SLAC NATIONAL ACCELERATOR LABORATORY

FACET-II Science Workshop 2017
17-20 Oct. 2017

Warp-X: a new exascale computing platform for Beam-Plasma Simulations

Jean-Luc Vay - Lawrence Berkeley National Laboratory

with A. Almgren[1], J. Bell[1], L. Ge[3], D. Grote[2], O. Kononenko[3], M. Hogan[3], R. Lehe[1], A. Myers[1], C. Ng[3], J. Park[1], R. Ryne[1], O. Shapoval[1], M. Thevenet[1], W. Zhang[1]

[1]Lawrence Berkeley National Laboratory
[2]Lawrence Livermore National Laboratory
[3]SLAC Accelerator National Laboratory

ECP EXASCALE COMPUTING PROJECT

NNSA National Nuclear Security Administration

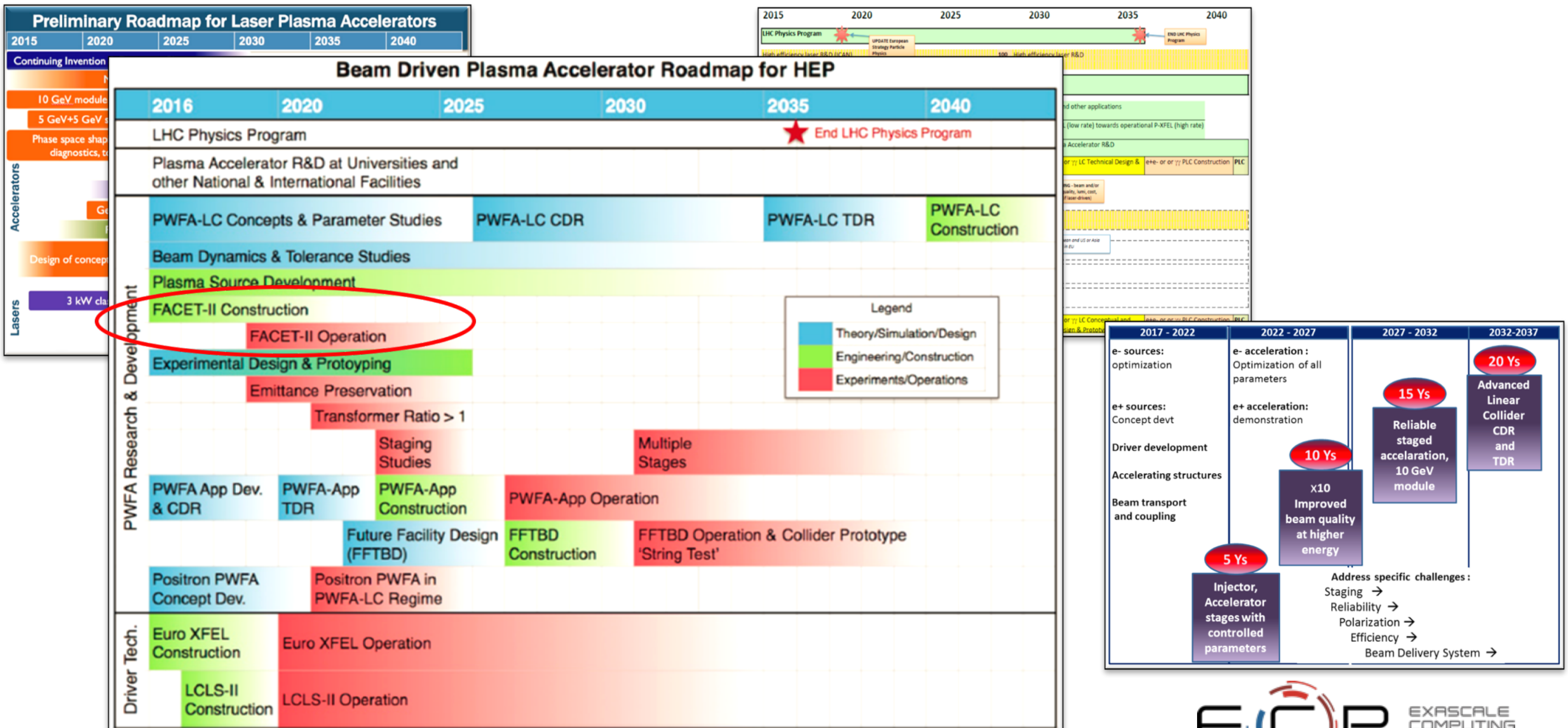
U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

Outline

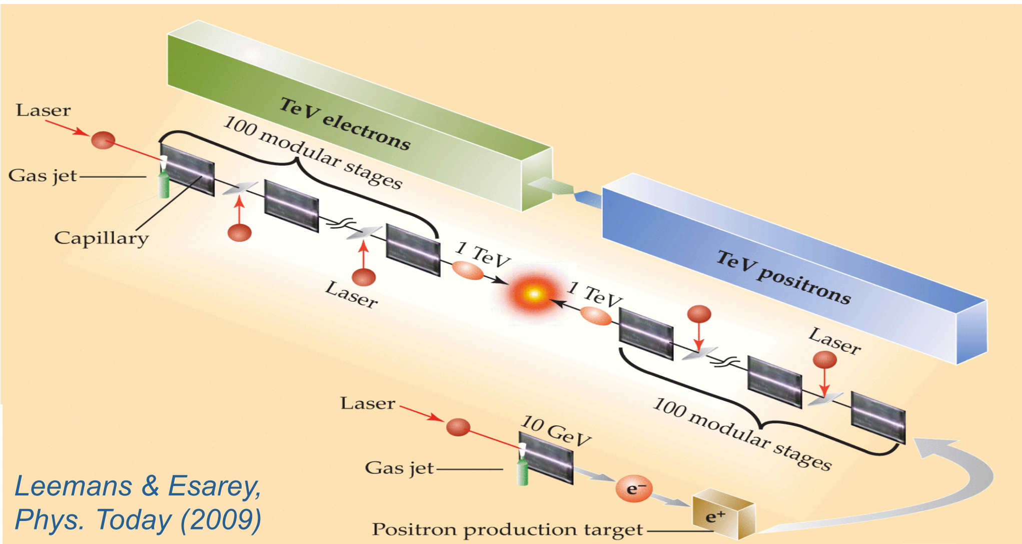
- Context & overview of the project
- Code structure
- Advanced algorithms
- Progress
- Next steps

Recent reports from US/Europe present roadmaps for plasma-based collider with design by 2035-2040



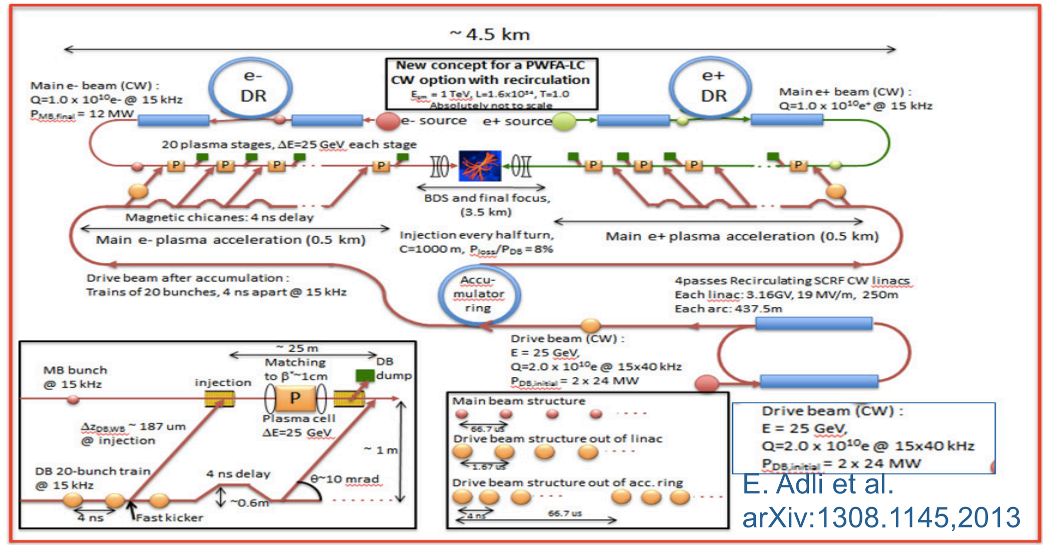
20-100 stages need to be lined up for e^-e^+ linear collider

LWFA



Leemans & Esarey, Phys. Today (2009)

PWFA



E. Adli et al. arXiv:1308.1145,2013

Simulations can currently take days for 1 stage (sometimes in RZ).

Need for ×100 stages ×100 ensemble ×1000 3D!

