Space Charge Physics in the Code ImpactX

Chad Mitchell
Lawrence Berkeley National Laboratory

BLAST
BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

ICFA Space Charge Workshop
Oxford, UK, Sept. 29-Oct. 3, 2026

BERKELEY LAB

SciDAC
Scientific Discovery through Advanced Computing

U.S. DEPARTMENT OF ENERGY | Office of Science

Acknowledgments

Thanks to the workshop organizers.

Thanks to all ImpactX collaborators, especially: A. Huebl, E. Stern, J. Qiang, A. Formenti, R. Lehe, W. Zhang, and J-L. Vay.

Funding acknowledgments:

This work was supported by the Director, Office of Science of the U.S. Department of Energy under Contracts No. DE-AC02-05CH11231 AND DE-AC02-07CH11359. This material is based upon work supported by the CAMPA Collaboration, a project of the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research and Office of High Energy Physics, Scientific Discovery Through Advanced Computing (SciDAC) Program. This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science user facility supported by the Office of Science of the U.S. Department of Energy under Contract. No. DE-AC02-05CH11231 using NERSC awards HEP-ERCAP002379 and HEP-ERCAP0014350.

BLAST
BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

Developed by an international, multidisciplinary team

WarpX open governance

open source initiative®

THE LINUX FOUNDATION

HIGH PERFORMANCE SOFTWARE FOUNDATION

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ATAP
ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION

AMCRD

NERSC

Jean-Luc Vay



Ji Qiang



Arianna Formenti



Axel Huebl



Rémi Lehe



Chad Mitchell



Olga Shapoval



Edoardo Zoni



David Grote



Justin Angus



Ann Almgren



Kevin Gott



Junmin Gu



Revathi Jambunathan



Andrew Myers



Weiqun Zhang



UR LLE

Kale Weichmann



Roelof Groenewald



HELION

REALTA FUSION

Eric Clark



Prabhat Kumar



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DESY.

Maxence Thévenet



Alexander Sinn



Ángel Ferran Pousa*



Rob Shalloo



France

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Igor Andriyash



Switzerland

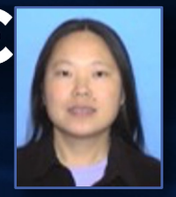
CERN

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Lixin Ge



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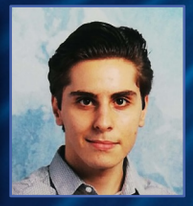
Henri Vincenti



Luca Fedeli



Thomas Clark



Pierre Bartoli*



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CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

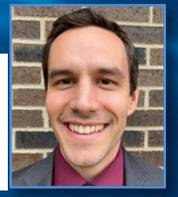
Franz Poeschel



*former members

tae TECHNOLOGIES

Ryan Sandberg



AVALANCHE

Marco Garten



over 120 **contributors,** incl. from the private sector

Software stack for the modern BLAST 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

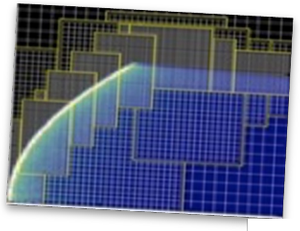
- s-based tracking with symplectic maps
- detailed RF cavity models and standard magnetic elements (w/soft-edge models)
- exact nonlinear maps for sbends, drifts
- translation/rotation errors and apertures
- radiation (CSR/ISR) and spin tracking

Space Charge Model

- space charge included using a split-operator approach
- 3D, 2D, and 2.5D models
- Multi-Level, Multi-Grid Poisson solver

Triple Acceleration Approach

- GPU support
- Mesh Refinement (AMReX)
- 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/**BLAST-ImpactX/impactx**

Space Charge Models Currently Supported in ImpactX

Space charge is included with symplectic tracking using a 2nd-order operator Hamiltonian splitting. Space charge fields are treated as electrostatic in the beam rest frame.

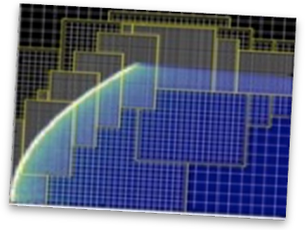
1. FFT-based Integrated Green's Function Solvers (open boundaries)

- 2D (transverse) and 3D PIC models
- 2.5D PIC model (cf. PyOrbit and Synergia)

J. Qiang *et al*, PRAB **9**, 044204 (2006)

2. AMReX Multi-Level Multigrid Poisson Solver (3D PIC)

- conducting or Neumann boundaries
- multi-level mesh refinement around the beam



W. Zhang *et al*, IJHPCA **35**, 508 (2021)

3. Quasi-Frozen (Gaussian) Models

- 3D and 2.5D Gaussian models
- nonlinear and fully symplectic, based on beam moments

J. Qiang, PRAB **28**, 114602 (2025)

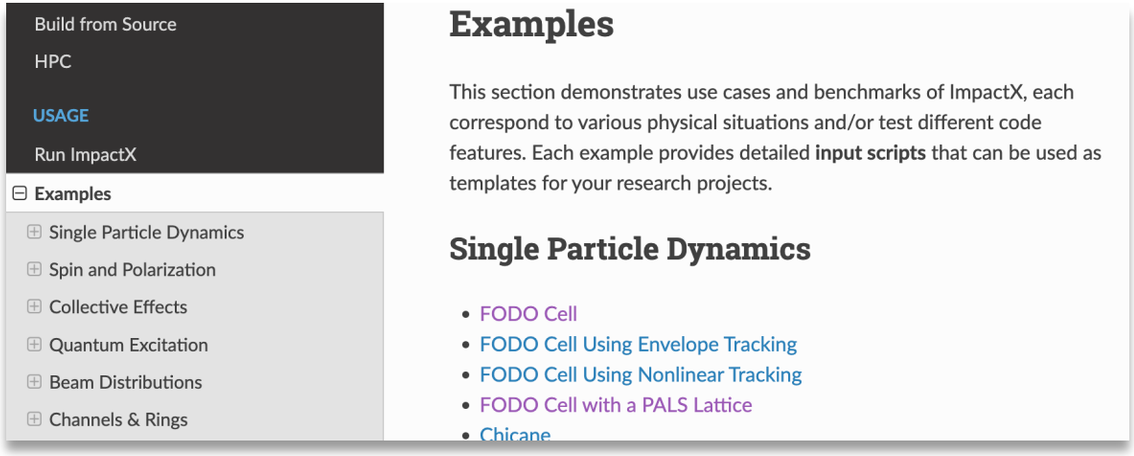
4. Envelope Tracking Models (2D and 3D)

- linear and fully symplectic, based on beam moments

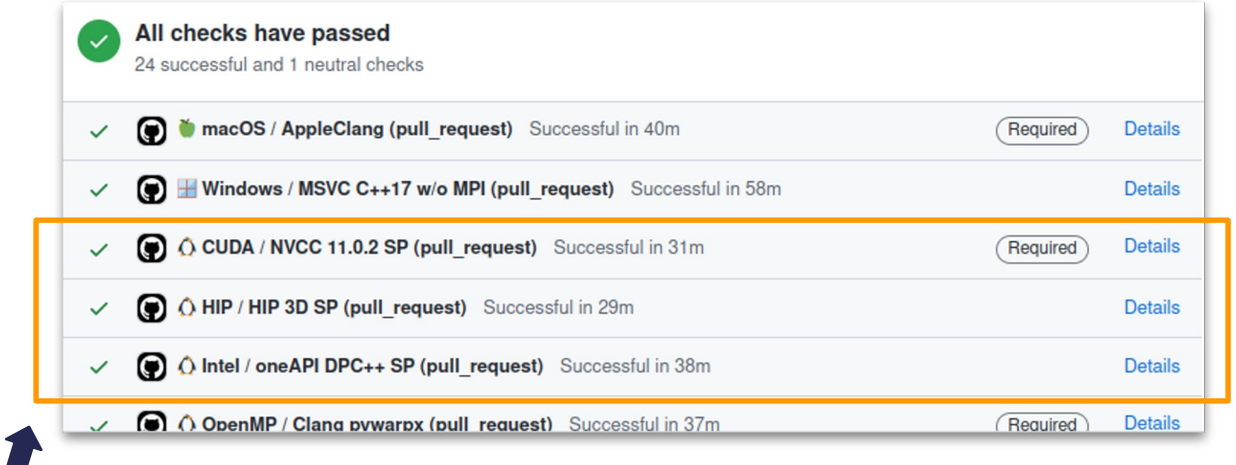
C. Mitchell, LBNL-2001685 (2025)

