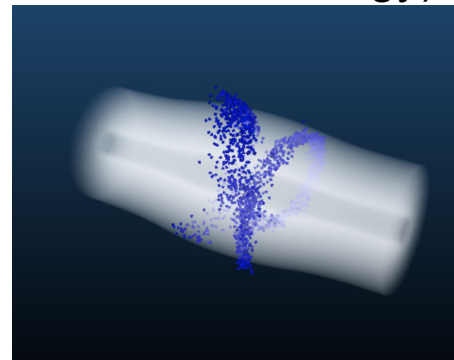


Plasma mirrors and high-field physics + QED (CEA Saclay/LBNL)

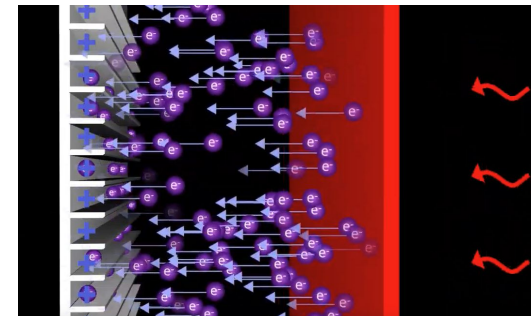


Laser-ion acceleration - laser pulse shaping (LLNL)

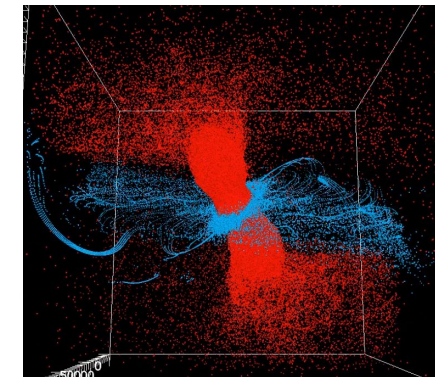
Plasma confinement, fusion devices (Zap Energy, Avalanche Energy)



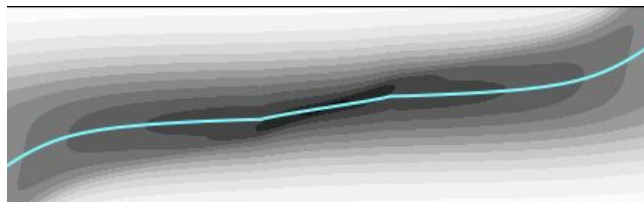
Thermionic converter (Modern Electron)



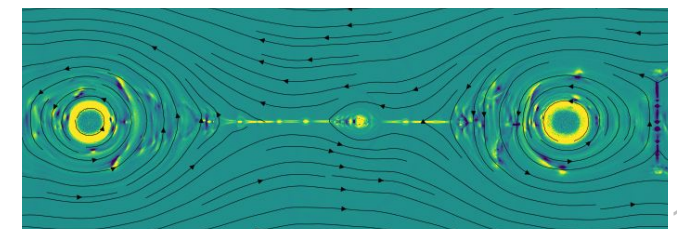
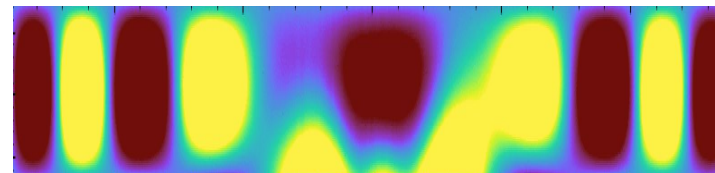
Pulsars, magnetic reconnection (LBNL)



Magnetic fusion sheaths (LLNL)



Microelectronics (LBNL) - ARTEMIS



ImpactX: GPU-, AMR- & AI/ML-Accelerated Beam Dynamics

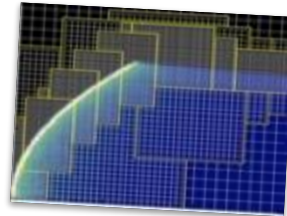
Last month, we open sourced ImpactX as an early developer preview.

Particle-in-Cell Loop

- electrostatic
 - with space-charge effects (in dev.)
- s-based
 - relative to a reference particle
 - elements: symplectic maps

Fireproof Numerics

based on IMPACT suite of codes, esp. IMPACT-Z and MaryLie



Triple Acceleration Approach

- GPU support
- Adaptive Mesh Refinement (in dev.)
- AI/ML & Data Driven Models (in dev.)



ImpactX: GPU-, AMR- & AI/ML-Accelerated Beam Dynamics

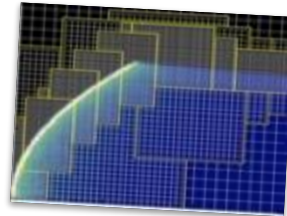
Last month, we open sourced ImpactX as an early developer preview.

Particle-in-Cell Loop

- electrostatic
 - with space-charge effects (in dev.)
- s-based
 - relative to a reference particle
 - elements: symplectic maps

Fireproof Numerics

based on IMPACT suite of codes, esp. IMPACT-Z and MaryLie



Triple Acceleration Approach

- GPU support
- Adaptive Mesh Refinement (in dev.)
- AI/ML & Data Driven Models (in dev.)

User-Friendly

- single-source C++, full Python control
- fully tested
- fully documented

Multi-Node parallelization

- MPI: 2D/3D domain decomposition
- dynamic load balancing (in dev.)

On-Node Parallelization

- GPU: CUDA, HIP and SYCL
- CPU: OpenMP

Scalable, Parallel I/O (in dev.)

- openPMD
- in situ analysis/visualization



ImpactX: Physics Benchmark Examples

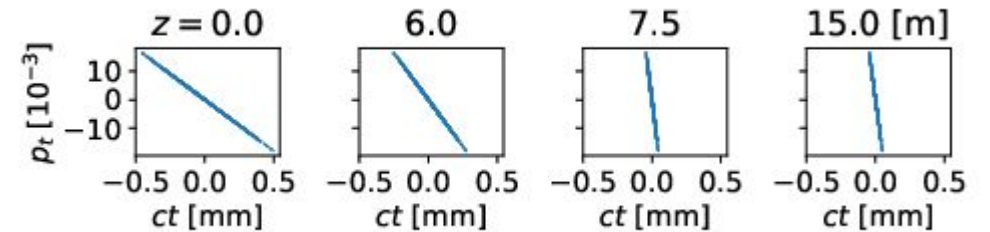
- FODO cell
- magnetic bunch compression chicane
- stationary beam in a const. focusing channel
- Kurth-distr. beam in periodic isotropic focusing channel
- stable FODO cell + short RF (buncher) cavities for longitudinal focusing
- chain of thin multipoles
- nonlin. focusing channel (IOTA nonlin. lens)
- Fermilab IOTA storage ring (linear optics)

ImpactX: Physics Benchmark Examples

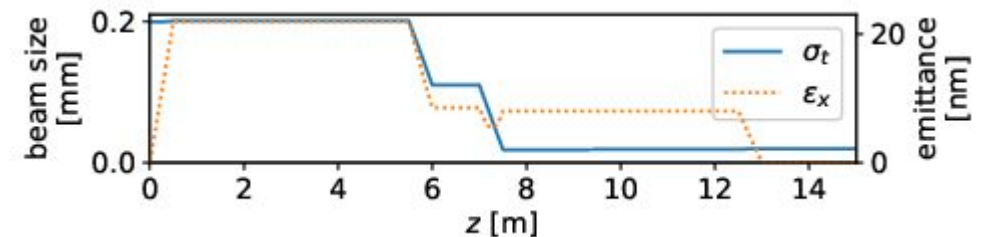
- FODO cell
- magnetic bunch compression chicane
- stationary beam in a const. focusing channel
- Kurth-distr. beam in periodic isotropic focusing channel
- stable FODO cell + short RF (buncher) cavities for longitudinal focusing
- chain of thin multipoles
- nonlin. focusing channel (IOTA nonlin. lens)
- Fermilab IOTA storage ring (linear optics)

Berlin-Zeuthen Chicane

- rms-matched 5 GeV electron beam with initial normalized transverse rms emittance of $1 \mu\text{m}$
- LCLS (@5GeV) & TESLA XFEL (@500MeV)-like



- longitudinal phase space: 10x compression
- emittance coupling: recovered at exit

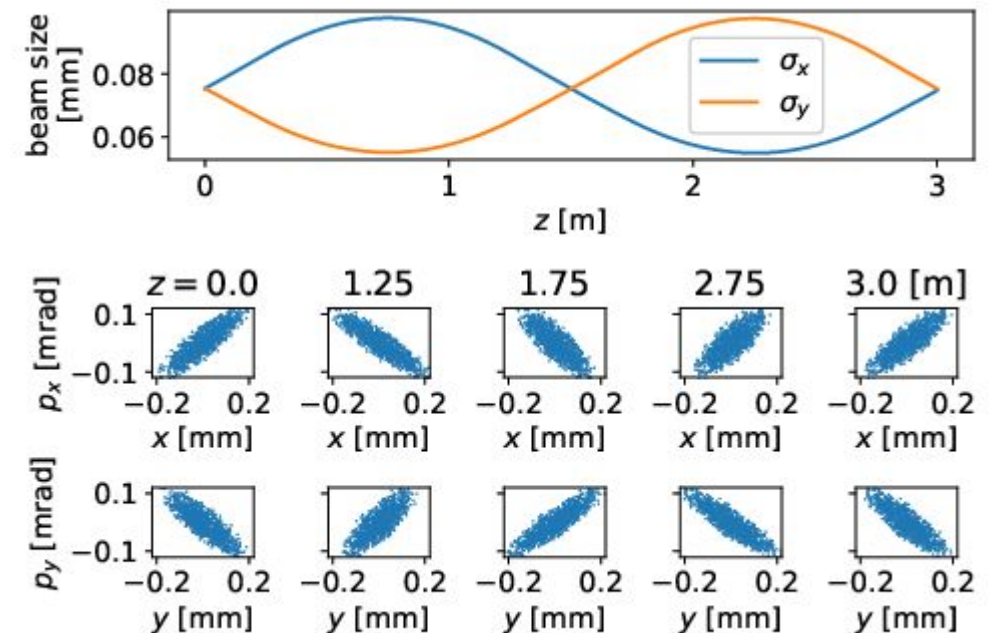


ImpactX: Physics Benchmark Examples

- FODO cell
- magnetic bunch compression chicane
- stationary beam in a const. focusing channel
- Kurth-distr. beam in periodic isotropic focusing channel
- stable FODO cell + short RF (buncher) cavities for longitudinal focusing
- chain of thin multipoles
- nonlin. focusing channel (IOTA nonlin. lens)
- Fermilab IOTA storage ring (linear optics)

