Community Modeling Tools for High Brightness Beam Physics

Chad Mitchell, Lawrence Berkeley National Laboratory
(on behalf of the BLAST team & collaborators)

BLAST
BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

Workshop on High-Intensity and High-Brightness Hadron Beams
CERN, October 9-13, 2023

BERKELEY LAB

SciDAC
Scientific Discovery through Advanced Computing

U.S. DEPARTMENT OF ENERGY | Office of Science

Acknowledgments

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*Special thanks to Axel Huebl, Jean-Luc Vay, Ji Qiang for many slides re-used here.

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U.S. DEPARTMENT OF ENERGY | Office of Science

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…& private sector

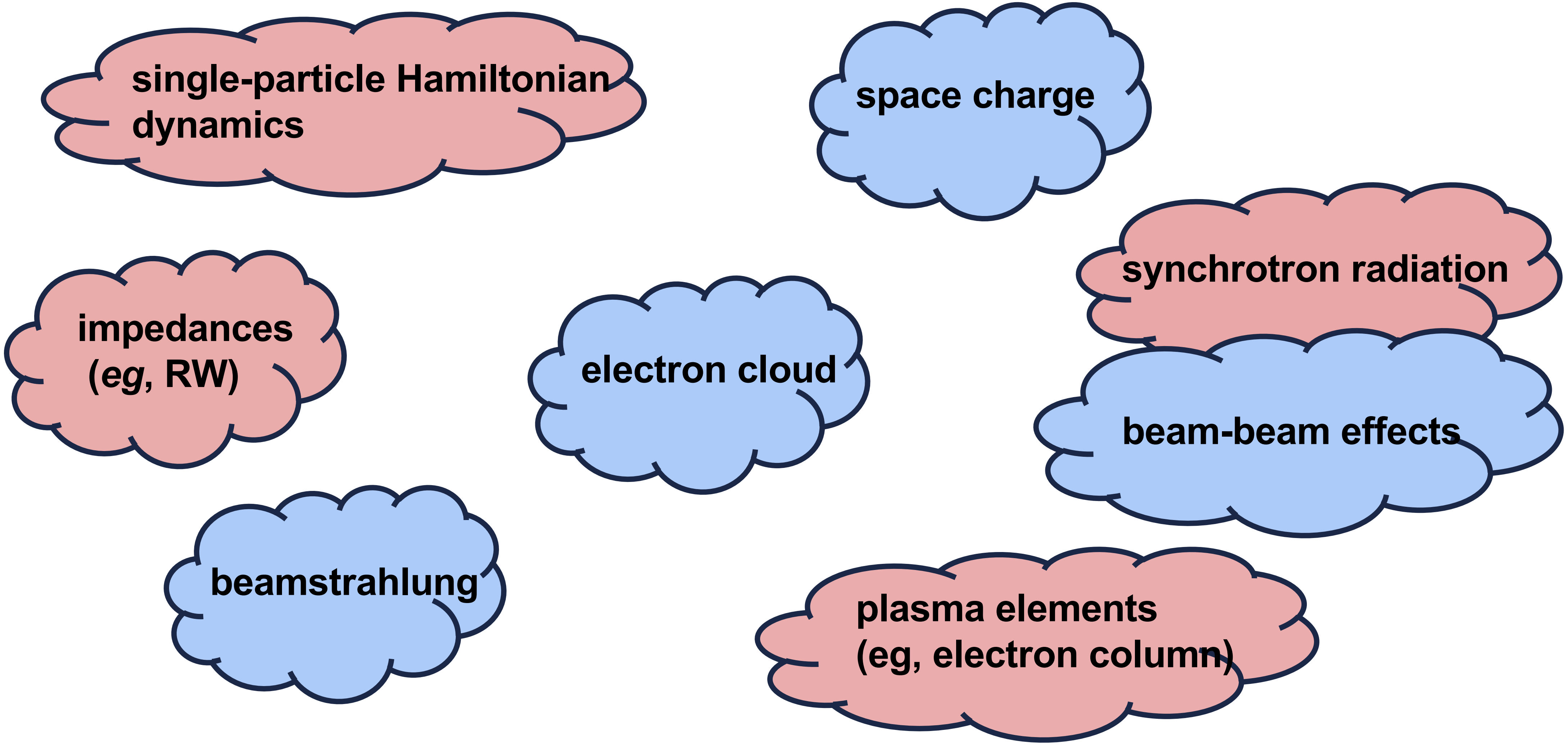
MODERN ELECTRON · Intense Computing · AVALANCHE · tae TECHNOLOGIES

Overview

- Modeling challenges for high-intensity, high-brightness beams
- BLAST toolkit and ImpactX development
- Toward an open community ecosystem
- Benchmarking and validation

- Modeling challenges for high-intensity, high-brightness beams

Broad range of physics effects at interplay



See, *eg*. E. Metral, IEEE Trans. on Nucl. Sci. **63**, p. 1001 (2016) and G. Iadarola *et al*, https://arxiv.org/abs/2310.00317

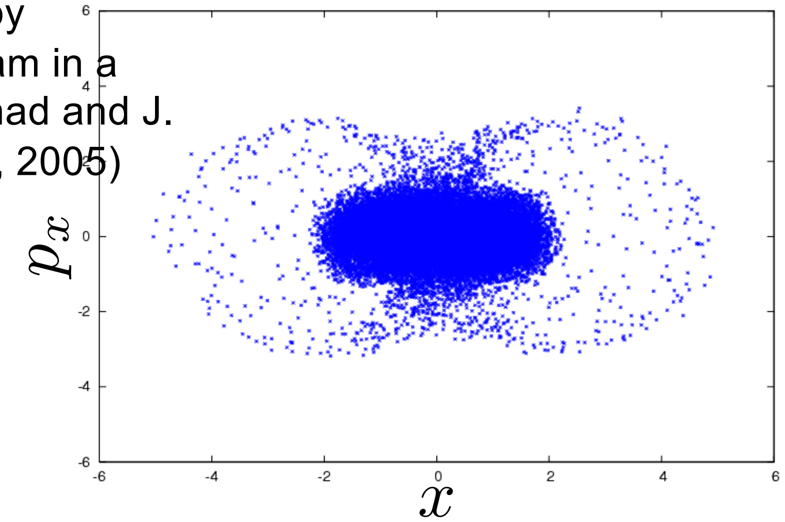
Space charge modeling at high fidelity and resolution

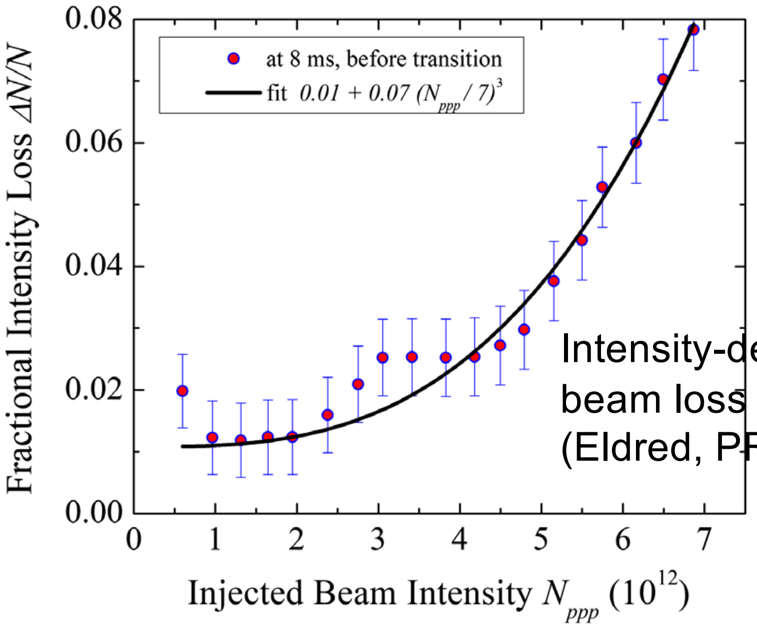
PIC modeling with high spatial resolution and good particle statistics is needed to:

- predict low-density beam halo formation
- understand intensity-dependent beam loss
- understand space charge induced emittance growth
- model and mitigate certain collective instabilities

Beam halo generated by mismatched proton beam in a linear channel (K. Sonnad and J. Cary, PRAB **8**, 064202, 2005)

Dynamic range can be >> 10^6





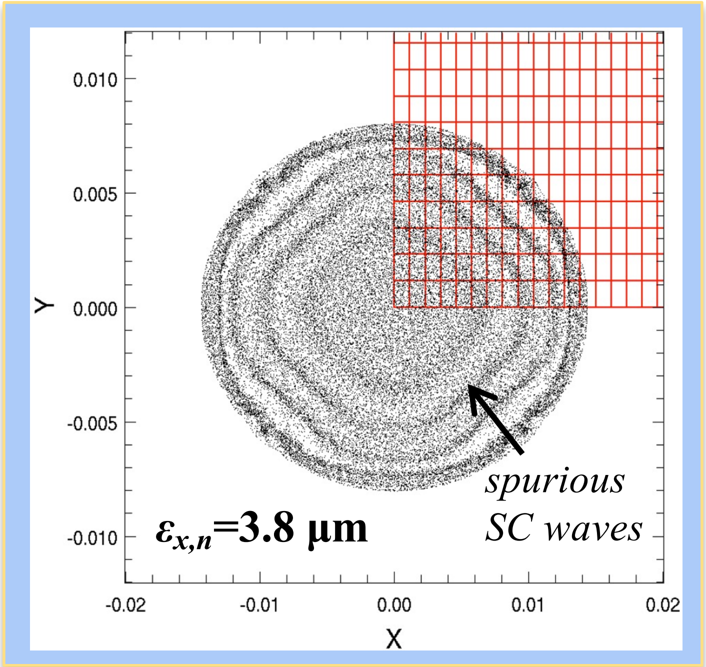
Intensity-dependent fractional beam loss in FNAL Booster (Eldred, PRAB **24**, 044001, 2021)

For large turn numbers in rings, PIC is subject to numerical artifacts (noise) and long computing times.

