Beam Dynamics with Space Charge in ImpactX: Code Design and IOTA Applications

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

BLAST
BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

IOTA/FAST Collaboration Meeting
Fermilab, March 12-14, 2024

BERKELEY LAB

SciDAC
Scientific Discovery through Advanced Computing

U.S. DEPARTMENT OF ENERGY | Office of Science

Acknowledgments

Thanks to the workshop organizers.

*Special thanks to Axel Huebl and Jean-Luc Vay for providing slides re-used here.

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Overview

- BLAST toolkit and ImpactX development
- Benchmarking and space charge validation
- Toward applications to IOTA

- Beam Plasma & Accelerator Modeling Toolkit (BLAST)

Multidisciplinary, Multi-Institutional Contributor Team

U.S. DEPARTMENT OF ENERGY | Office of Science
NNSA

ECP

BERKELEY LAB

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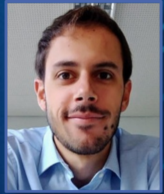

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BLAST
BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

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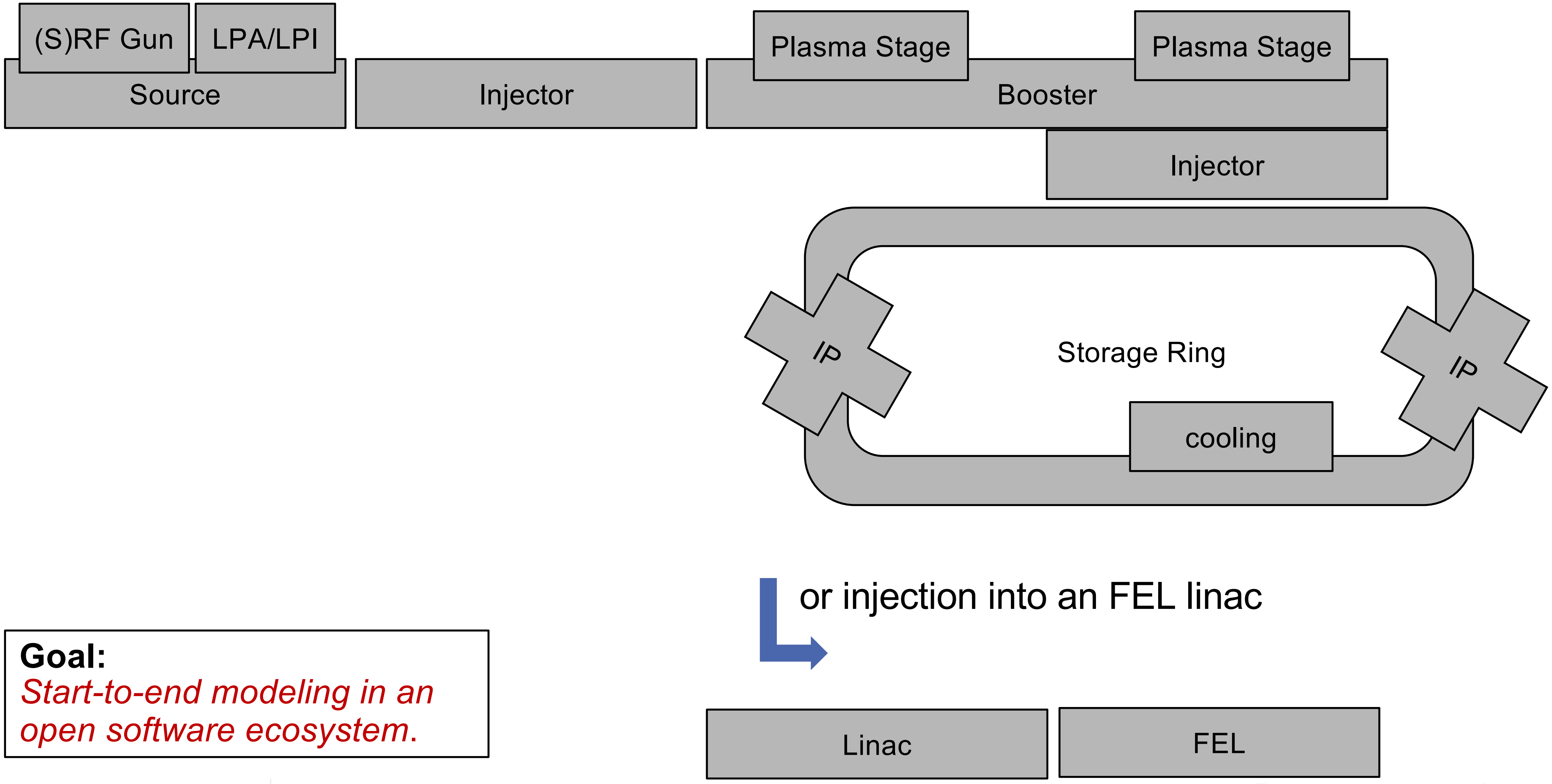
MODERN ELECTRON
Intense Computing
AVALANCHE
tae TECHNOLOGIES

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.

Legend

in BLAST

BLAST: Exascale

other

BLAST: integrated beam physics across accelerator subsystems

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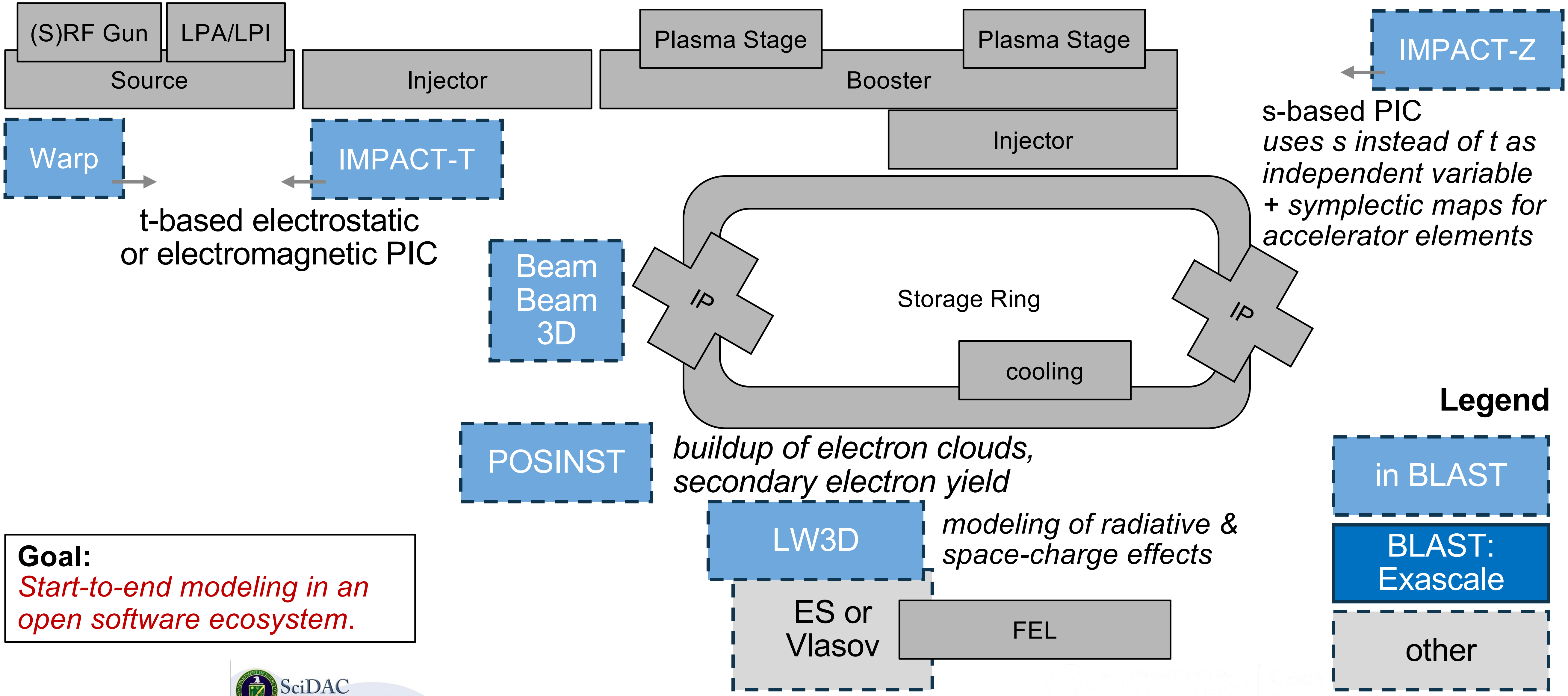

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BLAST: integrated beam physics across accelerator subsystems