FODO Cell

- stable FODO lattice with a zero-current phase advance of 67.8 degrees per cell
- rms-matched 2 GeV electron beam with initial unnormalized rms emittance of 2 nm
 - test also checks if emittance stays flat

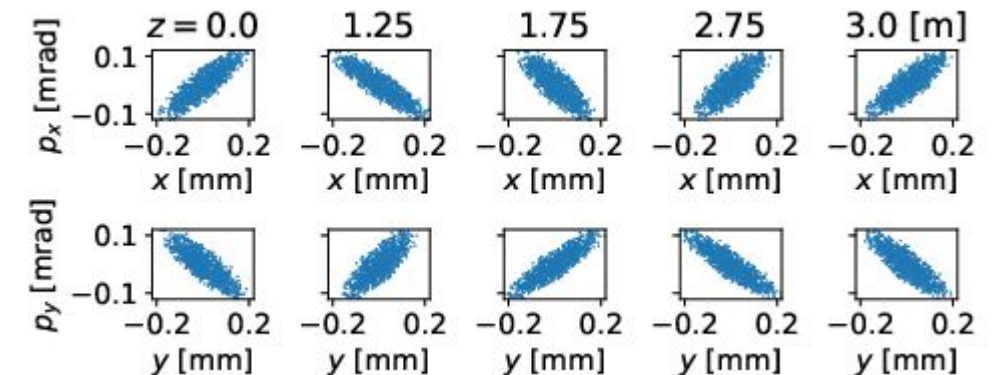
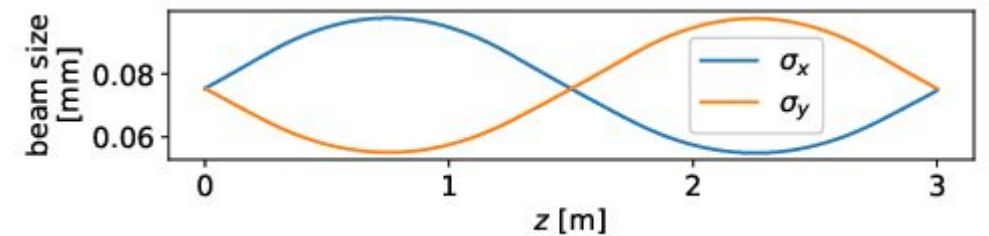


ImpactX: Physics Benchmark Examples

```
1 from impactx import ImpactX, RefPart, \
2     distribution, elements
3
4 sim = ImpactX() # simulation object
5
6 # set numerical parameters and IO control
7 sim.set_particle_shape(2) # B-spline order
8 sim.set_slice_step_diagnostics(True)
9 sim.set_space_charge(False)
10
11 # domain decomposition & space charge mesh
12 sim.init_grids()
13
14 # load a 2 GeV electron beam with an initial
15 # unnormalized rms emittance of 2 nm
16 energy_MeV = 2.0e3 # reference energy
17 charge_C = 1.0e-9 # used with space charge
18 mass_MeV = 0.510998950 # mass
19 qm_qeeV = -1.0e-6/mass_MeV # charge/mass
20 npart = 10000 # number of macro particles
21
22 distr = distribution.Waterbag(
23     sigmaX = 3.9984884770e-5,
24     sigmaY = 3.9984884770e-5,
25     sigmaT = 1.0e-3,
26     sigmaPx = 2.6623538760e-5,
27     sigmaPy = 2.6623538760e-5,
28     sigmaPt = 2.0e-3,
29     muxpx = -0.846574929020762,
30     muypy = 0.846574929020762,
31     mutpt = 0.0)
32 sim.add_particles(
33     qm_qeeV, charge_C, distr, npart)
34
35 # set the energy in the reference particle
36 sim.particle_container().ref_particle() \
37     .set_energy_MeV(energy_MeV, mass_MeV)
38
39 # design the accelerator lattice
40 ns = 25 # steps slicing through ds
41 fodo = [
42     elements.Drift(ds=0.25, nslice=ns),
43     elements.Quad(ds=1.0, k=1.0, nslice=ns),
44     elements.Drift(ds=0.5, nslice=ns),
45     elements.Quad(ds=1.0, k=-1.0, nslice=ns),
46     elements.Drift(ds=0.25, nslice=ns)
47 ]
48 # assign a fodo segment
49 sim.lattice.extend(fodo)
50
51 # run simulation
52 sim.evolve()
```

FODO Cell

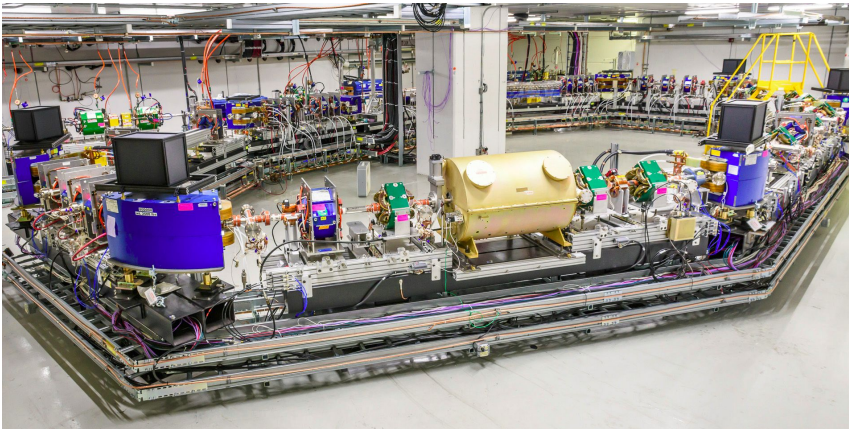
- stable FODO lattice with a zero-current phase advance of 67.8 degrees per cell
- rms-matched 2 GeV electron beam with initial unnormalized rms emittance of 2 nm
 - test also checks if emittance stays flat



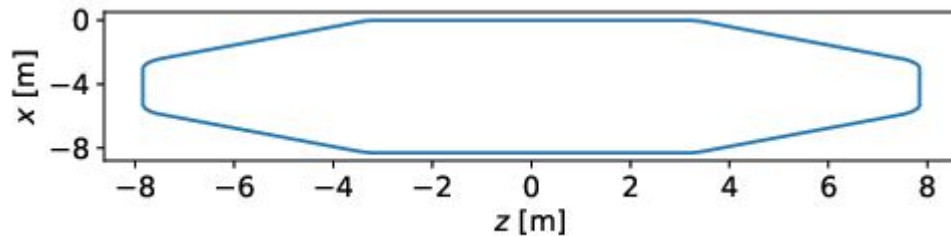
Same Script
CPU/GPU & MPI

ImpactX: IOTA (v8.4) Lattice Benchmark @2.5 MeV protons

bare (linear) lattice of the Fermilab IOTA storage ring; an rms-matched proton beam with an unnormalized emittance of $4.5 \mu\text{m}$ propagates over a single turn

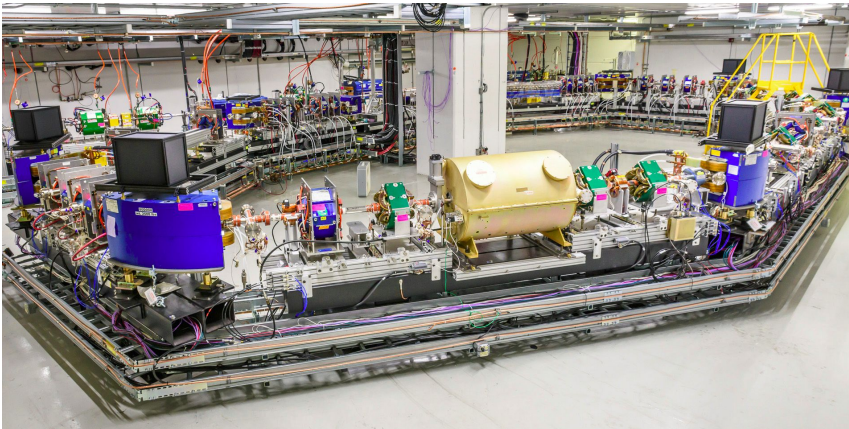


Reference Orbit

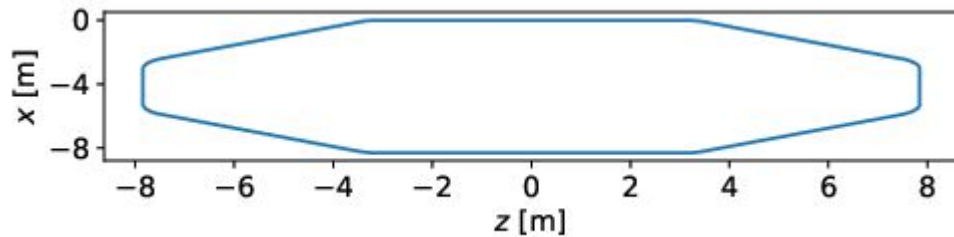


ImpactX: IOTA (v8.4) Lattice Benchmark @2.5 MeV protons

bare (linear) lattice of the Fermilab IOTA storage ring; an rms-matched proton beam with an un-normalized emittance of $4.5 \mu\text{m}$ propagates over a single turn



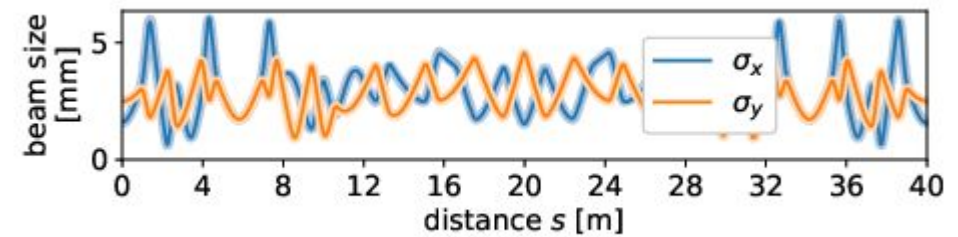
Reference Orbit



Preservation of Second Moments

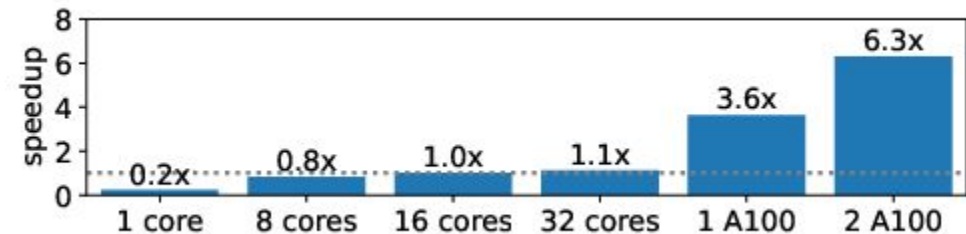
- nnl. element: conserve invariants of motion
- check emittance preservation
- rms beam size evolution:

IMPACT-Z vs ImpactX



Preliminary Performance

- on Perlmutter (NERSC) CPU / GPU
- order-of-magnitude perf. \nearrow w/o dyn. LB (yet)



An open interface with the community

Online Documentation:
warpX|hipace|impactx.readthedocs.io

USAGE

Run WarpX

Input Parameters

Python (PICMI)

Examples

- Beam-driven electron acceleration
- Laser-driven electron acceleration
- Plasma mirror
- Laser-ion acceleration
- Uniform plasma
- Capacitive discharge

For a complete list of all example input files, have a look at our [Examples/](#) directory. It contains folders and subfolders with self-describing names that you can try. All these input files are automatically tested, so they should always be up-to-date.

