

Our Road to Exascale:

Particle Accelerator & Laser-Plasma Modeling



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On behalf of the WarpX team (lead: J-L Vay @ LBNL)
LBNL, LLNL, SLAC

+ contributors external to ECP from labs,
universities & industry in USA, Europe & Asia

Webinar Series on Best Practices for
HPC Software Developers

virtual
March 15th, 2023



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Outline

- **Intro** - particle accelerator modeling
- **Then (<2016)** - Warp
- **The journey** - from Warp to WarpX (2016-2023)
- **Now (2023+)** - WarpX + ecosystem
- **Conclusion**

Particle Accelerators are Essential Tools in Modern Life

Medicine



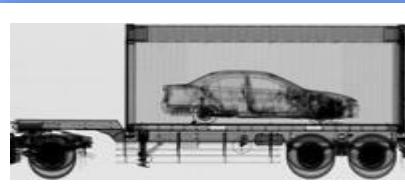
- ~9,000 medical accelerators in operation worldwide
- 10's of millions of patients treated/yr
- 50 medical isotopes, routinely produced with accelerators

Industry



- ~20,000 industrial accelerators in use
 - Semiconductor manufacturing
 - cross-linking/ polymerization
 - Sterilization/ irradiation
 - Welding/cutting
- Annual value of all products that use accel. Tech.: \$500B

National Security



- Cargo scanning
- Active interrogation
- **Stockpile stewardship:** materials characterization, radiography, support of non-proliferation

Discovery Science



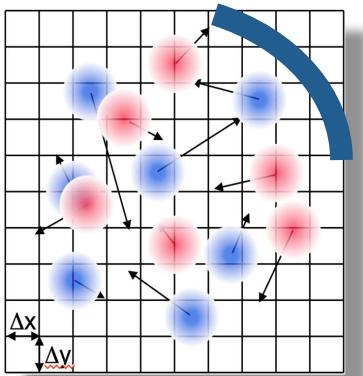
- ~30% of Nobel Prizes in Physics since 1939 enabled by accelerators
- 4 of last 14 Nobel Prizes in Chemistry for research utilizing accelerator facilities

Opportunity for much bigger impact by reducing size and cost.

Modeling: Exploration → Understanding → Design

The Modeling of Particle Accelerators is Very Complex

Macroparticles Surfaces



electromagnetic (EM)
fields on a grid

Involves the modeling of the intricate interactions of

- **relativistic particles:** beams, plasmas, halo, stray electrons
- **EM fields:** accelerating/focusing fields, beam self-fields, laser/plasma fields
- **structures:** metals, dielectrics.

Typical computer representations:

- **particles:** macroparticles representing each 1- 10^6 particles
- **fields:** electromagnetic, on a grid
- **structures:** surfaces interacting with grid and macroparticles

Many space and time scales to cover:

- from **μm** (e.g., plasma structures, e⁻-surface interactions) to **km** (e.g., LHC)
- from **ns** (beam passing one element) to **seconds or more** (beam lifetime)

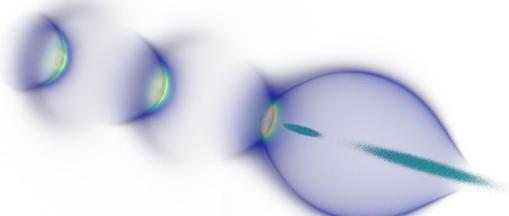
⇒ **needs best algorithms on largest & fastest computers**

AMP has pioneered algorithms to cut on

- # of meshes: adaptive mesh refinement for beams & plasmas¹
- # of time steps: Lorentz boosted frame method²

¹ J.-L. Vay *et al*, *Phys. Plasmas* **11**, 2928 (2004)

² J.-L. Vay, *Phys. Rev. Lett.* **98**, 130405 (2007)



All Accelerators in the World Rely on Modeling and Increasingly on *High-Performance Computing (HPC)*

HEP Accelerator and Beam Physics Grand Challenges*

#1 beam intensity: Increase beam intensities by orders of magnitude.

⇒ increase # of particles by orders of magnitude.

#2 beam quality: Increase beam phase-space density by orders of magnitude

**Next generation of accelerators needs
next generation of HPC modeling tools!**

#3 b

⇒ simulate all the particles.

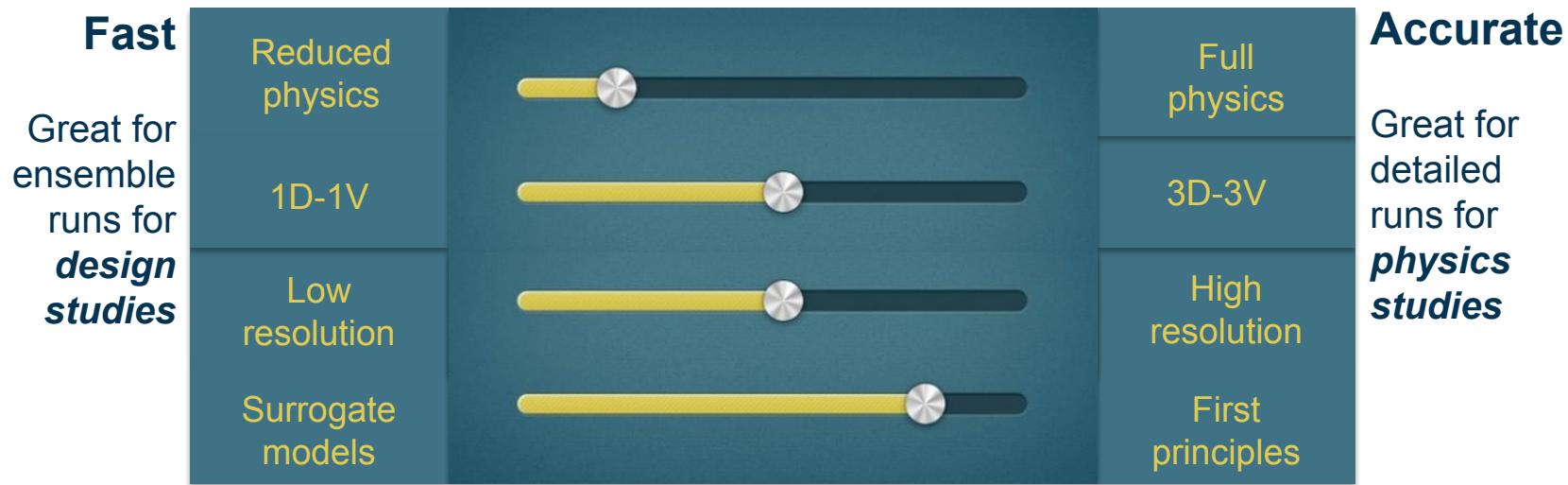
#4 beam prediction: Develop predictive “virtual particle accelerators”?

⇒ simulate everything: all the particles, conductors,
dark currents, many turns, ...

