# Open-source simulation ecosystem for laptop to Exascale modeling of high-gradient accelerators

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Expert Panel on High-Gradient Accelerator (Plasma/Laser) Townhall - May 31, 2021

BERKELEY LAB
ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION ATAP
U.S. DEPARTMENT OF ENERGY | Office of Science

# The *BLAST* suite offers a large set of open-source codes


## State-of-the-art simulation tools*:

- ***Multi-physics frameworks:*** IMPACT, Warp, WarpX.
- ***Specialized codes:*** BeamBeam3D, FBPIC, HiPACE++.
- ***Libraries & standards:*** PICSAR, openPMD, PICMI.

## Multiphysics:

- beams, plasmas, lasers, structures, beam-beam, $e^-$ clouds, …
- plasma/dielectric accelerators, linacs, rings, injectors, traps, …

## At the forefront of computing:

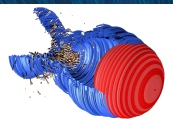
- ***Novel algorithms:*** boosted frame, spectral Maxwell solvers, …
- ***Supercomputing:*** Exascale, CPUs & GPUs.
- ***Advanced designs:*** genetic or ML (e.g., Bayesian) optimization

## Expanding applications, contributors

- Major contributors: LBNL, CEA, CERN, DESY, HZDR, LLNL, Radiasoft, UHH

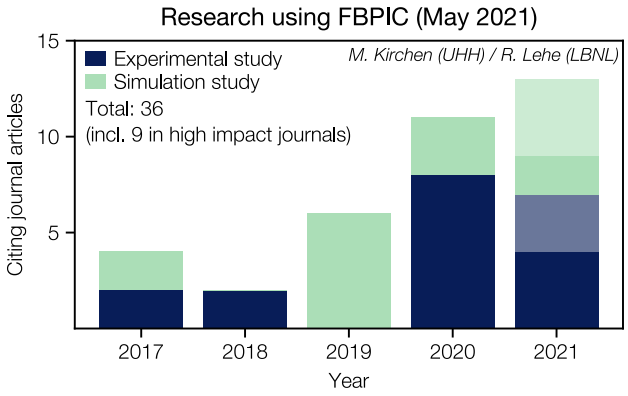
# BLAST flagship full PIC codes for plasma acceleration

## FBPIC

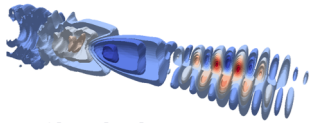


- **Geometry:** RZ + azimuthal decomp.
- **Languages:** Python (+numba)
- **Platforms:** CPUs, GPUs
- **Maxwell solvers:** PSATD, PSATD-Galilean
- **Grid:** static, moving window, boosted frame
- **Other physics:** ADK ionization, Compton emission

FBPIC is a very easy-to-use specialized code that is growing in popularity




## WarpX



- **Geometry:** 3D, 2D, RZ + azimuthal decomp.
- **Languages:** C++ (optional Python frontend)
- **Platforms:** CPUs, GPUs
- **Maxwell solvers:** FDTD, PSATD, PSATD-Galilean, PSATD-time averaged
- **Grid:** static, moving window, boosted frame, mesh refinement*
- **Other physics:** ADK ionization, QED, Coulomb collisions, embedded boundaries*
- **Other numerics:** dynamic load balancing

WarpX is a general purpose multiphysics (still easy-to-use) high-performance code

*in development

# WarpX: Multidisciplinary Multi-institutions Development Team
## physicists + applied mathematicians + computer scientists

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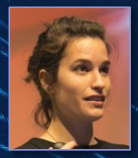
NNSA

ECP EXASCALE COMPUTING PROJECT

ATAP ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION

BERKELEY LAB


Jean-Luc Vay (PI)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Maxence Thévenet

DESY

DESY (Germany)


Marc Hogan (coPI)


Lixin Ge


Cho Ng

SLAC


Lorenzo Giacomel

CERN

CERN (Switzerland)

# Timeline for Exascale project WarpX

## From initial code coupling to ensemble of chains of multi GeV-scale stages

2030 - Collider designs

Modeling of chain of 50-100 multi-GeV-scale plasma accelerator stages 2023

Frontier (ORNL)
Aurora (ANL)
>1 ExaFlops

Modeling chain of 20-50 multi-GeV-scale plasma accelerator stages 2022

Modeling chain of 10-20 multi-GeV-scale plasma accelerator stages 2021

Now

Modeling chain of 5-10 multi-GeV-scale plasma accelerator stages 2020

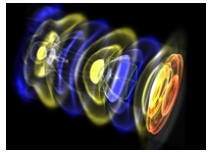
2019 Modeling chain of 3 multi-GeV-scale plasma accelerator stages

All C++
Port to GPUs.

2018 Modeling a single multi-GeV-scale plasma accelerator stage

Open source release to community.