Beam-driven electron acceleration

AMReX [inputs](#) :

- [2D case](#)
- [2D case in boosted frame](#)
- [3D case in boosted frame](#)

Open-Source Development & Benchmarks:
github.com/ECP-WarpX

All checks have passed
24 successful and 1 neutral checks

✓	macOS / AppleClang (pull_request)	Successful in 40m	Required	Details
✓	Windows / MSVC C++17 w/o MPI (pull_request)	Successful in 58m		Details
✓	CUDA / NVCC 11.0.2 SP (pull_request)	Successful in 31m	Required	Details
✓	HIP / HIP 3D SP (pull_request)	Successful in 29m		Details
✓	Intel / oneAPI DPC++ SP (pull_request)	Successful in 38m		Details
✓	OpenMP / Clang on warpX (pull_request)	Successful in 37m	Required	Details



188 physics benchmarks run on every code change of WarpX
8 physics benchmarks + 32 tests for ImpactX

An open interface with the community

Online Documentation:
warpX|hipace|impactx.readthedocs.io

For a complete list of all example input files, have a look at our [Examples/](#) directory. It contains folders and subfolders with self-describing names that you can try. All these input files are automatically tested, so they should always be up-to-date.

Beam-driven electron acceleration

AMReX [inputs](#) :

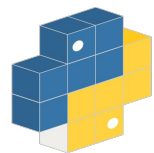
- [2D case](#)
- [2D case in boosted frame](#)
- [3D case in boosted frame](#)

Open-Source Development & Benchmarks:
github.com/ECP-WarpX

All checks have passed
24 successful and 1 neutral checks

✓	🍏 macOS / AppleClang (pull_request)	Successful in 40m	Required	Details
✓	🪟 Windows / MSVC C++17 w/o MPI (pull_request)	Successful in 58m		Details
✓	🔥 CUDA / NVCC 11.0.2 SP (pull_request)	Successful in 31m	Required	Details
✓	🍷 HIP / HIP 3D SP (pull_request)	Successful in 29m		Details
✓	🇮🇹 Intel / oneAPI DPC++ SP (pull_request)	Successful in 38m		Details
✓	🇧🇪 OpenMP / Clang nvwarpX (pull_request)	Successful in 37m	Required	Details

Rapid and easy installation on any platform:



`python3 -m pip install .`



`brew tap ecp-warpX/warpX`
`brew install warpX`



`conda install`
`-c conda-forge warpX`



`spack install warpX`
`spack install py-warpX`



`cmake -S . -B build`
`cmake --build build --target install`



`module load warpX`
`module load py-warpX`



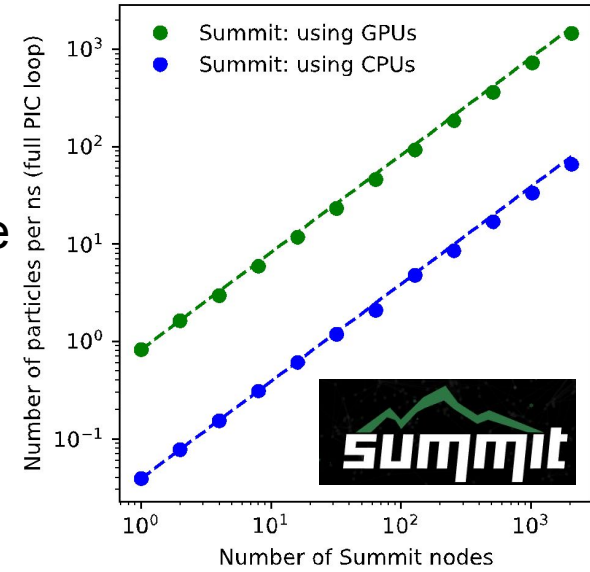
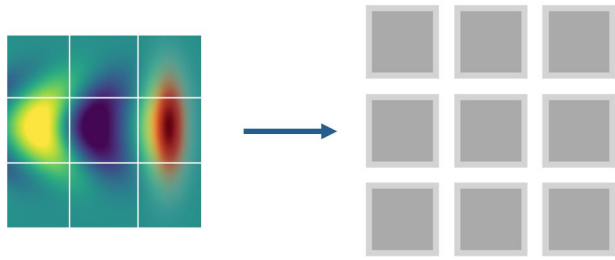
188 physics benchmarks run on every code change of WarpX
8 physics benchmarks + 32 tests for ImpactX

Portable Performance through Exascale Programming Model

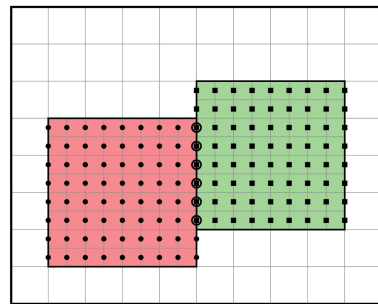
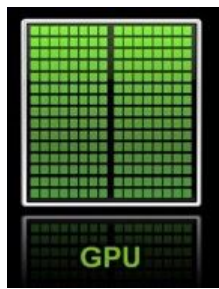
AMReX library



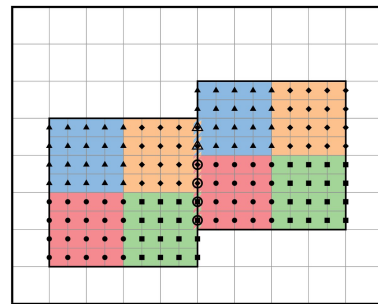
- Domain decomposition & MPI communications: MR & load balance



- Performance-Portability Layer: GPU/CPU/KNL



without tiling



with tiling



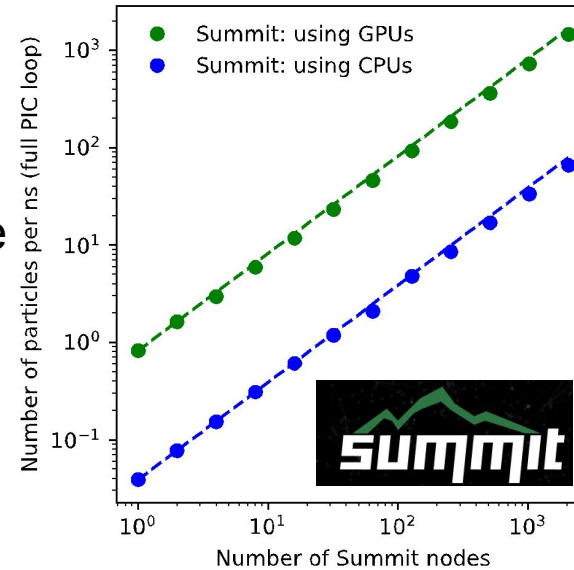
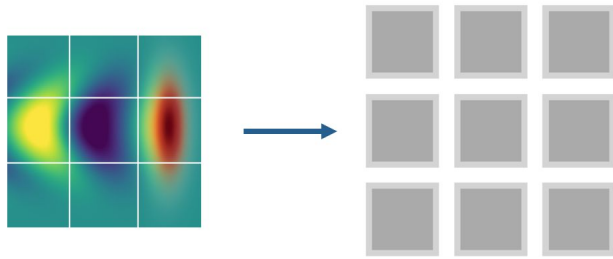
Data Structures

Portable Performance through Exascale Programming Model

AMReX library



- Domain decomposition & MPI communications: MR & load balance

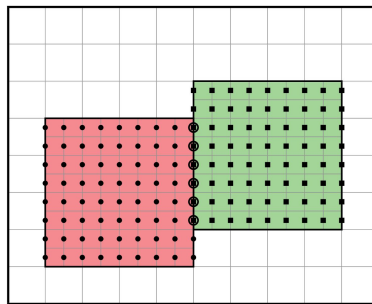
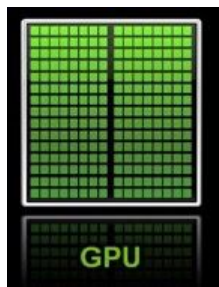


- Write the code once, specialize at *compile-time*

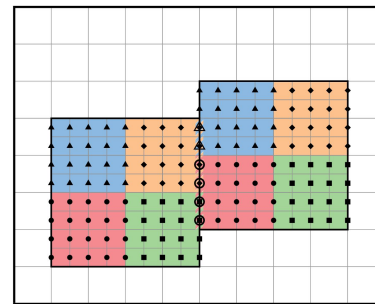
ParallelFor (/Scan/Reduce)

```
amrex::ParallelFor( n_particles,
    [=] AMREX_GPU_DEVICE (long i) {
        UpdatePosition( x[i], y[i], z[i],
            ux[i], uy[i], uz[i], dt );
    });
```

- Performance-Portability Layer: GPU/CPU/KNL



without tiling



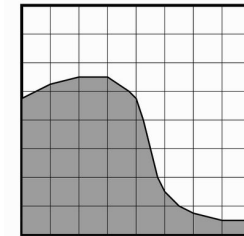
with tiling



Data Structures

- Parallel linear solvers (e.g. multi-grid Poisson solvers)

- Embedded boundaries



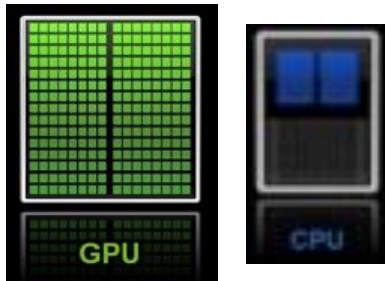
- Runtime parser for user-provided math expressions (incl. GPU)

A. Myers et al., "Porting WarpX to GPU-accelerated platforms," Parallel Computing 108, 102833 (2021)

Transitioning to an Integrated Ecosystem



Desktop
to
HPC



MPI

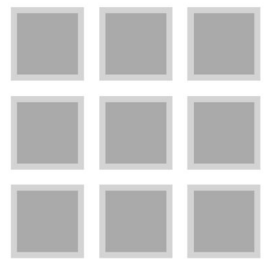
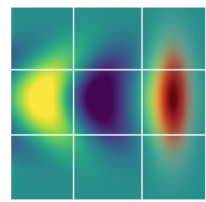
CUDA, OpenMP, SYCL, HIP