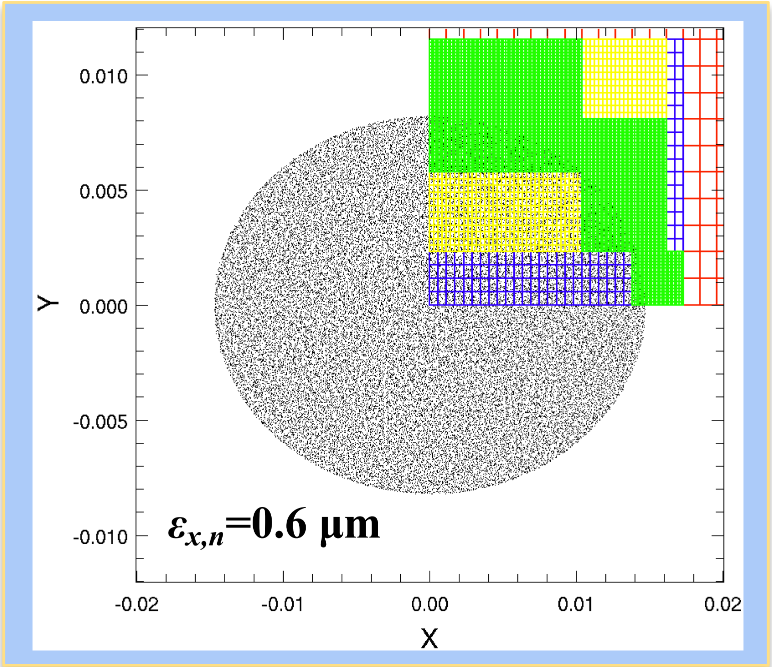
Toward efficient space charge modeling on long time scales

- Reduced-fidelity models for speed and noise suppression (frozen SC, AI/ML models)
- Novel PIC algorithms preserving the geometric structure of the Vlasov-Poisson system
- Fast *in-situ* numerical phase space diagnostics and scalable parallel I/O
- Higher-order interpolation schemes for charge deposition to aid in noise suppression
- Adaptive Mesh Refinement (AMR) for resolving density gradients, beam edge and halo

No AMR



With AMR



Example: initially KV beam (ε_{xn}= 0.5 μm) in a FODO lattice[1]

Simulation time:

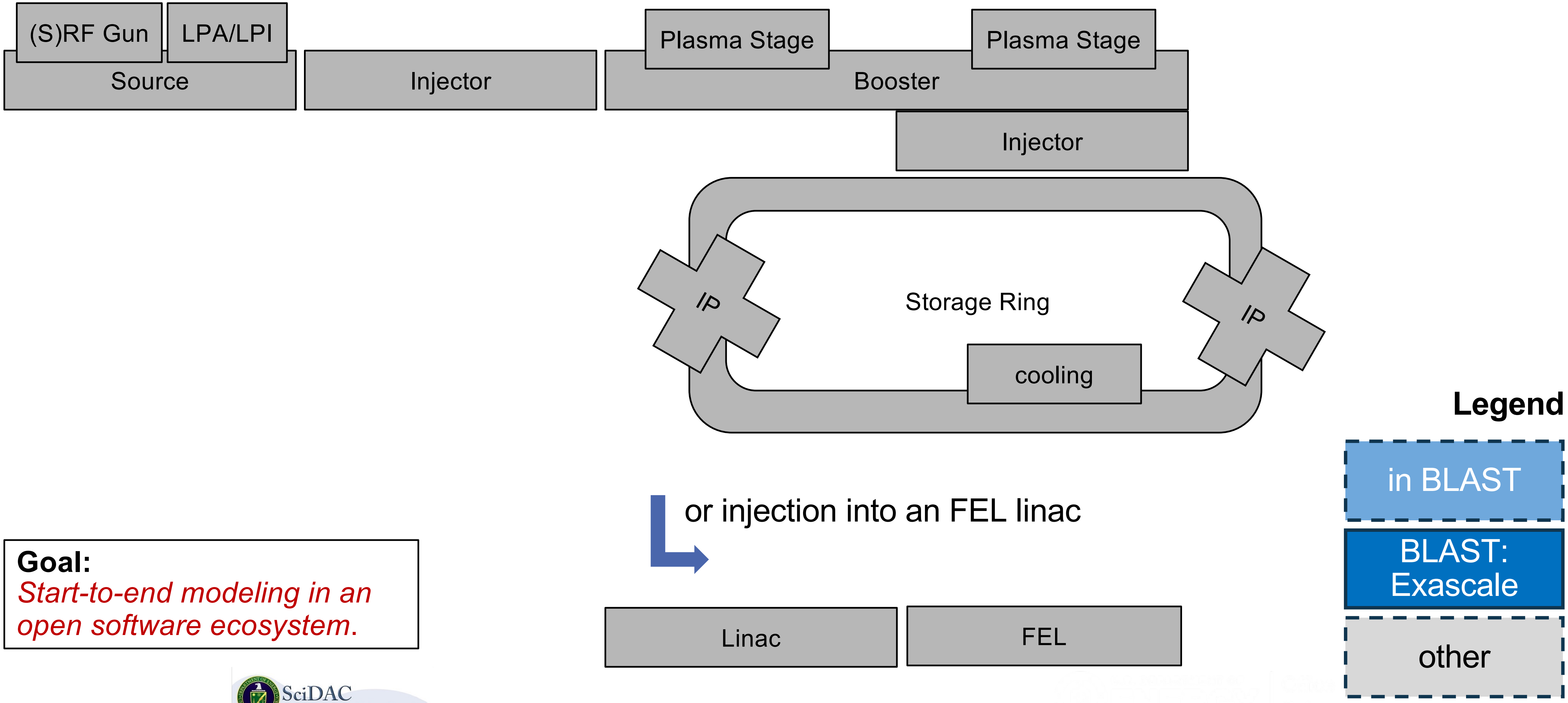
low resolution with AMR: 10.5 s
high resolution with no AMR: 30 s

[1]J-L. Vay, in WARP

- Beam Plasma & Accelerator Modeling Toolkit (BLAST)

BLAST: integrated beam physics across accelerator subsystems

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



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

BLAST: integrated beam physics across accelerator subsystems

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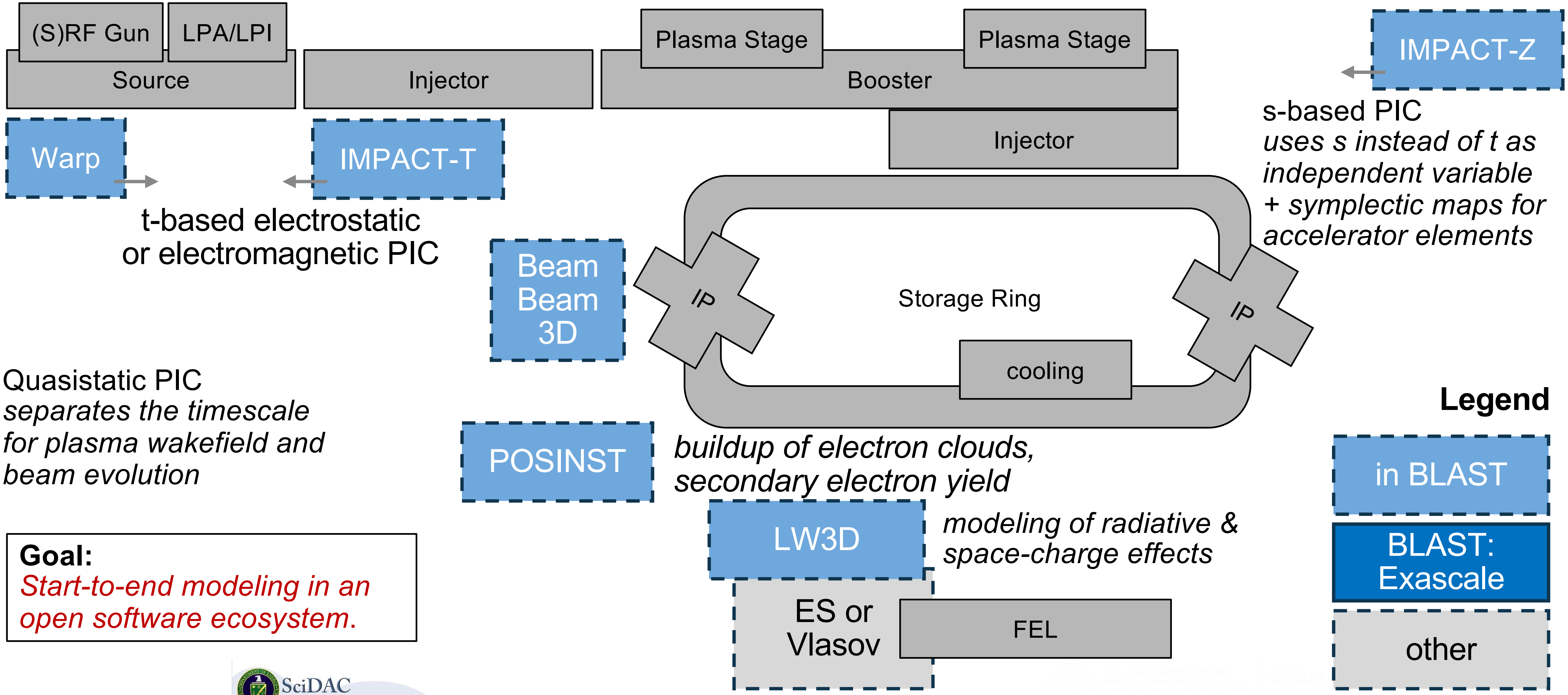