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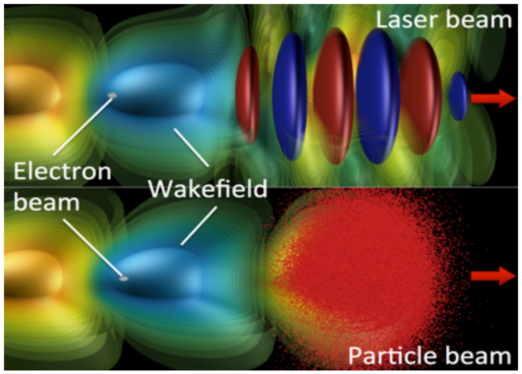
Plasma accelerators are challenging to model



Short driver/wake propagates through long plasma

➔ Many time steps.

For a 10 GeV LPA scale stage:

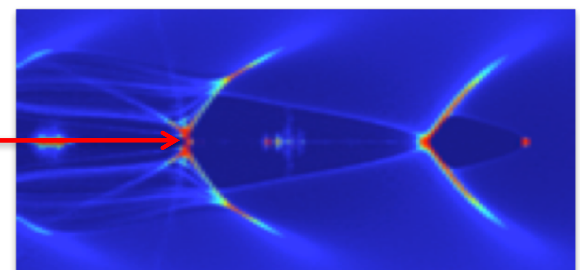
~**1μm** wavelength laser propagates into ~**1m** plasma

➔ millions of time steps needed

Non-linear regime:

very small features

➔ small grid cells

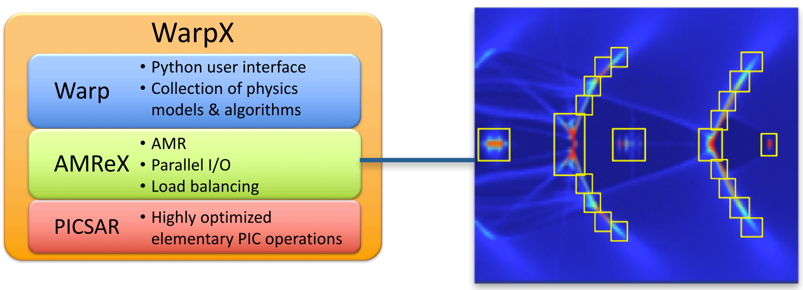


ECP Project WarpX: Exascale Modeling of Advanced Particle Accelerators

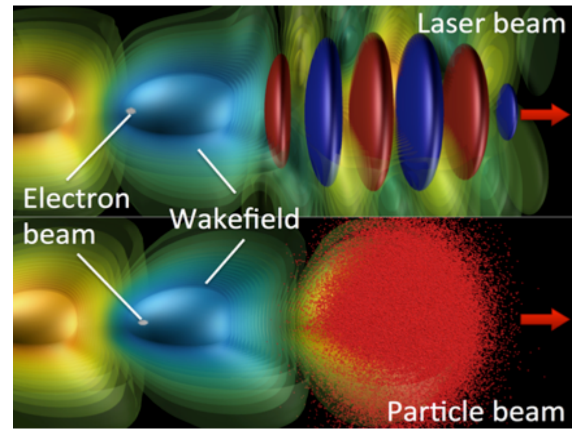
Goal (4 years): Convergence study in 3-D of 10 consecutive multi-GeV stages in linear and bubble regime, for laser- & beam-driven plasma accelerators.

How: ➔ Combination of most advanced algorithms

➔ Coupling of Warp+AMReX+PICSAR



➔ Port to emerging architectures (Intel KNL, GPU, ...)



Team: LBNL ATAP (accelerators) + LBNL CRD (computing science) + SLAC + LLNL

Ultimate goal: enable modeling of 100 stages by 2025 for 1 TeV collider design!

DOE Exascale Computing Project Applications (1ST ROUND)

Title	Team
Computing the Sky at Extreme Scales	Salman Habib (ANL)+LANL,LBNL
Exascale Deep Learning and Simulation Enabled Precision Medicine for Cancer	Rick Stevens (ANL)+LANL, LLNL, ORNL, NIH/NCI
Exascale Lattice Gauge Theory Opportunities and Requirements for Nuclear and High Energy Physics	Paul Mackenzie (FNAL)+BNL,TJNAF,Boston U.,Columbia U., U. of Utah,Indiana U., UIUC,Stony Brook,College of William & Mary
Molecular Dynamics at the Exascale: Spanning the Accuracy, Length and Time Scales for Critical Problems in Materials Science	Arthur Voter (LANL)+SNL, U. of Tennessee
Exascale Modeling of Advanced Particle Accelerators	Jean-Luc Vay (LBNL)+LLNL, SLAC
An Exascale Subsurface Simulator of Coupled Flow,Transport,Reactions and Mechanics	Carl Steefel (LBNL)+LLNL, NETL
Exascale Predictive Wind Plant Flow Physics Modeling	Steve Hammond (NREL)+SNL,ORNL, U. of Texas Austin
QMCPACK: A Framework for Predictive and Systematically Improvable Quantum-Mechanics Based Simulations of Materials	Paul Kent (ORNL)+ANL,LLNL,SNL,Stone Ridge Technology, Intel, Nvidia
Coupled Monte Carlo Neutronics and Fluid Flow Simulation of Small Modular Reactors	Thomas Evans (ORNL,PI)+ANL, INL, MIT
Transforming Additive Manufacturing through Exascale Simulation (TrAMEx)	John Turner (ORNL)+LLNL, LANL, NIST
NWChemEx: Tackling Chemical,Materials and Biomolecular Challenges in the Exascale Era	T. H. Dunning,Jr. (PNNL),+Ames, ANL, BNL, LBNL, ORNL, PNNL, Virginia Tech
High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasma	Amitava Bhattacharjee (PPPL)+ANL,ORNL, LLNL, Rutgers, UCLA, U. of Colorado
Data Analytics at the Exascale for Free Electron Lasers	Amedeo Perazzo (SLAC)+LANL, LBNL, Stanford
Transforming Combustion Science and Technology+Exascale Simulations	Jackie Chen (SNL)+LBNL, NREL, ORNL, U. of Connecticut
Cloud-Resolving Climate Modeling of the Earth's Water Cycle	Mark Taylor (SNL)+ANL, LANL, LLNL, ORNL, PNNL, UCI, CSU

U.S. DOE Exascale Computing Project (ECP)

- ECP's work encompasses
  - applications,
  - system software,
  - hardware technologies and architectures, and
  - workforce development to meet scientific and national security mission needs.

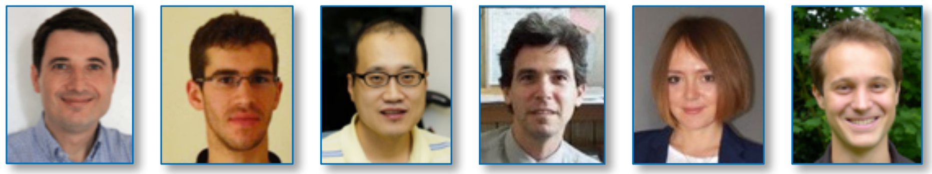
- As part of the National Strategic Computing initiative, ECP was established to accelerate delivery of a **capable exascale** computing system that integrates hardware and software capability to deliver approximately 50 times more performance than today's 20-petaflops machines on mission critical applications.

WarpX team

Main topics

LBNL ATAP

Jean-Luc Vay (PI) · Rémi Lehe · Jaehong Park · Robert Ryne · Olga Shapoval · Maxence Thevenet



- Management
- Algorithms
- Optimization
- Visualization & I/O
- LWFA

LBNL CRD

Ann Almgren (coPI) · John Bell · Andrew Myers · Weiqun Zhang

- AMR
- MPI, OpenMP
- Visualization & I/O

SLAC

Marc Hogan (coPI) · Lixin Ge · Cho Ng · Oleksiy Kononenko

- Optimization
- Visualization
- PWFA

LLNL

David Grote (coPI)