Transitioning to an Integrated Ecosystem



Desktop
to
HPC



AMReX
Containers, Communication,
Portability, Utilities

FFT
on- or
multi-
device

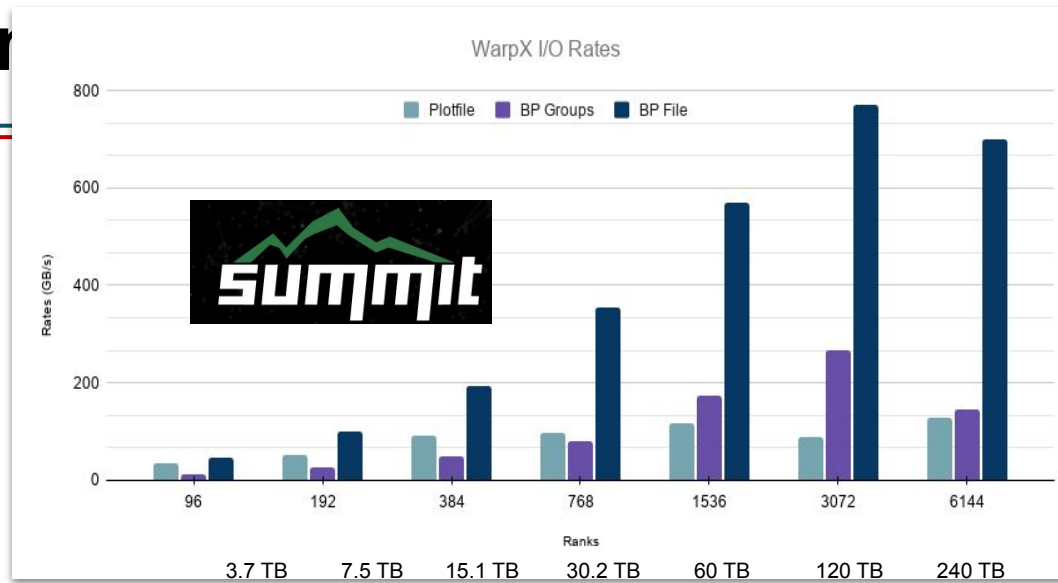
**Lin.
Alg.**
BLAS++
LAPACK++

MPI

CUDA, OpenMP, SYCL, HIP



Transitioning to an HPC



- PByte-scale
- TByte/s Bandwidth



Desktop
to
HPC



AMReX

Containers, Communication,
Portability, Utilities

Diagnostics
I/O
code coupling

openPMD

ADIOS S2 HD F5

ZFP

Asc ent

VTK -m

FFT

on- or
multi-
device

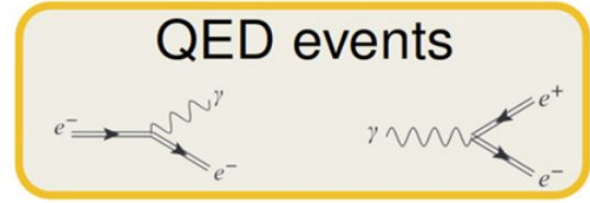
Lin. Alg.

BLAS++
LAPACK++

MPI

CUDA, OpenMP, SYCL, HIP

Transitioning to an Integrated Ecosystem



PICSAR
QED Modules

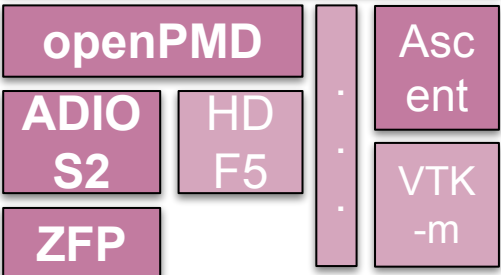
ABLASTR library: common PIC physics



Desktop
to
HPC

AMReX
Containers, Communication,
Portability, Utilities

Diagnostics
I/O
code coupling



FFT
on- or
multi-
device

Lin. Alg.
BLAS++
LAPACK++

MPI

CUDA, OpenMP, SYCL, HIP



Transitioning to an Integrated Ecosystem



Desktop
to
HPC



WarpX
full PIC, LPA/LPI

HiPACE++
quasi-static, PWFA

ARTEMIS
microelectronics

ImpactX
accelerator
lattice design

PICSAR
QED Modules

ABLASTR library: common PIC physics

AMReX
Containers, Communication,
Portability, Utilities

Diagnostics
I/O
code coupling

openPMD

ADIOS2

HD F5

ZFP

·
·
·

Asc
ent

VTK
-m

FFT
on- or
multi-
device

Lin. Alg.
BLAS++
LAPACK++

MPI

CUDA, OpenMP, SYCL, HIP

Transitioning to an Integrated Ecosystem



Desktop
to
HPC



Python: Modules, PICMI interface, Workflows

WarpX
full PIC, LPA/LPI

HiPACE++
quasi-static, PWFA

ARTEMIS
microelectronics

ImpactX
accelerator
lattice design

Object-Level
Python Bindings
extensible, AI/ML

pyAMReX

PICSAR
QED Modules

ABLASTR library: common PIC physics

AMReX
Containers, Communication,
Portability, Utilities

Diagnostics
I/O
code coupling

openPMD

ADIO
S2

HD
F5

ZFP

Asc
ent

VTK
-m

FFT
on- or
multi-
device

**Lin.
Alg.**
BLAS++
LAPACK++

MPI

CUDA, OpenMP, SYCL, HIP

- BLAST: Beam pLasma Accelerator Simulation Toolkit
- IO, Standardization & Open Development
- HPC: The Exascale Computing Project and Beyond



We Standardize & Develop Scalable Data Methods

Start-to-end accelerator modeling requires data compatibility and control usability

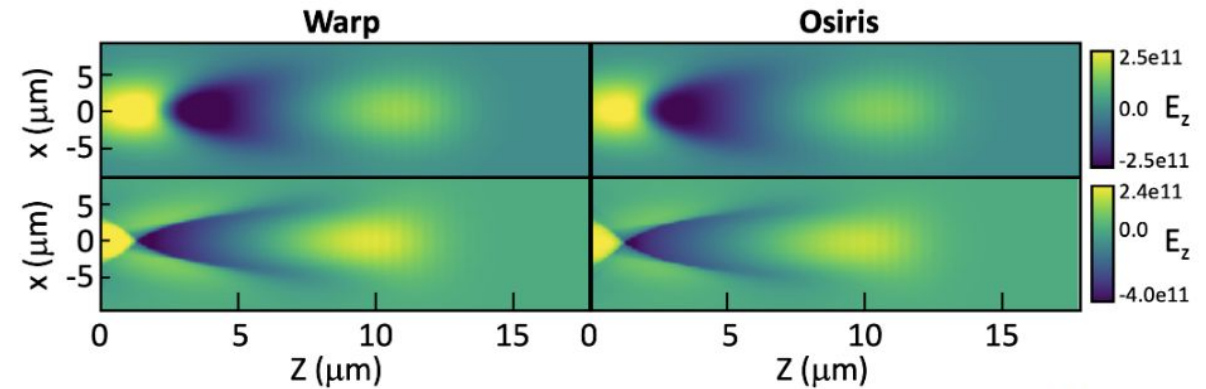
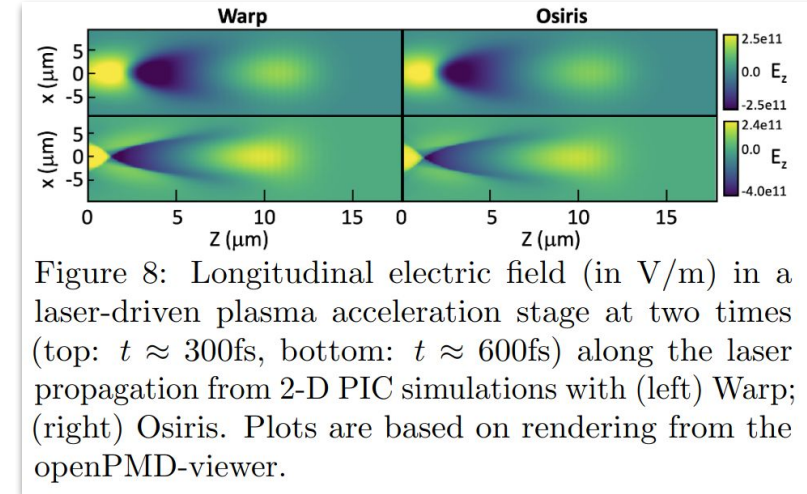
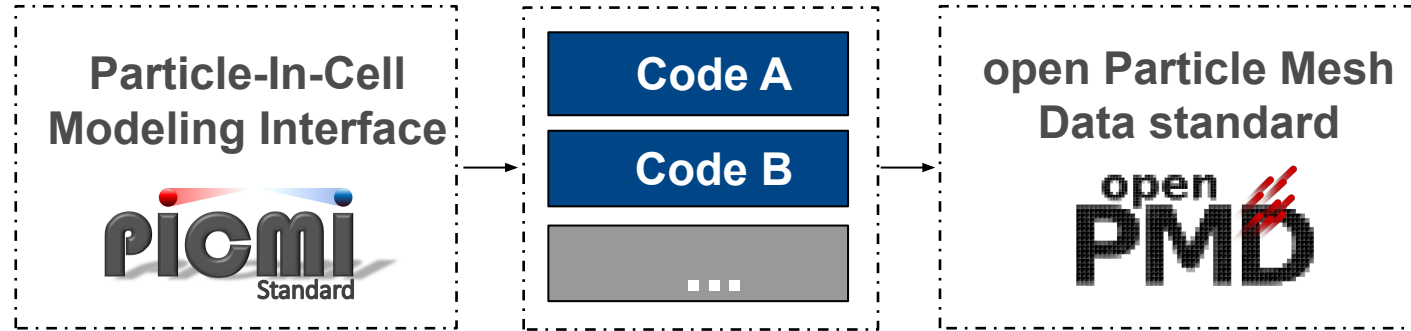


Figure 8: Longitudinal electric field (in V/m) in a laser-driven plasma acceleration stage at two times (top: $t \approx 300\text{fs}$, bottom: $t \approx 600\text{fs}$) along the laser propagation from 2-D PIC simulations with (left) Warp; (right) Osiris. Plots are based on rendering from the openPMD-viewer.