Fully open development and continuous benchmarking

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



Open-Source Development & Benchmarks: github.com/BLAST-ImpactX



262 automated tests *run on every code change* of ImpactX
22 space charge physics benchmarks

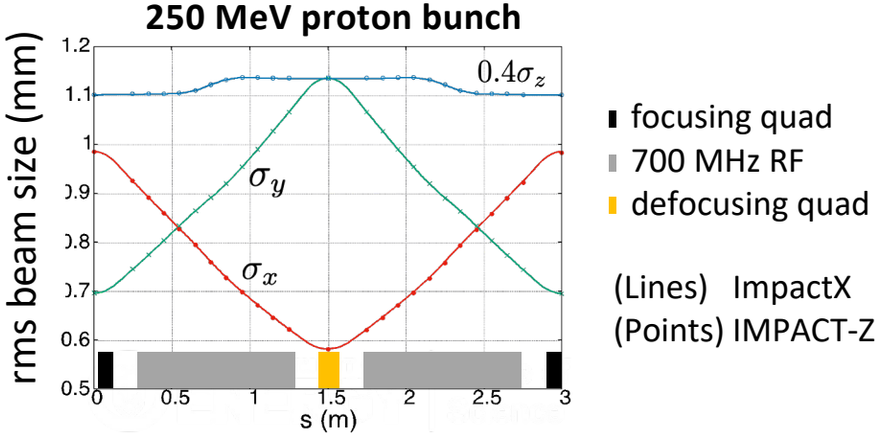
Rapid and easy installation on any platform:

conda create –n impactx
-c conda-forge impactx

python -m pip install impactx-noacc

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

Example:



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)*:

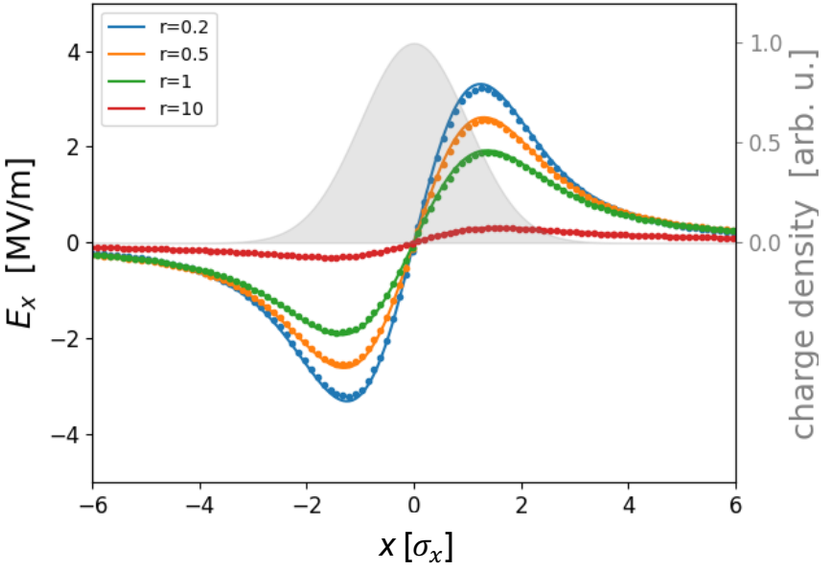
$$r = \sigma_z/\sigma_\perp, \quad \sigma_x = \sigma_y = \sigma_\perp = 1 \text{ mm}$$

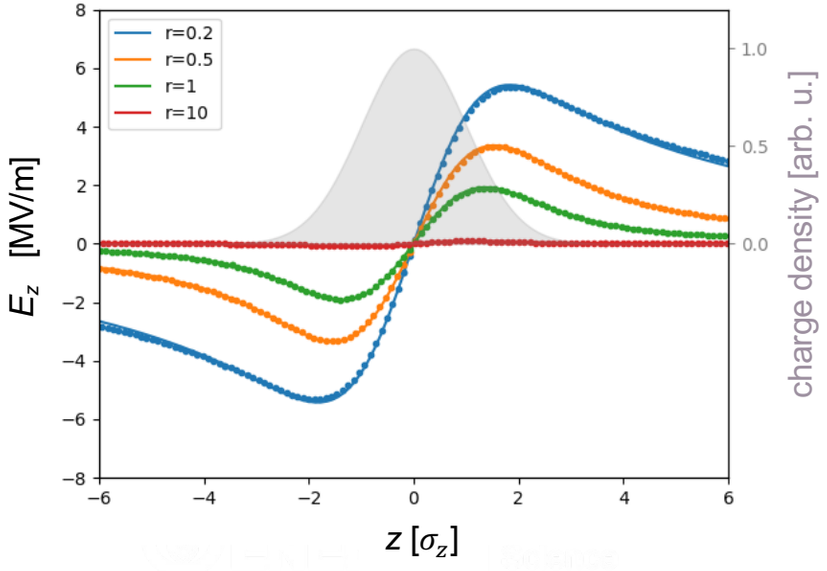
- Points – output from ImpactX. Lines – exact result.

$\vec{E} = -\nabla\phi$ 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: Expanding Coasting Beam

- Dynamics of a cold, uniform expanding bunch in free space (both 2D and 3D cases), protons:

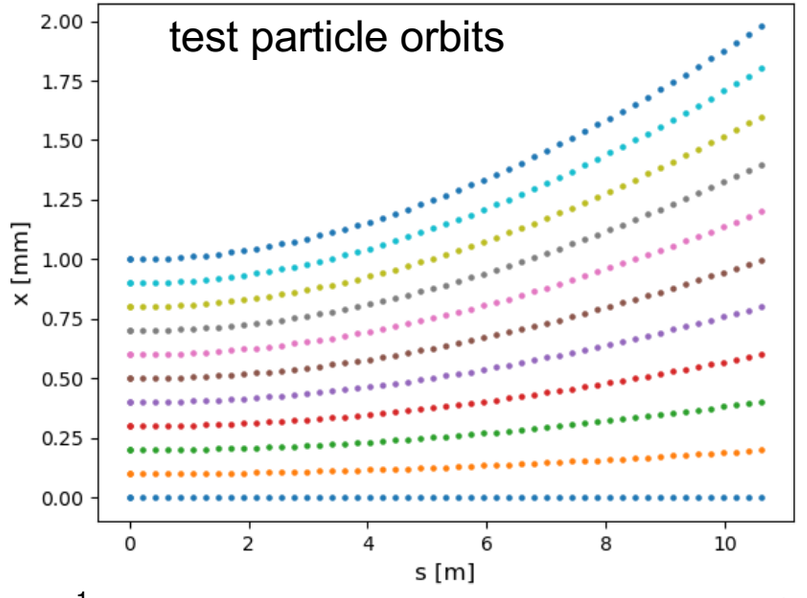
$$KE = 250\ \text{MeV}, \quad I_b = 0.15\ \text{A}, \quad R_0 = 1\ \text{mm}$$

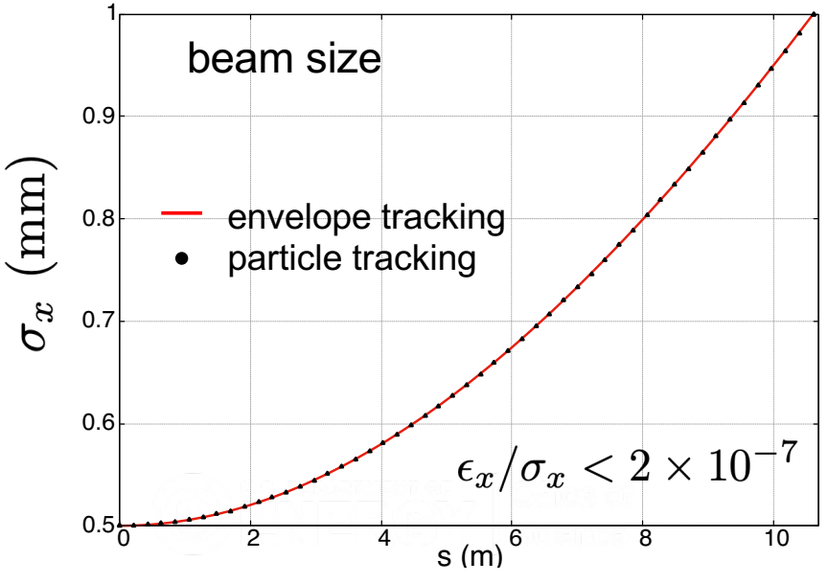
- Exact distance to radius doubling:

$$\Delta s_{2D} = \kappa_{2D}\sqrt{\frac{I_A(\beta\gamma)^3 R_0^2}{2I_b}}, \quad \Delta s_{3D} = \kappa_{3D}\sqrt{\frac{(\beta\gamma)^2 R_0^3}{r_c N_b}}$$

κ_{2D}, κ_{3D} are known constants.