*S. Nagaitsev et al., “Accelerator and Beam Physics: Grand Challenges and Research Opportunities,” Snowmass 2021 LOI



Ultimate goal: virtual accelerator with *on-the-fly tunability* of physics & numerics complexity to users



Mean toward goal
Open software ecosystem with tunable physics & numerics

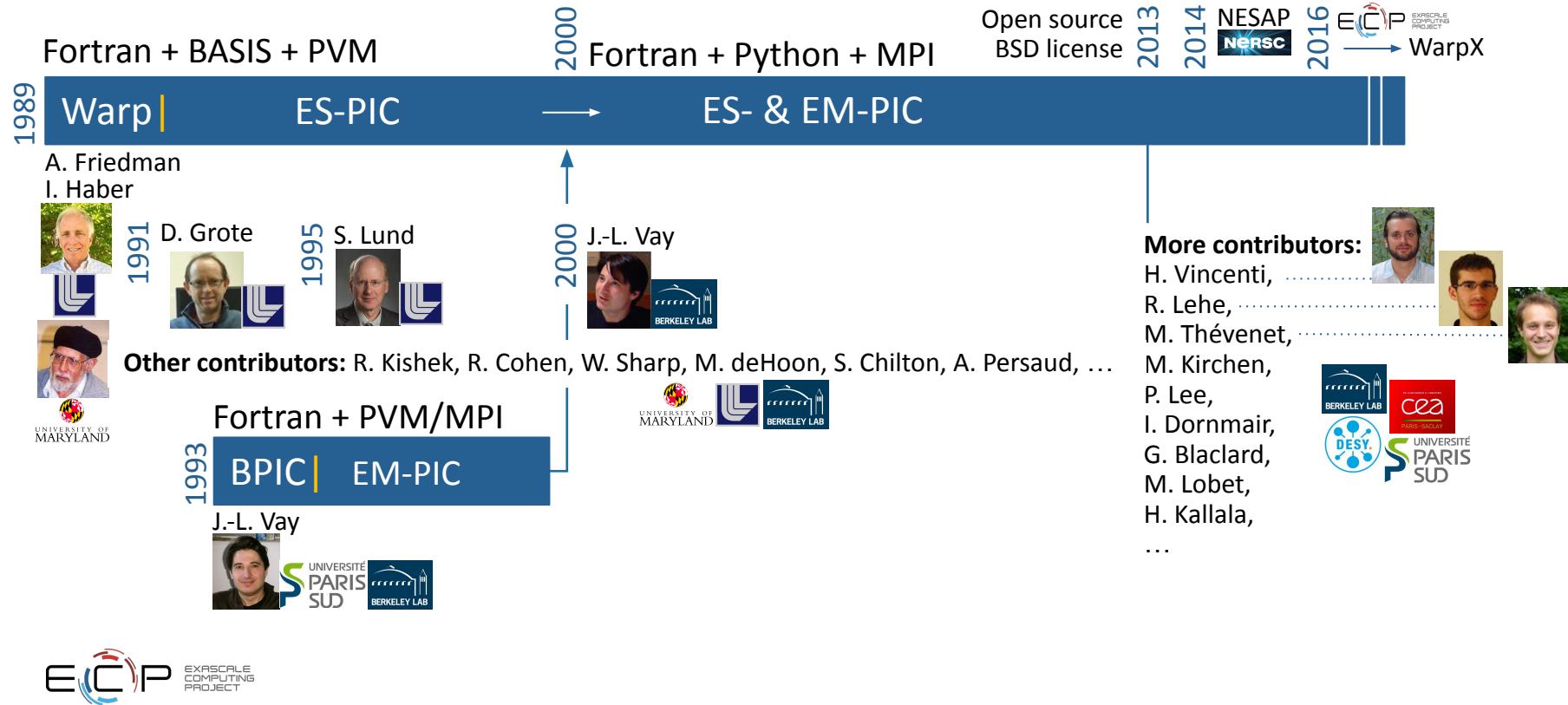


Start-to-End Modeling R&D

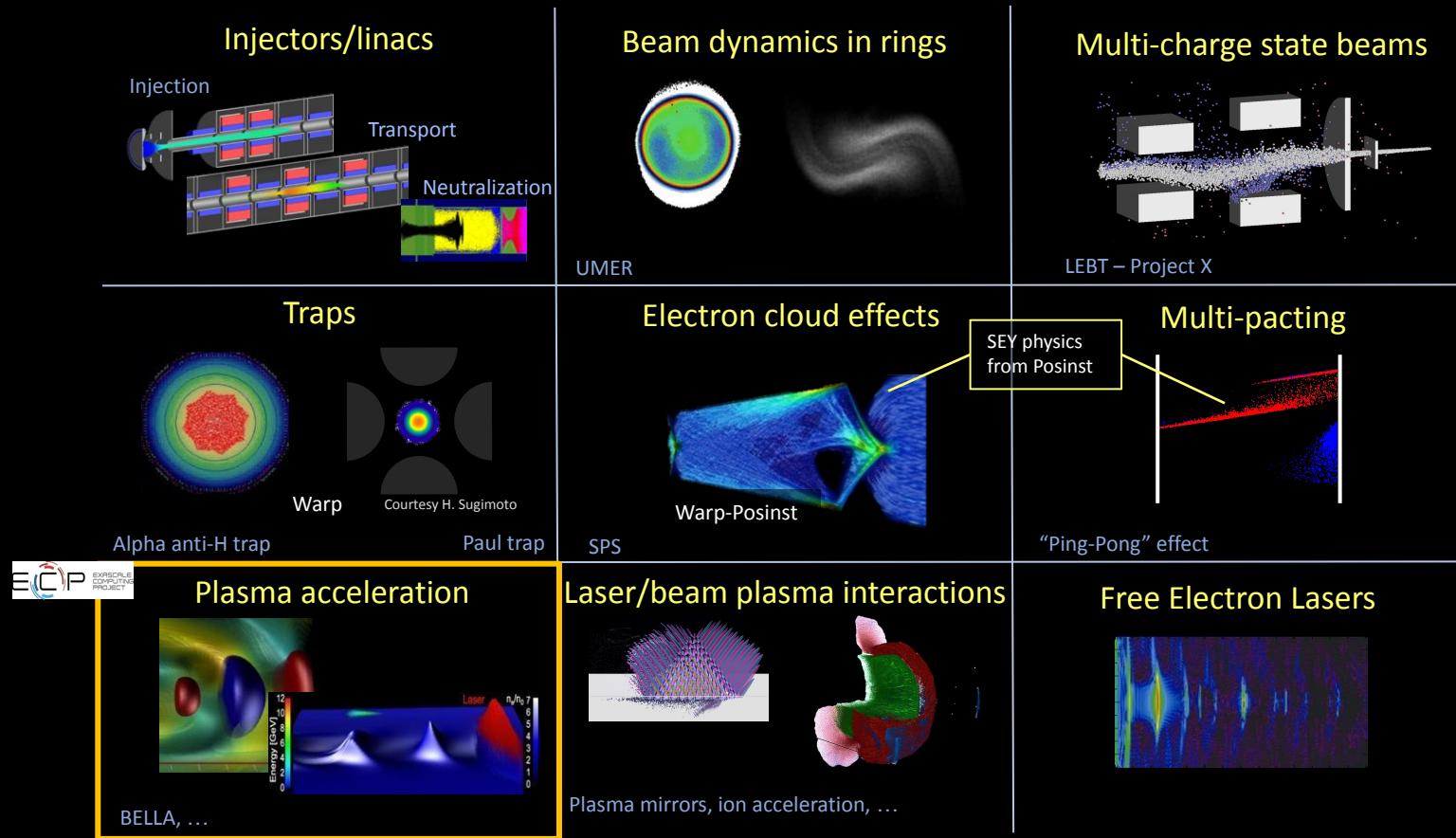
- advanced models: numerics, AI/ML surrogates
- speed & scalability: team science with computer sci.
- flexibility & reliability: modern software ecosystem

Then:
Warp prior to 2016

Warp: historical roadmap & funding

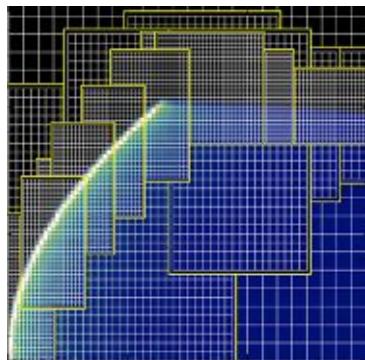


Warp had become a PIC framework with many applications



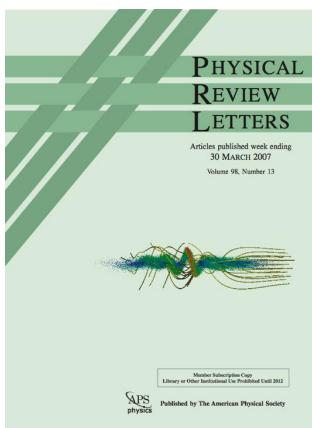
What made Warp unique: algorithmic innovation