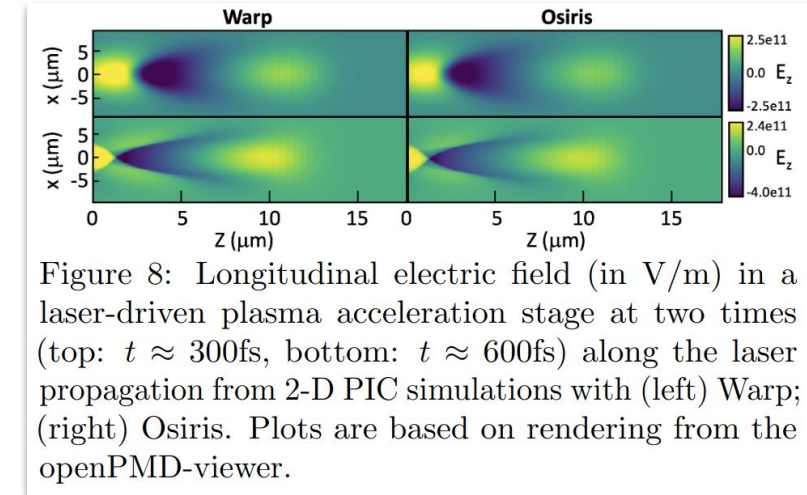
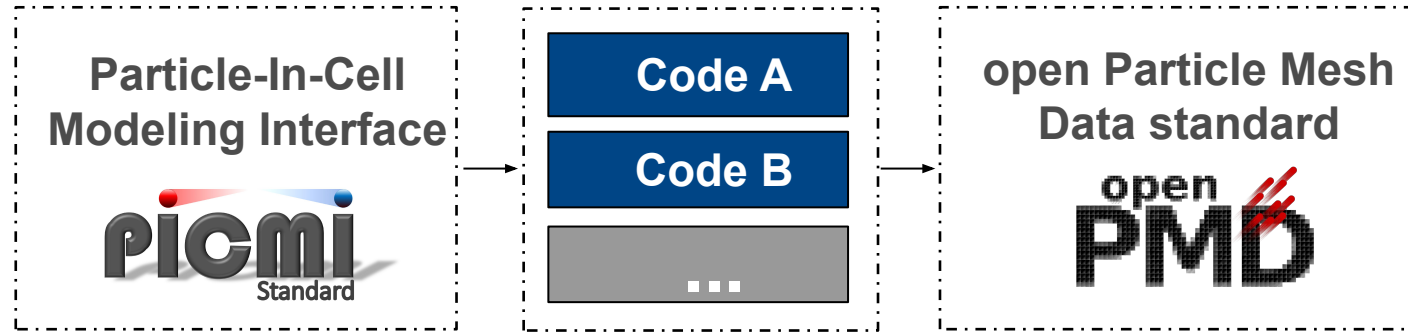
We Standardize & Develop Scalable Data Methods

Start-to-end accelerator modeling requires data compatibility and control usability



We Standardize & Develop Scalable Data Methods

Start-to-end accelerator modeling requires data compatibility and control usability



Communities

Consortium for Advanced Modeling of Particle Accelerators **CAMPA**

openPMD: Open Standard for Particle-Mesh Data



- **markup** / schema for arbitrary hierarchical data formats
- truly, scientifically **self-describing**
- basis for **open data workflows**

openPMD standard (1.0.0, 1.0.1, 1.1.0)

the underlying file markup and definition

A Huebl et al., DOI:10.5281/zenodo.33624

openPMD: Open Standard for Particle-Mesh Data



- **markup** / schema for arbitrary hierarchical data formats
- truly, scientifically **self-describing**
- basis for **open data workflows**

openPMD standard (1.0.0, 1.0.1, 1.1.0)

the underlying file markup and definition

A Huebl et al., DOI:10.5281/zenodo.33624

base standard

general description

wavefronts, particle species, particle beams, weighted particles, PIC, MD, mesh-refinement, CCD images, ...

extensions

domain specific

openPMD: Open Standard for Particle-Mesh Data



- **markup** / schema for arbitrary hierarchical data formats
- truly, scientifically **self-describing**
- basis for **open data workflows**

openPMD standard (1.0.0, 1.0.1, 1.1.0)

the underlying file markup and definition

A Huebl et al., DOI:10.5281/zenodo.33624

base standard

general description

wavefronts, particle species, particle beams, weighted particles, PIC, MD, mesh-refinement, CCD images, ...

extensions

domain specific



openPMD: Open Standard for Particle-Mesh Data



- **markup** / schema for arbitrary hierarchical data formats
- truly, scientifically **self-describing**
- basis for **open data workflows**

openPMD standard (1.0.0, 1.0.1, 1.1.0)

the underlying file markup and definition

A Huebl et al., DOI:10.5281/zenodo.33624

base standard

general description

wavefronts, particle species, particle beams, weighted particles, PIC, MD, mesh-refinement, CCD images, ...

extensions

domain specific



openPMD-viewer

quick visualization

explore, e.g., in Jupyter

openPMD-api

reference library

file-format agnostics API

openPMD-updater

auto-update to new standard, verify

openPMD-validator

We Standardize & Develop Scalable Data Methods

... and integrate them for scientific productivity

including data analytics frameworks & graphical user interfaces

In []: `ts_2d.slider()`

Calling this method will insert the following panel inside the notebook. (Note that the panel below is a **non-interactive image**, which is here for the use of this notebook online. Calling the `slider` method in a live notebook, will produce a truly **interactive** panel.)

- + t (fs) 33

Field type

Field: B E J rho

Coord: x y z

Plotting options

Always refresh Refresh now!

Particle quantities

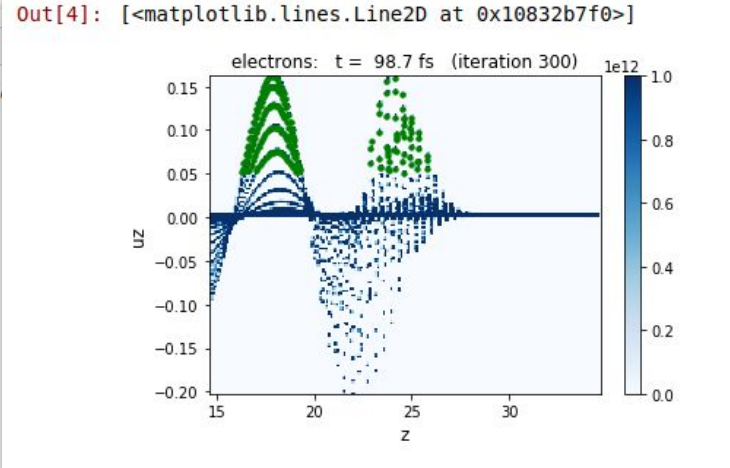
Hydrogen1+

x	y	z	ux	uy	uz	w	
x	y	z	ux	uy	uz	w	None

Particle selection

Plotting options

Out[4]: [`<matplotlib.lines.Line2D at 0x10832b7f0>`]

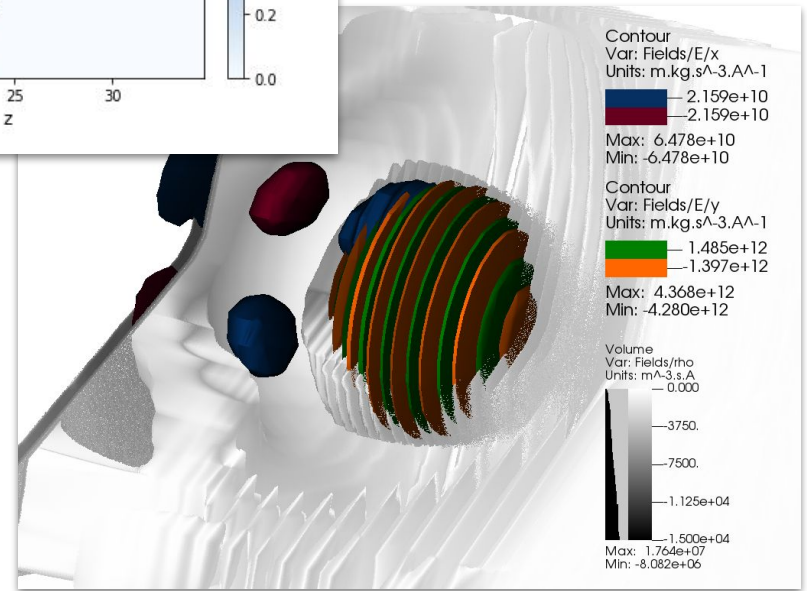
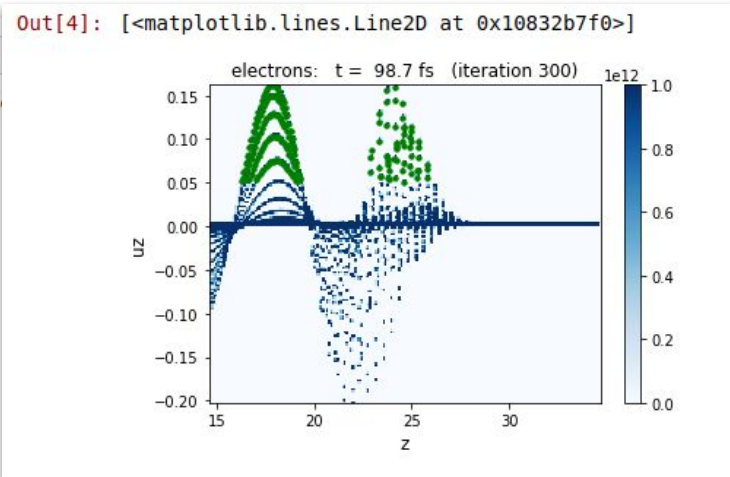


We Standardize & Develop Scalable Data Methods

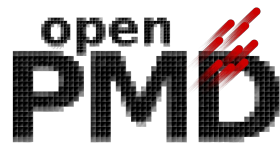
... and integrate them for scientific productivity
including data analytics frameworks & graphical user interfaces

In []: `ts_2d.slider()`

Calling this method will insert the following panel inside the notebook. (Note that the panel below is a **non-interactive image**, which is here for the use of this notebook online. Calling the `slider` method in a live notebook, will produce a truly **interactive** panel.)