2017 Modeling of single plasma accelerator stage with static mesh refinement



2016 Initial coupling of AMReX and Warp/PICSAR

# WarpX one of the very first codes on newest DOE supercomputer Perlmutter

Recording

Snapshot from inauguration via Zoom May 27, 2021

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# Development of high-gradient accelerators needs from ultrafast to very precise modeling tools

Great for ensemble runs for design studies


Many codes exist in the community that can fill the space. But there may be:

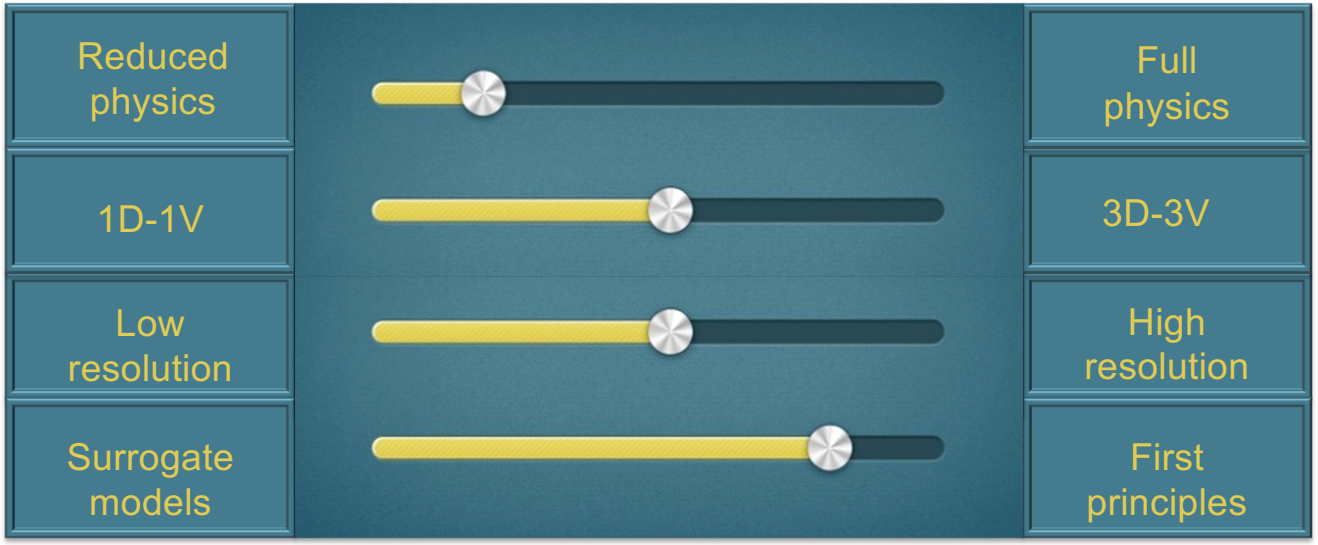
- Clustering with overlaps (aka duplication)
- Gaps (e.g., AI/ML)
- Need to change input scripts and data analysis for each code


Great for detailed runs for physics studies

➔ Need for development of integrated ecosystem of codes:

# Ultimate goal would be an integrated ecosystem that offers on-the-fly tunability of physics & numerics complexity to users

Great for ensemble runs for design studies




Great for detailed runs for physics studies

Consortium for Advanced Modeling of Particle Accelerators CAMPA

BERKELEY LAB SLAC Fermilab UCLA

DOE HEP GARD

Lawrence Livermore National Laboratory radiasoft TECH-X

Particle-In-Cell Modeling Interface

picmi Standard

Code A

Code B

...

open Particle Mesh Data standard

openPMD

HZDR BERKELEY LAB TECHNISCHE UNIVERSITÄT DRESDEN EUCALL Lawrence Livermore National Laboratory SLAC DESY UHH European XFEL UCLA ioq JENA CBG Fermilab OAK RIDGE plasmapy

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# Questions for the community – part 1

What is the role of your work here?

- Community support in theory and modeling
- Includes development, maintenance, distribution, support, training and usage of advanced simulation codes

What are the important milestones for the next 10 years to get there from today?

- Modeling of increasingly long chain of high-gradient stages toward readiness for conceptual design ~ 2030+

What additional support is needed to achieve these?

- Sustained support to teams of computational physicists + applied mathematicians + software engineers to develop, maintain, distribute, support, train & use core ecosystem of codes & novel algorithms
- Additional support is needed to (i) help transition codes to GPUs and future computing platforms, (ii) AI/ML

What should be proposed as deliverables until 2026?

- Faster, user-friendly codes running on GPUs and future platforms; ultrafast AI/ML surrogate models
- Development & adoption of standards for input scripts (e.g., PICMI) and output data (e.g., openPMD)
- Tunable ecosystem for ultrafast (reduced physics/1D/low resolution/surrogate) to detailed (full physics/3D/high res./first principles) modeling

# Questions for the community – part 2

Is the R&D work for each of those deliverables already funded and, if not, what additional resources / support would be needed?

- DOE Exascale Computing Project founds WarpX; ends in 2023. Follow-on funding not defined yet
- openPMD, PICMI supported by DOE HEP CAMPA but level of funding is modest and renewed yearly; many voluntary contributions by the community that could be funded together

Is a completely new ~~facility~~ code needed?

- Probably not but PIC codes tend to sprout like mushrooms, so new codes are likely

Are additional structures needed beyond existing networks and projects, e.g. a design study for a collider or an advanced accelerator stage?

- Advocating for (i) teams that include software engineers with (ii) better coordination of codes development to contain excessive duplication and foster interoperability and still (iii) foster creativity (e.g., novel algorithms) is needed
- Whether additional structures are needed is unclear. Existing structures to coordinate codes development, e.g., CAMPA, could be strengthened and grow

# Thank you for your attention