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BLAST: integrated beam physics across accelerator subsystems

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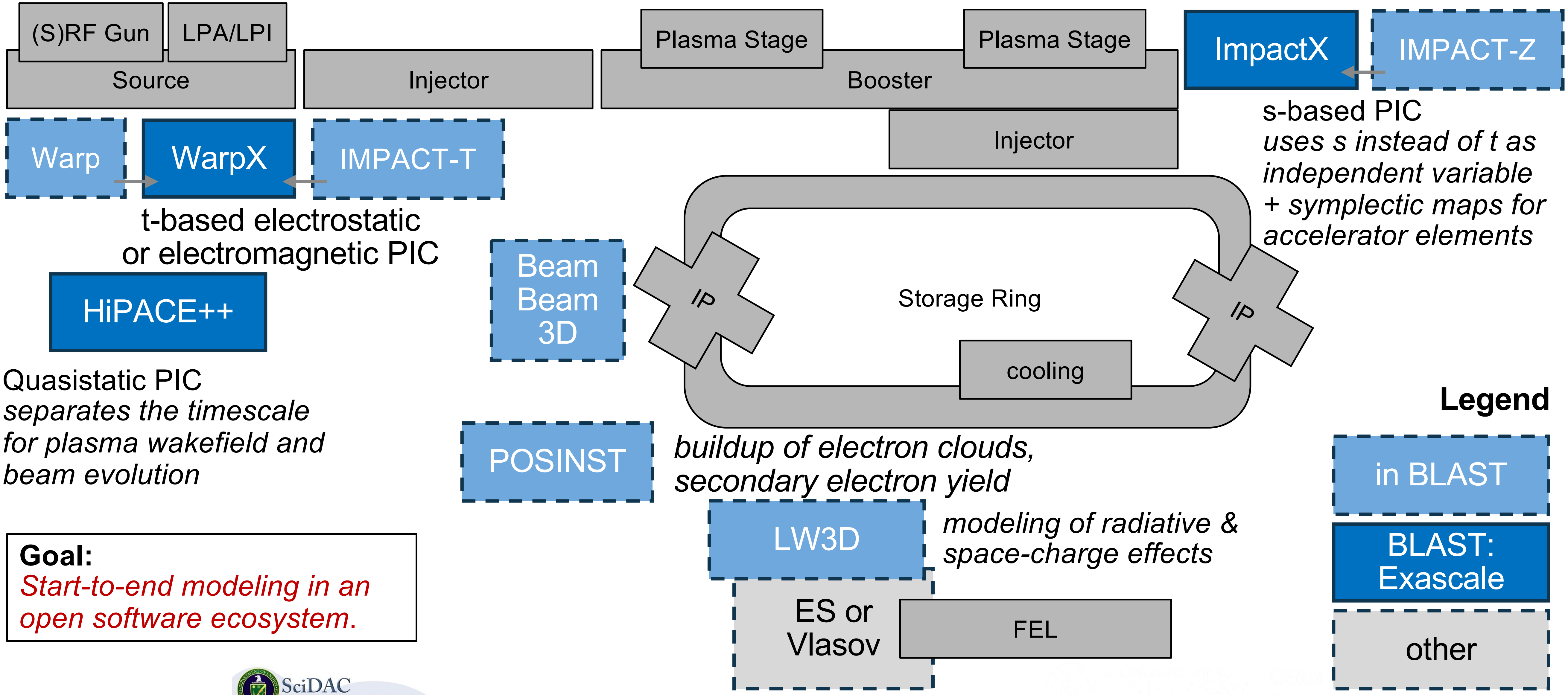
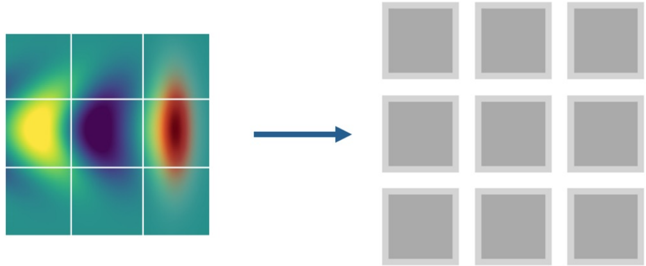


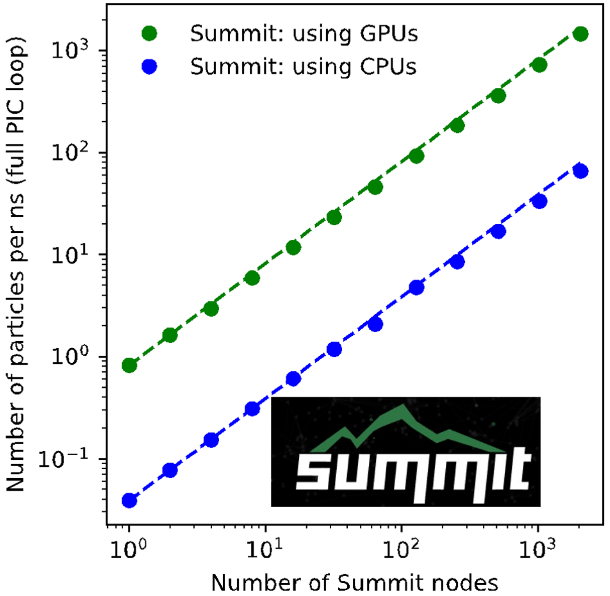
Goal:
Start-to-end modeling in an open software ecosystem.

Modernizing BLAST through an Exascale Programming Model

AMReX library

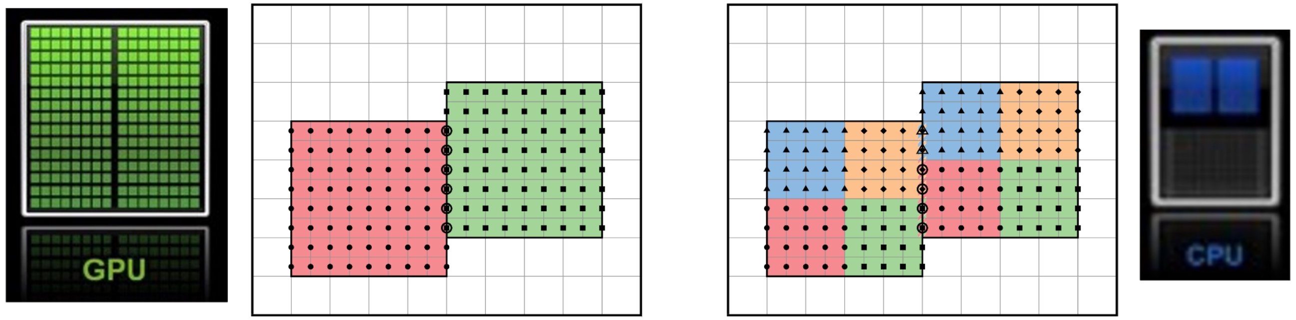
- Domain decomposition & MPI **communications:** MR & load balance





A100 gives additional ~< 2x

- **Performance-Portability Layer:** GPU/CPU/KNL



without tiling

with tiling

Data Structures

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

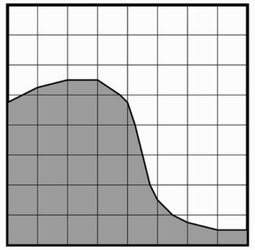
`ParallelFor(/Scan/Reduce)`

```
amrex::ParallelFor( n_particles,
    [=] AMREX_GPU_DEVICE (long i) {

        UpdatePosition( x[i], y[i], z[i],
                ux[i], uy[i], uz[i], dt );

    });
```

- **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 BLAST to an integrated ecosystem

Vendor

MPI multi-node comm.

CUDA, OpenMP, DPC++, HIP

Desktop to HPC

Transitioning BLAST to an integrated ecosystem

Computer Science

AMReX
Containers, Communication, Portability, Utilities

openPMD I/O, streaming, in situ: ADIOS/HDF5

Math
LinAlg., FFT

Vendor

MPI multi-node comm.

CUDA, OpenMP, DPC++, HIP

Desktop to HPC

Transitioning BLAST to an integrated ecosystem

Libraries	**pyAMReX**	**ABLASTR** common PIC components	**PICSAR** QED modules
Computer Science	**AMReX** Containers, Communication, Portability, Utilities	**openPMD** I/O, streaming, in situ: ADIOS/HDF5	**Math** LinAlg., FFT
Vendor	MPI multi-node comm.	CUDA, OpenMP, DPC++, HIP	

mac OS

Desktop to HPC

Transitioning BLAST to an integrated ecosystem

Apps: WarpX | HiPACE++ | ImpactX | ...