We Standardize & Develop Scalable Data Methods

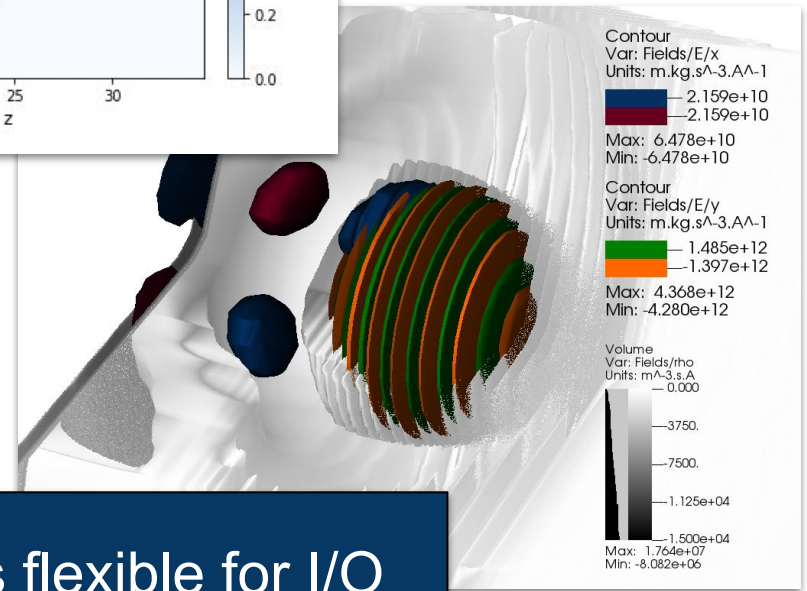
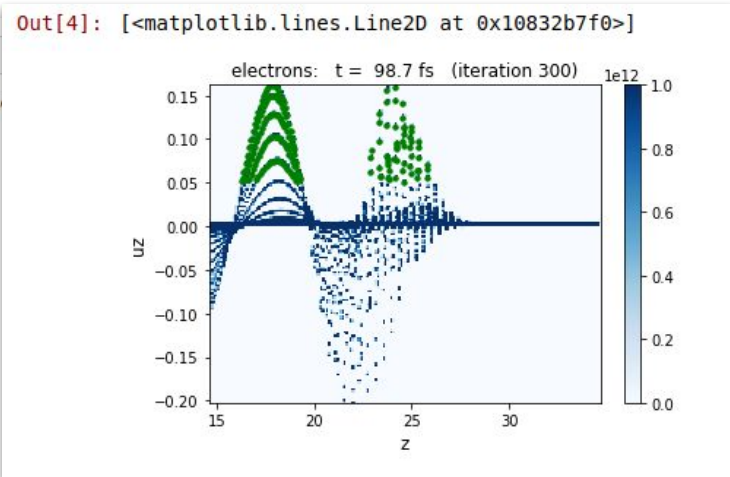


... and integrate them for scientific productivity
including data analytics frameworks & graphical user interfaces

In []: `ts_2d.slider()`

Calling this method will insert the following panel inside the notebook. (Note that the panel below is a **non-interactive image**, which is here for the use of this notebook online. Calling the `slider` method in a live notebook, will produce a truly **interactive** panel.)

The interface includes a slider for time t (fs) set to 33. It features sections for 'Field type' (with options B, E, J, rho and coordinates x, y, z), 'Particle quantities' (for Hydrogen1+ with axes x, y, z, ux, uy, uz, w), and 'Plotting options' (with 'Always refresh' and 'Refresh now!' buttons).



Open standardization, i.e. openPMD, makes us flexible for I/O libraries, tooling & domain-science needs.



- BLAST: Beam pLasma Accelerator Simulation Toolkit
- IO, Standardization & Open Development
- HPC: The Exascale Computing Project and Beyond

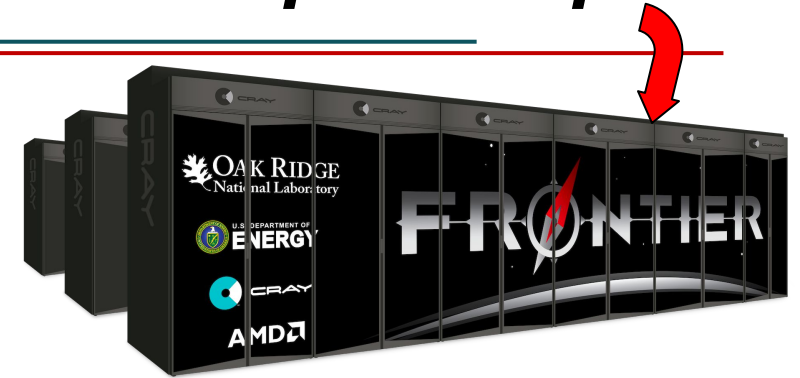


WarpX: Runs Efficiently on the *First Exascale Supercomputer*

April-July 2022: ran on **world's largest HPCs**
L. Fedeli, A. Huebl et al., *accepted* in SC'22, 2022

Note: Perlmutter & Frontier are pre-acceptance!

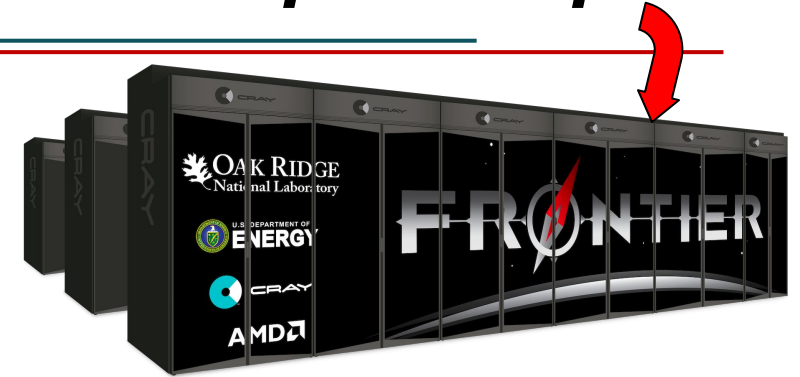
Demonstrated scaling **4-5 orders** of magnitude



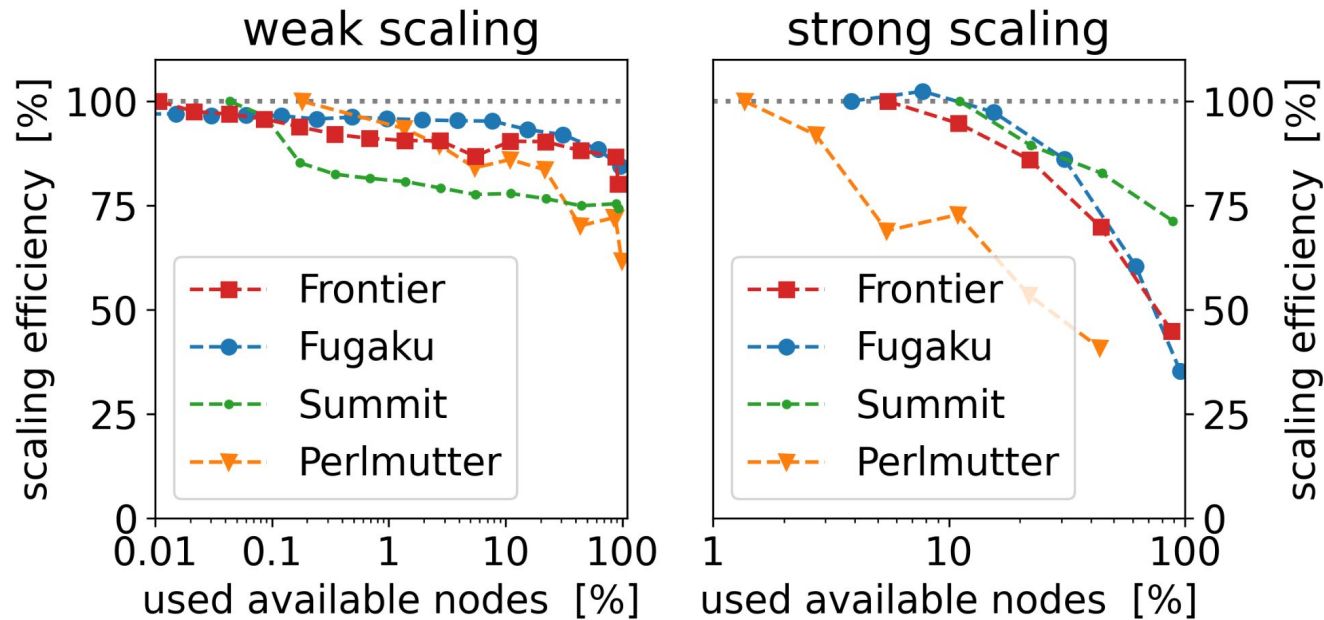
WarpX: Runs Efficiently on the *First Exascale Supercomputer*

April-July 2022: ran on **world's largest HPCs**
L. Fedeli, A. Huebl et al., *accepted* in SC'22, 2022

Note: Perlmutter & Frontier are pre-acceptance!



Demonstrated scaling **4-5 orders of magnitude**



WarpX: Runs Efficiently on the *First Exascale Supercomputer*

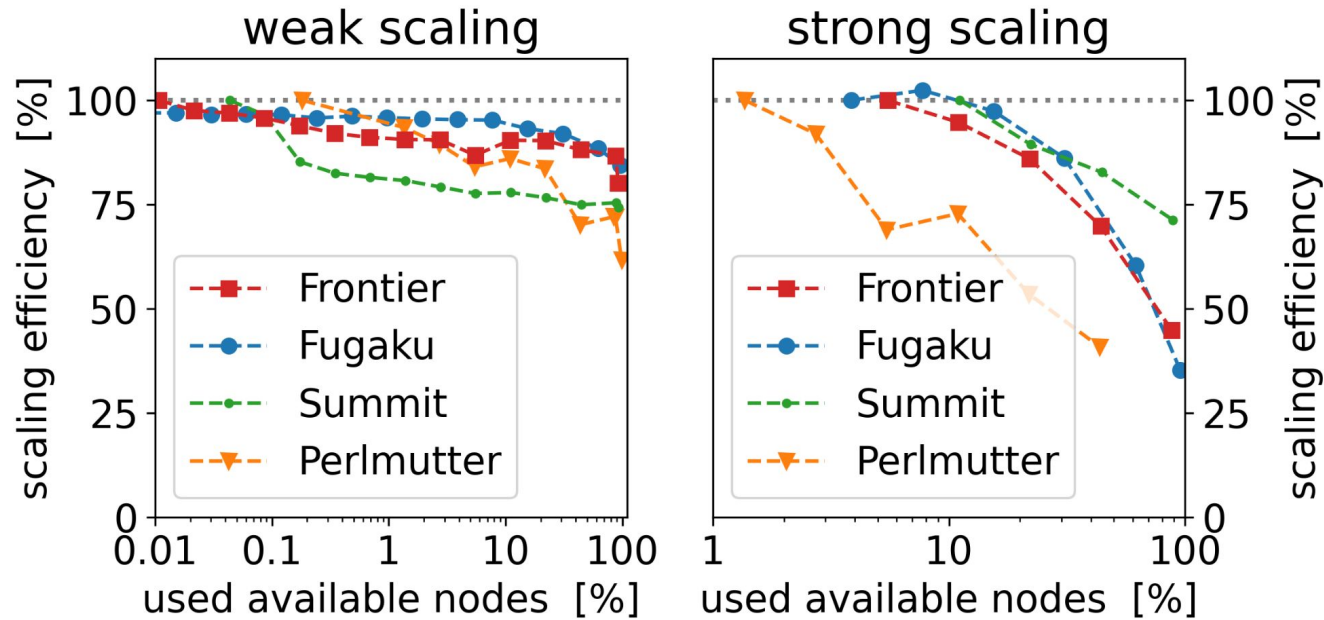
April-July 2022: ran on **world's largest HPCs**
 L. Fedeli, A. Huebl et al., *accepted in SC'22, 2022*

Note: Perlmutter & Frontier are pre-acceptance!