- Python interface

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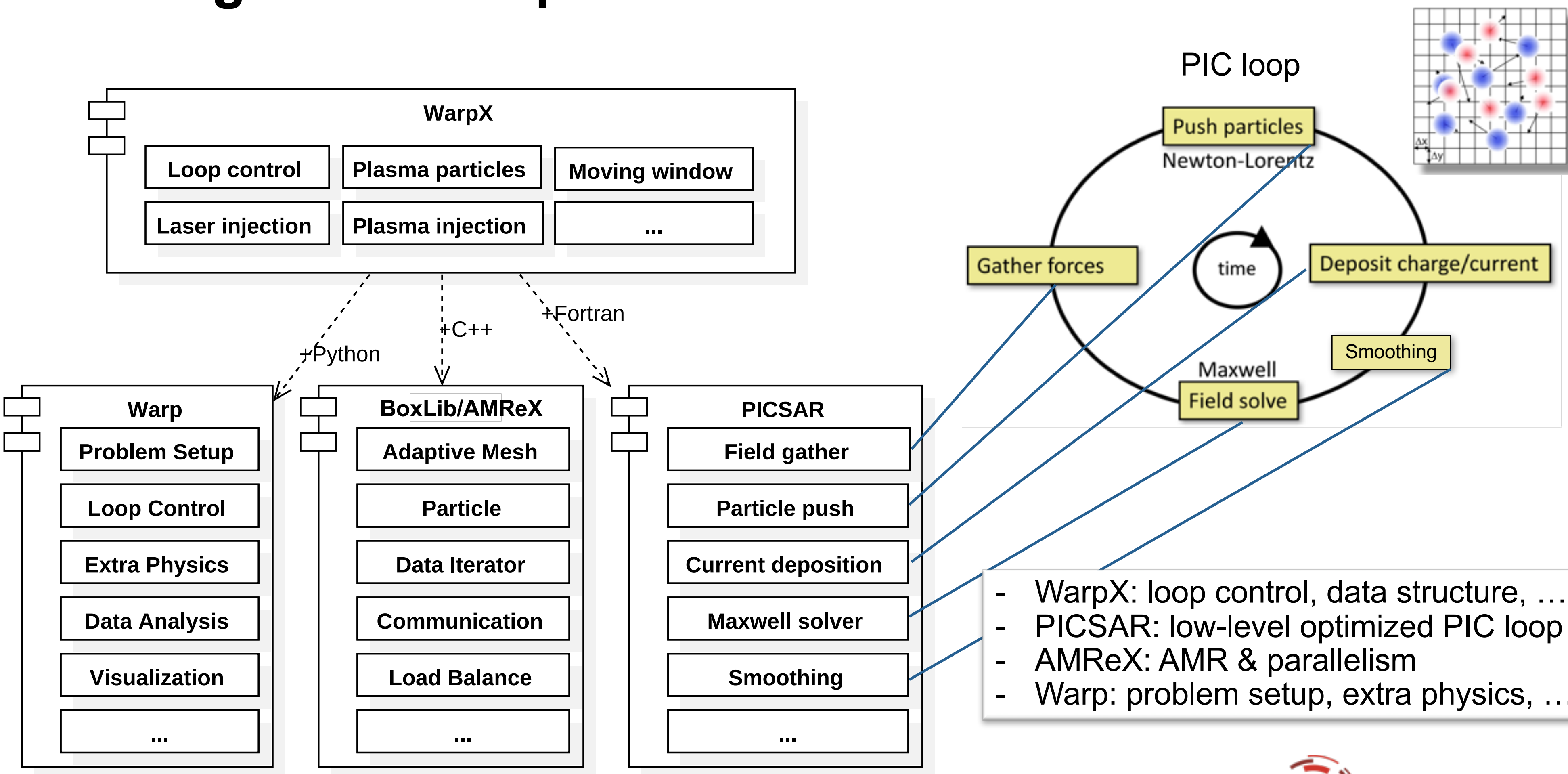
UML Diagram of WarpX details code structure



- WarpX: loop control, data structure, …
- PICSAR: low-level optimized PIC loop
- AMReX: AMR & parallelism
- Warp: problem setup, extra physics, …

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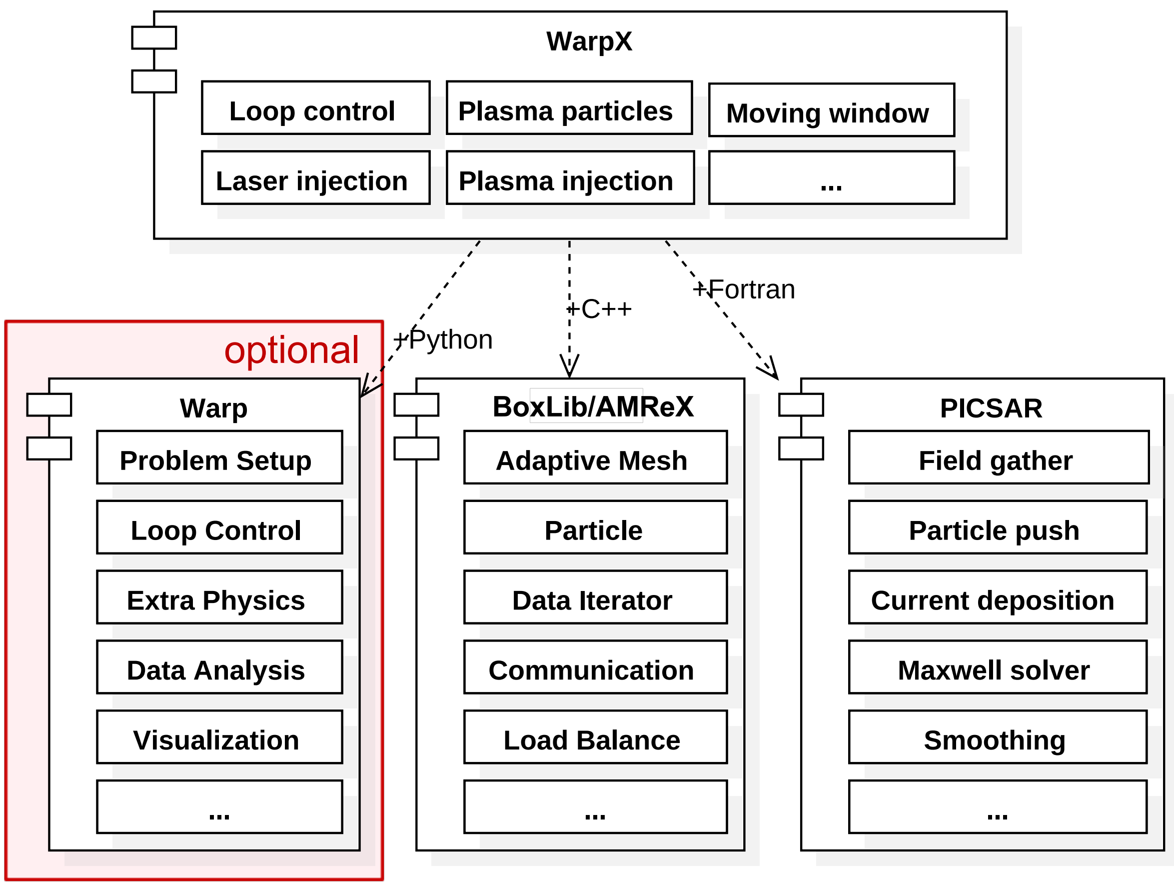
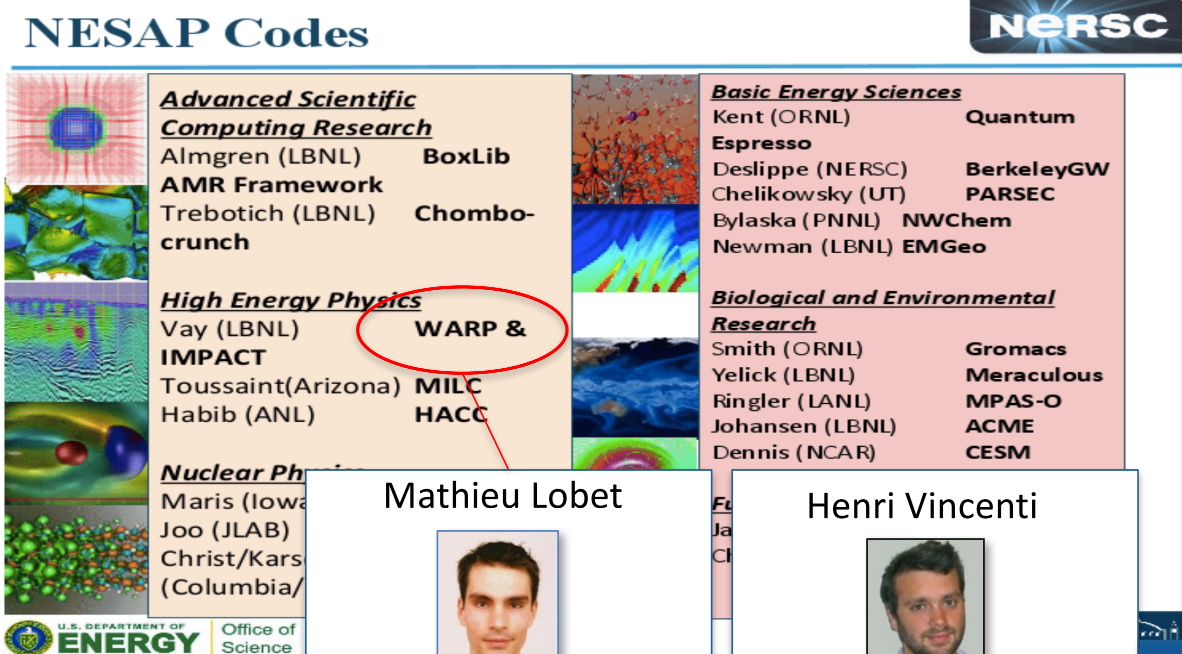
Python layer and connection to Warp are optional



WarpX can be run in 3 modes:

1. Compiled languages only: main in C++.
2. Compiled languages + Python: main in Python
   a. Standalone.
   b. With Warp.