Particle-In-Cell with Adaptive Mesh Refinement



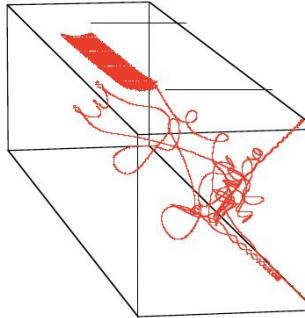
J.-L. Vay, et al, *Comput. Phys. Comm.* **164**, 171 & 297 (2004)

Use of special relativity to slash # time steps by orders of magnitude



J.-L. Vay, *Phys. Rev. Lett.* **98**, 130405 (2007)

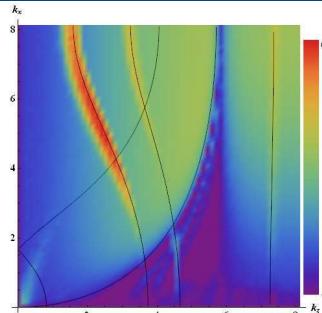
Novel particle pushers



R. Cohen, et al, *Phys. Plasmas* **12**, 056708 (2005)

J.-L. Vay, *Phys. Plasmas* **15**, 056701 (2008)

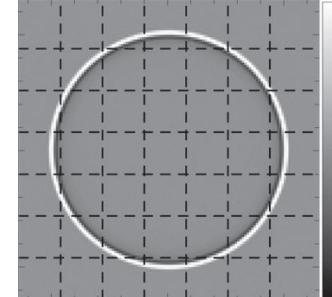
Control of numerical Cherenkov instability



B. Godfrey, et al, *J. Comp. Phys.* **248**, 33 (2013)

R. Lehe, et al, *Phys. Rev. E* **94**, 053305 (2016)

Scalable spectral Maxwell solvers w/ domain decomposition



J.-L. Vay, et al, *J. Comp. Phys.* **243**, 260 (2013)

H. Kallala, et al, *Comp. Phys. Comm.* **244**, 25 (2019)

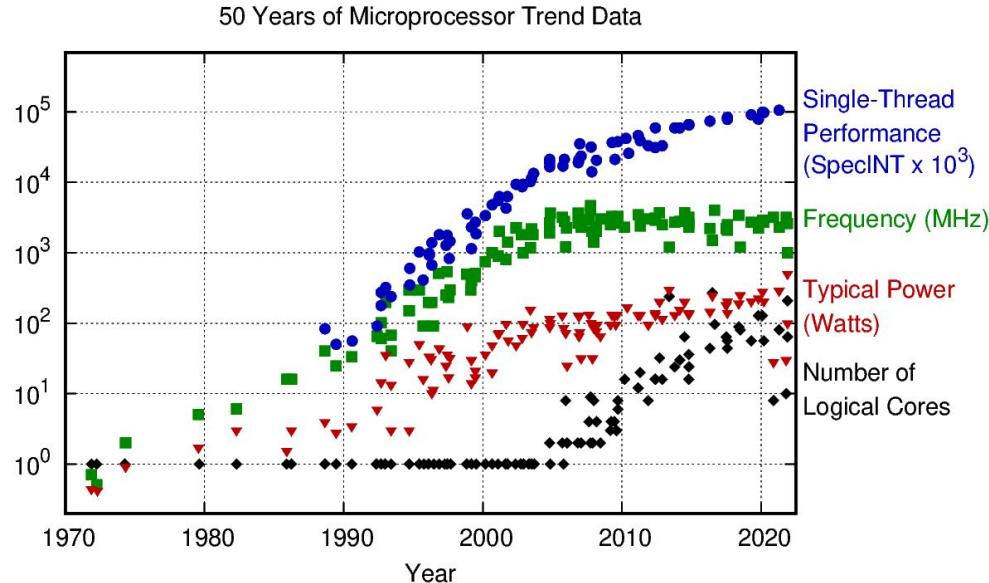
Sample algorithm innovations pioneered in Warp (some adopted in other codes)

Warp: limitations as of 2016

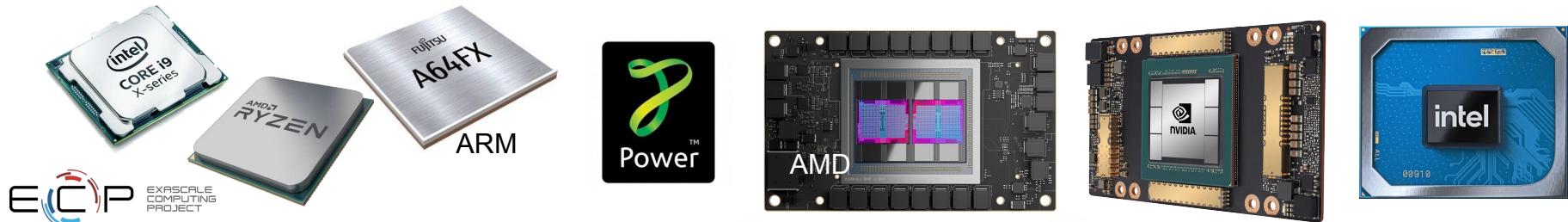
- **Half code in Fortran + half in Python**
 - Python: difficulty scaling on large supercomputers (>1 hour start time at scale)
 - Complicating transition to new hardware: manycore, GPUs, etc.
 - **Small core team (2+ physicists w/ science projects) made it difficult to**
 - Transition to new hardware
 - Keep up performance optimization with fast pace of algorithmic innovation
 - Support growing users (& developers) base
 - Maintain documentation, test suite
 - **SciDAC funding**
 - Supported a project that included 6+ (independent) Particle-In-Cell codes/frameworks with diverse science targets: dilution
- ⇒ ECP provided opportunity for focused effort with sufficient critical mass, & more...

The Journey: from Warp to WarpX (2016-2023)

Power-Limits Seed a Cambrian Explosion of Compute Architectures



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2021 by K. Rupp



Power-Limits Seed a *Cambrian Explosion* of Compute Architectures

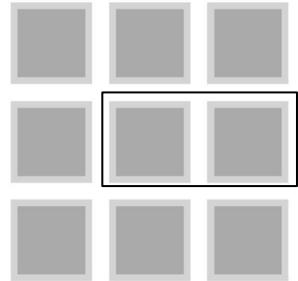
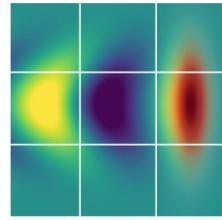
distribute one simulation

over

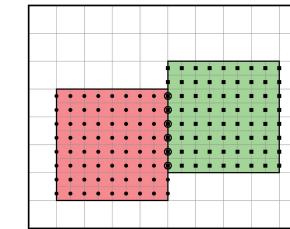
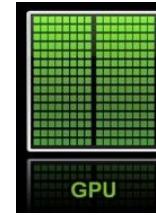
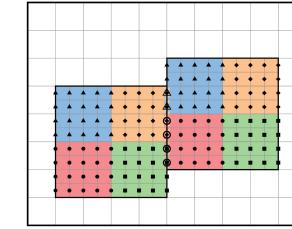
10,000s of computers

for

millions of cores



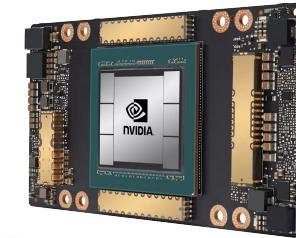
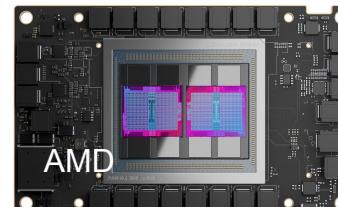
potential future



Field-Programmable Gate Array (FPGA)

Application-Specific Integrated Circuit (ASIC)

