Simulations of Next-Generation Colliders

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multi-stage LPA simulation in a boosted frame with WarpX *transversely focusing fields & beam*

Lisbon, March 19-22, 2024 5th ALEGRO (Advanced LinEar collider study GROup) Workshop



ACCELERATOR TECHNOLOGY & ATAP



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Simulations of Next-Generation Colliders



Algorithmic Options

From first principles to effective approximations and data models

Ecosystem of Simulation Codes

Collaboration for Advanced Modeling of Particle Accelerators

Modeling Staging: Levels of Realism

Number of stages modeled, plasma ramps, propagation & transport, more realistic beams, ...

Algorithmic Options From first principles to effective approximations and data models

General Algorithmic Choices



e.g., initial designs, optimization & operations

e.g., RZ geometry, quasi- and electro-static approximation, fluid background

e.g., stability proofs, exploration, ML training data

This requires an **ecosystem of models** ⇒ share models & data between codes ⇒ works best when standardized

Algorithmic Options for Modeling Plasma Sources



Algorithmic Options for Modeling Plasma Sources



Algorithmic Options for Modeling Plasma Stages



P5 Report: Exploring the Quantum Universe (2023); AGR Thomas and D Seipt, PRAB 24, 104602 (2021); B Foster et al., NJP 25,093037 (2023) Schroeder et al., PRSTAB (2010); Schroeder et al., NIMA (2016); Benedetti et al., arXiv:2203.08366 (2022); Schroeder et al., JINST (2023)

Algorithmic Options for Modeling Transport Between Stages



• space charge for >100pC charge

CA Lindstrom and E Adli, PRAB 19, 071002 (2016) A Huebl et al., NAPAC'22, DOI:10.18429/JACoW-NAPAC2022-TUYE2 (2022); A Huebl et al., AAC'22, in print, arXiv:2303.12873 (2022)

Algorithmic Options for the Interaction Point



Physics at Play

- disruption & beamstrahlung
- pair generation
- self-consistent pair plasmas
- hadron production
- crossing angles



Algorithmic Options for the Interaction Point

Source

Staging of ~800 elements

>10 TeV IP

Staging of ~800 elements

Source



Physics at Play

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Snowmass21: Beam-Beam Crossing Underexplored

- There is long-standing skepticism that such a machine is possible:
 - E.g., for e-/e+: "It is concluded that in the energy regime approaching 10 TeV the present single pass linear collider will probably be unsatisfactory due to high backgrounds, excessive power demand or both." [1]
- A Beam-Beam Collaboration has formed motivated by design and simulation needs for a future 10 TeV pCM wakefield collider, as recommended in the 2023 P5 report
 - T. Barklow, S. Gessner, M. Hogan, C.-K. Ng, D. Ntounis, M. Peskin, T. Raubenheimer, C. Vernieri, R. Watt (SLAC) S. Bulanov, A. Formenti, R. Lehe, C. Schroeder, J.-L. Vay (LBNL)
 W. Nguyen (Imperial College) L. Fedeli, H. Vincenti (CEA Saclay) G. Jiawei Cao, C. A. Lindstrøm (U. Oslo) L. Gray (CERN)

The goals for this collaboration include:

- Understand the limitations of particle collisions at large beamstrahlung parameter.
- Develop simulation tools that can accurately model these collisions.
- Explore methods for suppressing (or embracing) beamstrahlung to enable high luminosity-per-power linear colliders.

P5 Report: Exploring the Quantum Universe (2023)

Barklow et al., JINST 18 P09022 (2023) D0I:10.1088/1748-0221/18/09/P09022; [1] M Tigner, AIP Conf. Proc. 279, 1-15 (1992) D0I:10.1063

Algorithmic Options for Modeling the Whole Collider



Connections

- Record e⁻ and e⁺ beams (and fields if transition within a stage) histories at a given location.
- Inject beams in next simulation; if within a stage, inject fields using a virtual antenna.

A Huebl et al., openPMD, DOI:10.5281/zenodo.591699 (2015); DP Grote et al., Particle-In-Cell Modeling Interface (PICMI) (2021); M. Thévenet et al., LASY: an open-source Python library for easy interfacing of laser pulses between experiments and simulations, EAAC23, under review (2023)

forming open governance



Developed by an international, multidisciplinary team







WarpX is a GPU-Accelerated PIC Code for Exascale



Multiple Particle-in-Cell Loops

• electromagnetic or -static (time integration)



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, secondary emission

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Geometries

 1D3V, 2D3V, 3D3V and RZ (quasicylindrical)





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

- PICMI input
- openPMD (HDF5 or ADIOS)
- in situ: diagnostics & Python APIs





L Fedeli, A Huebl et al., SC22, ACM Gordon Bell Prize Winner (2022)

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

Particle-in-Cell Loop

- electrostatic
 - with space-charge effects
- s-based
 - relative to a reference particle Ο
 - elements: symplectic maps Ο



Fireproof Numerics

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

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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

Multi-Node parallelization

- MPI: domain decomposition ٠
- dynamic load balancing (in dev.)