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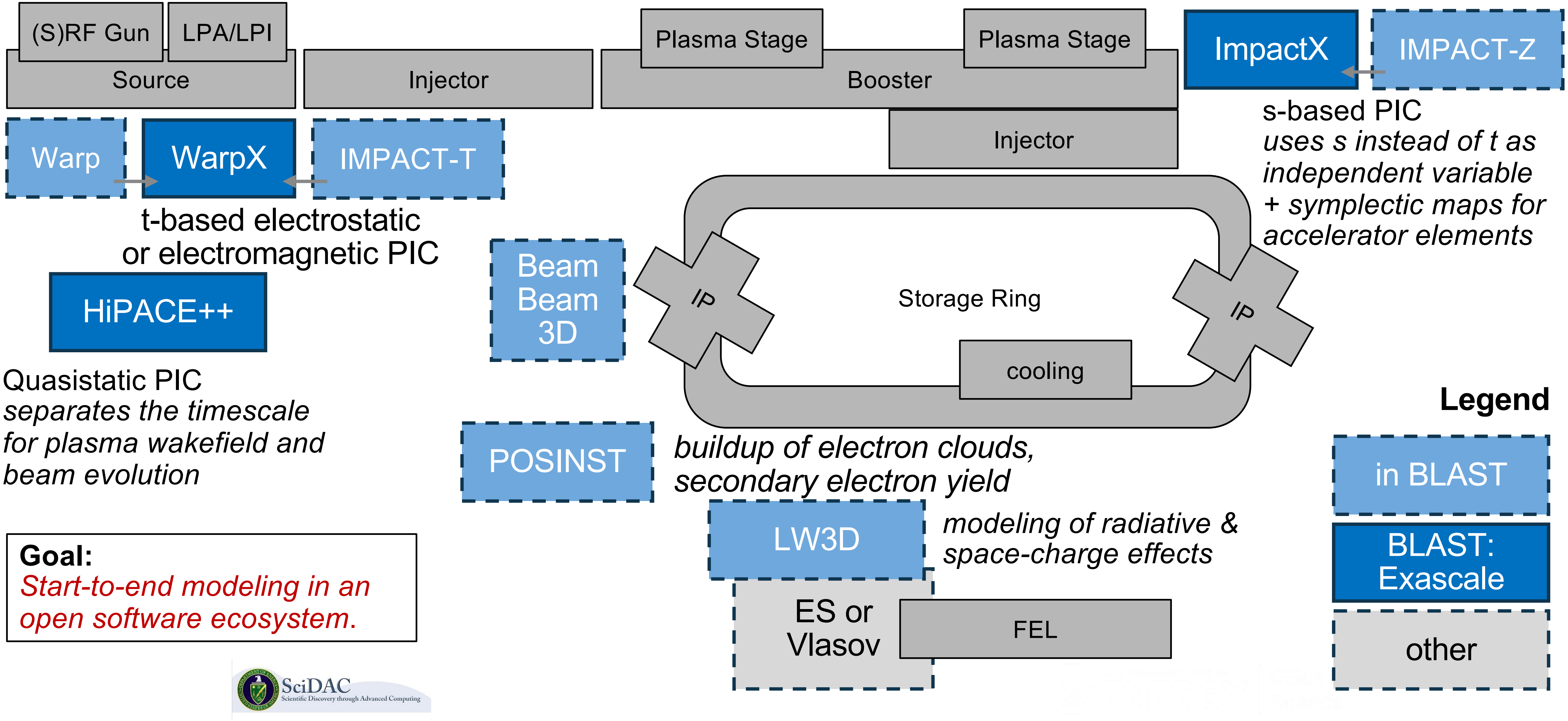
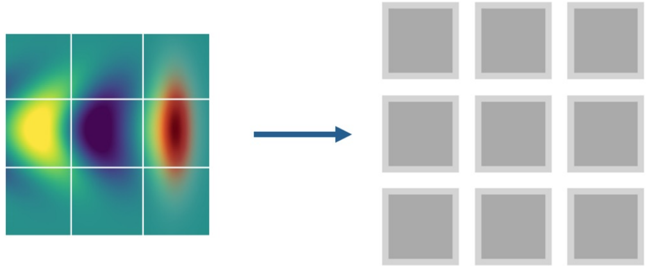


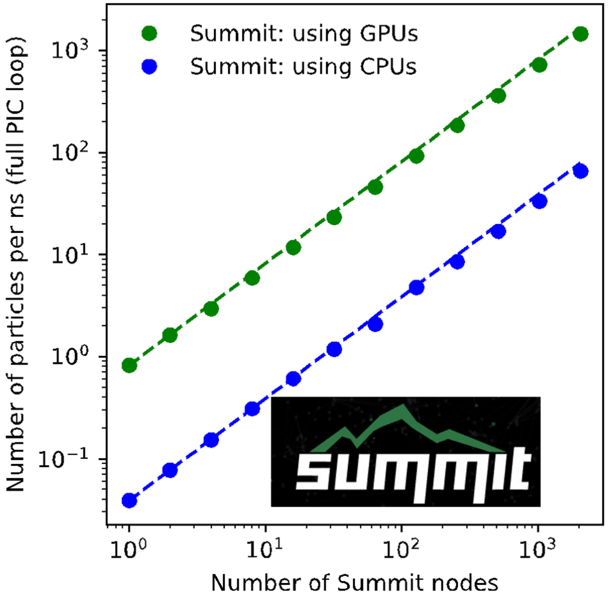
Modernizing BLAST through an Exascale Programming Model

AMReX library

EXASCALE COMPUTING PROJECT

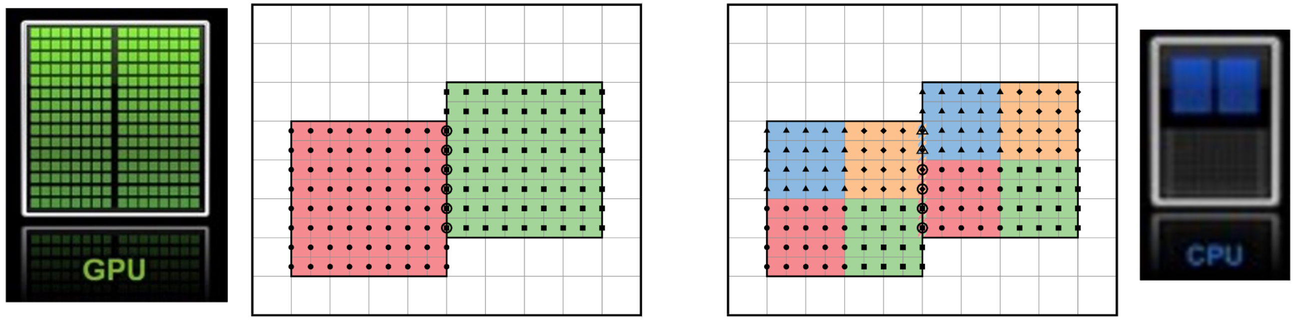
- Domain decomposition & MPI **communications:** MR & load balance