PICSAR created as part of NERSC Exascale Applications Program (NESAP)



Mathieu Lobet

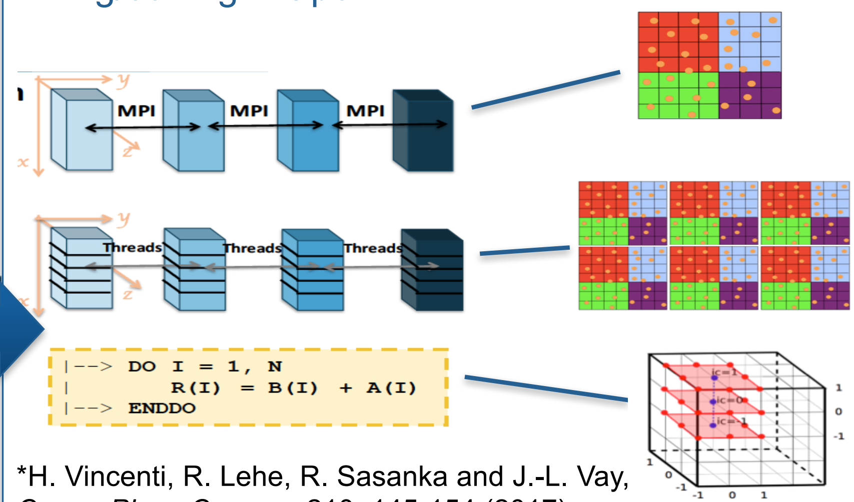
Ex-NESAP postdoc
(now at CEA, Saclay, France)

Henri Vincenti

Marie Curie postdoc fellowship
(now at CEA, Saclay, France)

Warp EM-PIC kernel extracted
➔ Particle-In-Cell Scalable Architecture Resources (PICSAR) library + miniapp

Optimized with new vectorization algo.* + tiling/sorting + OpenMP + MPI



*H. Vincenti, R. Lehe, R. Sasanka and J.-L. Vay, *Comp. Phys. Comm.* , 210, 145-154 (2017).

PICSAR is now open source: https://picsar.net
Used in Warp, WarpX & SMILEI.

EXASCALE COMPUTING PROJECT

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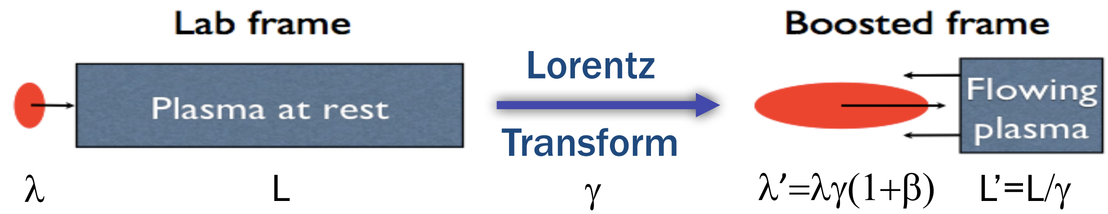
We are combining advanced algorithms

Lower # time steps:

- optimal Lorentz boosted frame



time steps α L/λ

time steps α L'/λ'

➔ Speedup ~ $\gamma^2(1+\beta)$

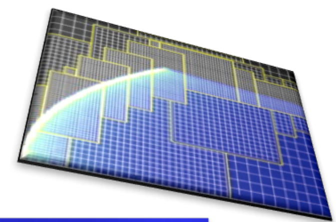
We are combining advanced algorithms

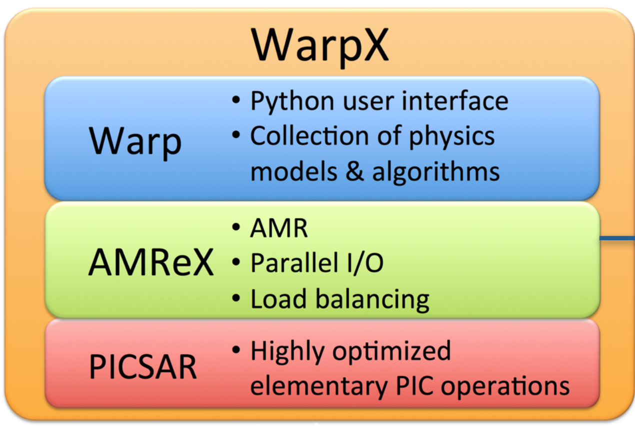
Lower # time steps:

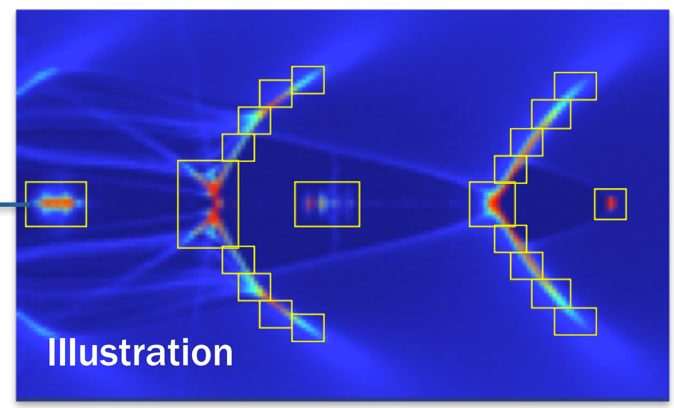
- optimal Lorentz boosted frame

Higher accuracy:

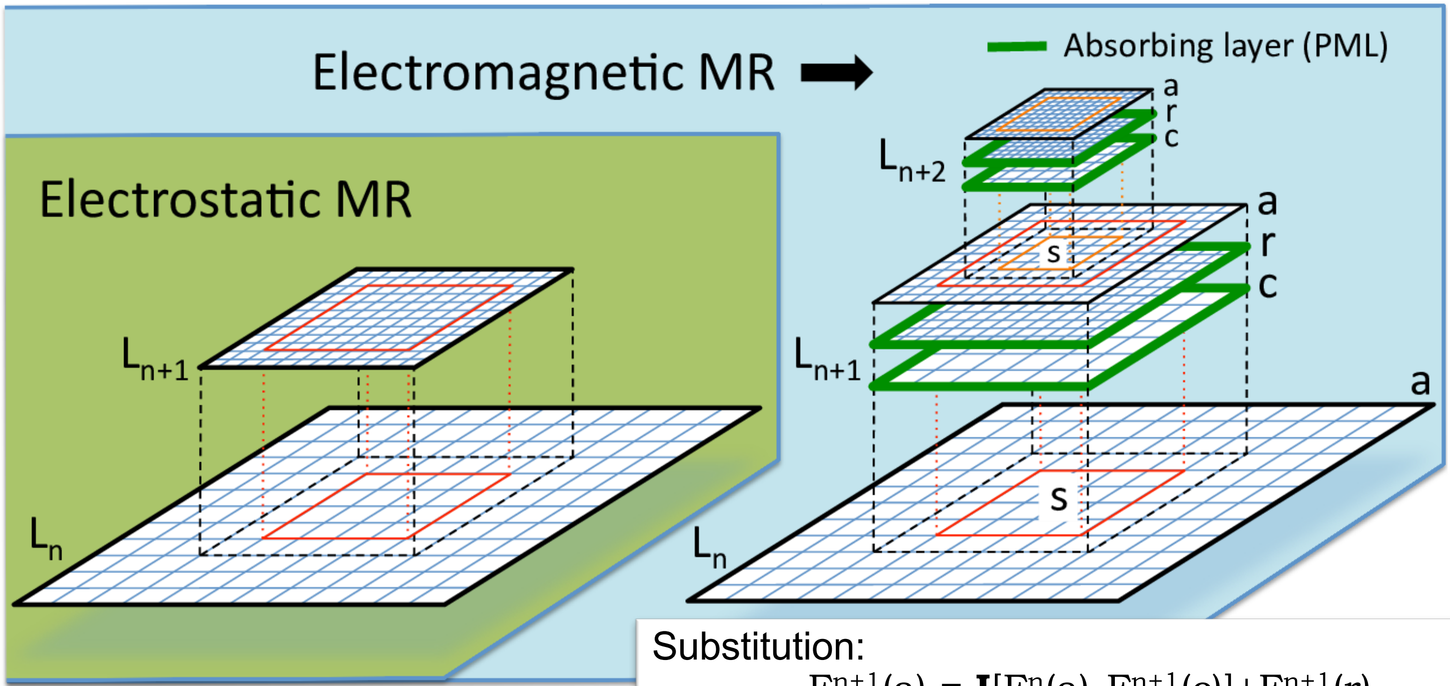
- AMR provided by BoxLib/AMReX library







Implementation of mesh refinement based on Warp algorithm



Substitution:
$F^{n+1}(a) = \mathbf{I}[F^n(a)-F^{n+1}(c)]+F^{n+1}(r)$

- Need to avoid spurious:
  1. self-forces
  2. wave reflections
  3. `ghost stuck' particles