Libraries: **pyAMReX** | **ABLASTR** common PIC components | **PICSAR** QED modules

Computer Science: **AMReX** Containers, Communication, Portability, Utilities | **openPMD** I/O, streaming, in situ: ADIOS/HDF5 | **Math** LinAlg., FFT

Vendor: MPI multi-node comm. | CUDA, OpenMP, DPC++, HIP

mac OS

Desktop to HPC

Transitioning BLAST to an integrated ecosystem

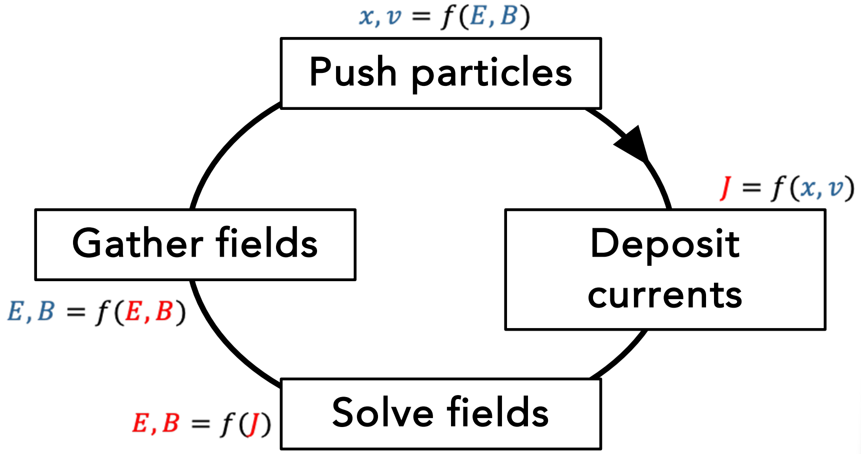
User Interfaces	Python Bindings & Particle-In-Cell Modeling Interface (PICMI)
Apps	WarpX · HiPACE++ · ImpactX · ...
Libraries	**pyAMReX** · **ABLASTR** common PIC components · **PICSAR** QED modules
Computer Science	**AMReX** Containers, Communication, Portability, Utilities · **openPMD** I/O, streaming, in situ: ADIOS/HDF5 · **Math** LinAlg., FFT
Vendor	MPI multi-node comm. · CUDA, OpenMP, DPC++, HIP

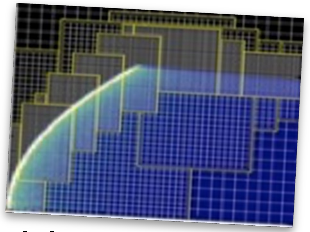
Desktop to HPC

WarpX is a GPU-Accelerated PIC Code for Exascale

Available Particle-in-Cell Loops

- electrostatic & electromagnetic (fully kinetic)





Advanced algorithms

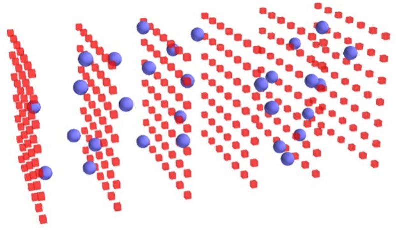
boosted frame, spectral solvers, Galilean frame, embedded boundaries + CAD, MR, ...

Multi-Physics Modules

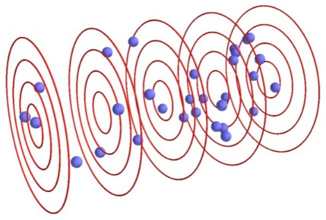
field ionization of atomic levels, Coulomb collisions, QED processes (e.g. pair creation), macroscopic materials

Geometries

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



3D Cartesian grid



Cylindrical grid (schematic)

Multi-Node parallelization

- MPI: 3D domain decomposition
- dynamic load balancing

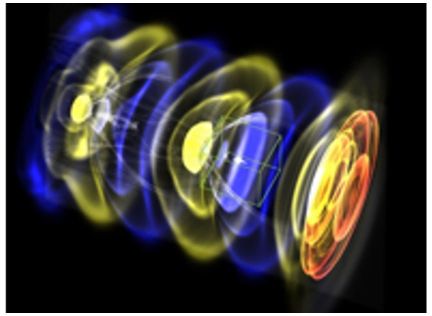
On-Node Parallelization

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

Scalable, Standardized I/O

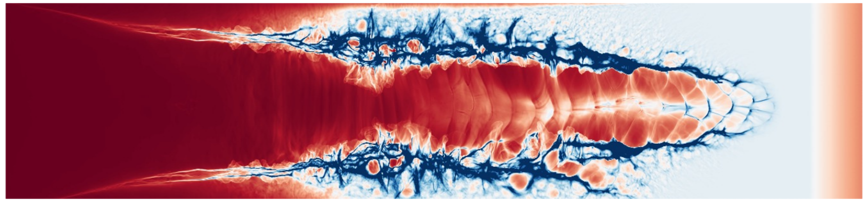
- PICMI Python interface
- openPMD (HDF5 or ADIOS)
- in situ diagnostics

WarpX supports a growing number of applications

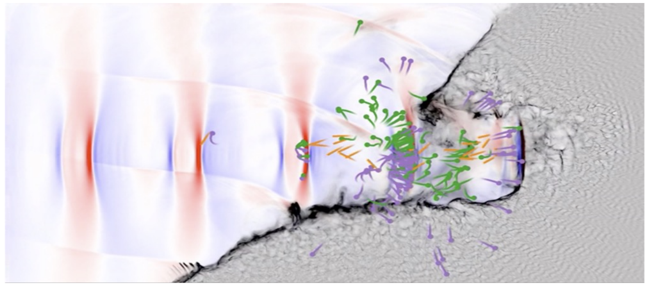


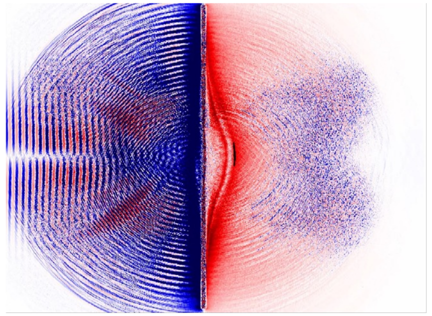
Plasma accelerators (LBNL, DESY, SLAC)

Laser-ion acceleration - advanced mechanisms (LBNL)



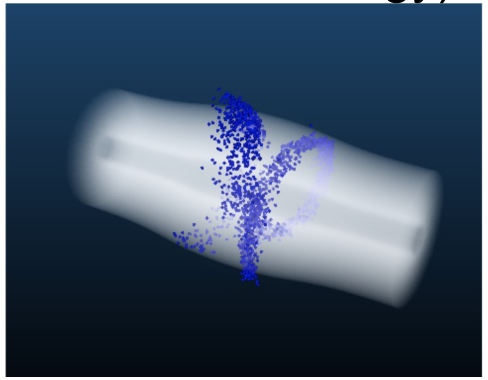
Plasma mirrors and high-field physics + QED (CEA Saclay/LBNL)



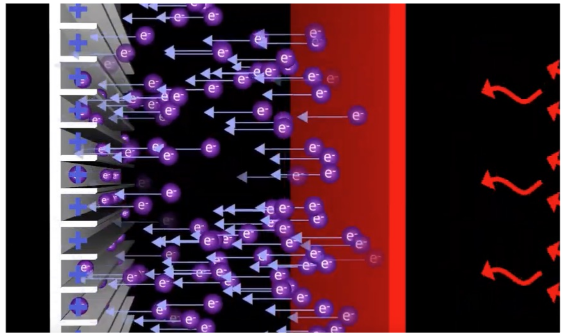


Laser-ion acceleration - laser pulse shaping (LLNL)

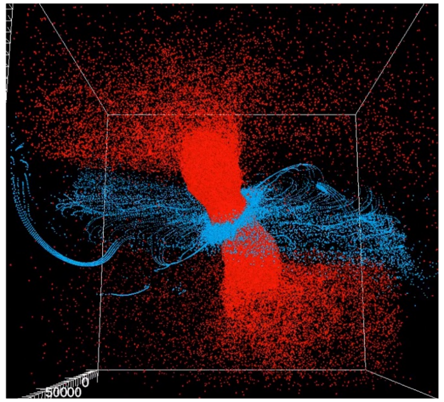
Plasma confinement, fusion devices (Zap Energy, Avalanche Energy)



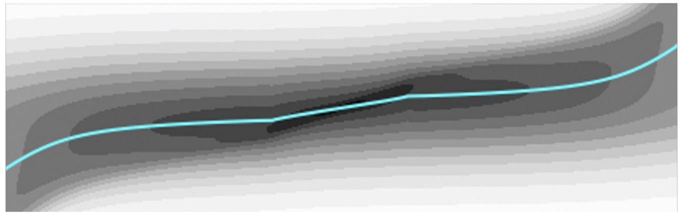
Thermionic converter (Modern Electron)



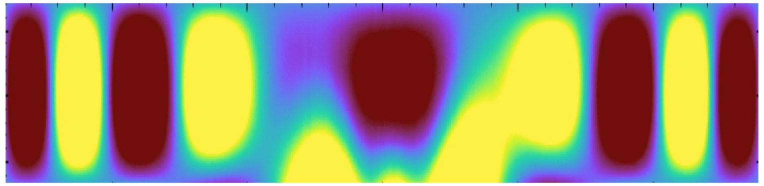
Pulsars, magnetic reconnection (LBNL)

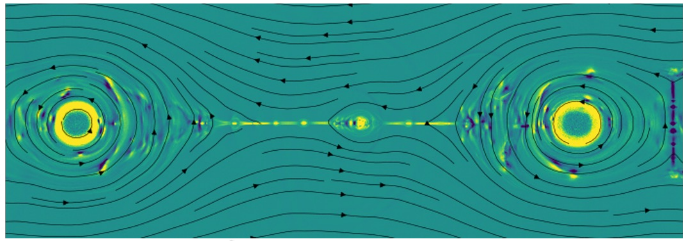


Magnetic fusion sheaths (LLNL)