Demonstrated scaling **4-5 orders of magnitude**

Figure-of-Merit over time



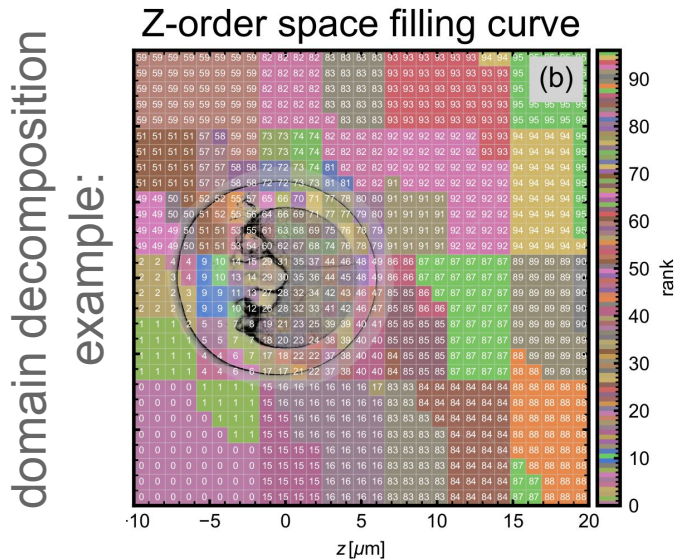
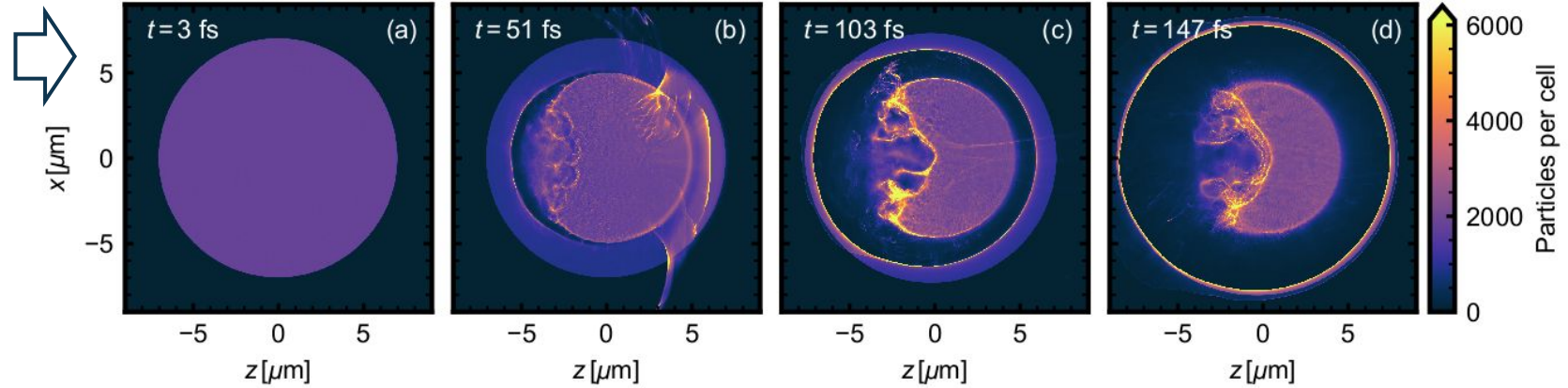
Date	Machine	N_c/Node	Nodes	FOM
3/19	Cori	0.4e7	6 625	1.0e11
6/19	Summit	2.8e7	1 000	7.8e11
9/19	Summit	2.3e7	2 560	6.8e11
1/20	Summit	2.3e7	2 560	1.0e12
2/20	Summit	2.5e7	4 263	1.2e12
6/20	Summit	2.0e7	4 263	1.4e12
7/20	Summit	2.0e8	4 263	2.5e12
3/21	Summit	2.0e8	4 263	2.9e12
6/21	Summit	2.0e8	4 263	2.7e12
7/21	Perlmutter	2.7e8	960	1.1e12
12/21	Summit	2.0e8	4 263	3.3e12
4/22	Perlmutter	4.0e8	928	1.0e12
4/22	Perlmutter†	4.0e8	928	1.4e12
4/22	Summit	2.0e8	4 263	3.4e12
4/22	Fugaku†	3.1e6	98 304	8.1e12
6/22	Perlmutter	4.4e8	1 088	1.0e12
7/22	Fugaku	3.1e6	98 304	2.2e12
7/22	Fugaku†	3.1e6	152 064	9.3e12
7/22	Frontier	8.1e8	8 576	1.1e13

110x

GPU Computing at Scale Requires Advanced Load Balancing

Application Challenges

- Plasma Mirrors & Laser-Ion Acceleration: moving front
- Laser Wakefield Accelerator: Injected Beam Particles

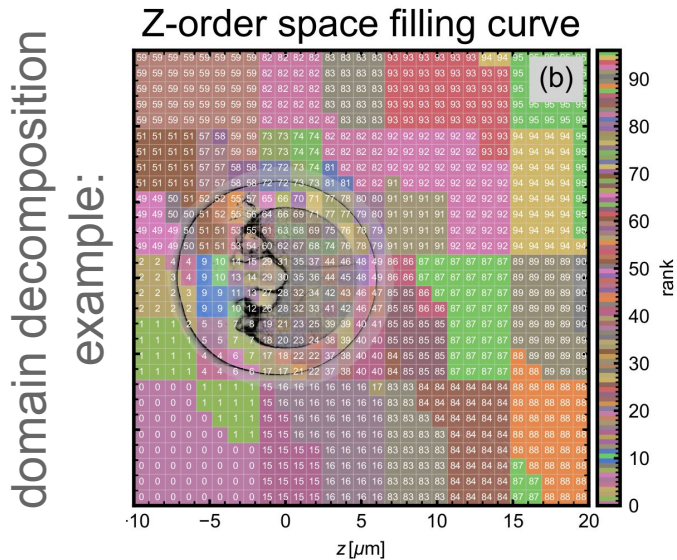
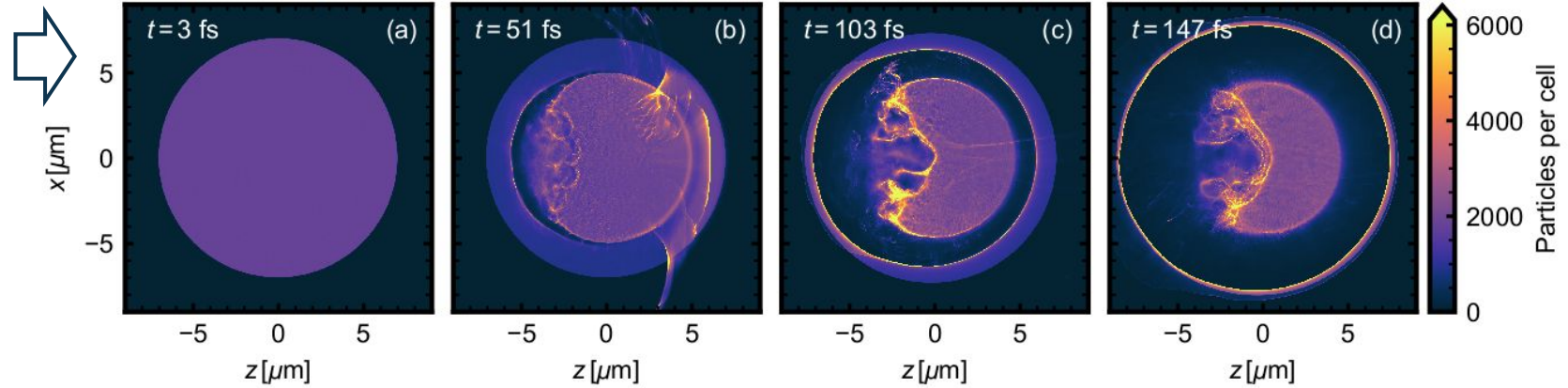


M. Rowan, A. Huebl, K. Gott, R. Lehe, M. Thévenet, J. Deslippe, J.-L. Vay, "In-Situ Assessment of Device-Side Compute Work for Dynamic Load Balancing in a GPU-Accelerated PIC Code," PASC21, DOI:10.1145/3468267.3470614 (2021)

GPU Computing at Scale Requires Advanced Load Balancing

Application Challenges

- Plasma Mirrors & Laser-Ion Acceleration: moving front
- Laser Wakefield Accelerator: Injected Beam Particles

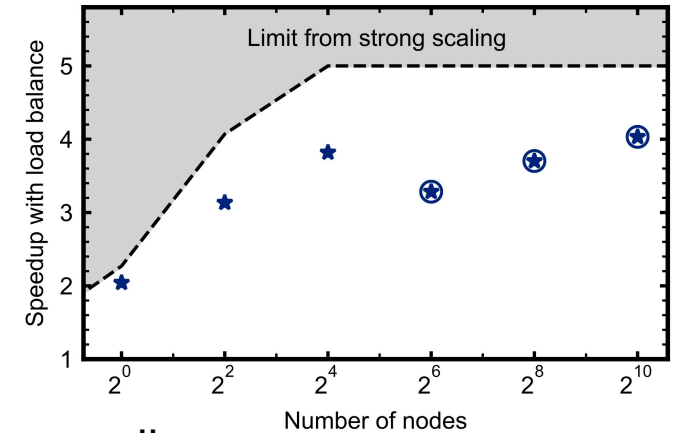


In Situ Cost Analysis

- basis for distribution functions
- realistic cost: kernel timing

Result: 3.8x speedup!