➔

  1. buffer regions
  2. PMLs around patches
  3. Extended Maxwell with divergence cleaning

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$
$$\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \mathbf{J} + \nabla F$$
$$\frac{\partial F}{\partial t} = \nabla \cdot \mathbf{E} - \rho$$

1. J.-L. Vay, P Colella, P Mccorquodale, B Van Straalen, A Friedman, and D. P. Grote. *Laser & Particle Beams* **20**, 569–575, (2002).
2. J.-L. Vay, J.-C. Adam, A. Héron, *Computer Physics Comm.* **164**, 171-177 (2004).
3. J.-L. Vay, D. P. Grote, R. H. Cohen, & A. Friedman, *Computational Science & Discovery* **5**, 014019 (2012).

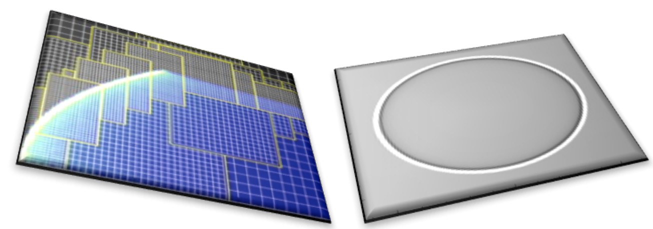
We are combining advanced algorithms

Lower # time steps:

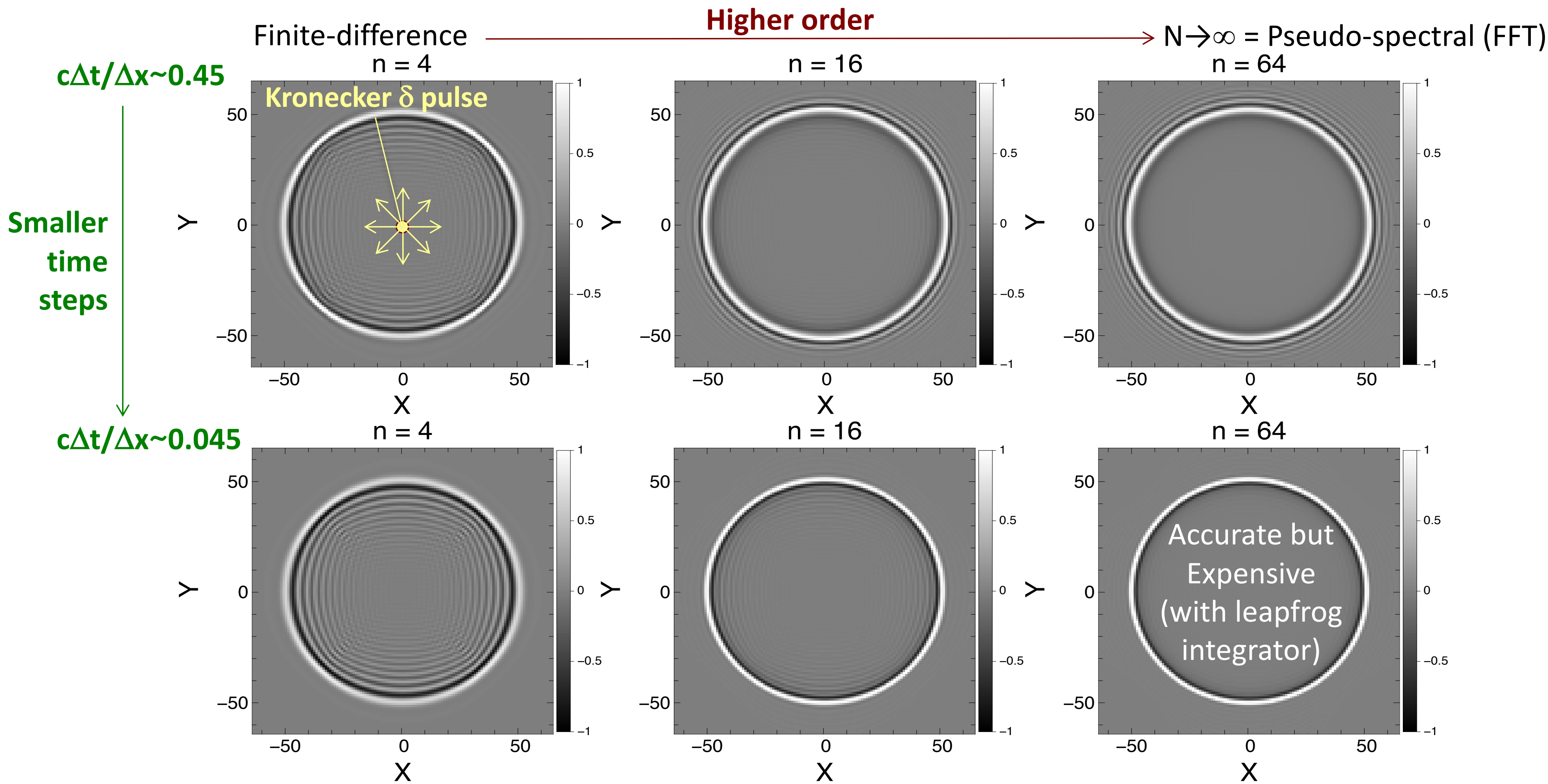
- optimal Lorentz boosted frame

Higher accuracy:

- AMR
- Arbitrary order & pseudo-spectral Analytical Maxwell solvers



Arbitrary-order Maxwell solver offers flexibility in accuracy
(on centered or staggered grids)

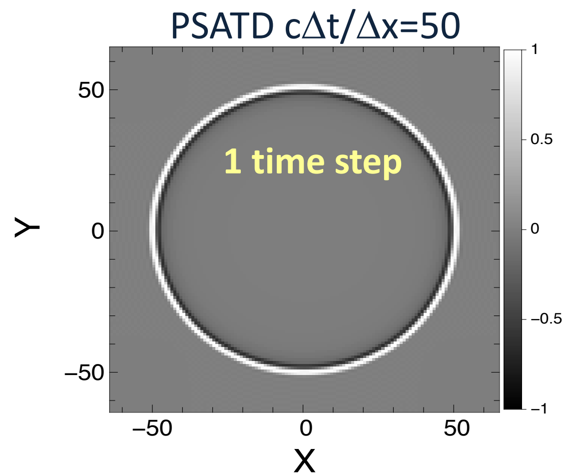


Analytical integration in Fourier space offers infinite order

Pseudo-Spectral Analytical Time-Domain[1] (PSATD)

$$B_z^{n+1} = \mathcal{F}^{-1}\left(C\mathcal{F}\left(B_z^n\right)\right) + \mathcal{F}^{-1}\left(iSk_y\ \mathcal{F}\left(E_x\right)\right) - \mathcal{F}^{-1}\left(iSk_x\ \mathcal{F}\left(E_y\right)\right)$$

with $C = \cos\left(kc\Delta t\right); \quad S = \sin\left(kc\Delta t\right); \quad k = \sqrt{k_x^2 + k_y^2}$



Easy to implement arbitrary-order *n* with PSATD ($k=k^{\infty} \rightarrow k^n$).

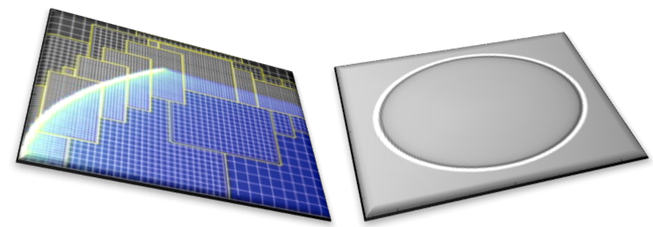
Both arbitrary order FDTD and PSATD to be implemented in WarpX.