Quantum-Circuit

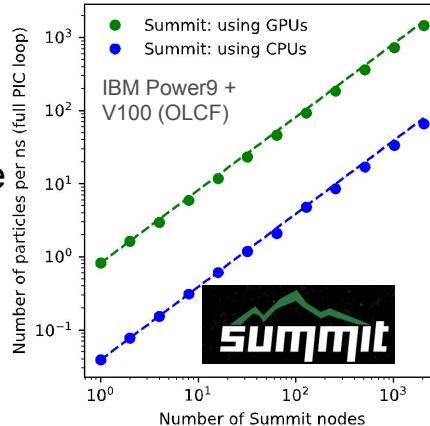
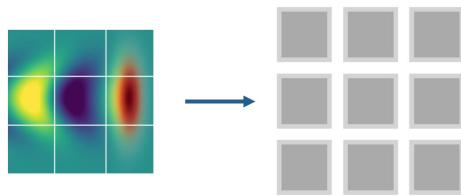


Portable Performance through Exascale Programming Model

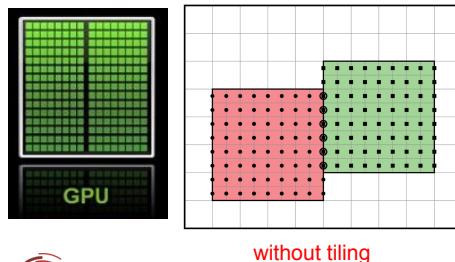
AMReX library



- Domain decomposition & MPI communications: MR & load balance



- Performance-Portability Layer: GPU/CPU/KNL



without tiling

with tiling

Data Structures

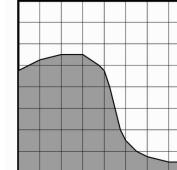
- Write the code once, specialize at *compile-time*

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



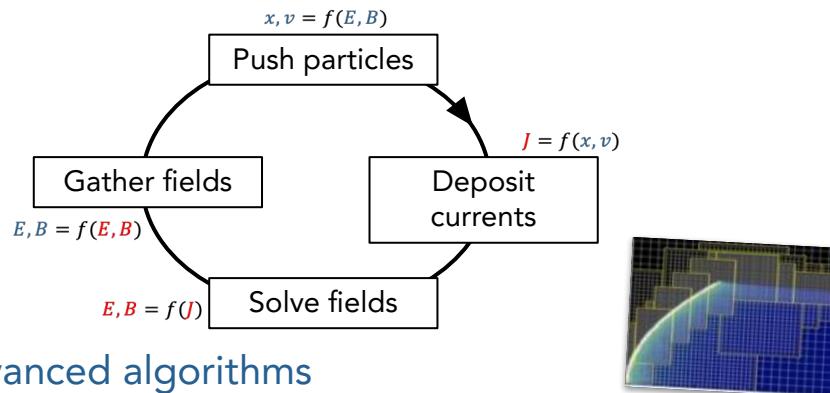
- Runtime parser for user-provided math expressions (incl. GPU)

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, ...

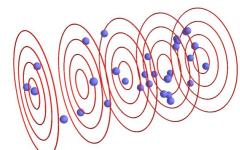
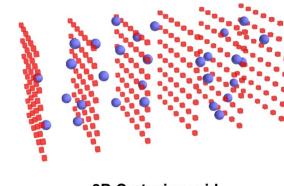
Multi-Physics Modules

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



Developed by a multidisciplinary, multi-institution team

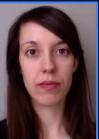


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Pierre
Bartoli



Maxence
Thévenet



(Germany)



(Switzerland)

...& private
sector



Warp to WarpX: the journey

2014 NESAP



Warp | ES- + EM-PIC



PICSAR | EM-PIC library

H. Vincenti, et al



Python + Numba

2015 FBPIC | EM-PIC

R. Lehe, M. Kirchen, et al



2010 C++ + Alpaka + openPMD-api

PIConGPU | EM-PIC

A. Huebl, H. Burau, M. Bussmann, et al



Fortran

C++



PICSAR-QED | High-Field Physics

AMReX | C++



AMR library

NESAP



WarpX | C++ + optional Python frontend



Software Productivity & Sustainability



Sustainable *documentation/knowledge, code and maintenance* (e.g., testing)

Online Documentation:

warpx|hipace|impactx.readthedocs.io

The screenshot shows the WarpX documentation interface. On the left, there's a sidebar with links for 'USAGE', 'Run WarpX', 'Input Parameters', 'Python (PICMI)', and 'Examples'. Under 'Examples', there are links for 'Beam-driven electron acceleration', 'Laser-driven electron acceleration', 'Plasma mirror', 'Laser-ion acceleration', 'Uniform plasma', and 'Capacitive discharge'. The main content area displays the 'Beam-driven electron acceleration' example. It includes a note about example input files, a code snippet for AMReX inputs, and a list of download links for 2D and 3D cases.

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

The screenshot shows a GitHub Actions CI status page. It lists several build configurations: macOS / AppleClang (pull_request), Windows / MSVC C++17 w/o MPI (pull_request), CUDA / NVCC 11.0.2 SP (pull_request), HIP / HIP 3D SP (pull_request), Intel / oneAPI DPC++ SP (pull_request), and OpenMP / Cland ovwarzdx (pull request). All checks have passed successfully. A blue arrow points from the '188 physics benchmarks' text below to this section.

PSIP processes: onboarding, etc.

Productivity and Sustainability
Improvement Planning

RateYourProject.org
bssw.io/psip



188 physics benchmarks run on every code change of WarpX
13 physics benchmarks + 32 tests for ImpactX

Automated Performance on Targets

- OLCF Ascent: IBM w/ V100
- NERSC GitLab: Cray w/ A100

Continuous Deployment

Rapid and easy installation on any platform:



```
conda install  
-c conda-forge warpx
```



```
spack install warpx  
spack install py-warpx
```



```
python3 -m pip install .
```



```
brew tap ecp-warpx/warpx  
brew install warpx
```



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



```
module load warpx  
module load py-warpx
```

WarpX

Azure Pipelines succeeded | nightly packages succeeded | docs passing | spack v23.01 | conda-forge v23.01 | chat on gitter
platforms linux | osx | win | commits since 23.01 10 | supported by ECP | language C++17 | language Python
license BSD-3-Clause-LBNL | DOI (source) 10.5281/zenodo.4571577 | DOI (paper) 10.1016/j.parco.2021.102833

Summary

Jobs

Name

- ✓ Ubuntu pip from dev w/ OpenMPI
- ✓ Ubuntu pip from dev
- ✓ Ubuntu conda
- ✓ Ubuntu conda w/ OpenMPI
- ✓ Ubuntu mamba
- ✓ Ubuntu mamba w/ OpenMPI
- ✓ Ubuntu spack
- ✓ Ubuntu spack CUDA
- ✓ Ubuntu spack w/o MPI
- ✓ macOS pip from dev w/ OpenMPI
- ✓ macOS pip from dev w/o OMP
- ✓ macOS conda
- ✓ macOS conda w/ OpenMPI
- ✓ macOS mamba
- ✓ macOS mamba w/ OpenMPI
- ✓ macOS spack
- ✓ macOS spack from dev w/o MPI
- ✓ Windows pip from dev
- ✓ Windows conda
- ✓ Windows mamba