Microelectronics (LBNL) - ARTEMIS

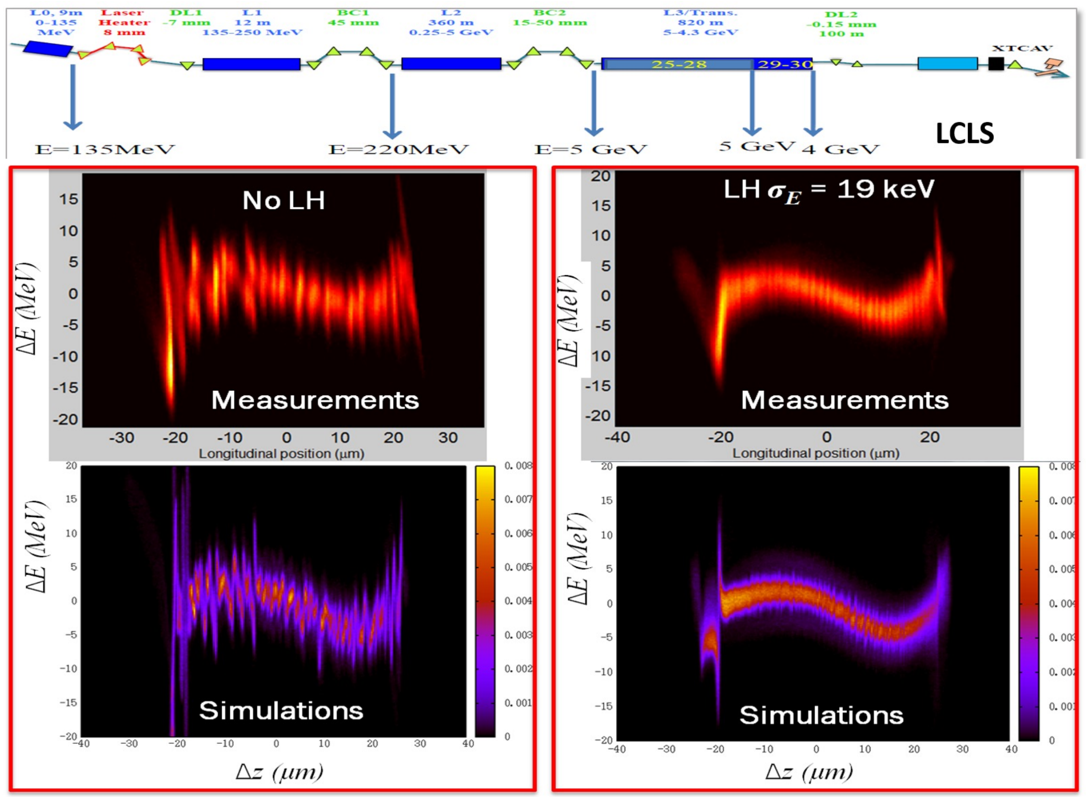




IMPACT: Multi-Physics High-Intensity and High Brightness Beam Dynamics Code Suite

- **Key features include:**
  - *time-dependent and position dependent PICs*
  - *serial and massive parallelization*
  - *detailed 3D RF accelerating and focusing model*
  - *standard elements: dipole, solenoid, multipole, etc.*
  - *multiple charge states, multiple bunches*
  - *3D space charge effects*
  - *structure and resistive wall wakefields*
  - *coherent synchrotron radiation (CSR)*
  - *incoherent synchrotron radiation (ISR)*
  - *photo-electron emission*
  - *machine errors and steering*
- **The IMPACT code suite is used by > 40 institutes worldwide**
  - *successfully applied to both electron & proton machines:*
    - ***CERN PS2 ring, SNS linac, …***
    - *LCLS-II linac*
  - *unprecedented resolution: ~2B macroparticles*

Start-to-end simulation of the Linac Coherent Light Source



J. Qiang et al., Phys. Rev. Accel. Beams 20, 054402 (2017).

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

Physical Model based on IMPACT-Z

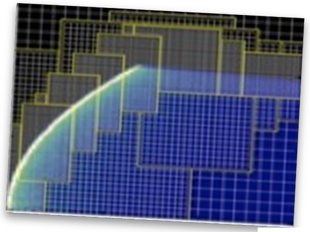
- s-based tracking with symplectic maps
- detailed RF cavity models and standard magnetic elements (w/soft-edge models)
- exact nonlinear maps for sbends, drifts
- space charge included using a split-operator approach

Space Charge Model

- 3D electrostatic in the bunch rest frame
- Multi-Level, Multi-Grid Poisson solver based on AMReX

Triple Acceleration Approach

- GPU support
- Adaptive Mesh Refinement
- AI/ML & Data Driven Models



User-Friendly

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

Same Script
CPU/GPU & MPI

Multi-Node parallelization

- MPI: domain decomposition
- dynamic load balancing (in dev.)

On-Node Parallelization

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

Scalable, Parallel I/O

- openPMD
- in situ analysis

mac OS

github.com/**ECP-WarpX/impactx**

BERKELEY LAB LDRD
SciDAC Scientific Discovery through Advanced Computing

- Toward an open community ecosystem

Integration with standardized I/Os toward a Community Accelerator Simulations Ecosystem (CASE)

C A S E

Particle-In-Cell Modeling Interface

PICMI Standard

→

Code A

Code B

...

→

open Particle Mesh Data standard

openPMD

MAISON DE LA SIMULATION

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF
BERKELEY LAB
TECHNISCHE UNIVERSITÄT DRESDEN
EUCALL
Lawrence Livermore National Laboratory
SLAC NATIONAL ACCELERATOR LABORATORY
DESY
UHH
European XFEL
UCLA
CBG Max Planck Institute of Molecular Cell Biology and Genetics
IOQ JENA Friedrich-Schiller-Universität
Fermilab
OAK RIDGE
plasmapy

BLAST BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

WarpX/FBPIC
HiPACE++
Wake-T
ImpactX

UCLA
Osiris
QuickPIC
QPAD

Synergia
Fermilab

Integration with standardized I/Os toward a Community Accelerator Simulations Ecosystem (CASE)

C A S E

Particle-In-Cell Modeling Interface

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→

open Particle Mesh Data standard

openPMD

BLAST – Beam Plasma & Accelerator Simulation Toolkit:
- WarpX/FBPIC
- HiPACE++
- Wake-T
- ImpactX

UCLA:
- Osiris
- QuickPIC
- QPAD

Fermilab:
- Synergia

- openPMD is already fairly mature and widely adopted:
  - undergoing further development and improvements under CAMPA with v2.0 scheduled for FY24
- PICMI is more recent and also more challenging: redesign is planned for FY24
- Discussions underway within CAMPA & beyond for accelerator lattice standard (AMI)

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 *general description*
standard extensions *domain specific*
wavefronts, particle species, particle beams,weighted particles, PIC, MD, mesh-refinement, CCD images, ...

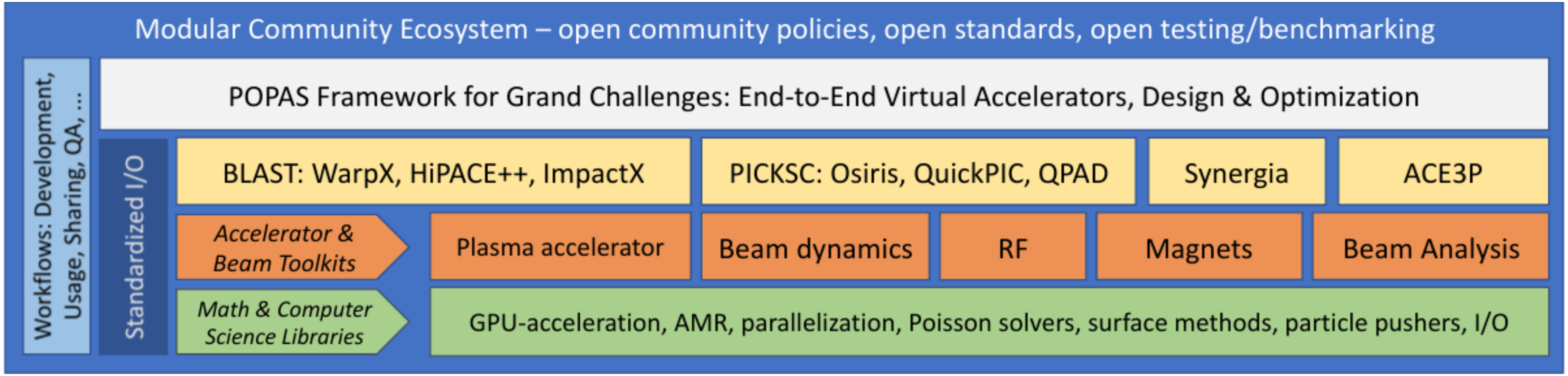
openPMD-viewer
quick visualization
explore, e.g., in Jupyter

openPMD-api
reference library
file-format agnostics API

openPMD-updater
auto-update to new standard, verify
openPMD-validator

Software Stack for a Community Accelerator Simulations Ecosystem (CASE)

Collaborative mult-institutional effort supported by SciDAC-5 (U.S. DOE) for HEP accelerator design