- Figures of merit:
  - exact envelope evolution
  - preservation of (zero) emittance
  - test particle orbits (shown right)



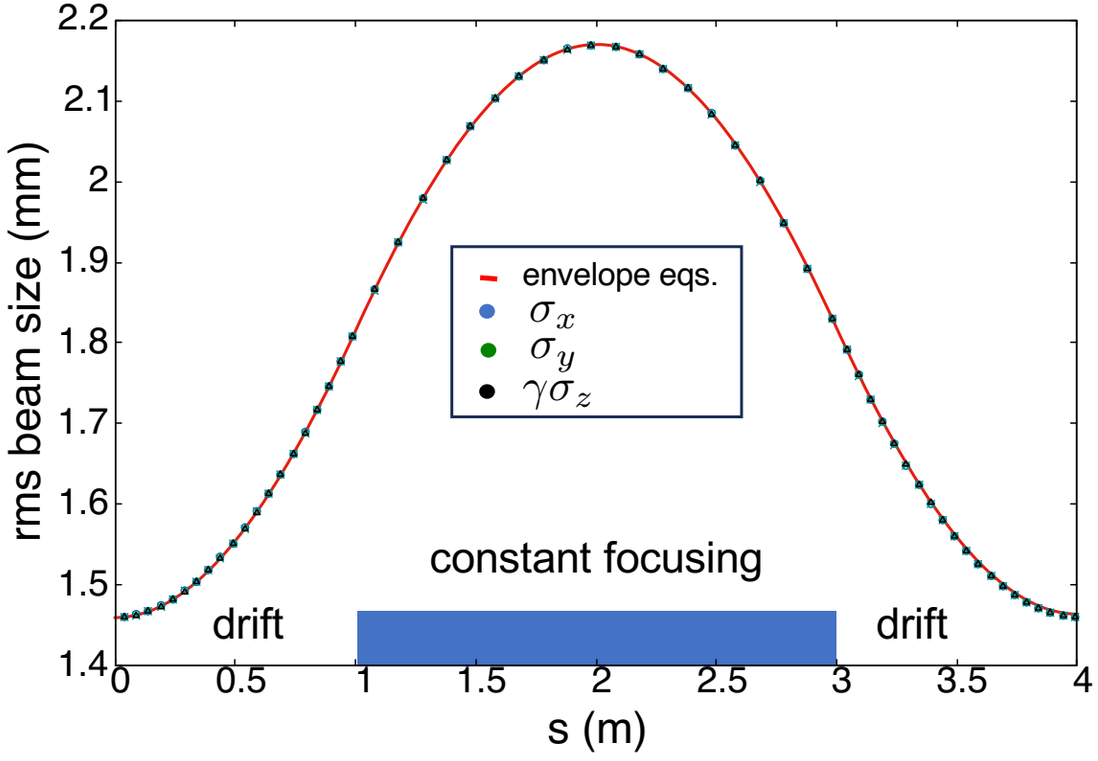


*R. Ryne et al, EPAC2004, WEPLT047 (2004)
C. Mitchell et al, HB2023, THBP44 (2023)

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



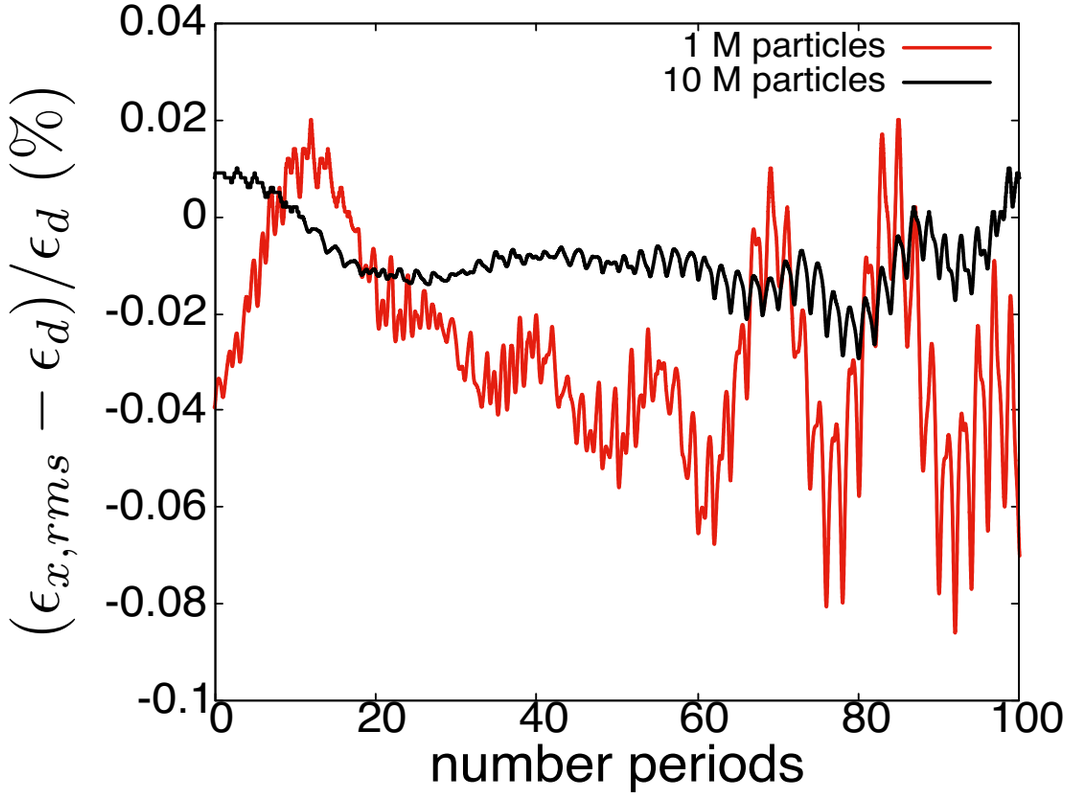
R. Kurth, Quart. Appl. Math. 36, pp. 325-329 (1978), C. Mitchell et al, IPAC2021, pp. 3213-3216 (2021).