A100 gives additional ~< 2x

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



without tiling

with tiling

Data Structures

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

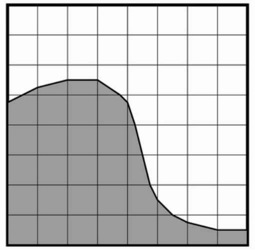
`ParallelFor(/Scan/Reduce)`

```
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)

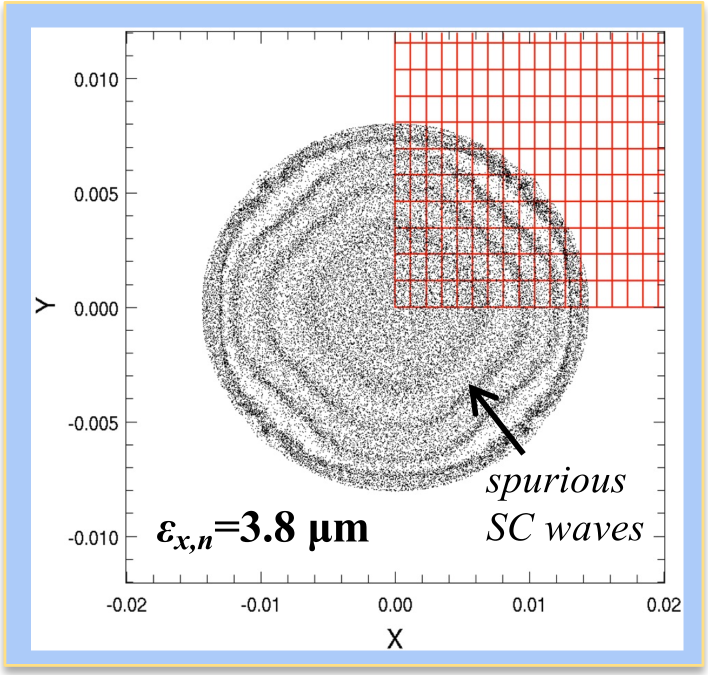
A. Myers et al., "Porting WarpX to GPU-accelerated platforms," Parallel Computing **108**, 102833 (2021)

Space charge capabilities supported by BLAST codes using the AMReX software framework

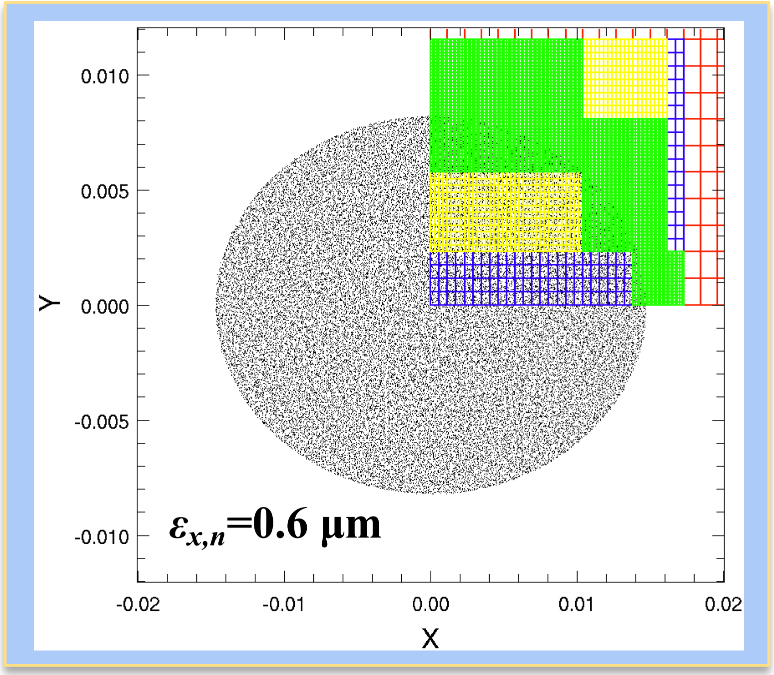
- Higher-order interpolation schemes for charge deposition to aid in noise suppression
- Parallel iterative Multi-Level Multi-Grid Poisson solver for performance scalability
- Adaptive Mesh Refinement (AMR) for resolving density gradients, beam edge and halo

Example: Using AMR can reduce computation time

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

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

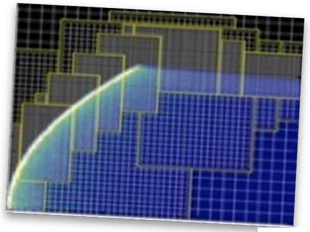
Desktop to HPC

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
- support for transverse machine errors
- apertures and lost particle diagnostics

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

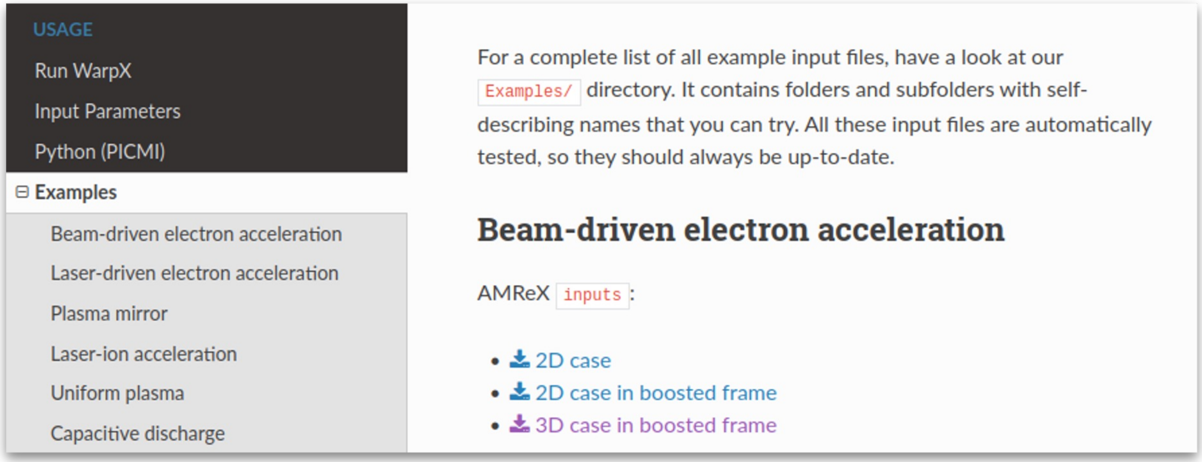
github.com/**ECP-WarpX/impactx**

BERKELEY LAB LDRD
SciDAC Scientific Discovery through Advanced Computing

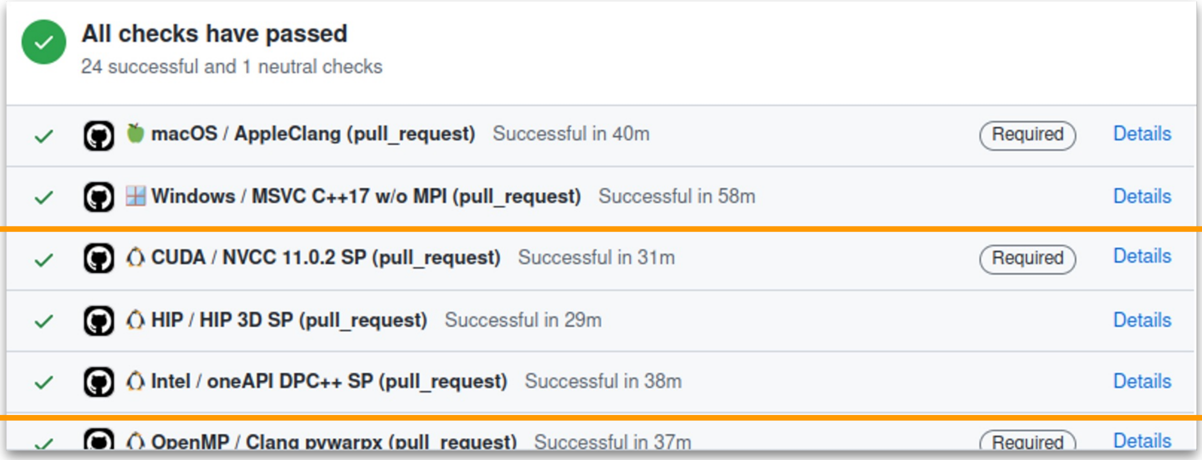
- Benchmarking and space charge validation

Fully open development and continuous benchmarking

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
34 physics benchmarks + 106 tests *for* ImpactX

Rapid and easy installation on any platform:

conda create –n impactx
-c conda-forge impactx

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
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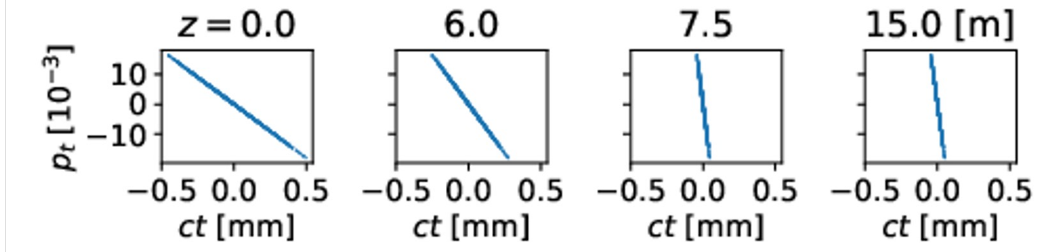