- production-quality, easy-to-use
- larger simulation: mitigate local memory spikes

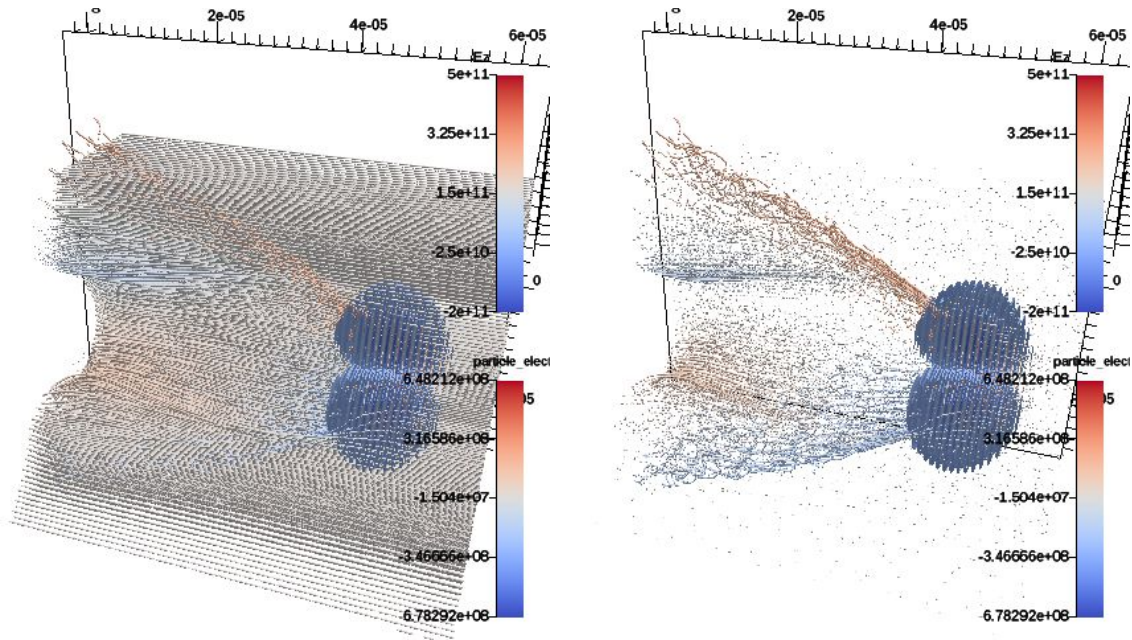


M. Rowan, A. Huebl, K. Gott, R. Lehe, M. Thévenet, J. Deslippe, J.-L. Vay, "In-Situ Assessment of Device-Side Compute Work for Dynamic Load Balancing in a GPU-Accelerated PIC Code," PASC21, DOI:10.1145/3468267.3470614 (2021)

Novel Visualization Techniques

Particle *Adaptive Sampling*

- **emphasis** on “uncommon” properties
- inverse sampling to incidence of a property

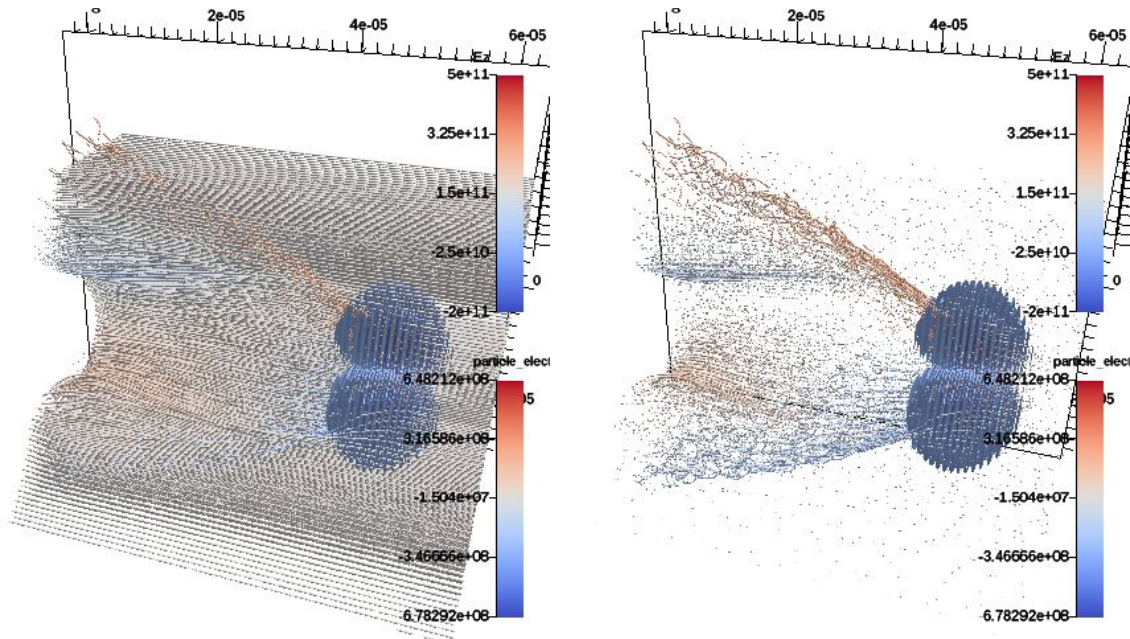


A. Biswas et al., “In Situ Data-Driven Adaptive Sampling for Large-scale Simulation Data Summarization,” ISAV18 @SC18 (2018)

Novel Visualization Techniques

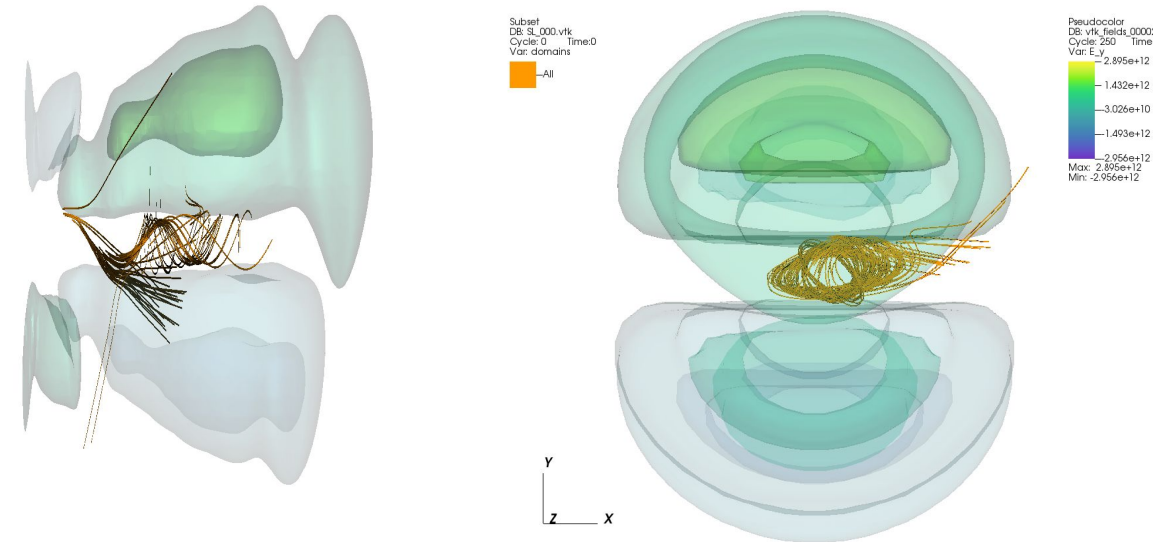
Particle Adaptive Sampling

- **emphasis** on “uncommon” properties
- inverse sampling to incidence of a property



Physics-Informed Flow Tracelines

- traditional flow vis. depends only on *local field values*
- plasma particles:
 - **inert**: track *relativistic momentum* on a traceline
 - **Lorentz-Force**: 6 fields (electromag.), leap-frog
- chance to **significantly reduce particle I/O** in real-life workflows through savings on **temporal fidelity**



A. Biswas et al., “In Situ Data-Driven Adaptive Sampling for Large-scale Simulation Data Summarization,” ISAV18 @SC18 (2018)

Postdocs Welcome - Come work with us!

jobs.lbl.gov/jobs/search/3151872

- **Modeling & Theory**

- Exascale & Wakefields
#92244
- Beam Dynamics & ML
#96603

- **Experiment**

- Wakefields, kHz-MHz (LPA)
#96321 #93729
- Laser-Proton/Ion (LPI)
#95498

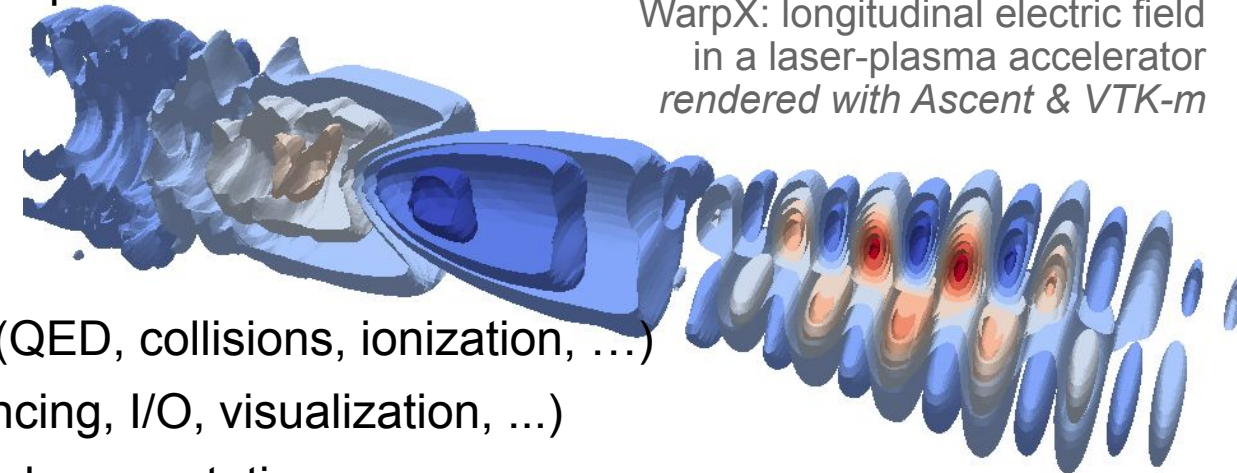


- **BLAST** is an open suite of PIC codes for **particle accelerator modeling**, increasingly build on top of the AMReX library, using code-sharing through the ABLASTR library and leveraging the U.S. DOE Exascale software stack. **ECP WarpX** is our first Exascale app, for relativistic plasma & beam modeling; **ImpactX** enhances these developments with AI/ML for s-based beam dynamics.



- **AMReX** for CPU/GPU Mesh-Refinement, **ABLASTR** shares PIC methods

- Portable CPU/GPU frameworks that avoid code duplication
- Efficient data structures, memory & comms.
- Reuse numerical methods in various PIC loops



- **Vibrant Ecosystem and Contributions**

- Runs on any platform: Linux, macOS, Windows
- Specialized codes & advanced physics modules (QED, collisions, ionization, ...)
- Advanced computer science research (load-balancing, I/O, visualization, ...)
- Public development, automated testing, review & documentation
- Friendly, open & helpful community



github.com/ECP-WarpX