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- Phase advance 121° ➡ 74°

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

Emittance fluctuations over 100 periods

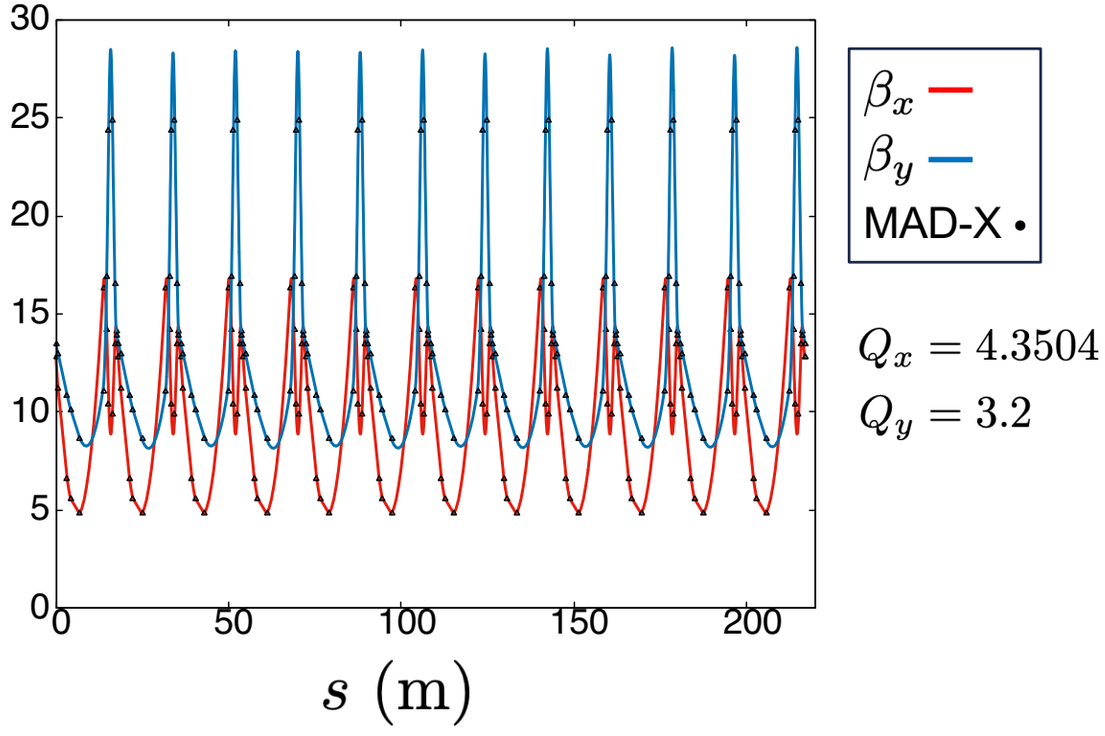


R. Kurth, Quart. Appl. Math. 36, pp. 325-329 (1978), C. Mitchell et al, IPAC2021, pp. 3213-3216 (2021).

GSI SIS18 Space Charge Benchmark of Resonance Trapping

- Confirm the space charge induced trapping of particles in a bunch during long term storage.
- Began to explain CERN PS experimental results*.
- Based on a simplified 12 cell SIS18 lattice

https://web-docs.gsi.de/~giuliano/research_activity/trapping_benchmarking/main.html



$Q_x = 4.3504$

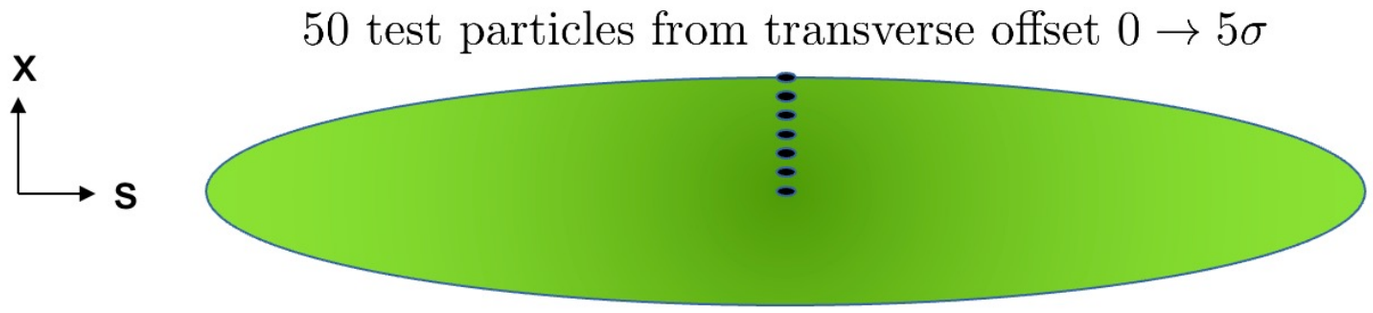
$Q_y = 3.2$

Lattice SIS18	
Strength of the sextupole (when used)	$K_2 = 0.2\ m^{-2}$
Maximum tuneshift	$\Delta Q_x = 0.1$
Horizontal transverse size (rms)	$X_{rms} = 5$ mm
Vertical transverse size (rms)	$Y_{rms} = 5$ mm
Longitudinal size (rms)	$Z_{rms} = 40.35$ m
Horizontal emittance (2 σ)	$\varepsilon_x = 12.57$ mm mrad
Vertical emittance (2 σ)	$\varepsilon_y = 9.30$ mm mrad
Turns for 1 synchrotron oscillation	$N_{synch} = 15000$
Bunch length (4 σ_z)	$\tau = 3472.7$ ns
Kinetik energy	$E_k = 11.4$ MeV/u
Gamma transition	$\gamma_t = 5$
momentum spread at $3\sigma_z$	$\Delta p/p = 2.5 \times 10^{-4}$

Sextupole may be energized to excite 3rd order resonance.

*G. Franchetti et al, PRST-AB 6, 124201 (2003)

GSI SIS18 Space Charge Benchmark: Test particles and tunes

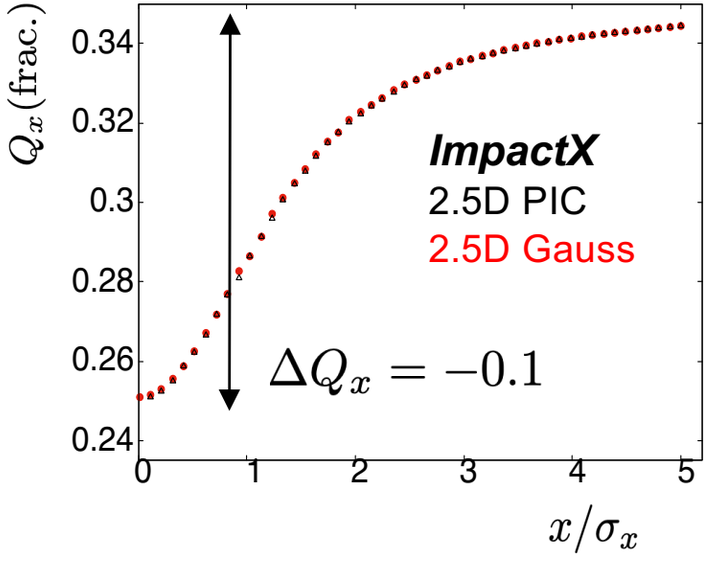


Gaussian bunch
11.4 MeV protons
matched to SIS18 lattice

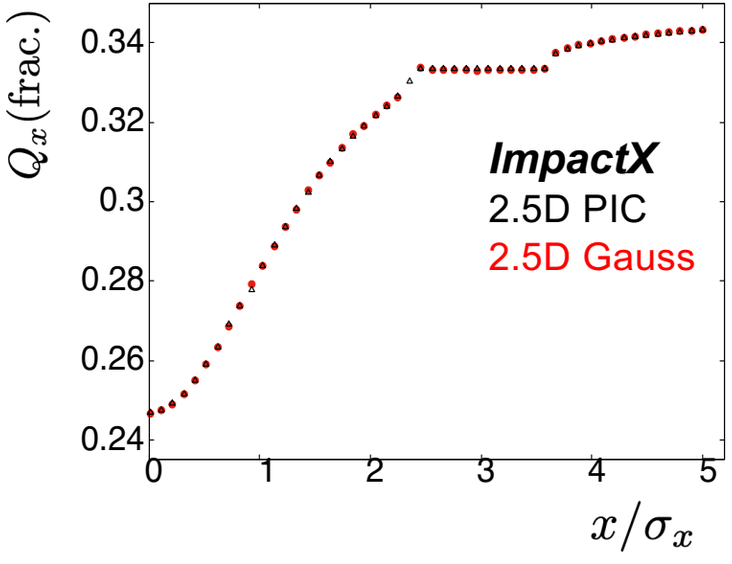
$$\sigma_x = \sigma_y = 5 \text{ mm}$$
$$\sigma_t = 870 \text{ ns}$$
$$\sigma_z = 40.3 \text{ m}$$