- Chain of thin multipoles
- A nonlinear focusing channel based on the IOTA nonlinear lens
- The “bare” linear lattice of the Fermilab IOTA storage ring
- Solenoid channel
- Drift using a Pole-Face Rotation
- Soft-edge solenoid
- Soft-Edge Quadrupole
- Positron Channel
- Cyclotron
- Combined Function Bend
- Ballistic Compression Using a Short RF Element
- Test of a Transverse Kicker

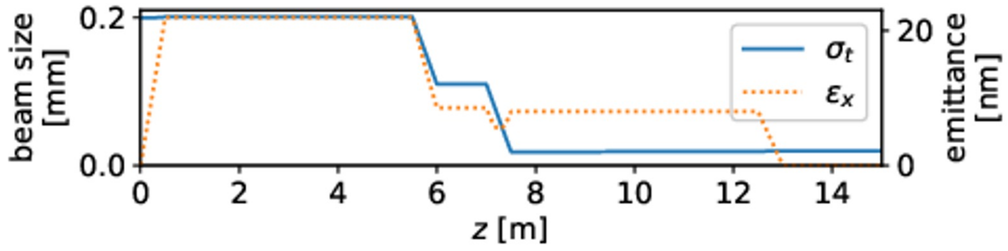
currently 34

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 3D Space Charge Validation: E field in a 3D Gaussian bunch

- Electric field in a 1 nC Gaussian bunch at rest for several values of aspect ratio (1M particles)*:

$$r = \sigma_z/\sigma_\perp, \quad \sigma_x = \sigma_y = \sigma_\perp = 1\ \mathrm{mm}$$

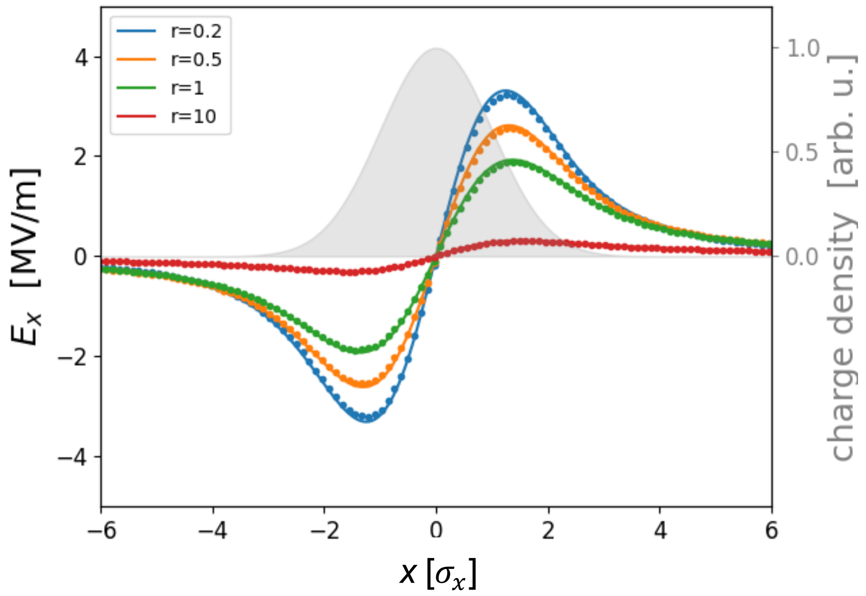
- Points – output from ImpactX. Lines – exact result.

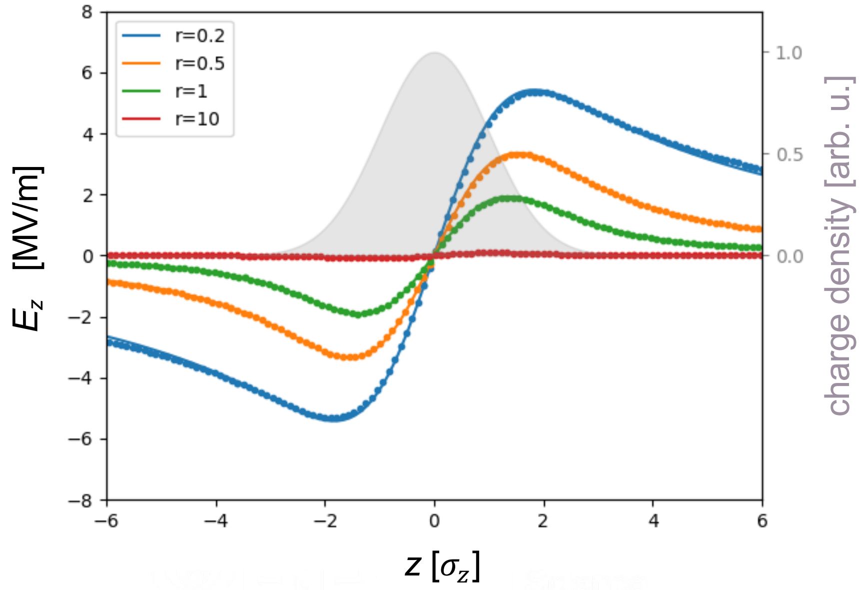
$\vec{E} = -\nabla\phi$ where:

$$\phi = \frac{Q}{4\pi\epsilon_0}\sqrt{\frac{2}{\pi}}\int_0^\infty \frac{e^{\frac{-\lambda^2 x^2}{2(\lambda^2\sigma_x^2+1)}} e^{\frac{-\lambda^2 y^2}{2(\lambda^2\sigma_y^2+1)}} e^{\frac{-\lambda^2 z^2}{2(\lambda^2\sigma_z^2+1)}}}{\sqrt{(\lambda^2\sigma_x^2+1)(\lambda^2\sigma_y^2+1)(\lambda^2\sigma_z^2+1)}} d\lambda$$

- Convergence becomes more challenging for large aspect ratio ➞ need Integrated Green Function (IGF) approach.

*C. Mayes et al, IPAC2018, THPAK085 (2018)
C. Mitchell et al, HB2023, THBP44 (2023)





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

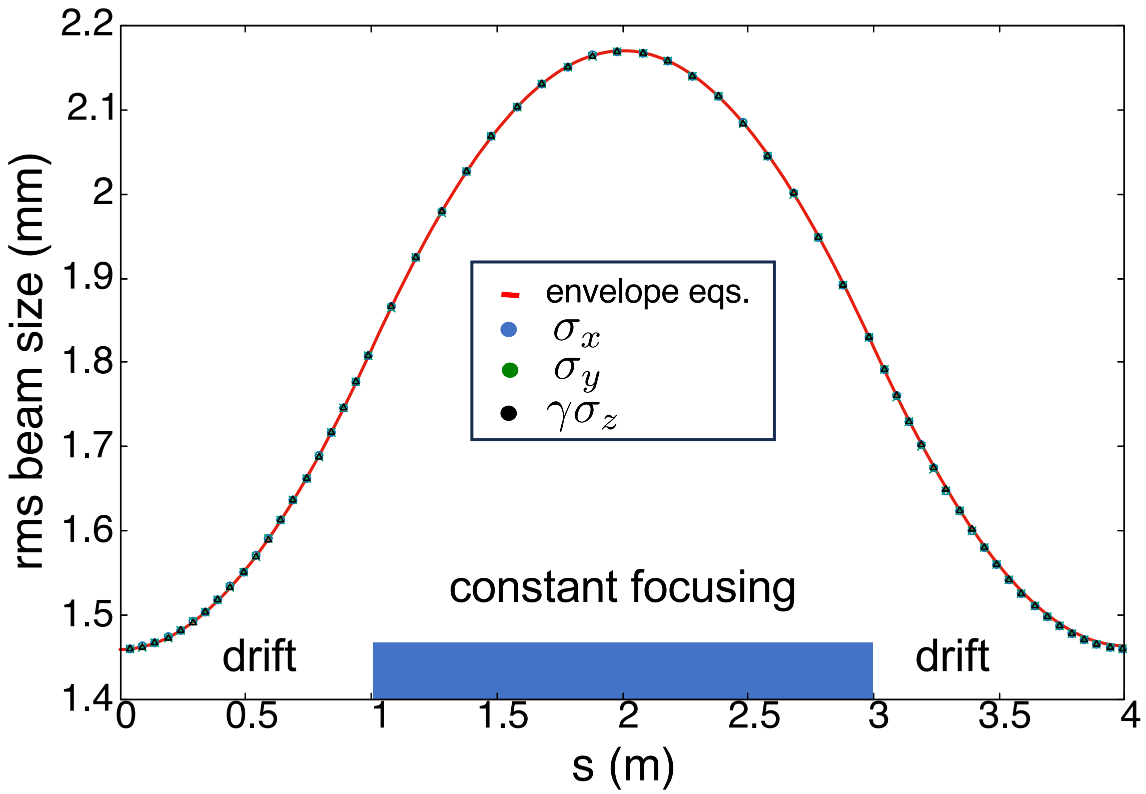
- Analogous to a K-V beam in a FODO channel, but appropriate for 3D bunched beams.

- 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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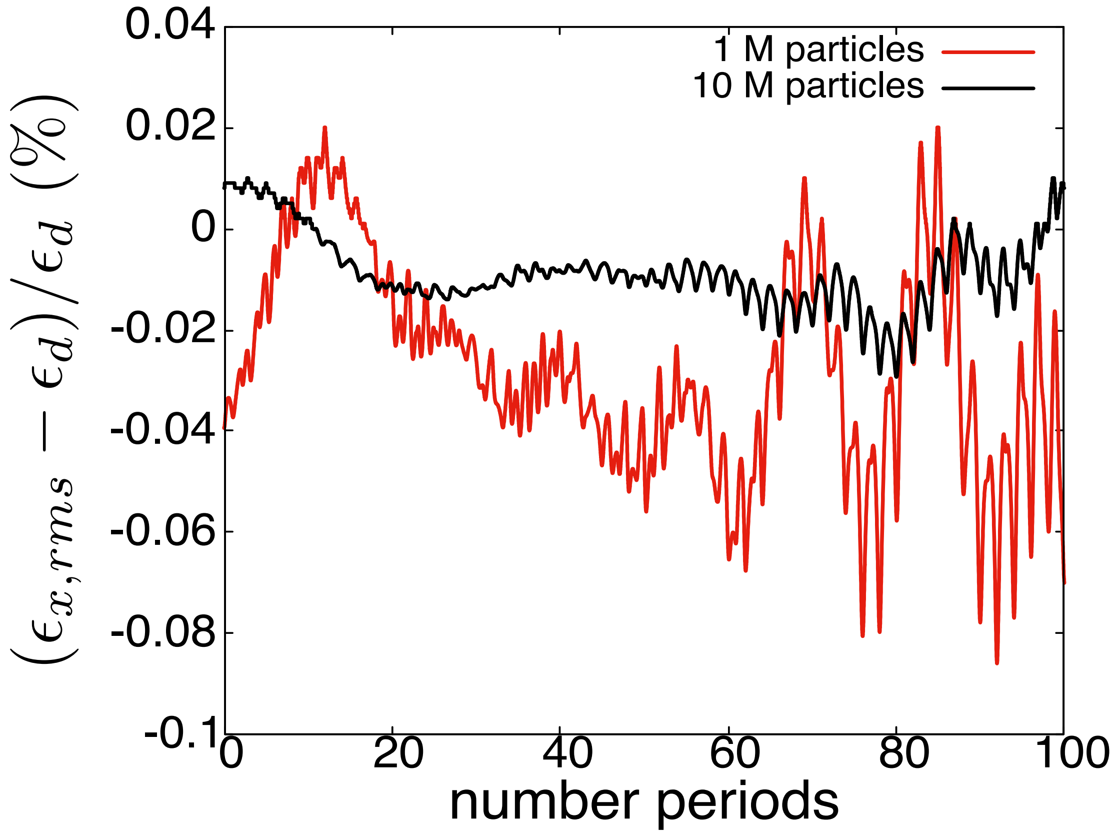
1 M particles, [72,72,72] grid