Now (2023+):
WarpX + Ecosystem

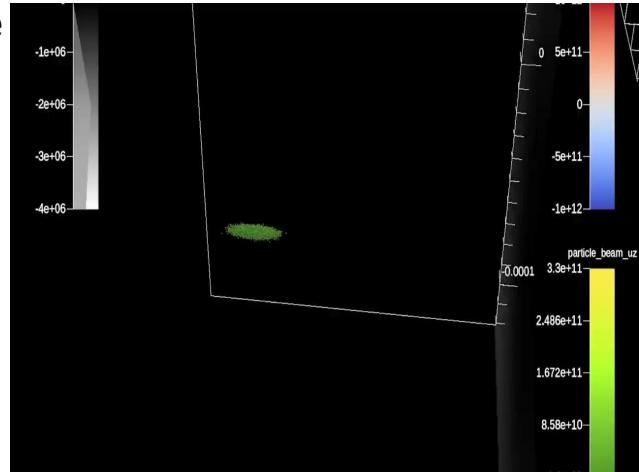
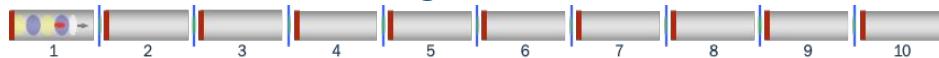
WarpX in ECP: Staging of Laser-Driven Plasma Acceleration

Goal: deliver & scientifically use the nation's first exascale systems

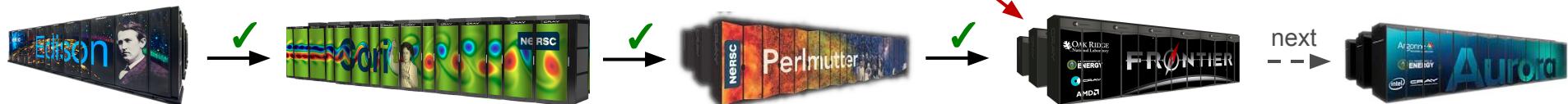
- **ExaFLOP:** a quintillion (10^{18}) calculations per second
- ensure *all* the necessary pieces are *concurrently* in place

Our DOE science case is in **HEP**, our methods are **ASCR**:

first 3D simulation of a chain of plasma
accelerator stages for future colliders



First-of-their-kind platforms: NERSC (Intel, then Nvidia) → Exascale: OLCF (AMD), ALCF (Intel)



J.-L. Vay, A. Huebl et al., ISAV'20 Workshop Keynote (2020) and PoP 28.2, 023105 (2021); L. Fedeli, A. Huebl et al., SC22 (2022)



2022 ACM Gordon Bell Prize: using the First Exascale Supercomputer

April-July 2022: WarpX on world's largest HPCs

L. Fedeli, A. Huebl et al., *Gordon Bell Prize Winner at SC'22, 2022*



modeling of novel
plasma e- beam injection
scheme

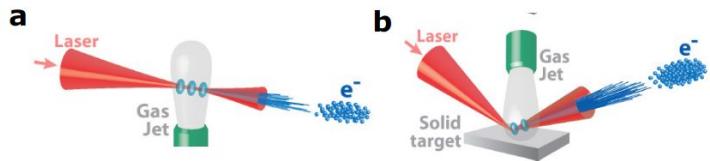


Fig. 1: Sketches showing the focusing of a high-power femtosecond laser (a) into a gas jet (b) onto a hybrid solid-gas target.



A success story of a multidisciplinary,
multi-institutional team!

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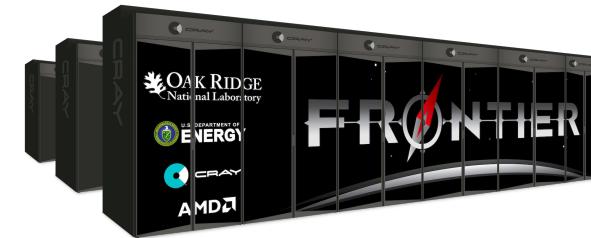
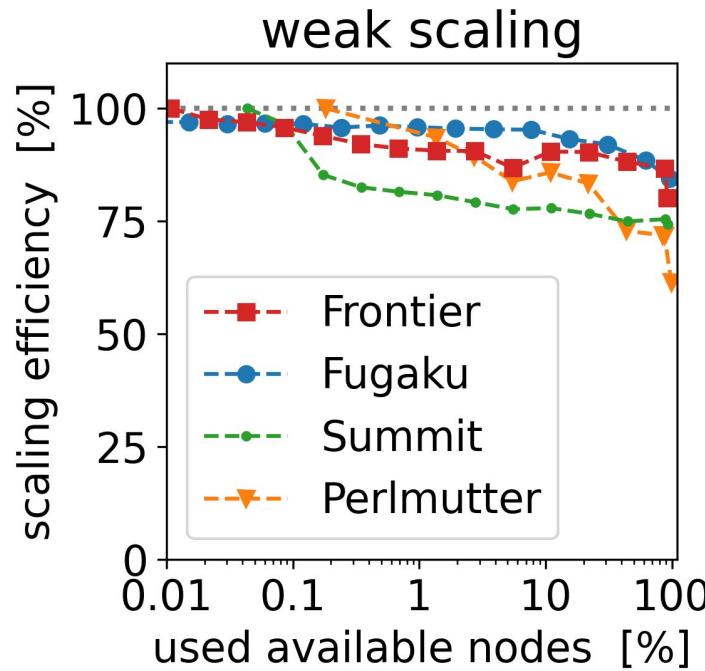


Figure-of-Merit: weighted updates / sec

Date	Code	Machine	N _c /Node	Nodes	FOM
3/19	Warp	Cori	0.4e7	6 625	2.2e10
3/19	WarpX	Cori	0.4e7	6 625	1.0e11
6/19	WarpX	Summit	2.8e7	1 000	7.8e11
9/19	WarpX	Summit	2.3e7	2 560	6.8e11
1/20	WarpX	Summit	2.3e7	2 560	1.0e12
2/20	WarpX	Summit	2.5e7	4 263	1.2e12
6/20	WarpX	Summit	2.0e7	4 263	1.4e12
7/20	WarpX	Summit	2.0e8	4 263	2.5e12
3/21	WarpX	Summit	2.0e8	4 263	2.9e12
6/21	WarpX	Summit	2.0e8	4 263	2.7e12
7/21	WarpX	Perlmutter	2.7e8	960	1.1e12
12/21	WarpX	Summit	2.0e8	4 263	3.3e12
4/22	WarpX	Perlmutter	4.0e8	928	1.0e12
4/22	WarpX	Perlmutter†	4.0e8	928	1.4e12
4/22	WarpX	Summit	2.0e8	4 263	3.4e12
4/22	WarpX	Fugaku†	3.1e6	98 304	8.1e12
6/22	WarpX	Perlmutter	4.4e8	1 088	1.0e12
7/22	WarpX	Fugaku	3.1e6	98 304	2.2e12
7/22	WarpX	Fugaku†	3.1e6	152 064	9.3e12
7/22	WarpX	Frontier	8.1e8	8 576	1.1e13

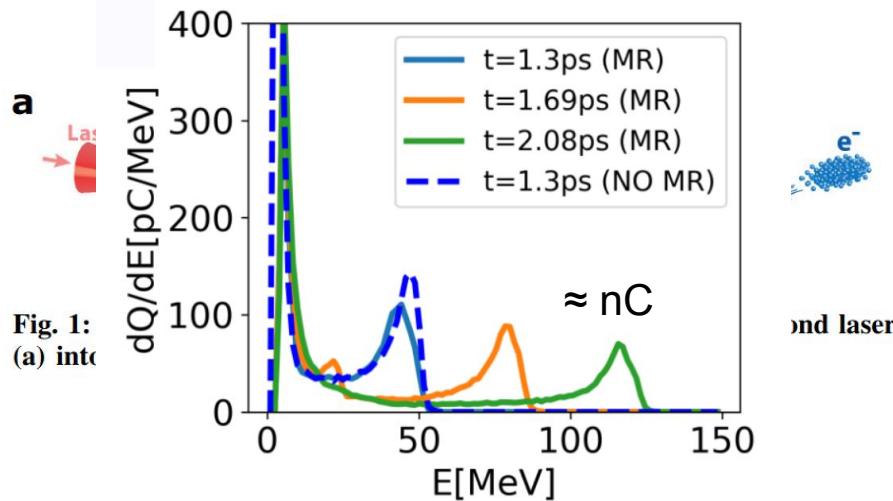
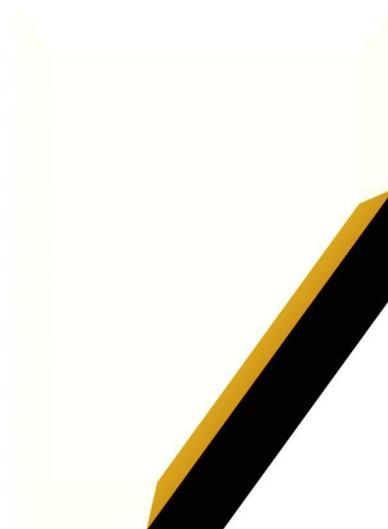


Note: Perlmutter & Frontier are pre-acceptance measurements!