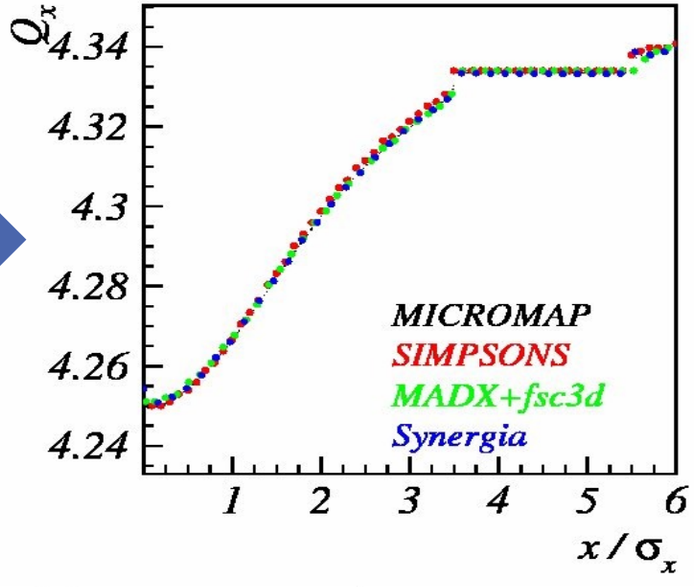
Propagate 1024 turns, calculate the tune of each test particle

Sextupole off



Sextupole on (with trapping)

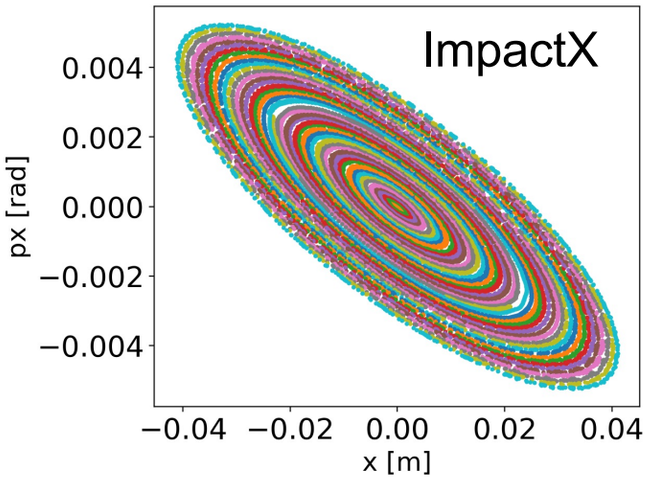




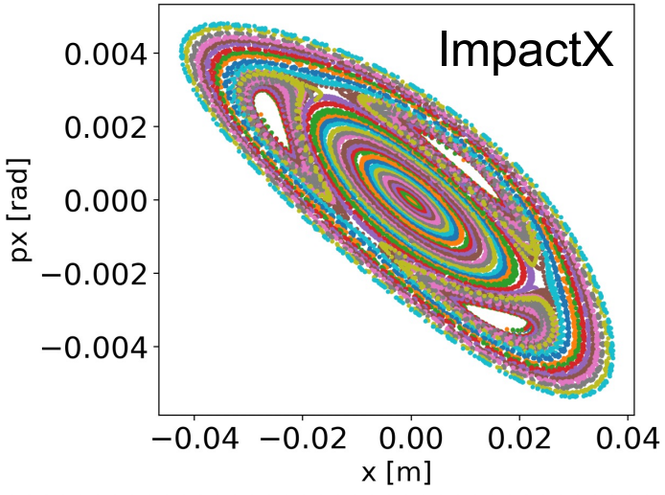
1M particles, 128x128 grid, 64 long. bins

GSI SIS18 Space Charge Benchmark: Phase space of trapped particles

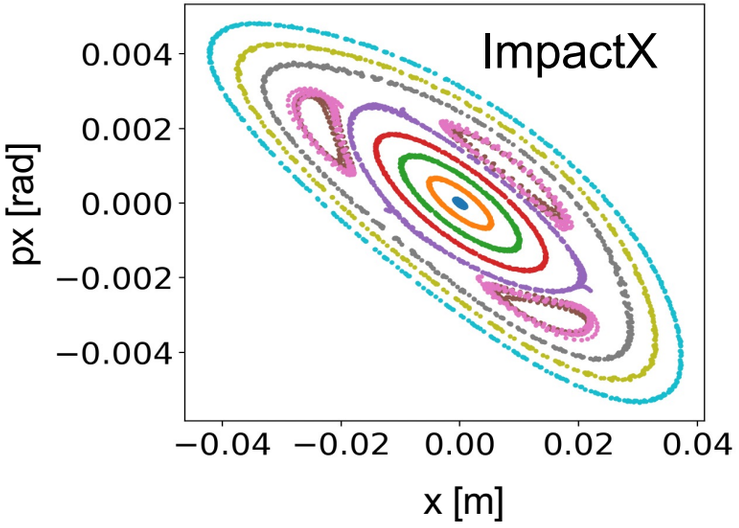
Sextupole off



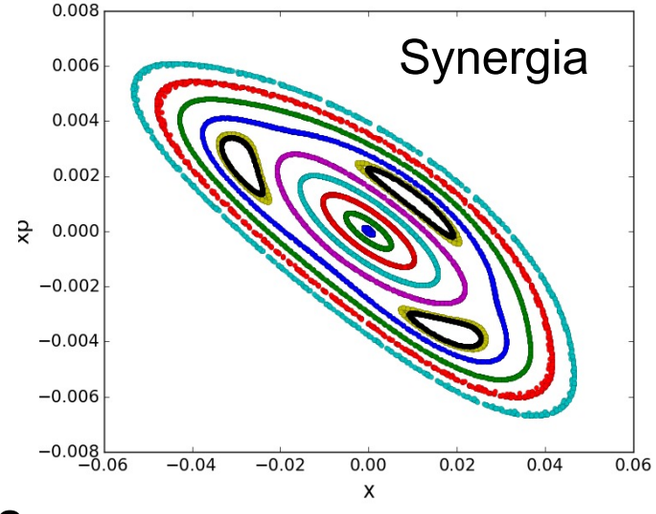
Sextupole on (with trapping)

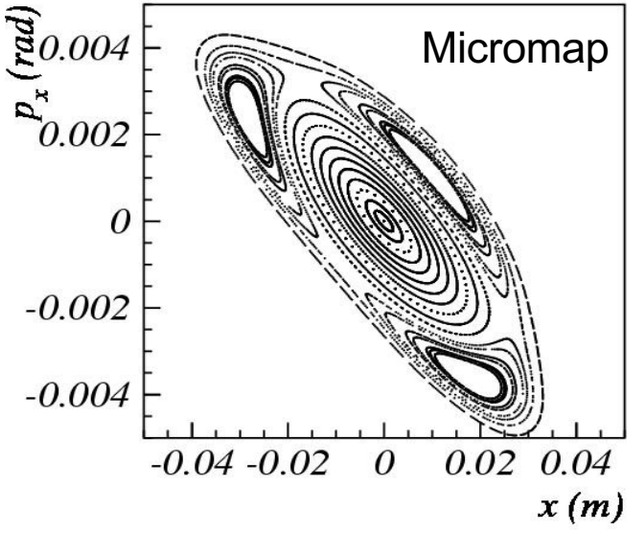


Sampling 10 initial conditions



- ImpactX simulation using 2.5D space charge (particle-in-cell)
- Poincare section of phase space over 500 turns
- Distinct colors denote distinct particle orbits