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).

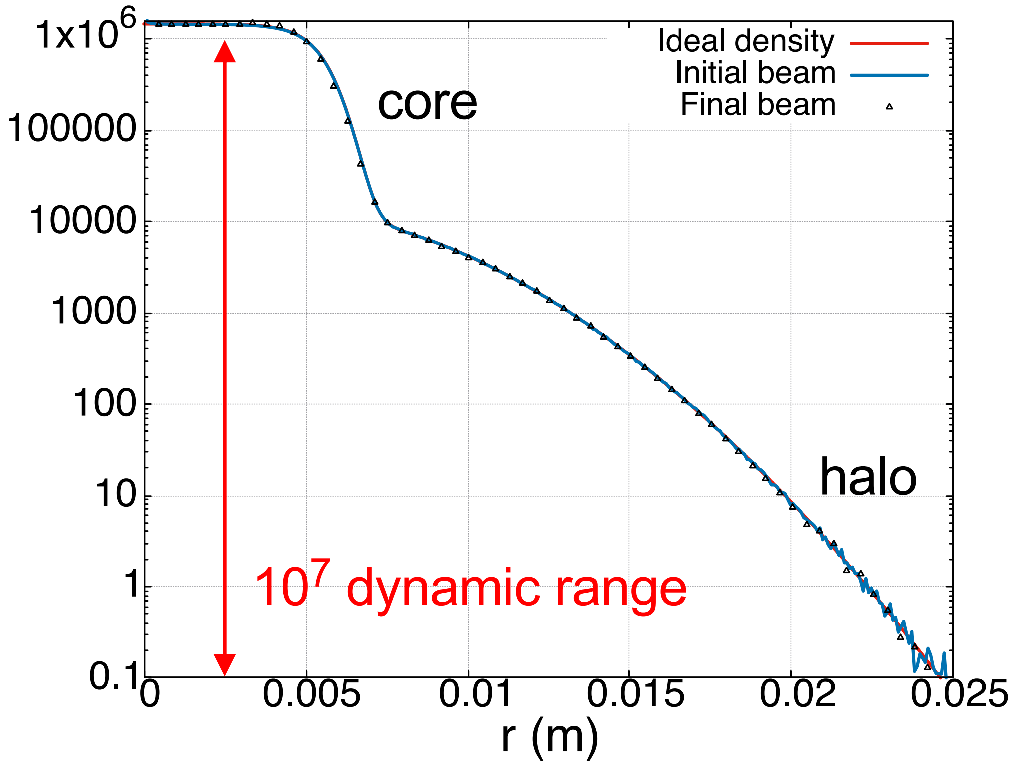
ImpactX 3D Space Charge Validation: bithermal beam in a CF channel

- 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

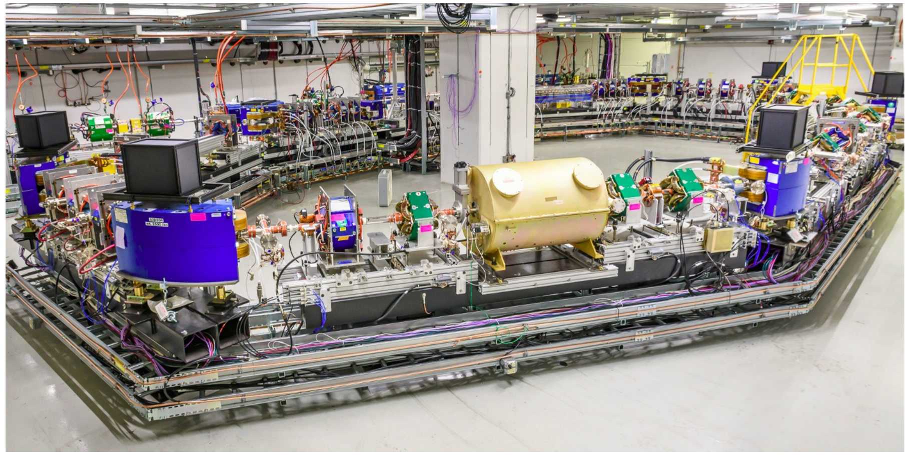
*R. Ryne et al, EPAC2004, WEPLT047 (2004)
C. Mitchell et al, HB2023, THBP44 (2023)

Zenodo: doi.org/10.5281/zenodo.8395849

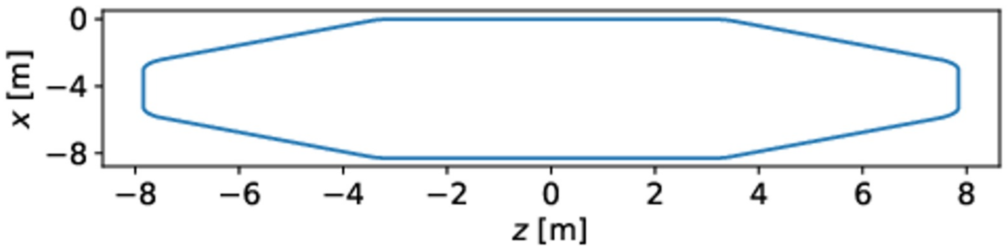
- Toward ImpactX applications to IOTA

IOTA (v. 8.4) Bare 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



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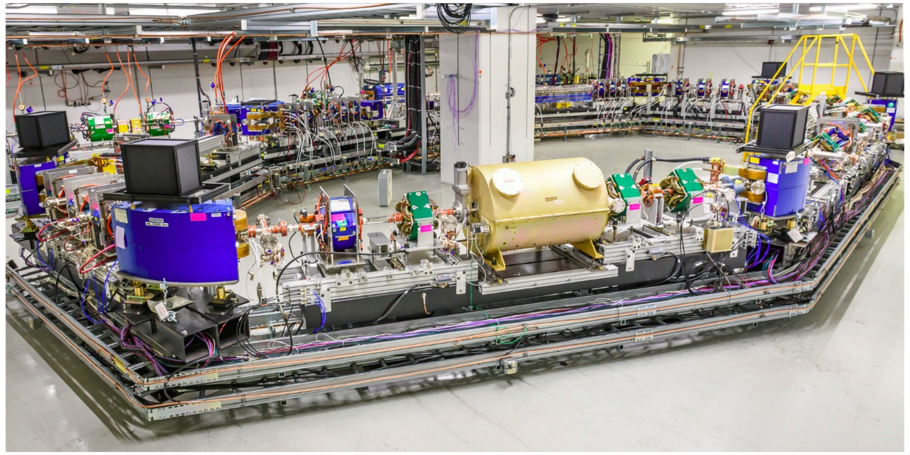

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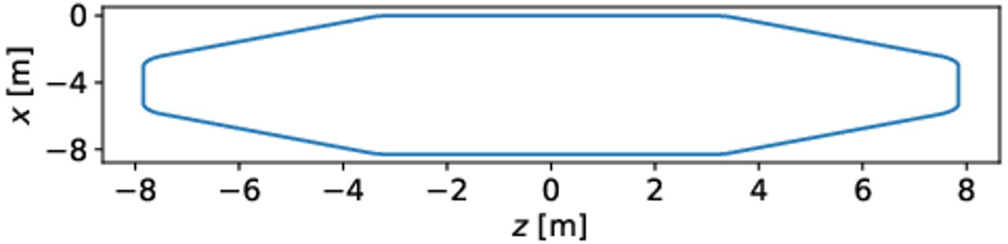
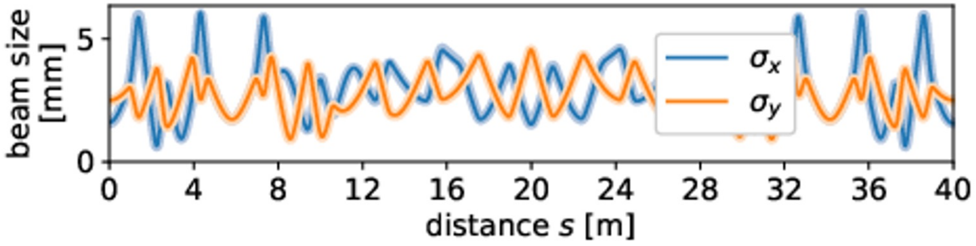


Second Moments / Linear Optics

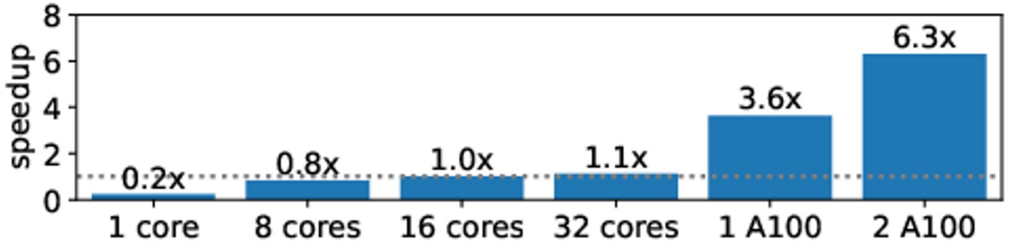
- check emittance preservation
- check rms beam envelopes:

IMPACT-Z vs ImpactX



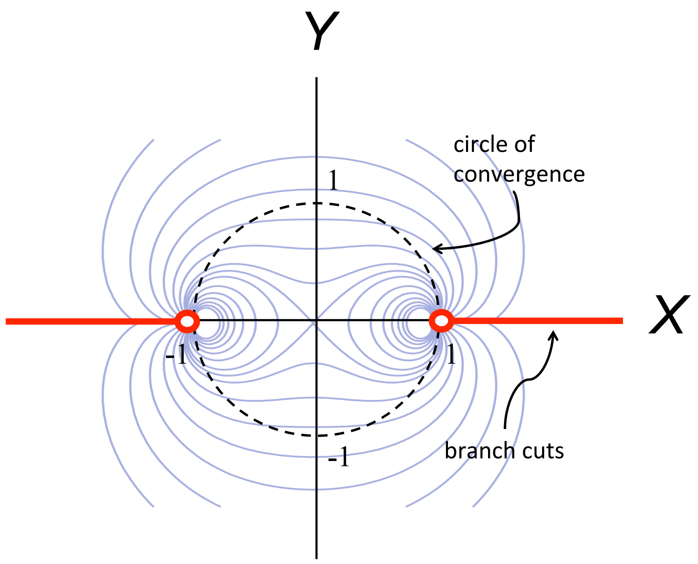
Preliminary Performance

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



Modeling of IOTA nonlinear integrable optics

Magnetic field lines in the NLI (transverse plane)



Coordinates normalized by $c\sqrt{\beta_x} = c\sqrt{\beta_y}$,

$c = 0.01\ \mathrm{m}^{1/2}$

- ImpactX contains a model of the IOTA nonlinear magnetic element*

V. Danilov and S. Nagaitsev, PRAB 13, 084002 (2010)

C. Mitchell *et al*, PRAB 23, 064002 (2020), & arXiv.1908.0036 (2019)

Modeling of IOTA nonlinear integrable optics

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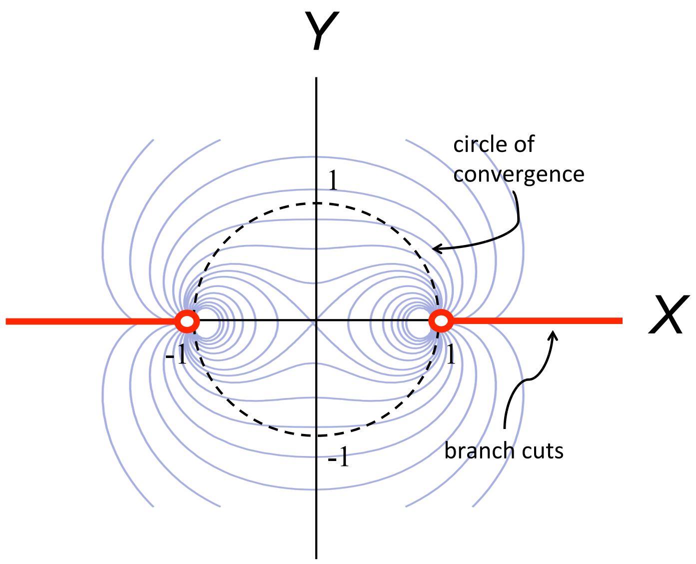
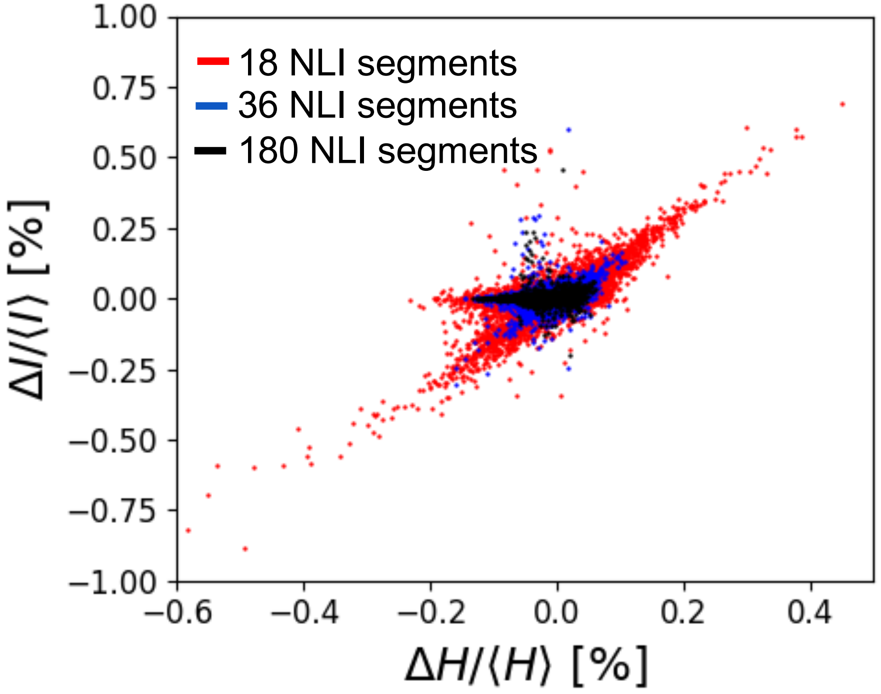


Coordinates normalized by $c\sqrt{\beta_x} = c\sqrt{\beta_y}$, $c = 0.01\ \mathrm{m}^{1/2}$

Preservation of nonlinear invariants

change in (H,I) after 100 turns



Increasing the number of NLI segments results in improved preservation of (H,I).