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L. Fedeli, A. Huebl et al., *Gordon Bell Prize Winner at SC'22, 2022*

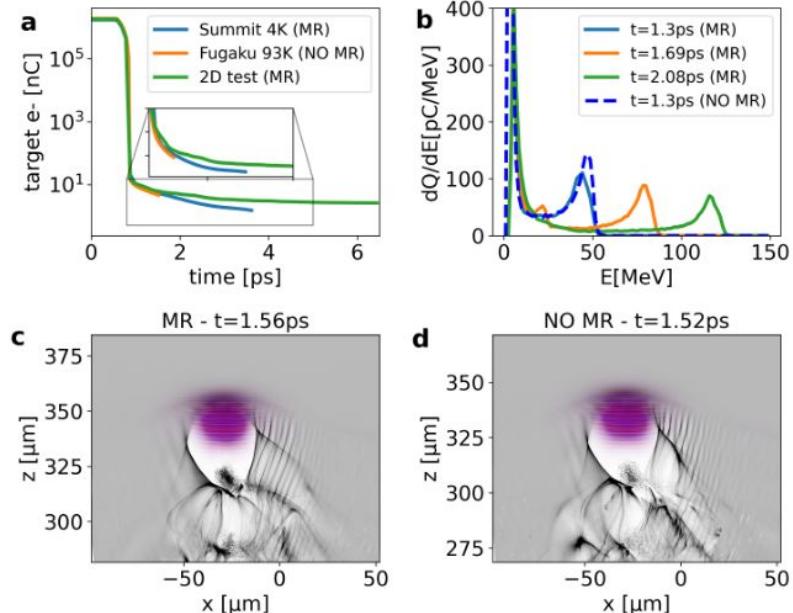
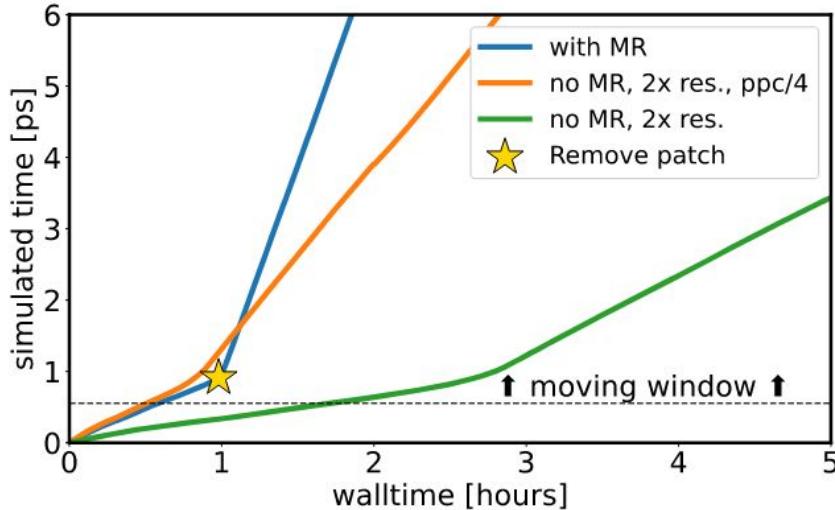


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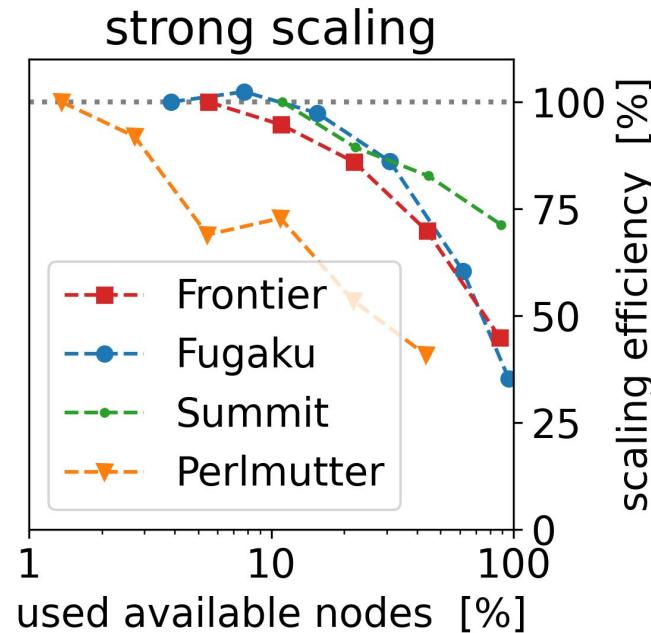
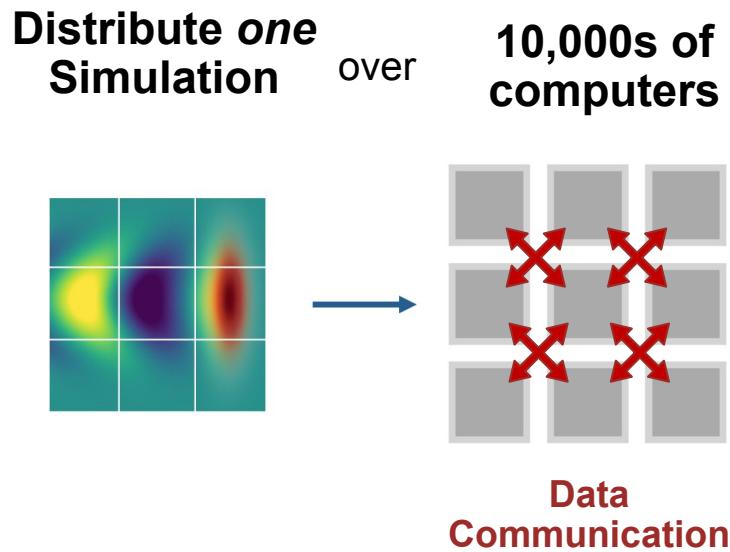
L. Fedeli, A. Huebl et al., *Gordon Bell Prize Winner at SC'22, 2022*



A success story of a multidisciplinary, multi-institutional team!

Is an ExaFlop/s (2022) 1,000x “faster” than a PetaFlop/s (2008)?

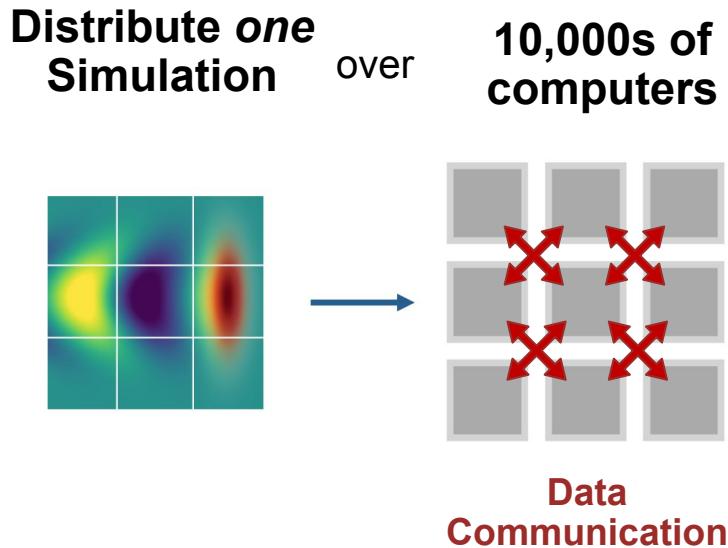
For the **exact same simulation size**, time-to-solution is *at best down by 20-100x!*



Note: Perlmutter & Frontier are pre-acceptance measurements!