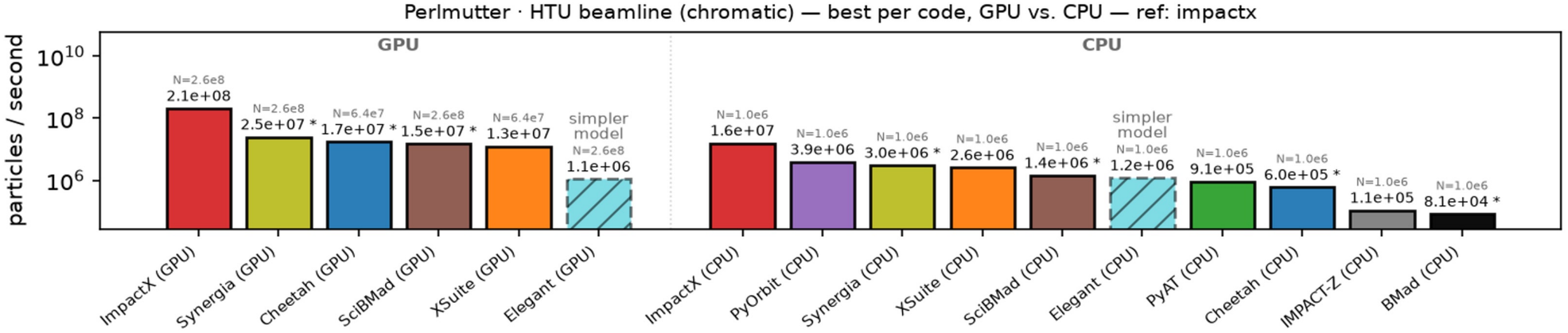




Data: **doi.org/10.5281/zenodo.22964778**

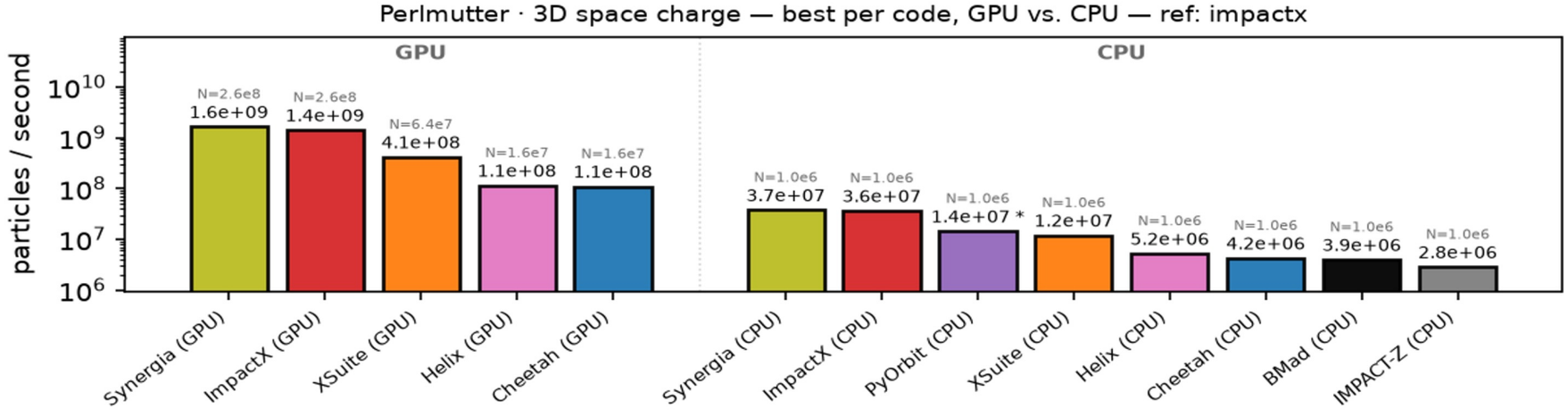
Comments on Performance Benchmarking (LLM-assisted)

Measurements here are very preliminary, please expect them to change. Higher is better.
Note the log scale: over 2000x performance difference.



Nonlinear tracking in a chromatic beamline*

*S. Barber et al, PRL 135, 055001 (2025)



Performance of a single 3D space charge kick

Optimization of Green's function calculation and caching are in progress.

Reproduce, improve, or contribute: github.com/**BLAST-ImpactX/impactx-benchmarks**

A. Huebl

Conclusions

- ImpactX is an s-based PIC code for beam dynamics modeling in linacs and rings
  - high-performance GPU successor to IMPACT-Z and Synergia (SciDAC-5 HEP)
  - strength is multi-node, multi-GPU support for high resolution space charge simulations
- Open public development, automated testing, review & documentation.
- A variety of 2D, 2.5D, and 3D space charge models is supported.
- Validation includes analytical models, community benchmarks (GSI benchmark ongoing).
- LLM agents can assist with large-scale campaigns for accuracy and performance benchmarking. These must be checked by human experts!
- Input from the community is encouraged.

Thank you for your attention!

Questions?

Contact: ChadMitchell@lbl.gov

Integrated Green's Function Approach

3D space-charge using an FFT-based Poisson solver (open boundaries):

$$\phi(\vec{r}) = \int \rho(\vec{r}')G(\vec{r}-\vec{r}')d\vec{r}' \rightarrow \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}' \quad \text{convolution integral}$$

$$\phi_{i,j,k} = h_x h_y h_z \sum_{i'=1}^{i'_{max}} \sum_{j'=1}^{j'_{max}} \sum_{k'=1}^{k'_{max}} \overline{\rho}_{i',j',k'} \overline{G}_{i-i',j-j',k-k'} \quad \text{cyclic convolution}$$

$$\phi_{i,j,k} = h_x h_y h_z \mathcal{F}^{bbb}\{(\mathcal{F}^{fff}\overline{\rho}_{i,j,k})(\mathcal{F}^{fff}\overline{G}_{i,j,k})\} \quad \text{FFT evaluation}$$

Integrated Green's function (constant basis functions):

$$\overline{G}_{i-i',j-j',k-k'} = \int_{x_{i'}-h_x/2}^{x_{i'}+h_x/2} dx' \int_{y_{i'}-h_y/2}^{y_{i'}+h_y/2} dy' \int_{z_{i'}-h_z/2}^{z_{i'}+h_z/2} dz' G(x_i - x', y_j - y', z_k - z') = F(x,y,z)|_{\text{limits}}$$

$$F(x,y,z) = -\frac{x^2}{2}\tan^{-1}\left(\frac{yz}{x\sqrt{x^2+y^2+z^2}}\right) + xy\sinh^{-1}\left(\frac{z}{\sqrt{x^2+y^2}}\right) + \text{cyclic permutations of } x,y,z$$

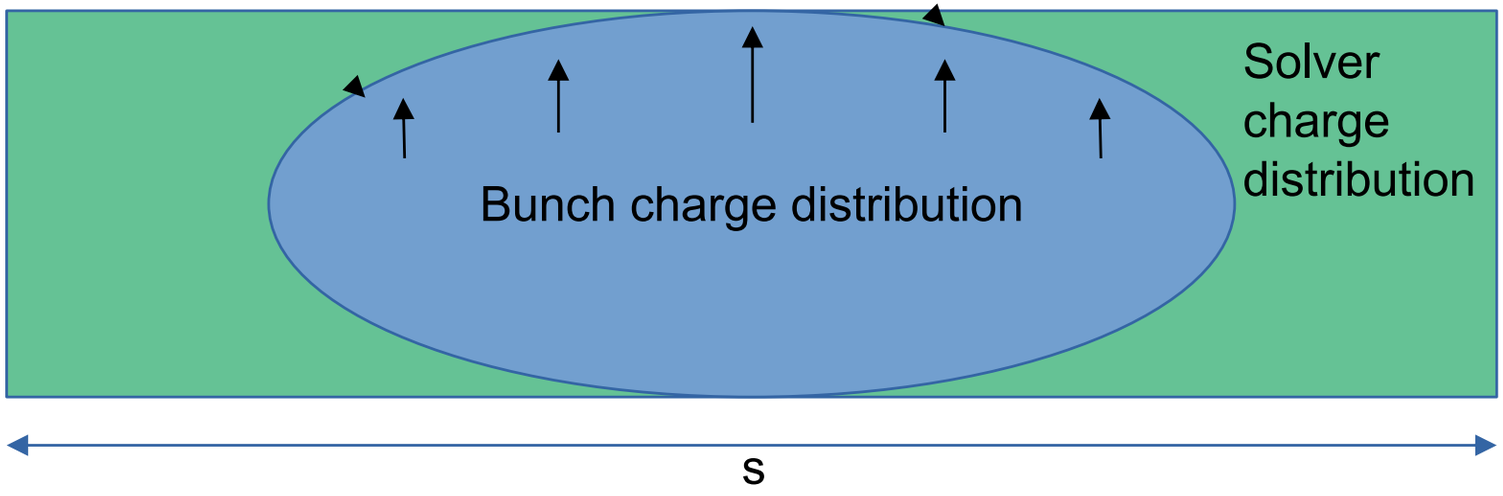
- requires resolving only the 3D charge density
- Green's function singularity is treated analytically
- large accuracy improvements for high aspect ratio beams