[1]I. Haber,R. Lee,H. Klein & J. Boris,*Proc. Sixth Conf. on Num. Sim. Plasma,* Berkeley, CA, 46-48 (1973)

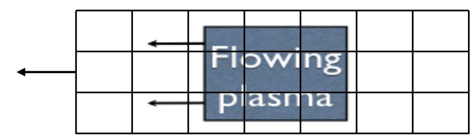
We are combining advanced algorithms

Lower # time steps:
- optimal Lorentz boosted frame

Higher accuracy:
- AMR
- Pseudo-spectral Analytical Maxwell solvers



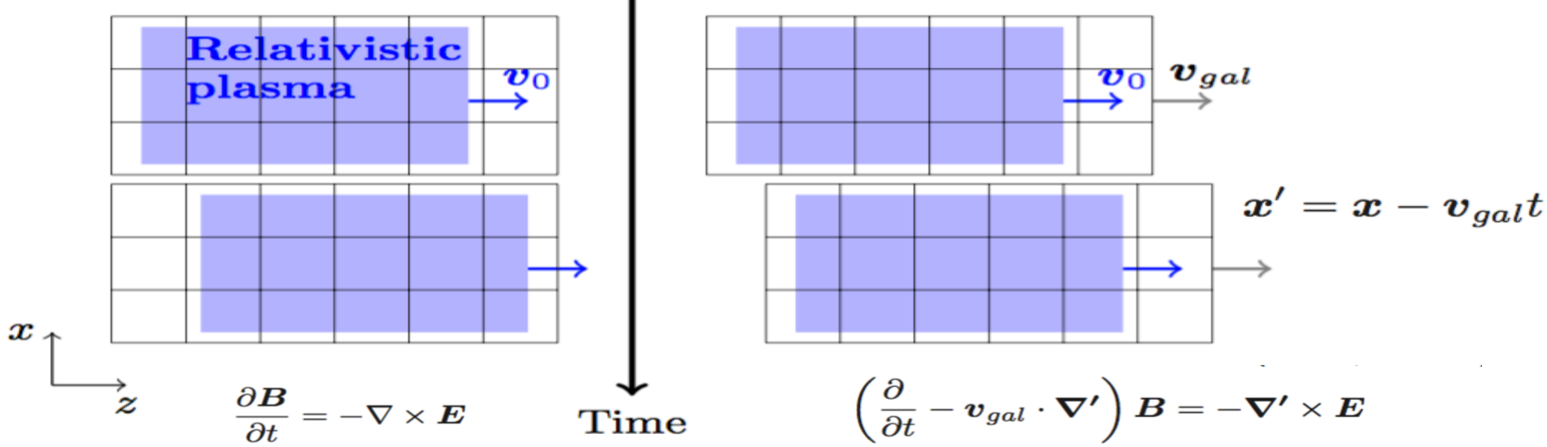
Higher stability
- Galilean T. to suppress Numerical Cherenkov Instability



PSATD also enables integration in Galilean frame

Use Galilean coordinates that follow the relativistic plasma.

Standard PSATD PIC | **Galilean PSATD PIC**



$$\frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E}$$
$$\frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} = \nabla \times \boldsymbol{B} - \mu_0 \boldsymbol{j}$$

$$\left(\frac{\partial}{\partial t} - \boldsymbol{v}_{gal} \cdot \boldsymbol{\nabla}'\right) \boldsymbol{B} = -\boldsymbol{\nabla}' \times \boldsymbol{E}$$
$$\frac{1}{c^2}\left(\frac{\partial}{\partial t} - \boldsymbol{v}_{gal} \cdot \boldsymbol{\nabla}'\right) \boldsymbol{E} = \boldsymbol{\nabla}' \times \boldsymbol{B} - \mu_0 \boldsymbol{j}$$

+ integrate analytically, assuming $\boldsymbol{j}(\boldsymbol{x}, t)$ $\boldsymbol{j}(\boldsymbol{x}', t)$ is constant over one timestep.

Original idea by Manuel Kirchen (PhD student at U. Hamburg)
Concept and applications: *Kirchen et al., Phys. Plasmas 23, 100704 (2016)*

Derivation of the algorithm: *Lehe et al., Phys. Rev. E 94, 053305 (2016)*

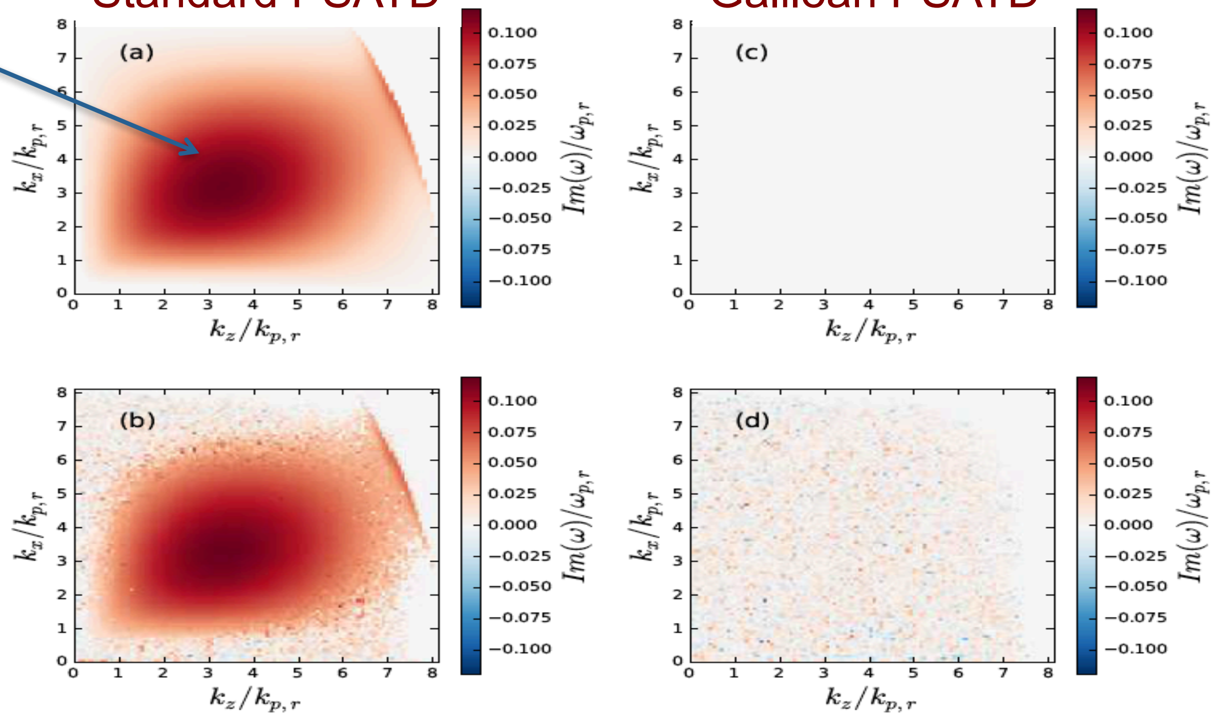
Galilean PSATD is stable for uniform relativistic flow

Uniform plasma streaming in 2D periodic box

Instability growth rate

Standard PSATD

Galilean PSATD



Analysis

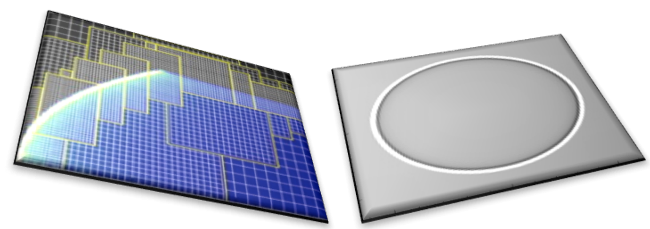
Simulation

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

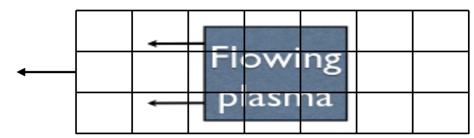
We are combining advanced algorithms

Lower # time steps:
- optimal Lorentz boosted frame

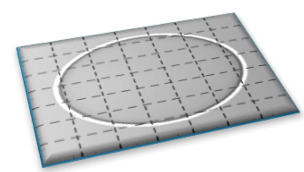
Higher accuracy:
- AMR
- Pseudo-spectral Analytical Maxwell solvers