- ImpactX contains a model of the IOTA nonlinear magnetic element*
- Example shown for a 2.5 MeV p beam initially matched to the bare lattice linear optics with $\epsilon_{x,y} = 3\ \mu\mathrm{m}$

V. Danilov and S. Nagaitsev, PRAB 13, 084002 (2010)

C. Mitchell *et al*, PRAB 23, 064002 (2020), & arXiv.1908.0036 (2019)

Modeling of IOTA nonlinear integrable optics

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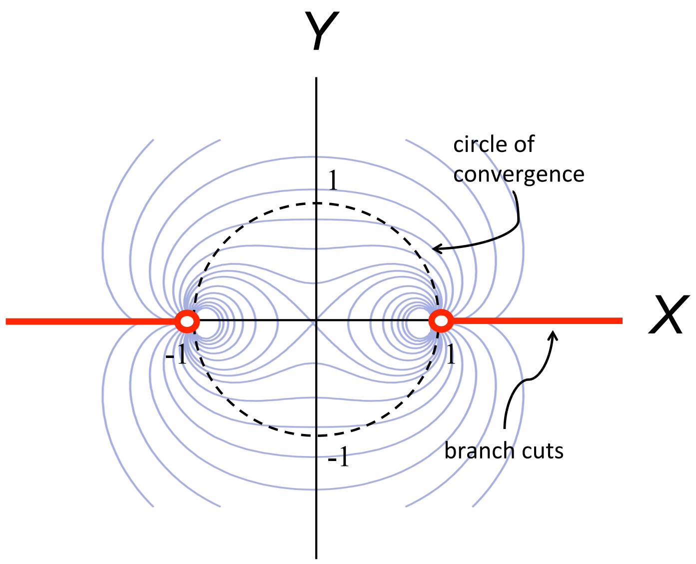

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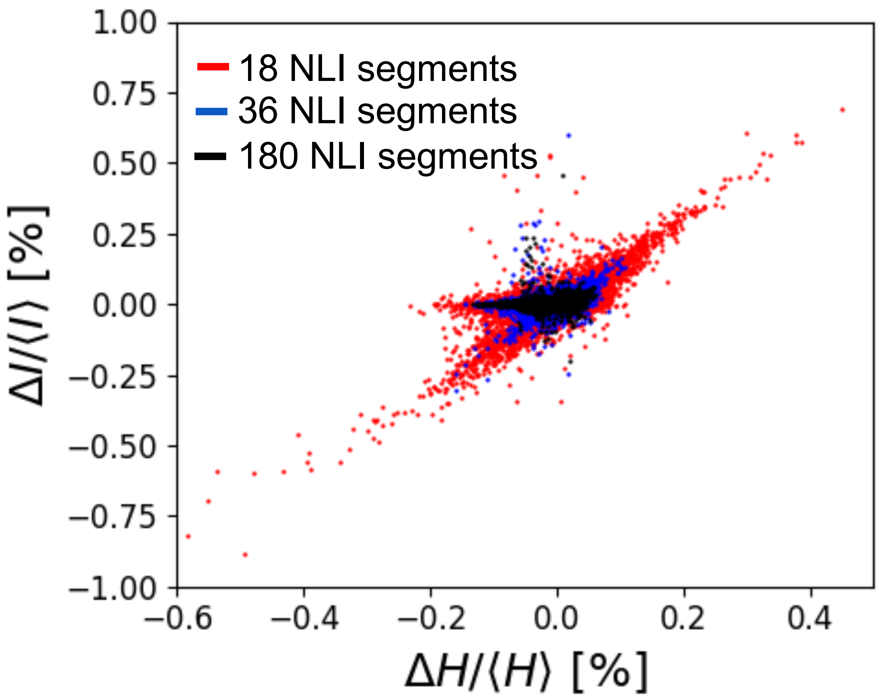
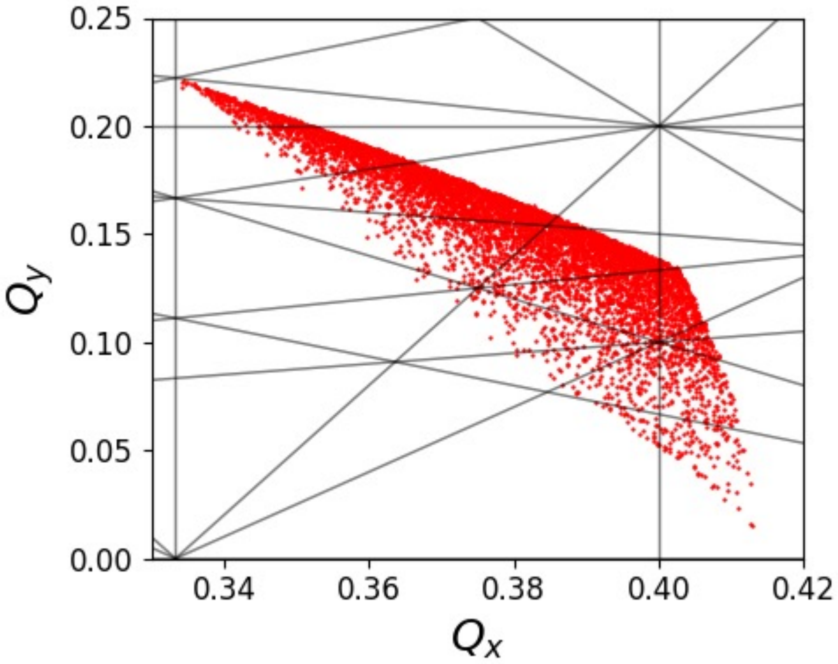


Increasing the number of NLI segments results in improved preservation of (H,I).

Fractional tune footprint

resonance lines through order 5

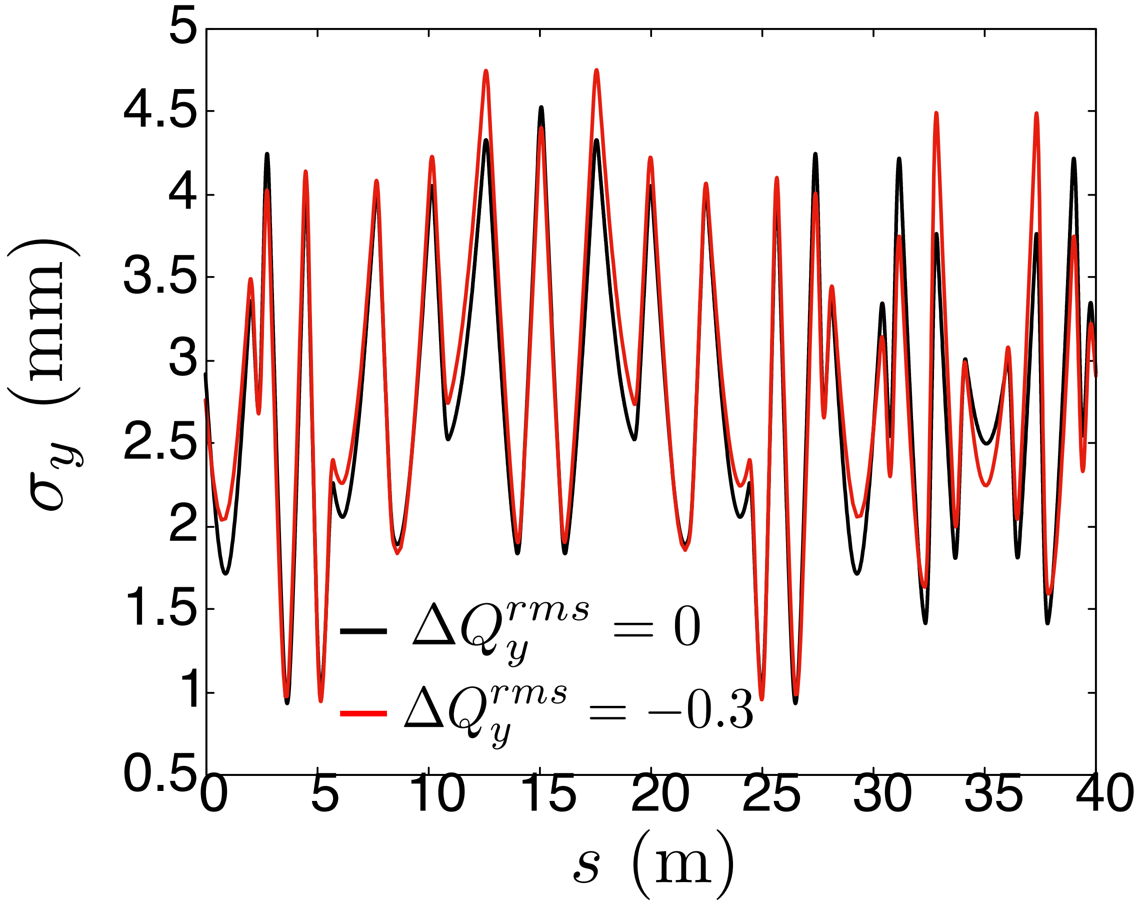


Nonlinear tune spread from TBT data.

Cf. bare linear lattice: $(Q_x, Q_y) = (0.3, 0.3)$

Examples of IOTA space charge modeling in ImpactX*

RMS matching w/ space charge (via Python interface)



- Using the Python interface, the user can couple ImpactX space charge runs with optimization.
- Vertical beam envelope for a beam matched to the bare linear lattice at nominal emittance with space charge tune depression -0.3.

*Using a bunched beam with $E_z^{SC} = 0$ to avoid debunching.

Examples of IOTA space charge modeling in ImpactX*

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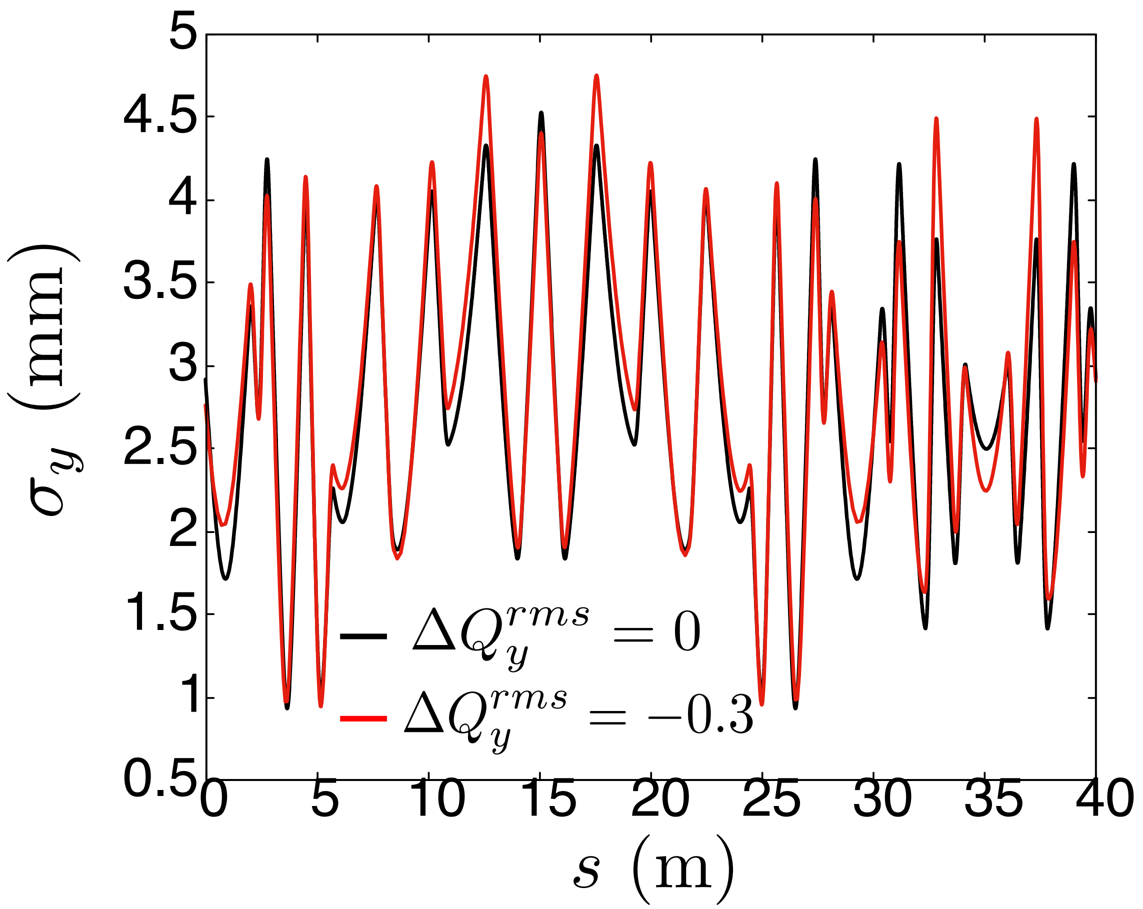
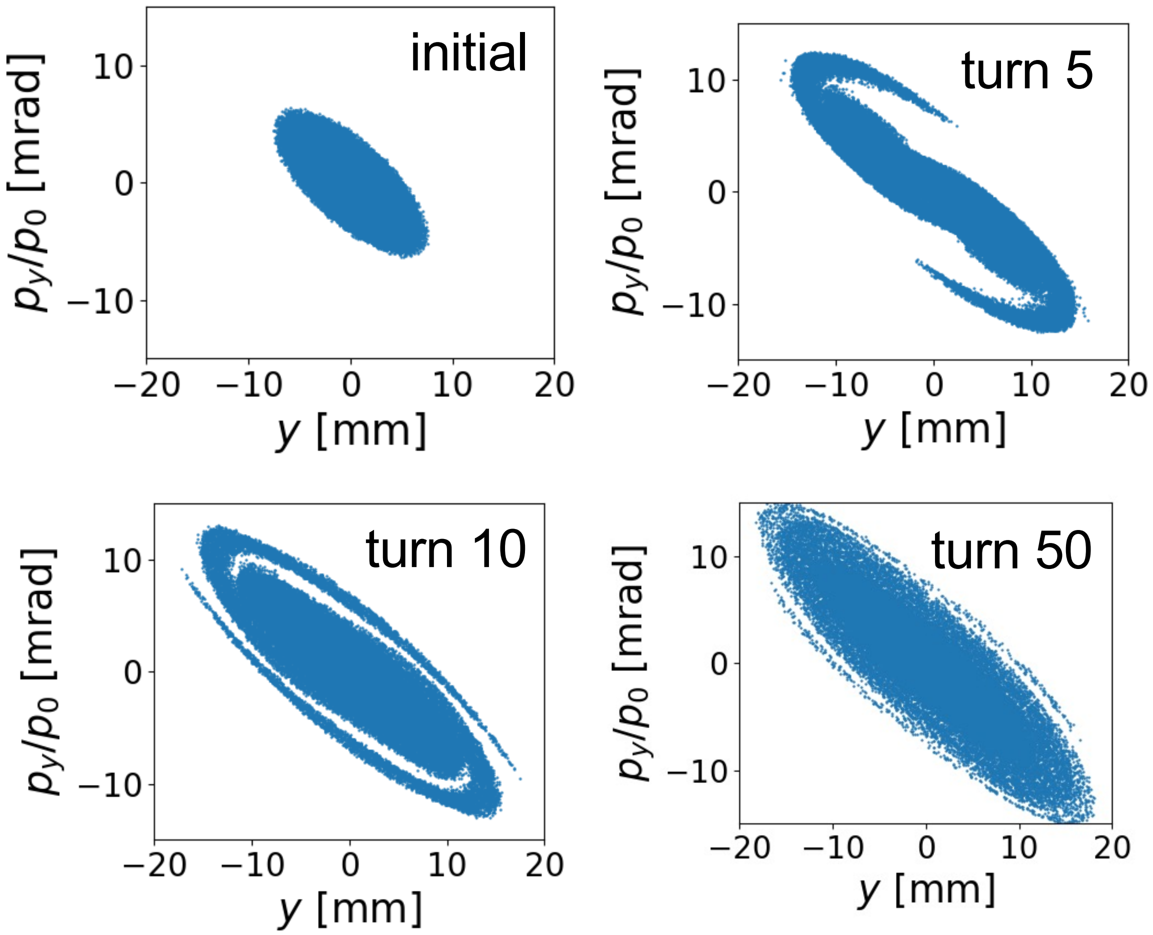


*Using a bunched beam with $E_z^{SC} = 0$ to avoid debunching.

Vertical phase space in the presence of space charge & nonlinear optics



For an initial SC tune shift $\Delta Q_y^{rms} = -0.3$

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:
  - Implementation of 2D and/or 2.5D space charge models for long and unbunched beams