J. Qiang et al, Phys. Rev. ST – Accel. Beams **9**, 044204 (2006)
J. Qiang et al, J. Software Eng. and Appl. **17**, 740-749 (2024)

SciDAC Scientific Discovery through Advanced Computing

Comments on 2.5D Space Charge PIC Model

E. Stern



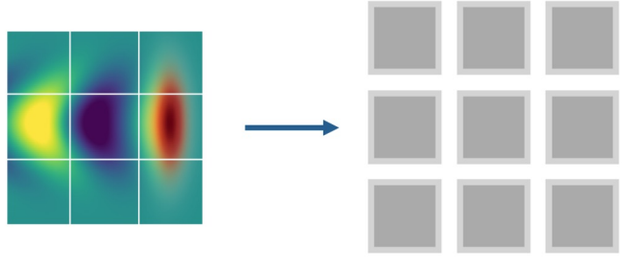
- The 2.5D PIC solver was developed for ORBIT and adopted in Synergia -> ImpactX
- The charge distribution is projected longitudinally, to obtain a 2D distribution in (x,y). A 2D IGF-based Poisson solver is used to calculate the space charge field.
- The resulting transverse momentum kicks are modulated by the longitudinal line charge density.
- A longitudinal kick based on the derivative of the longitudinal line charge density may be (optionally) applied. Note: the longitudinal kick is required by 6D symplecticity.

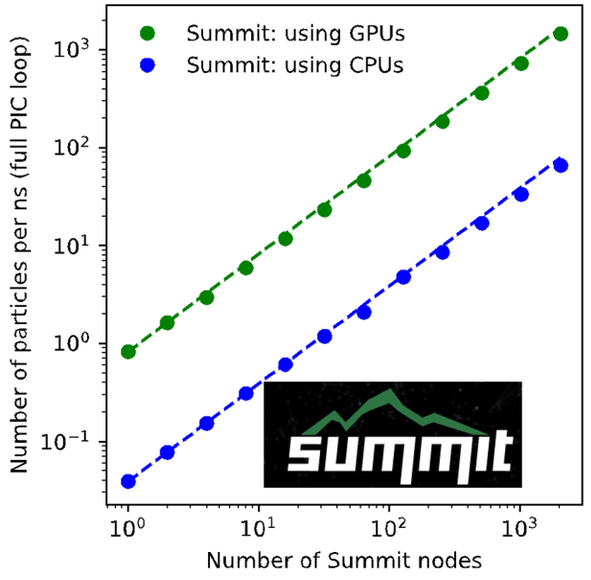
Modernizing BLAST through an Exascale Programming Model

AMReX library



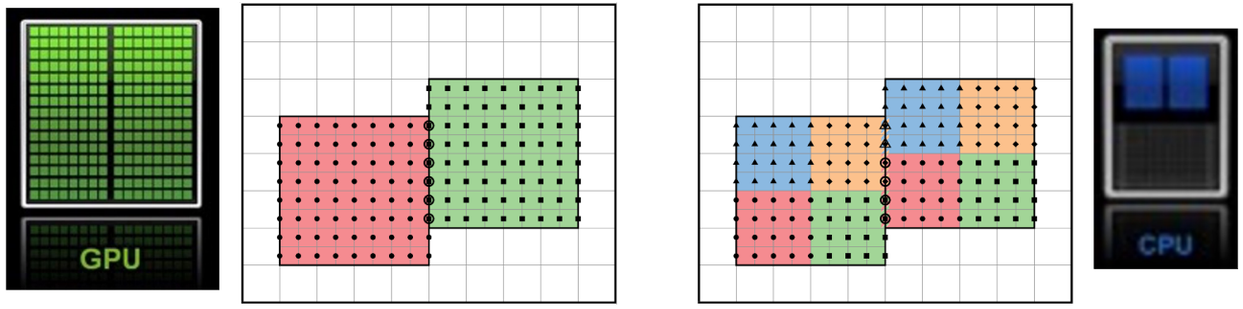
- Domain decomposition & MPI **communications:** MR & load balance