On-Node Parallelization

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





Scalable & Standardized

- openPMD (HDF5 or ADIOS)
- in situ: diagnostics & Python APIs





A Huebl et al., NAPAC22 (2022)

CAMPA Collaboration for Advanced Modeling of Particle Accelerators

Collaboration for Advanced Modeling of Particle Accelerators





CAMPA is to boost accelerator research & designs

Overarching purpose of CAMPA: accelerate and expand the scope of discoveries from high energy physics (HEP) particle accelerators by enabling the design of accelerators that are significantly more compact and cheaper to build and run



RF cavities in metallic vacuum tubegradient constrained by breakdown< 100 MV

Emphasis: design of advanced plasma-based colliders and the conventional accelerators in the Fermilab complex, enabling DUNE to access previously unreachable parameters of the Standard Model neutrino sector

Main goals:

(i) develop **HPC accelerator & beam modeling capabilities** to **design the full range** of systems required

(ii) develop **community simulation ecosystems** that seamlessly **integrate accelerator elements** to facilitate the **design and control** of the next-generation of particle accelerators

Very synergistic with ALEGRO

Community Accelerator Simulations Ecosystem (CASE)



A Huebl et al., DOI:10.5281/zenodo.591699 (2015); DP Grote et al., Particle-In-Cell Modeling Interface (PICMI) (2021); LD Amorim et al., GPos (2021); M Thévenet et al., EAAC23, arXiv:2403.12191 (2023); A Ferran Pousa et al., DOI:10.5281/zenodo.7989119 (2023); RT Sandberg et al., IPAC23, DOI:10.18429/JACoW-IPAC-23-WEPA101 (2023)

PICMI enables (90%) same input script with different codes



Modeling Staging: Levels of Realism number of stages modeled, plasma ramps, propagation & transport, realistic beams, ...

Systematically Increasing the Realism for Start-to-End Modeling

Start-to-End Physics Goals

The HEP community expects us to prove our machines in high-fidelity modeling **robust start-to-end designs**.

- Maximize energy gain & conserve charge transport
 - o plasma profile/channel design
 - o matching into plasma stages
 - o transverse beam stability
- Minimize energy spread
 - Requires flattening of wakefield over LPA length
 → bunch current profile
- Minimize Emittance growth, e.g.,
 - low phase mixing from energy-spread + betatron motion,
 - o controlled beam expansion at plasma exit
 - o reduce collision with background plasma, ...
- Compactness and energy efficiency
 - What is the best transport on a realistic length
 scale that allows for beam exit, coupling in a new laser pulse, beam matching to a new stage
- Robustness: realistic fluctuations & uncertainties in ops.

Modeling Capability & Workflow Needs

The community started with **exploratory LPA elements**, it is time to expand and model their interplay with and operation in beamlines that are **available now and in the next decade**.

- **Codes**: start w/ speed, then proof in high fidelity
- Exploration and **optimization workflows**: parameters can depend on previous stage
 - Single stage design
 - o Transport design
 - o Multi-stage design

ptimas

- ⇒ reproduce, automate & repeat, memorize (ML), abstract away
- Systematically removing idealizations
 - o laser profiles & coupling,
 - o realistic beam (charge, profile, spreads),
 - o transport distances, ...

LASY____

P5 Report: Exploring the Quantum Universe (2023); AGR Thomas and D Seipt, PRAB 24, 104602 (2021); M Thévenet et al., EAAC23, arXiv:2403.12191 (2023); Schroeder et al., PRSTAB (2010); Schroeder et al., NIMA (2016); Benedetti et al., arXiv:2203.08366 (2022); Schroeder et al., JINST (2023)

Level of Realism: 3 multi-GeV Stages Modeled in 3D





Movie from boosted frame data. Aspect ratio different from lab.

Focus was on numerics: performance, numerical convergence, etc.

WarpX

Focus was not on science, e.g., emittance preservation ⇒ some tuning of plasma lens amplitude performed but not optimized.

Video: M Thévent et al. (2019); J-L Vay et al., EAAC2019 (2019); J-L Vay, A Huebl et al., Phys. Plasmas 28, 023105 (2021) DOI:10.1063/5.0028512

Level of Realism: 50 multi-GeV Stages Modeled in 3D



Emittance Preservation for Plasma-Vacuum Coupling



Emittance Preservation for Plasma-Vacuum Coupling

Source

>10 TeV IP

Staging of ~800 elements

Source

Optimized Emittance: Stages at GeV...TeV Range

E ₀	1 GeV	10 GeV	100 GeV	1 TeV	10 TeV
Δείε	0.3%	3.0%	0.4%	1e-6	1e-6
Δε/ε (10 pC & 0.5% ΔΕ/Ε ₀)	0.5%	3.6%	1.3%	0.1%	0.2%

Betatron wavelength



P. Antici et al., JAP (2012) M. Migliorati et al., PRAB (2013)



Appropriate length scale increases with energy but emittance growth is also reduced

According to this preliminary RZ study, if we controllably expand the beam in the plasma ramp, adiabatic matching

of the ramps L~ \sqrt{y} might not be needed!