  - Addition of 1D resistive wall + CSR wakefield models (already in IMPACT-Z)

- *Comments welcome on additional capabilities relevant to FAST/IOTA modeling.*

Thank you for your attention!

Questions?

Contact: ChadMitchell@lbl.gov

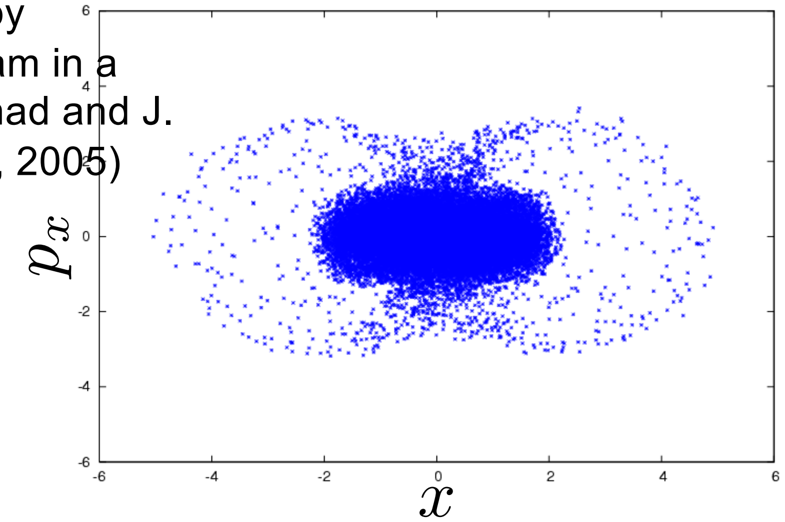
- Backup Slides

Space charge modeling at high fidelity: a community effort

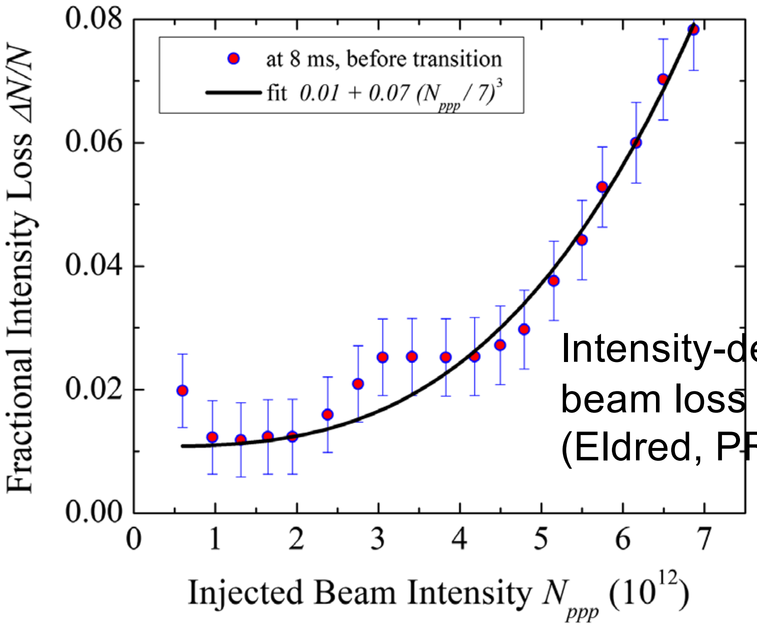
PIC modeling with high spatial resolution and good particle statistics is needed to:

- 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



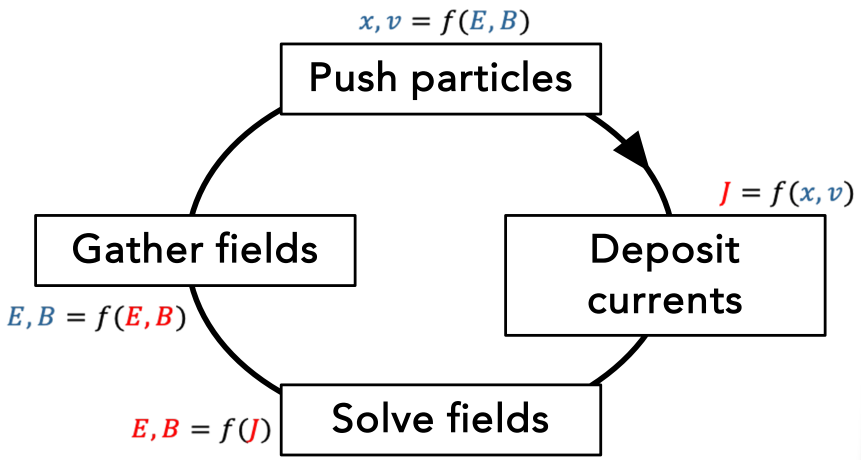
Intensity-dependent fractional beam loss in FNAL Booster (Eldred, PRAB **24**, 044001, 2021)

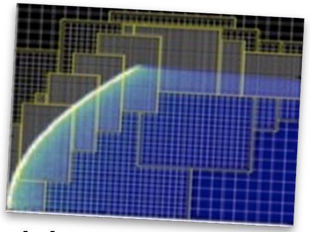
For large turn numbers in rings, PIC is subject to numerical artifacts (noise) and long computing times ➡ fast tools exploiting GPU architectures + integrated workflows + AI/ML

WarpX is a GPU-Accelerated PIC Code for Exascale

Available Particle-in-Cell Loops

- electrostatic & electromagnetic (fully kinetic)





Advanced algorithms

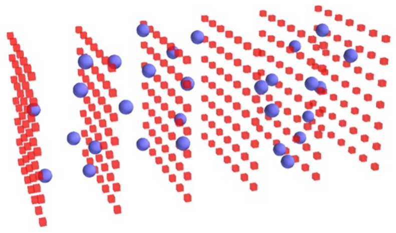
boosted frame, spectral solvers, Galilean frame, embedded boundaries + CAD, MR, ...

Multi-Physics Modules

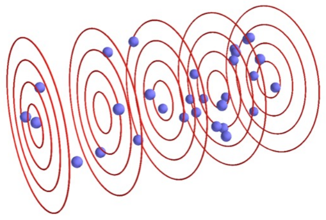
field ionization of atomic levels, Coulomb collisions, QED processes (e.g. pair creation), macroscopic materials

Geometries

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



3D Cartesian grid



Cylindrical grid (schematic)

Multi-Node parallelization

- MPI: 3D domain decomposition
- dynamic load balancing

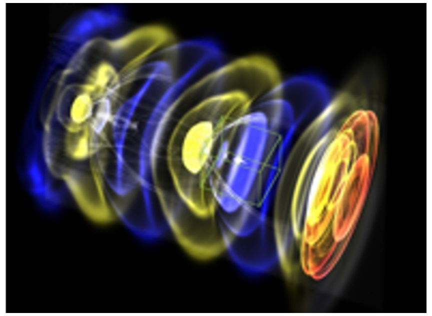
On-Node Parallelization

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

Scalable, Standardized I/O

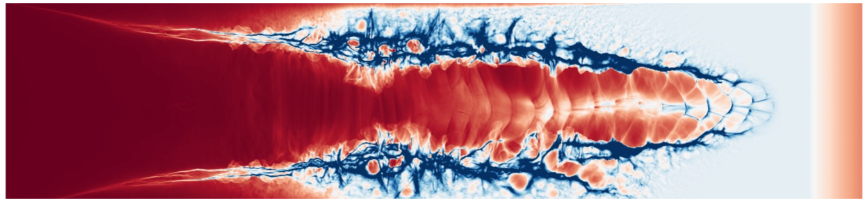
- PICMI Python interface
- openPMD (HDF5 or ADIOS)
- in situ diagnostics

WarpX supports a growing number of applications