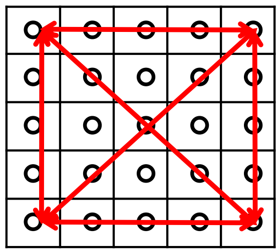
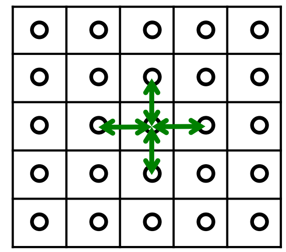
Higher stability
- Galilean T. to suppress Numerical Cherenkov Instability



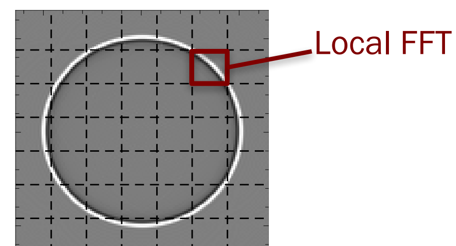
Higher scalability
- FFT Maxwell solvers on local domains + domain decomposition



Spectral solvers involve global operations ➔ harder to scale to large # of cores

Spectral		Finite Difference (FDTD)
global "costly" communications		local "cheap" communications
	vs	
Harder to scale		Easier to scale

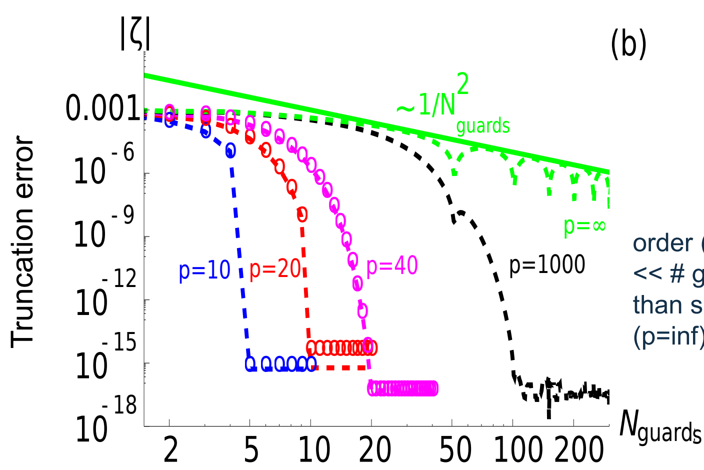
Finite speed of light ➔ local FFTs ➔ spectral accuracy+FDTD scaling!



J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260 (2013)
H. Vincenti, J.-L. Vay, *Comput. Phys. Comm.* **200**, 147 (2016)

Finite-order stencil offers scalable ultra-high order solver

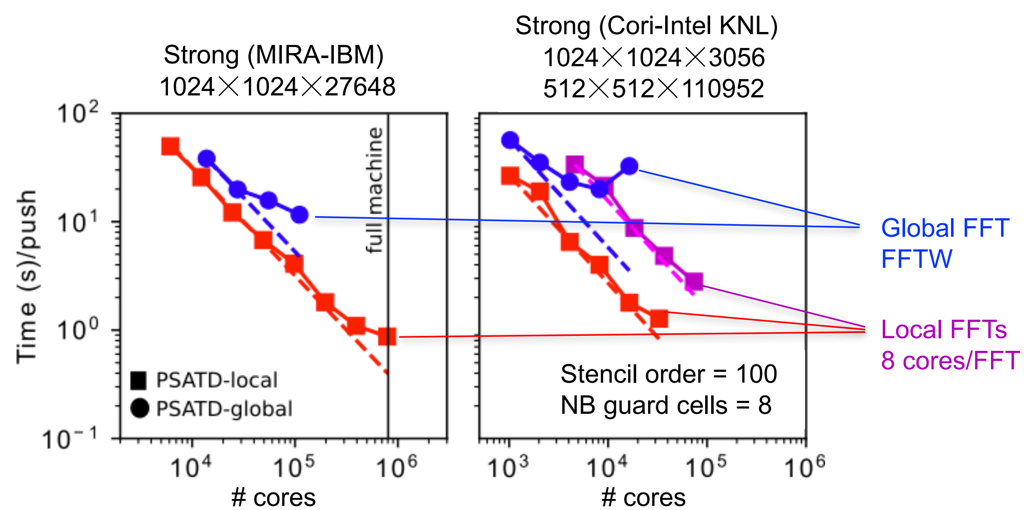
Truncation error analysis ➔ ultra-high order possible with much improved stability



order (p) requires << # guard cells than spectral (p=inf).

H. Vincenti et al., *Comput. Phys. Comm.* 200, 147 (2016).

Enabled demonstration of novel spectral solver with local FFTs scaling to ~1M cores



H. Vincenti, J.-L. Vay, "Ultrahigh-order Maxwell solver with extreme scalability for electromagnetic PIC simulations of plasmas.", http://arxiv.org/abs/1707.08500.

Applied successfully to modeling of LPAs at DESY[1] and plasma mirrors at CEA Saclay[2,3] in cases where standard second-order FDTD solvers fail.

[1] S. Jalas, I. Dornmair, R. Lehe, H. Vincenti, J.-L. Vay, M. Kirchen, A. R. Maier, *Phys. Plasmas* **24**, 033115 (2017).
[2] G. Blaclard, H. Vincenti, R. Lehe, J. L. Vay, Phys. Rev. E **96**, 033305 (2017)
[3] A. Leblanc, S. Monchoce, H. Vincenti,S. Kahaly, J-L. Vay, F.Quere, Phys. Rev. Lett. (in press)

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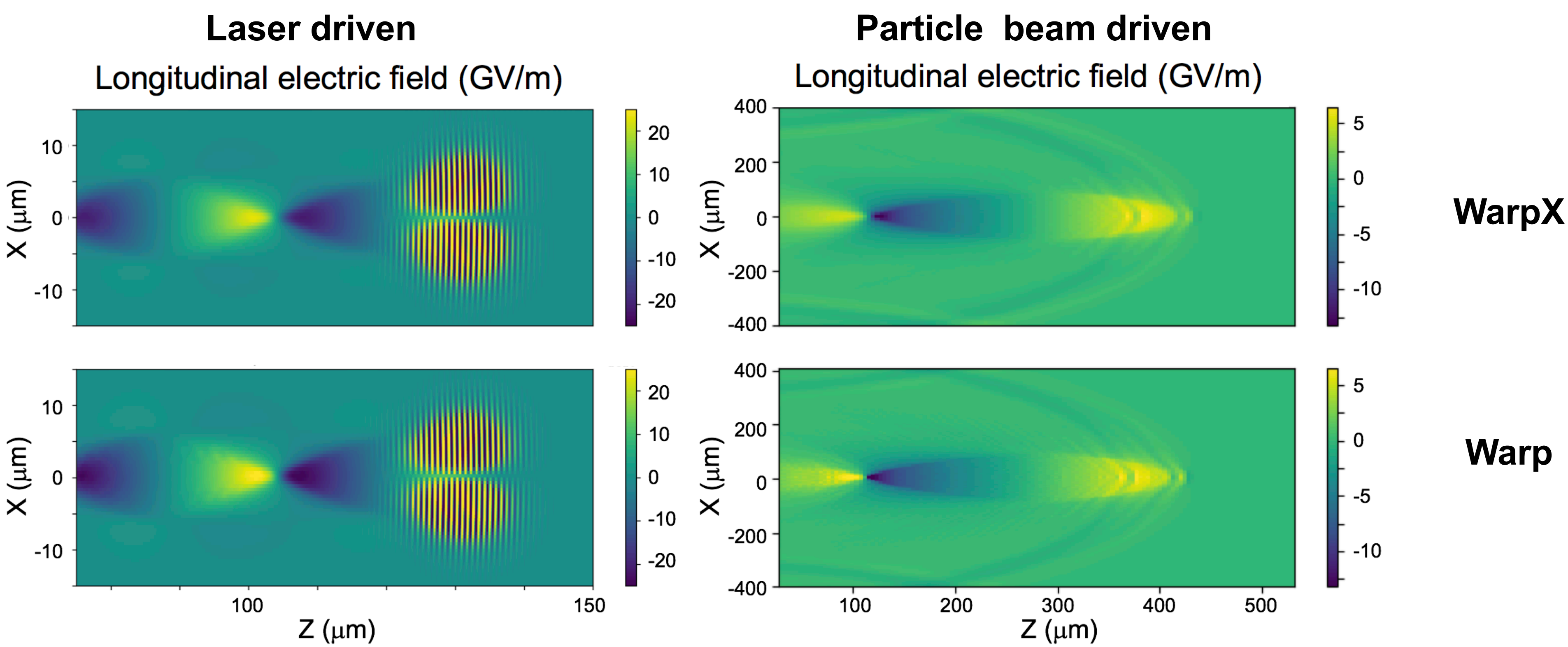
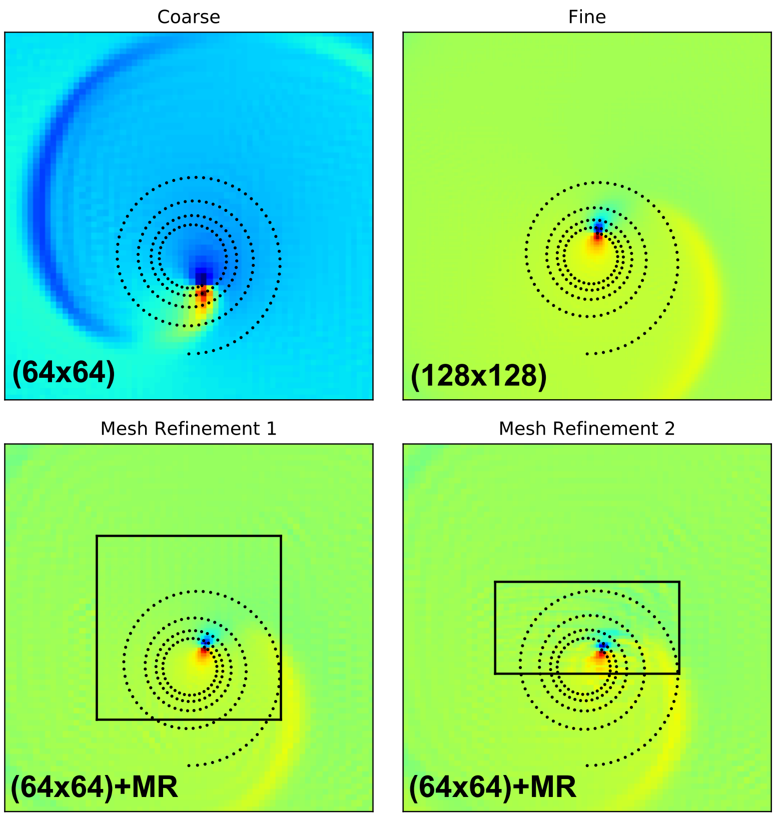
First simulations of plasma-based accelerators with WarpX (03/17)