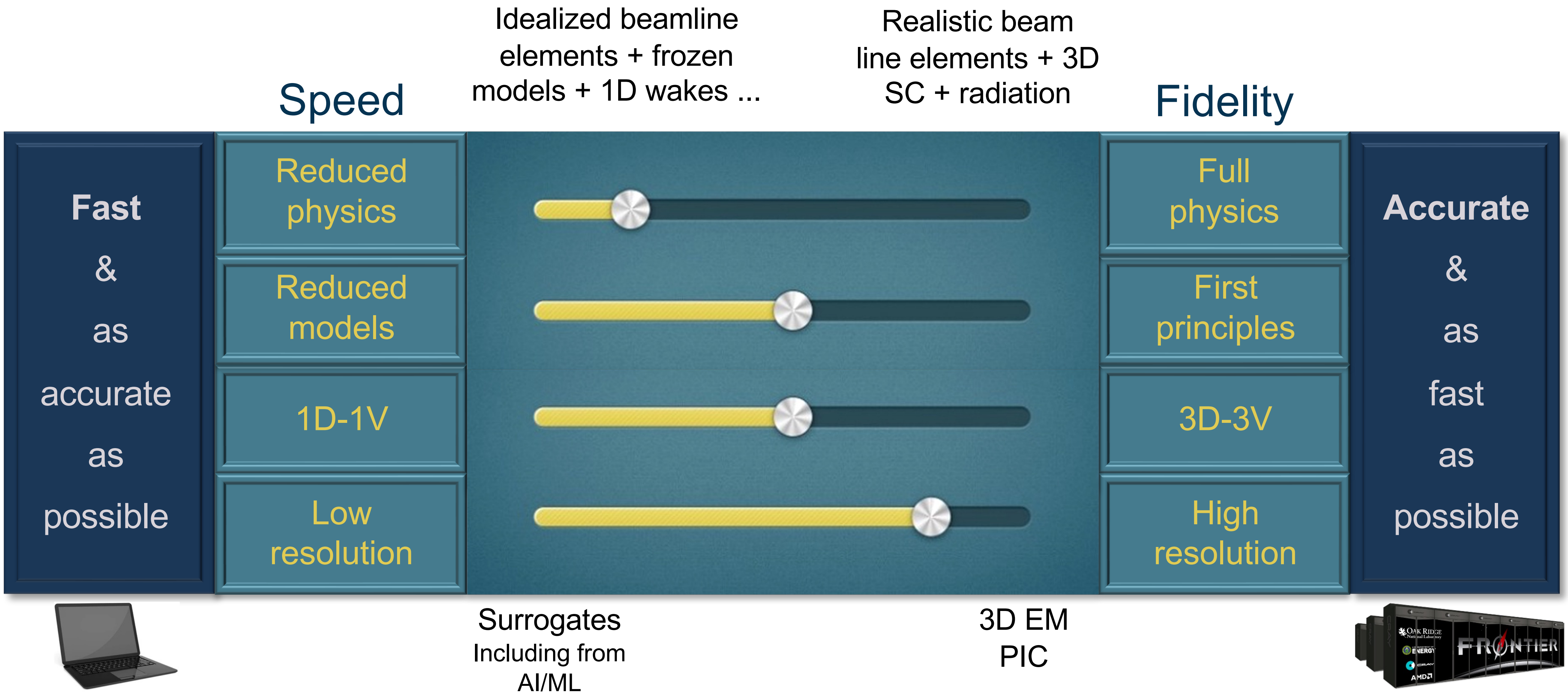
Fermilab SLAC NATIONAL ACCELERATOR LABORATORY
BERKELEY LAB CAMPA UCLA
Argonne NATIONAL LABORATORY OAK RIDGE National Laboratory

SciDAC Scientific Discovery through Advanced Computing

- standardized I/O and data layouts and common workflows
- top level: framework for optimization (CAMPA's Platform for Optimization of Particle Accelerators at Scale)

J-L Vay, "Collaboration for Advanced Modeling of Particle Accelerators," 2023 SciDAC PI Meeting, Sept. 12-14, 2023, Rockville, MD

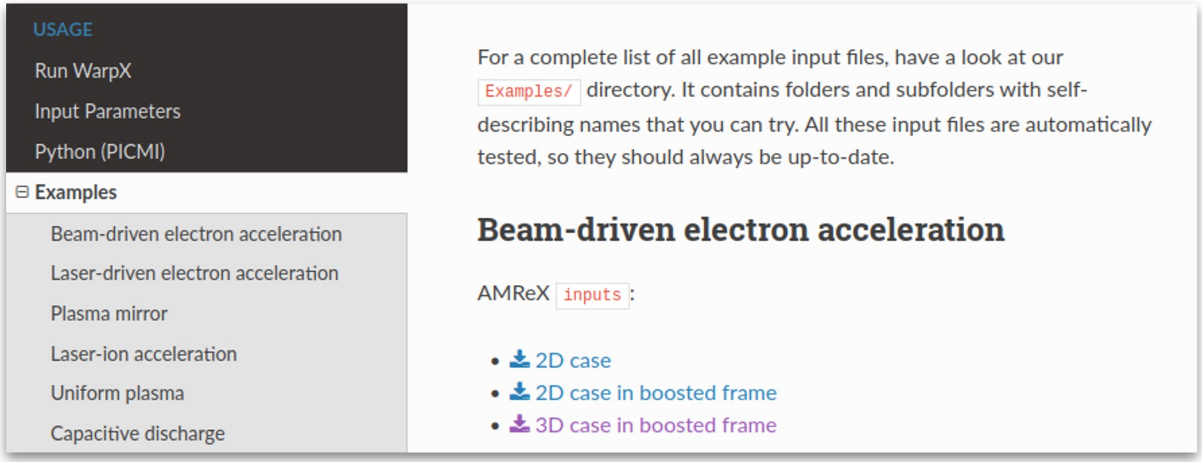
Goal: provide user an integrated ecosystem with on-the-fly tunability



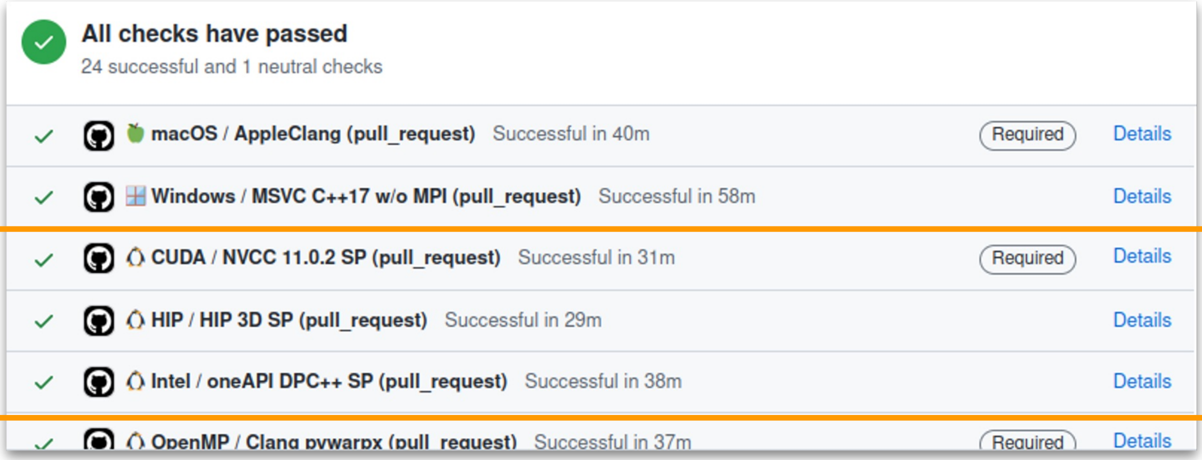
- Benchmarking and validation

We Develop Openly with the Community

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



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



230 physics benchmarks *run on every code change* of WarpX
19 physics benchmarks + 106 tests *for* ImpactX

Rapid and easy installation on any platform:

conda install -c conda-forge warpx

spack install warpx
spack install py-warpx

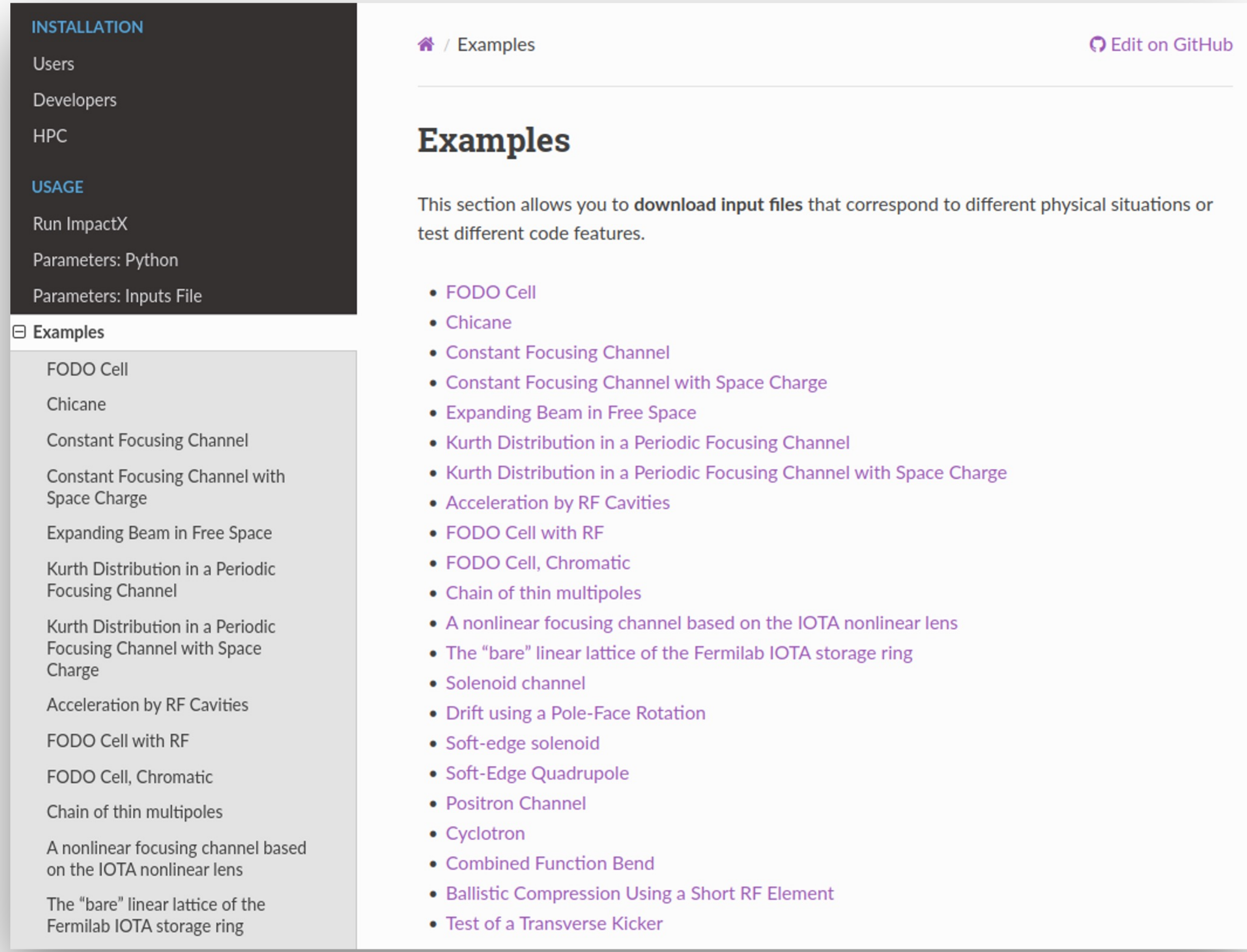
cmake -S . -B build
cmake --build build --target install

python3 -m pip install .