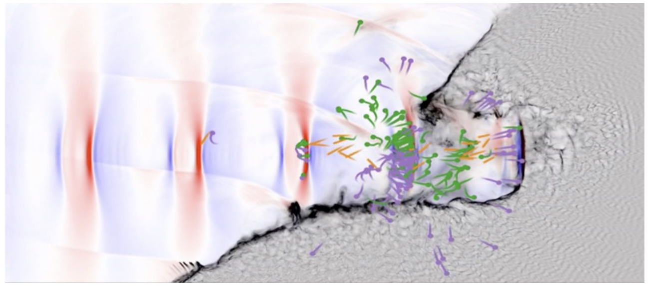


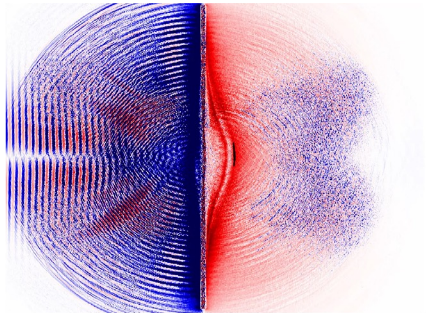
Plasma accelerators (LBNL, DESY, SLAC)

Laser-ion acceleration - advanced mechanisms (LBNL)



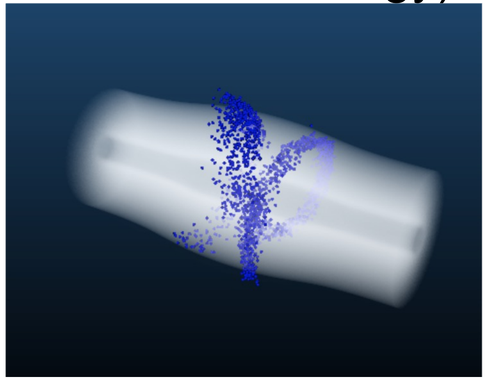
Plasma mirrors and high-field physics + QED (CEA Saclay/LBNL)



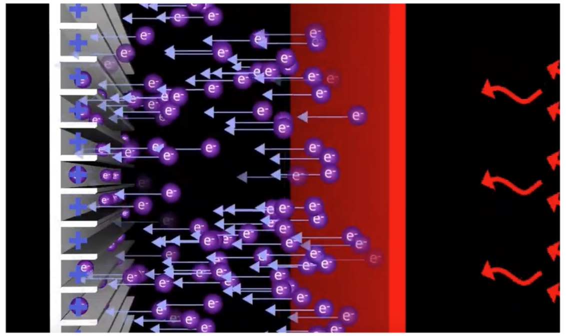


Laser-ion acceleration - laser pulse shaping (LLNL)

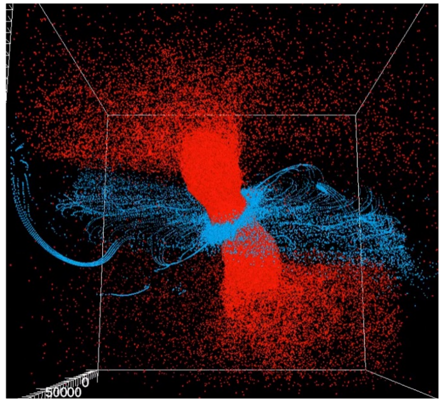
Plasma confinement, fusion devices (Zap Energy, Avalanche Energy)



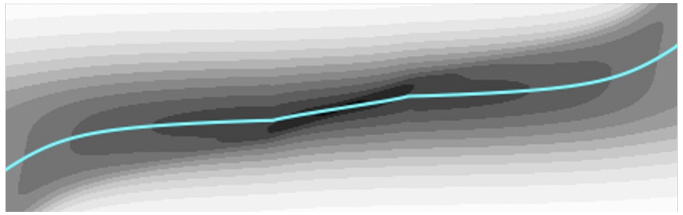
Thermionic converter (Modern Electron)



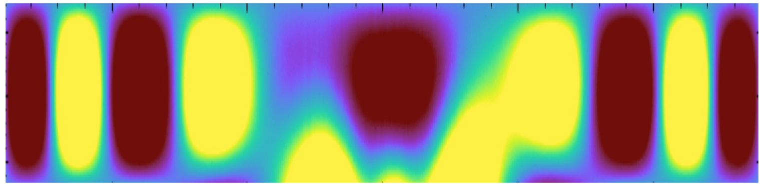
Pulsars, magnetic reconnection (LBNL)

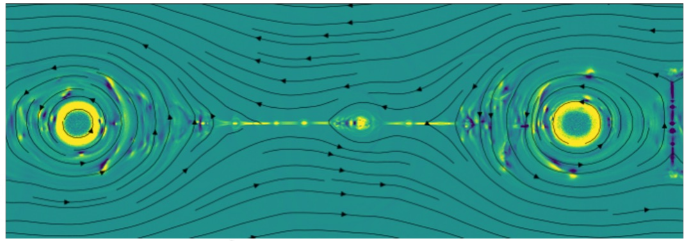


Magnetic fusion sheaths (LLNL)



Microelectronics (LBNL) - ARTEMIS





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

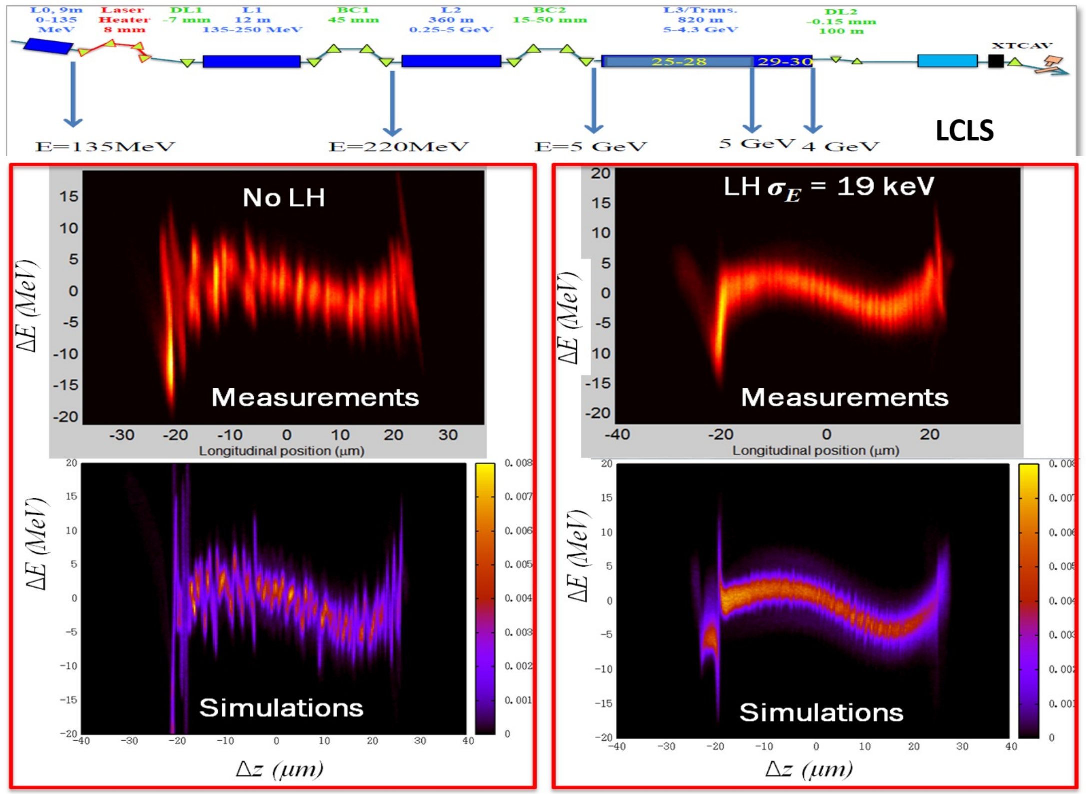
openPMD-api
reference library
file-format agnostics API

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

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).

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

BLAST — BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

WarpX/FBPIC
HiPACE++
Wake-T
ImpactX

UCLA: Osiris, QuickPIC, QPAD

Synergia — Fermilab

HZDR, Berkeley Lab, Technische Universität Dresden, EUCALL, Lawrence Livermore National Laboratory, SLAC, DESY, UHH, European XFEL, Cornell University, UCLA, CBG, IOQ Jena, Fermilab, Oak Ridge National Laboratory, plasmapy, Maison de la Simulation

SciDAC — Scientific Discovery through Advanced Computing

- Collaborative multi-institutional effort supported by SciDAC-5 for HEP applications
- openPMD standard is already fairly mature and widely adopted
- PICMI is more recent and also more challenging: redesign is planned for FY24
- Discussions underway/welcome regarding an accelerator lattice standard (AMI)