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For the **exact same simulation size**, time-to-solution is *at best* down by 20-100x!



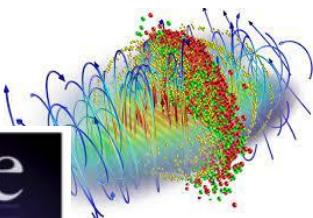
We now have **more parallelism!**
Let's model **more physics**:

- higher grid resolution
- more particles
- resolve ion motion & collisions
- resolve emittance growth from collisions
- 2D → 3D
- long-term stable, advanced solvers
- add high-field effects
- ...

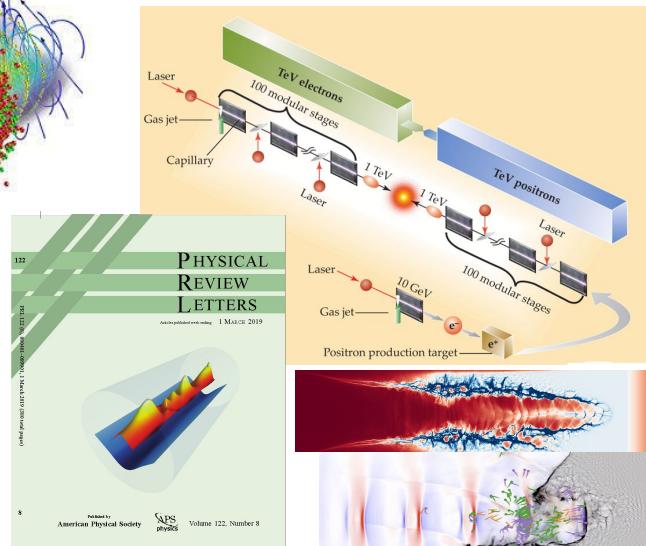
HEP Science Drivers Require Exascale

AAC Linear collider design: PBA & LWFA

PBA XFELs design
Extreme field science



High-Field Physics
Advanced ion sources



+ LLE, Beijing Normal, Tsinghua



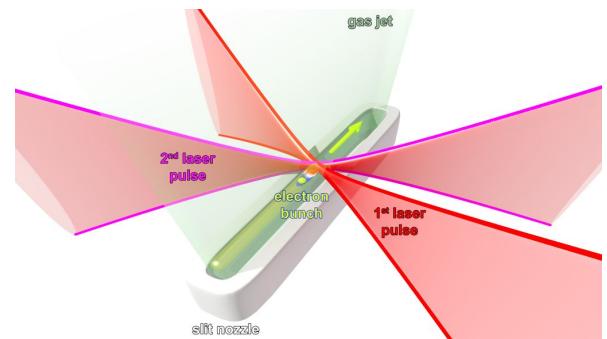
LEADERSHIP COMPUTING
FACILITY



Energy-scalable plasma accelerators

Traveling-wave electron acceleration (TWEAC) simultaneously circumvents the LWFA limitations of diffraction, dephasing and depletion.