A100 gives additional ~< 2x

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



Data Structures

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

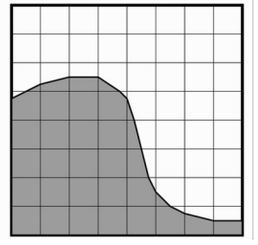
`ParallelFor(/Scan/Reduce)`

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

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

    });
```

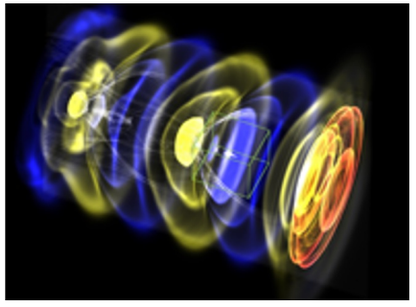
- **Parallel linear solvers** (e.g. multi-grid Poisson solvers)
- **Embedded boundaries**



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

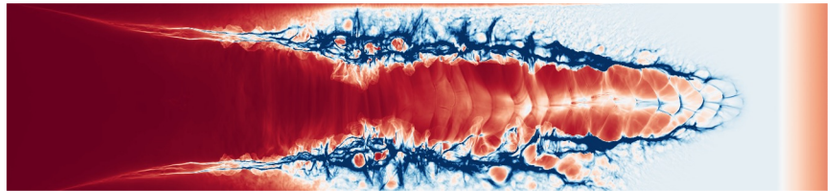
A. Myers et al., "Porting WarpX to GPU-accelerated platforms," Parallel Computing **108**, 102833 (2021)

WarpX supports a growing number of applications

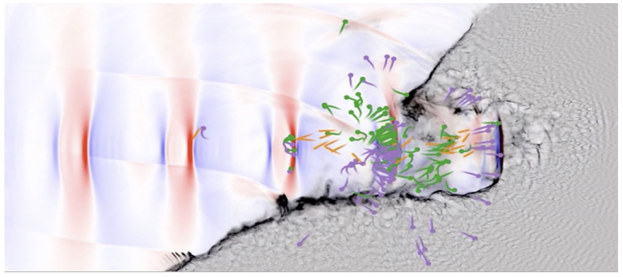


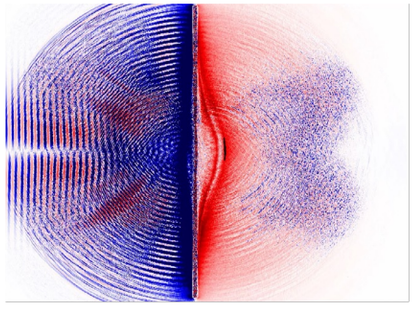
Plasma accelerators (LBNL, DESY, SLAC)

Laser-ion acceleration - advanced mechanisms (LBNL)



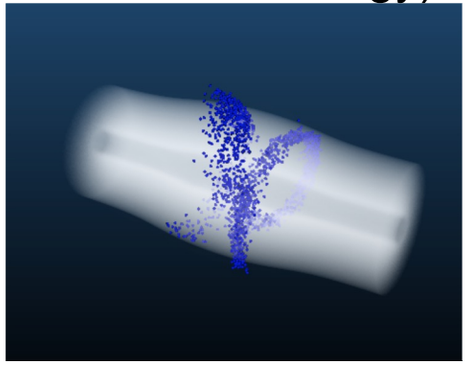
Plasma mirrors and high-field physics + QED (CEA Saclay/LBNL)



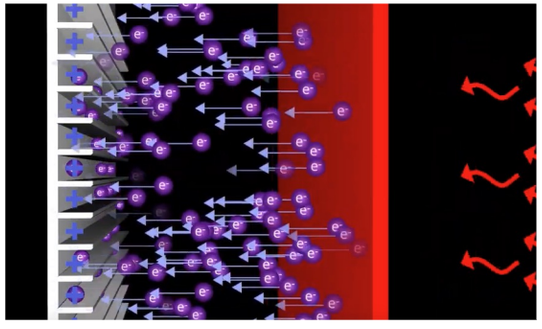


Laser-ion acceleration - laser pulse shaping (LLNL)

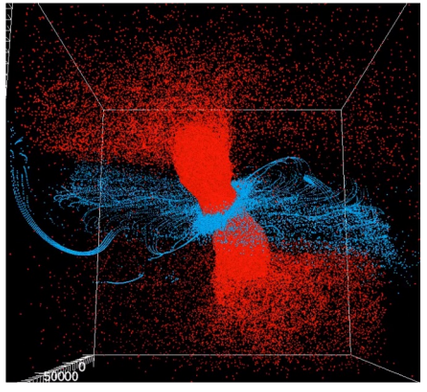
Plasma confinement, fusion devices (Zap Energy, Avalanche Energy)



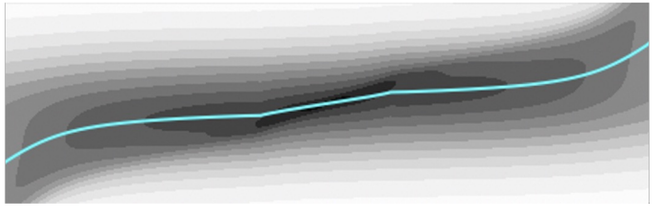
Thermionic converter (Modern Electron)



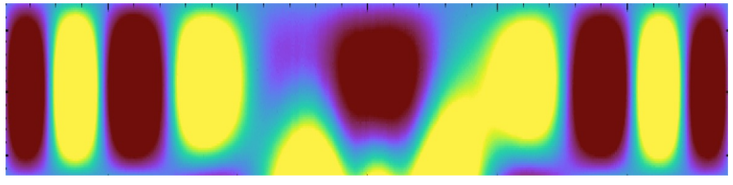
Pulsars, magnetic reconnection (LBNL)

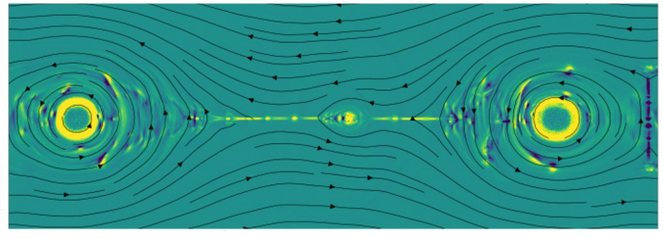


Magnetic fusion sheaths (LLNL)



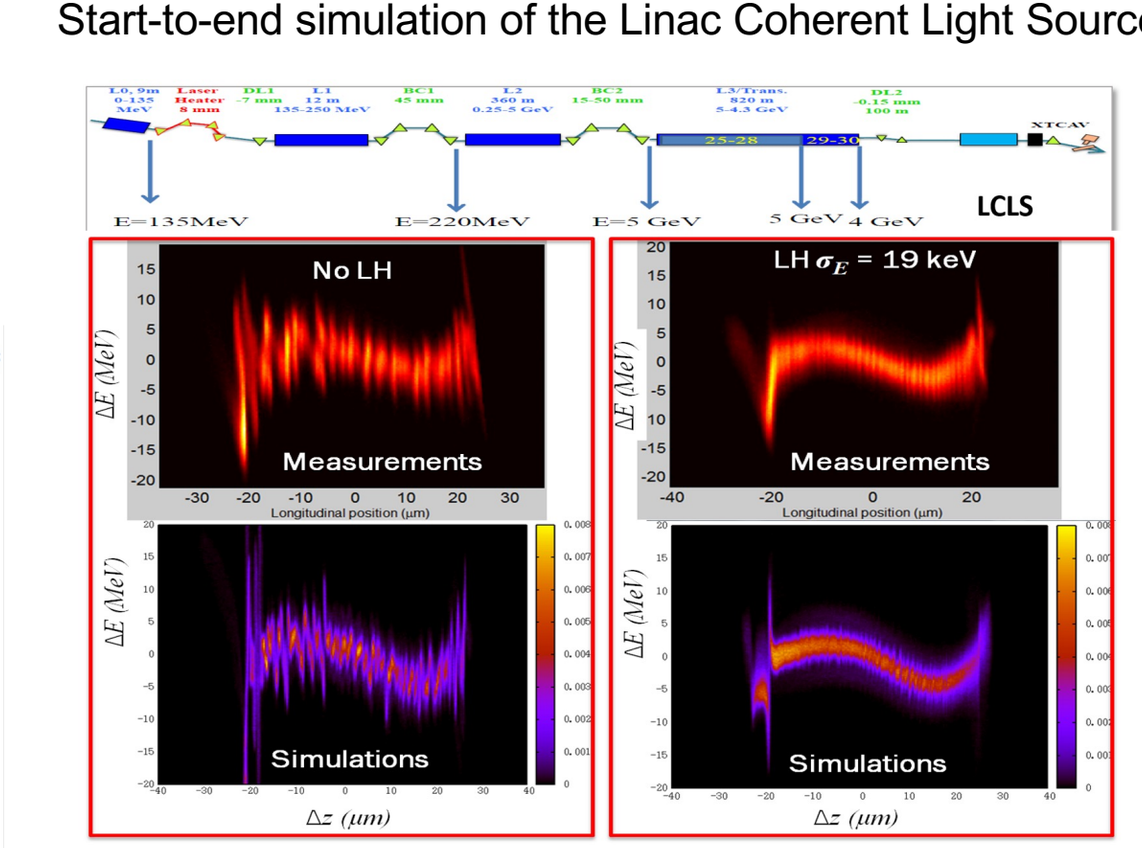
Microelectronics (LBNL) - ARTEMIS





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*



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

Courtesy of J. Qiang

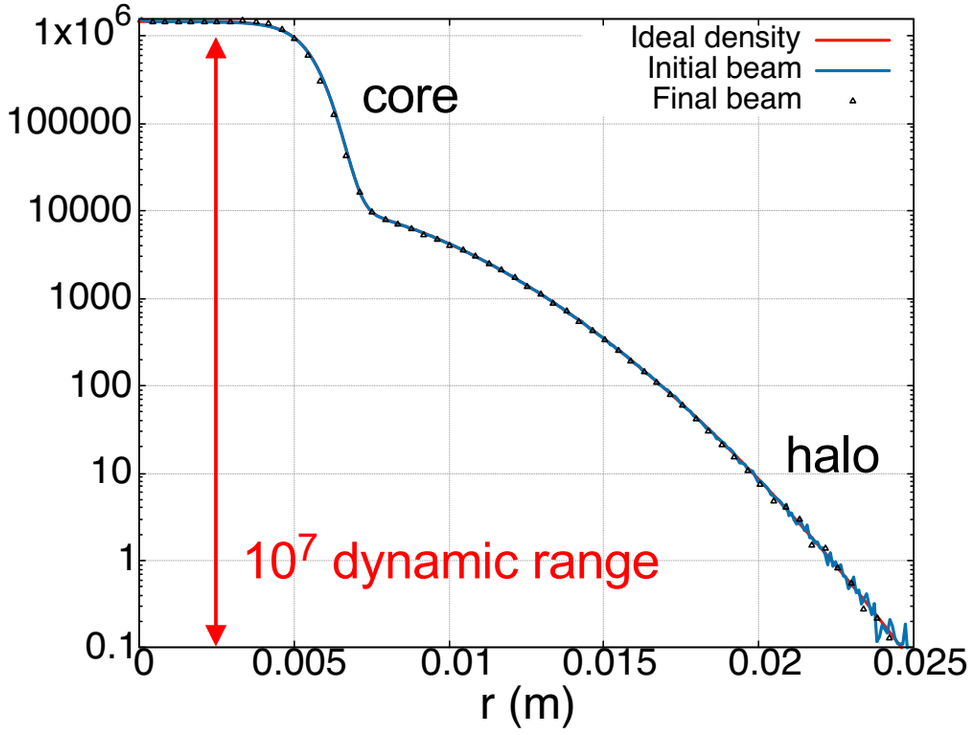
ImpactX 3D Space Charge Validation: bithermal beam in a CF channel

- 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
- $kT_1 = 36{\times}10^{-6}$, $kT_2 = 900{\times}10^{-6}$
- 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)

Data: **doi.org/10.5281/zenodo.8395849**

Overview

- BLAST tools and ImpactX
- Space charge models and validation
- GSI space charge benchmark
- Comments on HPC performance
- Summary and conclusions