brew tap ecp-warpx/warpx
brew install warpx

module load warpx
module load py-warpx

ImpactX: Physics Benchmark Examples


INSTALLATION
Users
Developers
HPC

USAGE
Run ImpactX
Parameters: Python
Parameters: Inputs File

⊟ Examples
FODO Cell
Chicane
Constant Focusing Channel
Constant Focusing Channel with Space Charge
Expanding Beam in Free Space
Kurth Distribution in a Periodic Focusing Channel
Kurth Distribution in a Periodic Focusing Channel with Space Charge
Acceleration by RF Cavities
FODO Cell with RF
FODO Cell, Chromatic
Chain of thin multipoles
A nonlinear focusing channel based on the IOTA nonlinear lens
The "bare" linear lattice of the Fermilab IOTA storage ring

/ Examples — Edit on GitHub

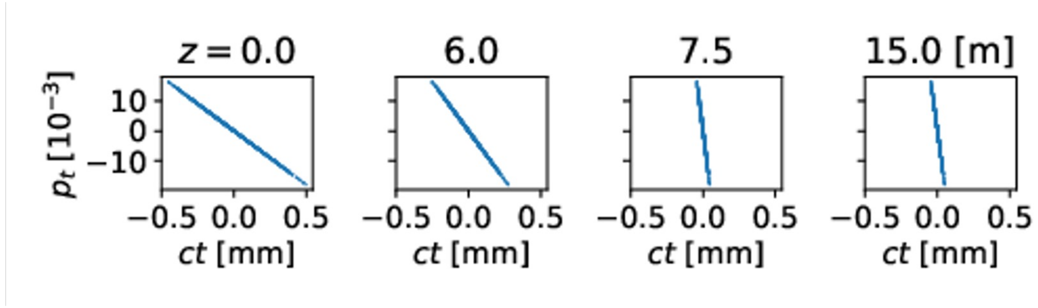
Examples

This section allows you to **download input files** that correspond to different physical situations or test different code features.

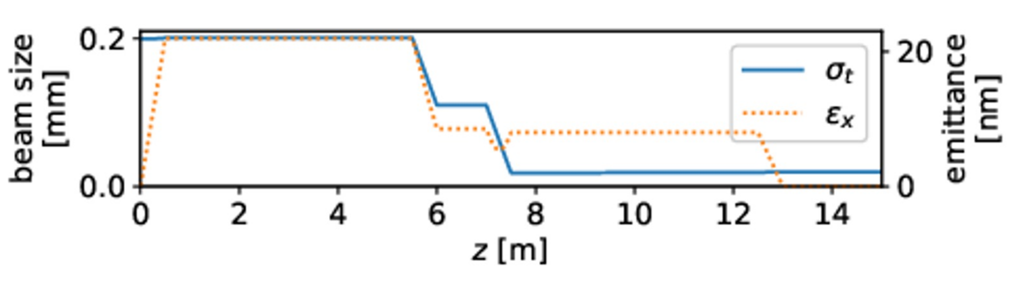
- FODO Cell
- Chicane
- Constant Focusing Channel
- Constant Focusing Channel with Space Charge
- Expanding Beam in Free Space
- Kurth Distribution in a Periodic Focusing Channel
- Kurth Distribution in a Periodic Focusing Channel with Space Charge
- Acceleration by RF Cavities
- FODO Cell with RF
- FODO Cell, Chromatic
- Chain of thin multipoles
- A nonlinear focusing channel based on the IOTA nonlinear lens
- The "bare" linear lattice of the Fermilab IOTA storage ring
- Solenoid channel
- Drift using a Pole-Face Rotation
- Soft-edge solenoid
- Soft-Edge Quadrupole
- Positron Channel
- Cyclotron
- Combined Function Bend
- Ballistic Compression Using a Short RF Element
- Test of a Transverse Kicker

Berlin-Zeuthen Chicane

- rms-matched 5 GeV electron beam with initial normalized transverse rms emittance of 1 μm
- LCLS (@5GeV) & TESLA XFEL (@500MeV)-like



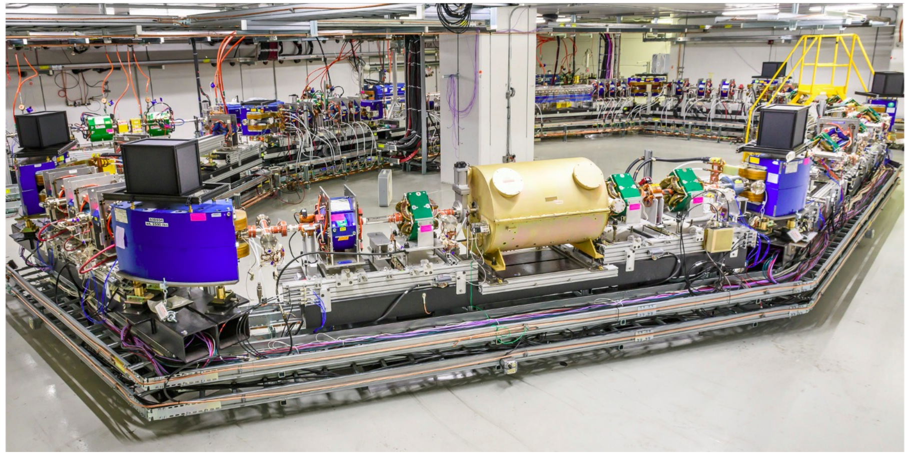
- longitudinal phase space: 10x compression
- emittance coupling: recovered at exit



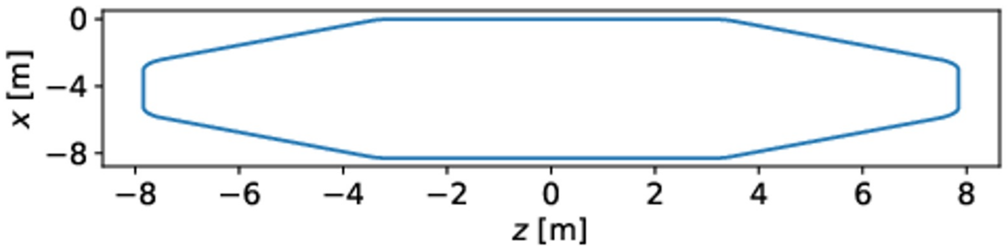
github.com/**ECP-WarpX/impactx**

ImpactX: IOTA (v. 8.4) 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 μm propagates over a single turn



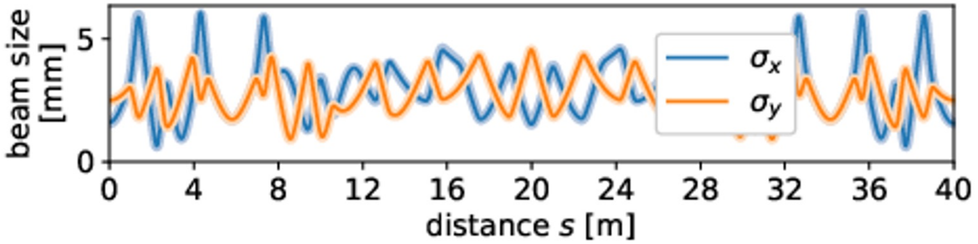
Reference Orbit



Preservation of Second Moments

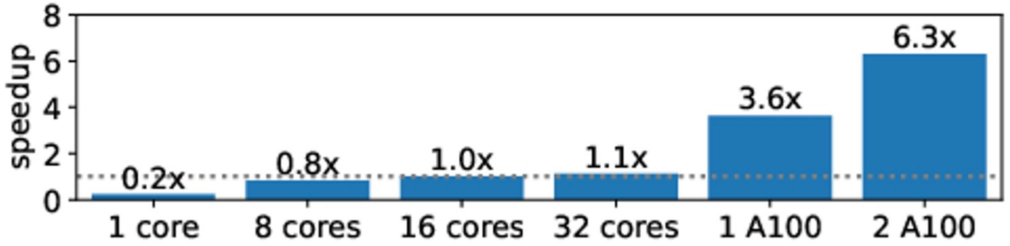
- check emittance preservation
- rms beam size evolution:

IMPACT-Z vs ImpactX



Preliminary Performance

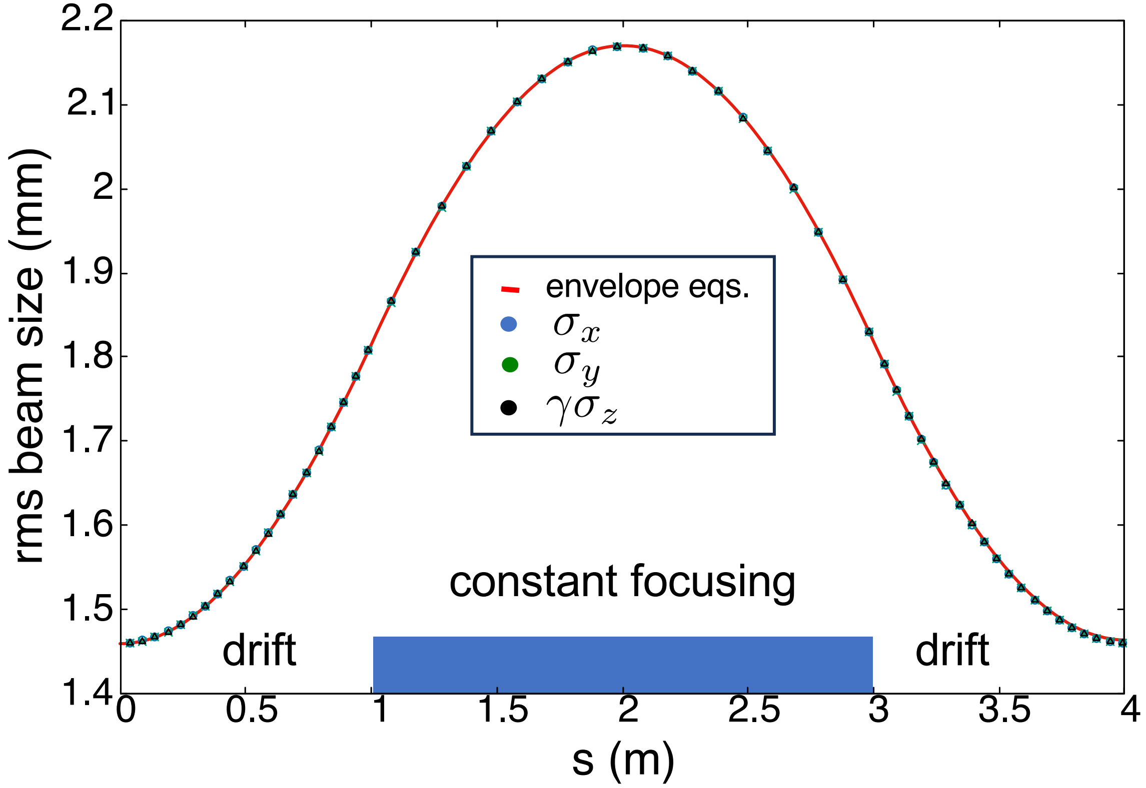
- on Perlmutter (NERSC) CPU / GPU
- order-of-magnitude perf.↗ w/o dyn. LB (yet)



ImpactX 3D Space Charge Validation: Kurth beam in periodic focusing

- Analogous to a K-V beam in a FODO channel, but appropriate for 3D bunched beams.
- Space charge forces are linear: fully described by 3D envelope equations
- 10 nC proton bunch @ 2 GeV
- unnormalized emittance $\epsilon_d = 1\ \mu$m (all planes)
- Phase advance 121° ➡ 74°

Matched rms envelopes over a single period



R. Kurth, Quart. Appl. Math. 36, pp. 325-329 (1978), C. Mitchell et al, IPAC2021, pp. 3213-3216 (2021).

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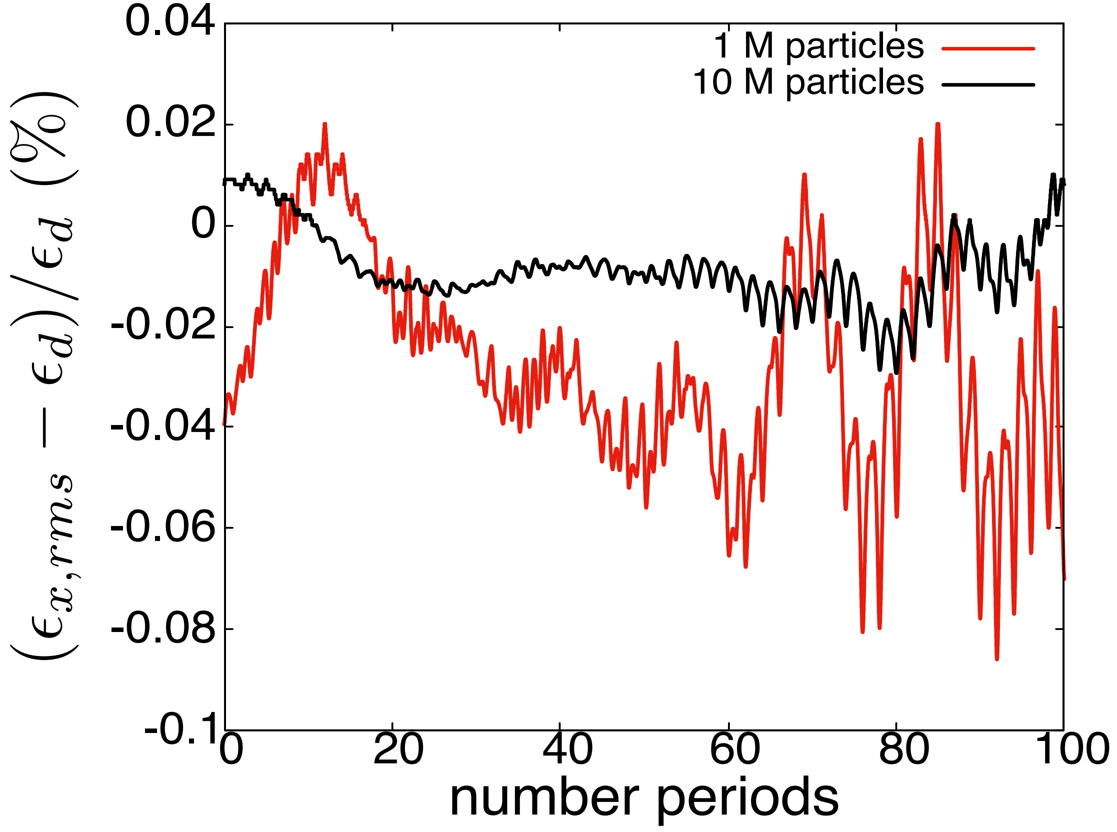
1 M particles, [72,72,72] grid
10 M particles, [128,128,128] grid

Emittance fluctuations over 100 periods



R. Kurth, Quart. Appl. Math. 36, pp. 325-329 (1978), C. Mitchell et al, IPAC2021, pp. 3213-3216 (2021).

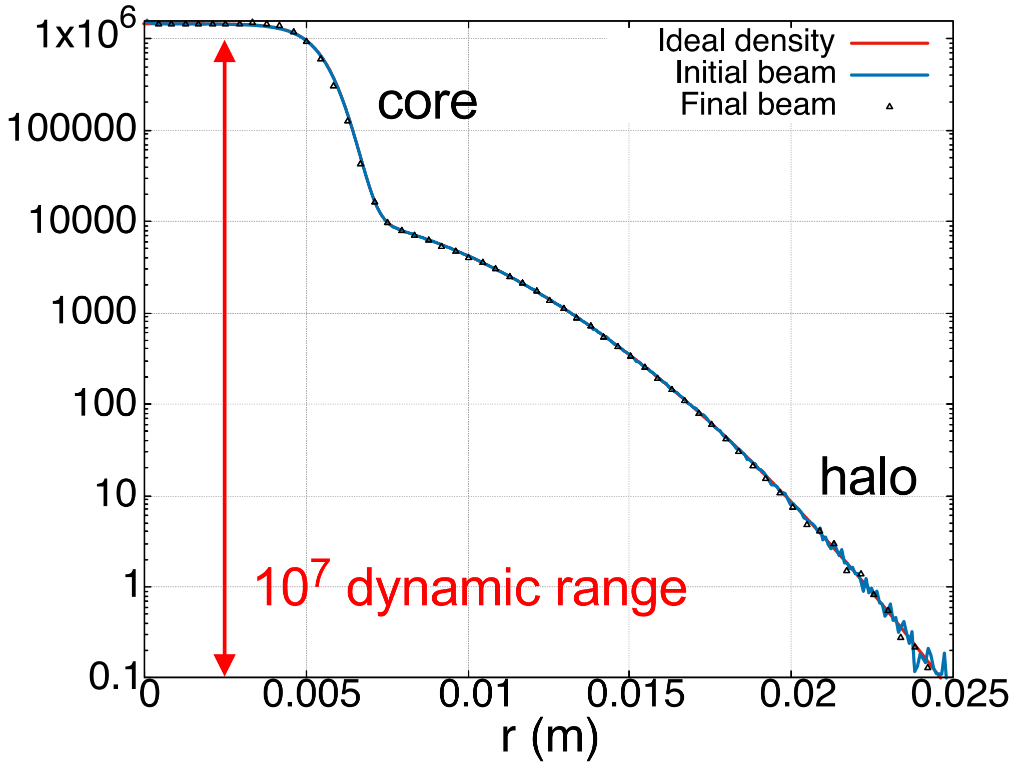
ImpactX 3D Space Charge Validation: bithermal beam in a CF channel

- Self-consistent model of a 3D bunch with a stationary core-halo distribution.

$$f = c_1 \exp(H/kT_1) + c_2 \exp(H/kT_2)$$

- Bunch is radially symmetric in the beam rest frame.
- A system of ODEs is solved for the space charge potential and radial density in equilibrium.
- 10 nC proton bunch @ 0.1 MeV
- $kT_1 = 36\times10^{-6}$, $kT_2 = 900\times10^{-6}$
- 95% of charge in core, 5% of charge in halo
- Beam is stationary over 10 focusing periods.

Spatial beam density as a function of radius



10 M particles, [128,128,128] grid

See poster THBP44 for additional details. All benchmarks are archived on Zenodo.

Conclusions

- A community approach to code development (*eg*, based on shared standards, common code interfaces, and shared benchmarks) is needed to address the challenges of high-intensity and high brightness beam modeling.

- BLAST is an open interoperable ecosystem of PIC codes for particle accelerator modeling
  - WarpX – for relativisitic t-based laser-plasma and beam modeling
  - ImpactX – for s-based beam dynamics modeling in linacs and rings, ...

- Runs on any platform: Linux, macOS, Windows

- Open public development, automated testing, review & documentation GitHub

- Future plans for ImpactX development include:
  - Detailed exploration of SC benchmark tests with mesh refinement
  - Implementation of 2D and/or 2.5D space charge models for long and unbunched beams
  - Import additional (1D) collective effects from IMPACT-Z (including resistive wall wakefields and CSR models)

Thank you for your attention!

Questions?

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