- non-rotationally symmetric 3D geometry
- long acceleration lengths



Exascale PIC Modeling Benefits Plasma Science Beyond HEP

Light Sources for Basic Energy Science & National Security

LPA beams for light sources

all-optical undulators

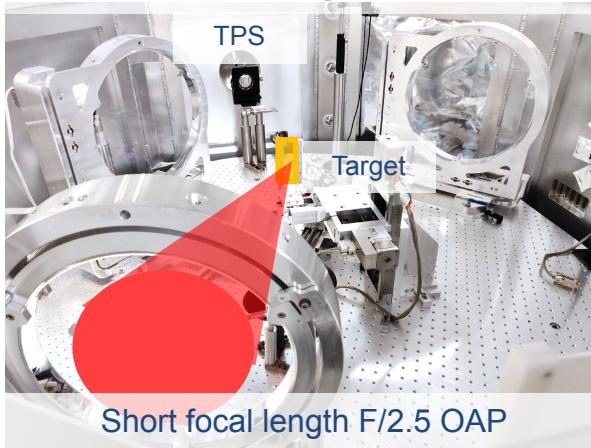
Industry

EUV semiconductor lithography

commercial fusion energy research

Fusion-Energy Sciences

BELLA iP2 target chamber

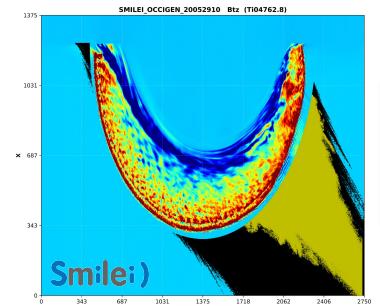


Life Sciences & Medicine

FLASH radio-biology

Astrophysics

origin of strong astrophysical fields & largest energy electrons



em. radiation, turbulence & electron beams from solar flares

magnetic reconnection

Our ECP Software Stack

Spack

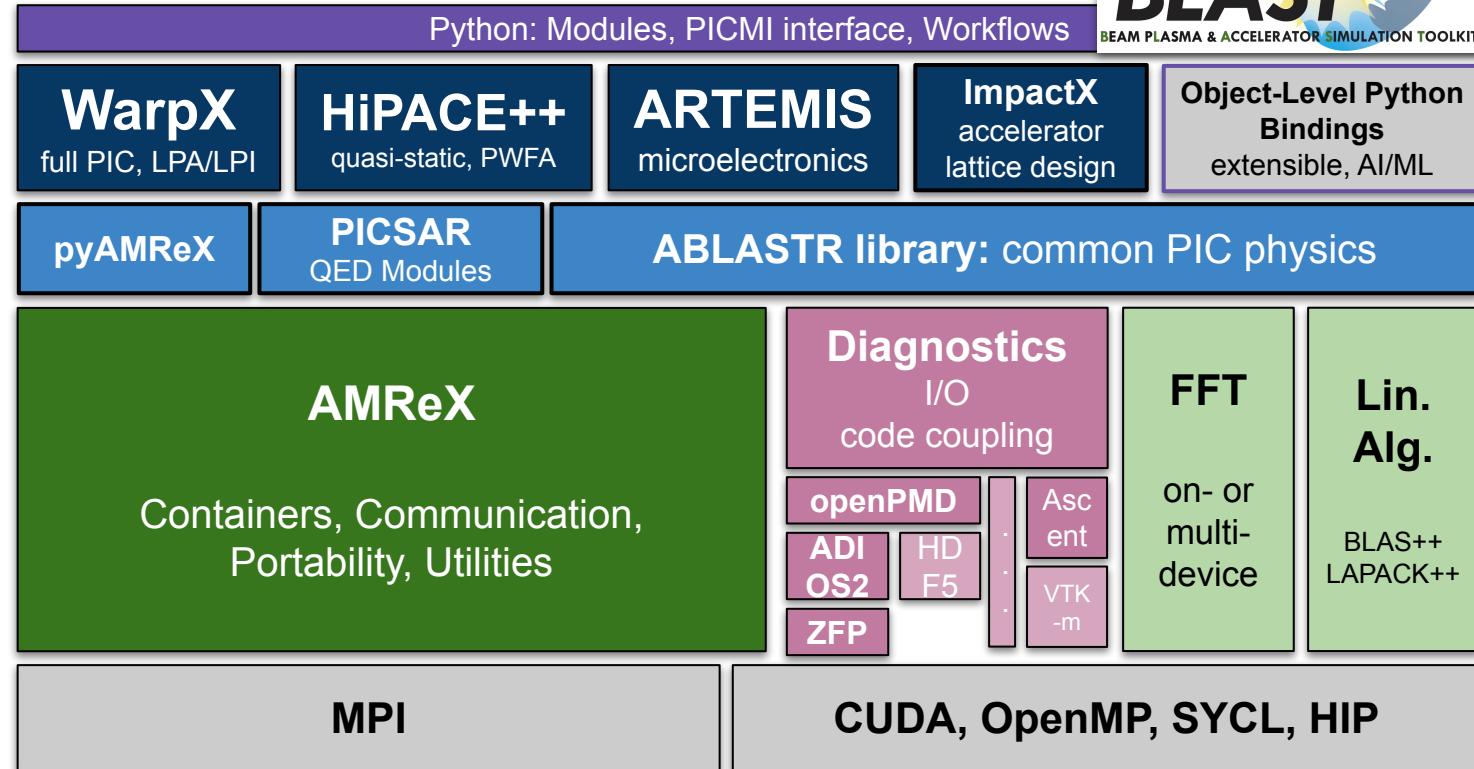
E4S



mac
OS



Desktop
to
HPC



Conclusions

The ECP *multi-year* strategy enabled

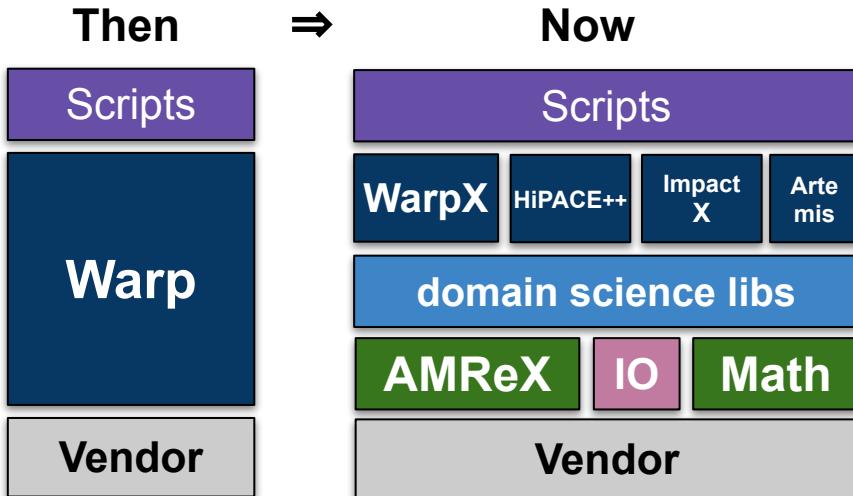
- **integration**: dependencies on vendors and ST require iteration
 - continuous improvements through ***multiple release cycles***
 - coherent, feature-complete, algorithmically innovative ***software products***
- **redesigns**: adjustments to technical execution were possible
 - compilers lacked support: decided for a Fortran to C++ migration mid project
 - Python infrastructure overhaul to GPU-capable methods
 - performance optimizations led to redesign of particle data structures
- **risk mitigation**: e.g., replace self-made with better I/O *methods from ECP ST*
 - *Contingency Funding Requests*: efficient process & funds
- **trust & collaboration**: attracted national & internat. contributors
 - trusted us: their FOSS contributions will be maintained
 - enabled us: leveraging of investment in WarpX spin-off/follow-up projects that *contribute back*



Write strategies: plotfiles → ADIOS BP per rank & step → ADIOS BP w/ append to subfiles

Dependencies become “*Team of Teams*”

- vendors, ST, centers, ...
- own sub-libs/modules, contributions
- machines & deployed environments



Incentives to integrate at all levels

- part of KPP's
- aimed at *production level*, not just prototypes

Prioritization of vendor bugs & features

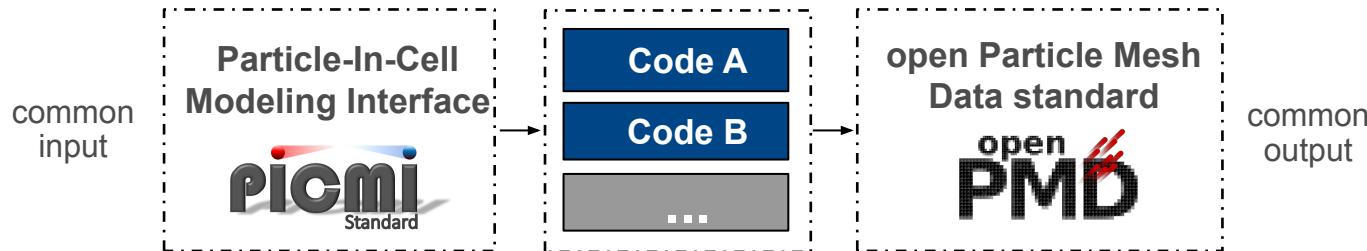
- AMD: CMake scripts, Compiler
- Intel: DPC++ compiler
- Nvidia: compiler bugs, warn host mem access

7yrs ECP vs. shorter multi-yr projects:

- **Scalable collaboration:** easy to add partners
- **Multiple iterations** over release cycles with partners
- **Deep SW stack** that is continuously developed together

We are Establishing an Open Community Ecosystem with Standards

Complexities in accelerator modeling **require to work together**



We established a **leadership role** in our community

- push to **organize**: enhance cooperation, avoid duplication
- **sustainable** development: code ecosystem

We lead the
Consortium for Advanced
Modeling of Particle Accelerators

US

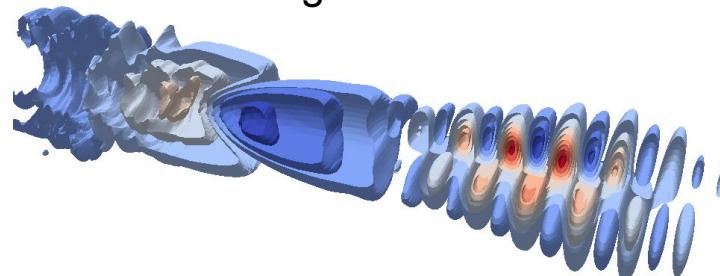


Internationally

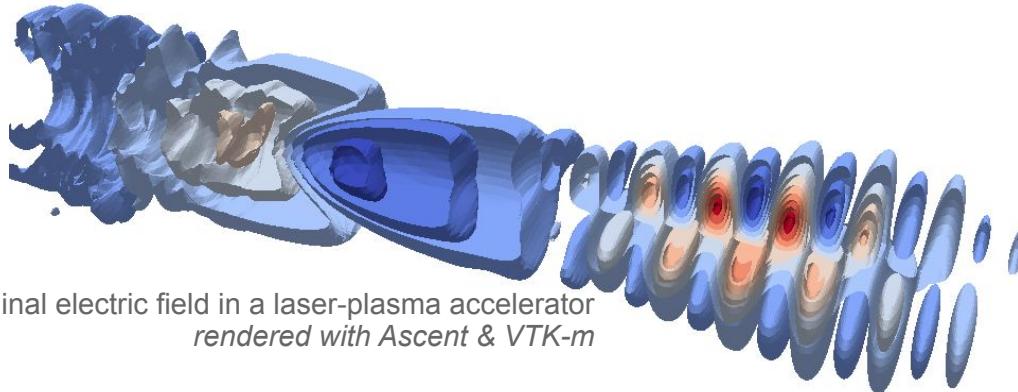


Conclusion

- **ECP enabled**
 - Complete rewrite of efficient code for CPUs+GPUs for focused area of research
 - Ability to combine innovation in algorithms with very efficient implementation
 - Collaboration WarpX+AMReX is the best that many of us have experienced
⇒ great outcome: **500x FOM** for Laser-Particle Acceleration; **Gordon Bell Prize '22**
- **Sustainable development over nearly a decade**
 - across teams, labs and technologies: **one “felt” as a part a community**
 - integrated teams of comput. phys. + applied math. + comput. sc. + software eng.
- **Management Structure**
 - Focused main deliverables, flexibility to correct course, **freedom to innovate**
 - Felt a good balance between oversight and overhead



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