Density Ramps: Next Steps

- Redo scans with beam loading (100s of pC)
- Reproduce emittance preservation in high fidelity (3D WarpX)
- Try other optimizers to explore minima

Associated Challenges

- Current profiles for flattened wakefield require additional optimization for every stage
- 3D simulations demand more resources (model ion motion \rightarrow suppress hosing for high-charge, low-emittance beams)



Emittance growth from chromaticity in drifts:

Modeling of Propagation & Transport

ML boosted: for a *specific* problem



- start-to-end collider modeling
- digital twin / 'real-time'

Model Speed: for accelerator elements



Simulation time: full geometry, full physics

5 hrs	<sec< th=""></sec<>
256 GPUs	1 GPU



RT Sandberg et al. and A Huebl, *accepted to PASC24*, arXiv:2402.17248 (2024) RT Sandberg et al and A Huebl, IPAC23, DOI:10.18429/JACoW-IPAC-23-WEPA101 (2023)

We Trained a Neural Net with WarpX for Staging of Electrons



Training time: 2-2.2 hrs on 1 GPU

WarpX

RT Sandberg et al and A Huebl, IPAC23, DOI:10.18429/JACoW-IPAC-23-WEPA101 (2023)

Modeling + ML Inference are Fully GPU Accelerated



	stage 1	stage 2	stage 15
σ _x	0.12%	1.8%	3.2%
σ _{px}	0.54%	2.1%	2.8%
٤ _x	0.43%	0.38%	0.39%
σ _y	0.03%	1.5%	1.2%
$\sigma_{_{py}}$	0.3%	1.9%	3.2%
ε _y	0.3%	0.44%	2.1%

ImpactX

Training data: 1M particles / beam Training time: 2-2.2 hrs on 1 GPU

RT Sandberg et al. and A Huebl, *accepted to PASC24*, arXiv:2402.17248 (2024) RT Sandberg et al and A Huebl, IPAC23, DOI:10.18429/JACoW-IPAC-23-WEPA101 (2023)



15th stage, ct=4.62e+00

Modeling + ML Inference are Fully GPU Accelerated



Modeling + ML Inference: Rapid Start-to-End Optimization



Rapid Start-to-End Optimization for Transport Design



GPU inference time: 63ns / particle / stage ImpactX tracking >1M particles



RT Sandberg et al. and A Huebl, *accepted to PASC24*, arXiv:2402.17248 (2024) RT Sandberg et al and A Huebl, IPAC23, DOI:10.18429/JACoW-IPAC-23-WEPA101 (2023) 30

Modeling + ML Inference: Enables Complex Transport Design Studies



Tune Calculation in a Periodic FODO Channel

github.com/ECP-WarpX/impactx

CA Lindstrøm and E Adli, PRAB 19, 071002 (2016); A Huebl et al., NAPAC'22, DOI:10.184 29/JACoW-NAPAC2022-TUYE2 (2022); A Huebl et al., AAC'22, in print, arXiv:2303.12873 (2022); RT Sandberg et al. and A Huebl, accepted to PASC24, arXiv:2402.17248 (2024)

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Source

Model Level of Realism: Benchmarking Interaction Point Physics



Summary

Source

Staging of ~800 elements

>10 TeV IP

Staging of ~800 elements

Source

Algorithmic Options

- particle-in-cell codes for plasma and transport
- Different levels of fidelity for different purposes: initial design, exploration, stability & scalability proof, start-to-end design, ...

Community Ecosystems

- Modeling must go through all stages of demonstration, reduced to high-fidelity, so our designs can be taken seriously by the HEP community.
- **Compatibility** (data/input) between codes is important: benchmarks & rapid collider design iterations are needed!

Levels of Realism for Staging

- Progress: 3D (50 stages, TeV level), need 10x for new CoM goals Good e- progress, more optimization & realism potential
- Transport designs: active can we find compact solutions?
- IP & sources: use Exascale codes exploration ongoing

Start-to-End: Community Codes

- Developed openly, well-documented, standardized
- Feature-rich: many algorithms •
- Continuously benchmarked
- GPU-accelerated options (Nvidia/AMD/Intel)
- Scalable: desktop study to HPC

github.com/ECP-WarpX github.com/Hi-PACE github.com/openPMD www.openPMD.org github.com/AMReX-Codes github.com/picmi-standard github.com/UCLA-Plasma-Simulation-Group github.com/fnalacceleratormodeling





Contacts & Funding Acknowledgements

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