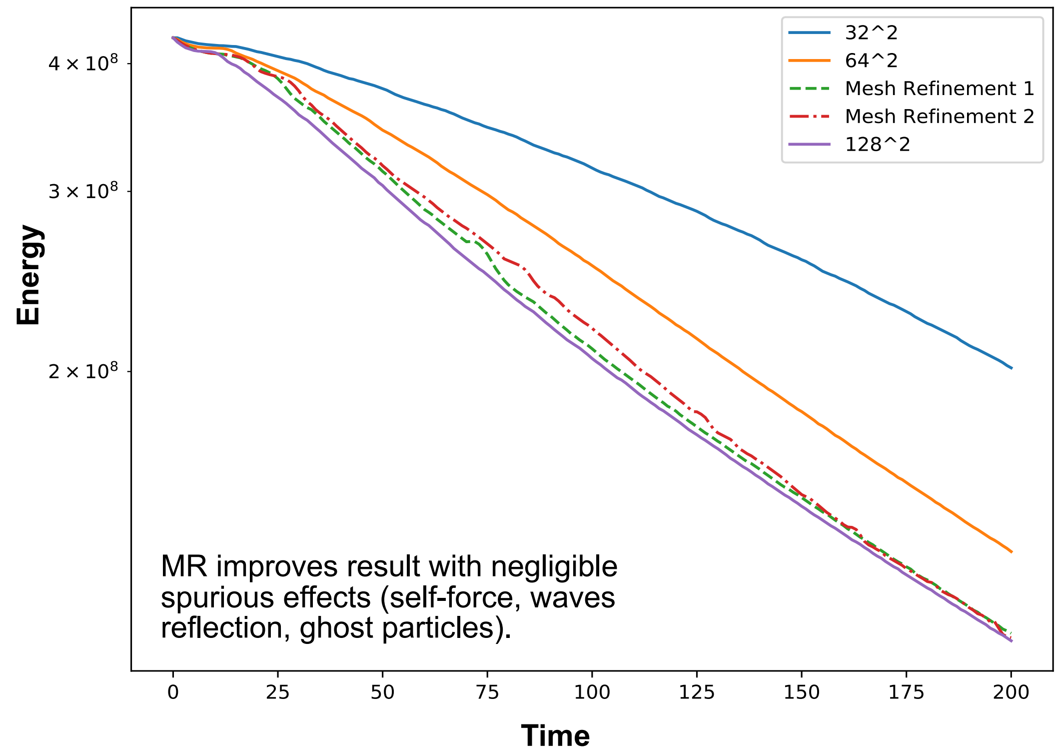


WarpX successfully benchmarked against Warp.

Electromagnetic MR was implemented and tested (06/17)

Single particle orbiting around an external magnetic field, emitting synchrotron radiation





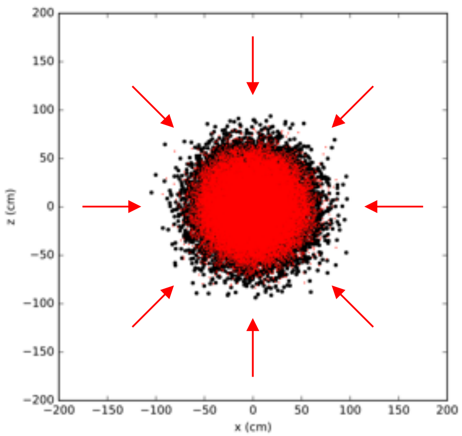
Note: buffer region not implemented yet; expected to improve results once implemented.

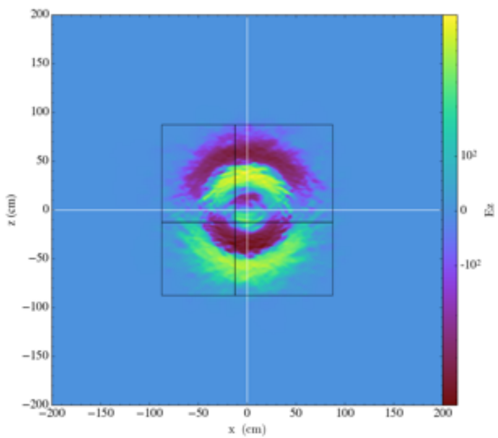
Validation on many particles `beam breathing' test

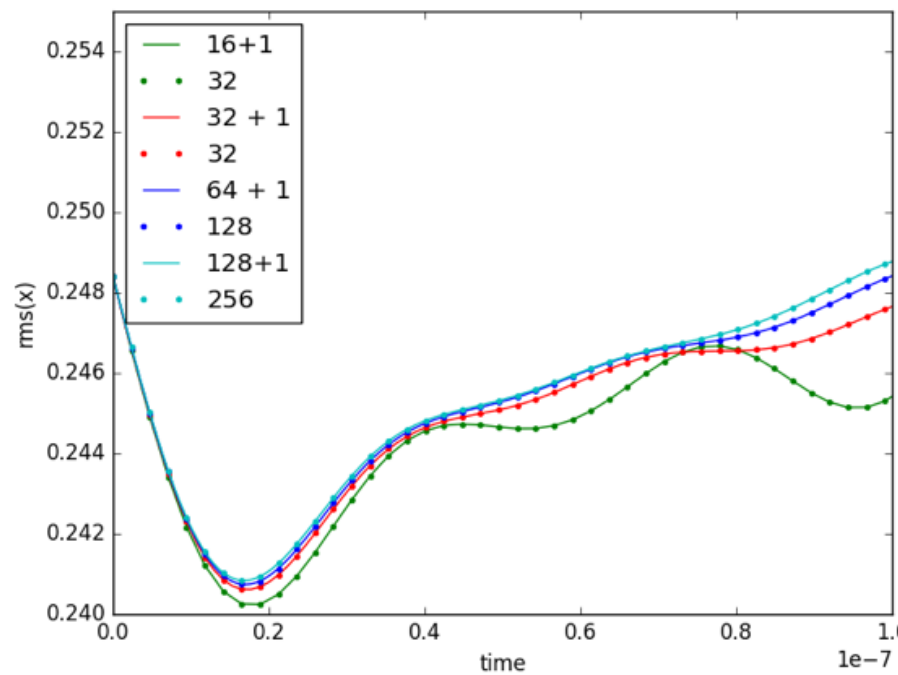
Electron Gaussian distribution with inward initial radial velocity on top of static proton dist.

Electron beam contraction/expansion depends on resolution.

MR enables higher accuracy, covering fraction of box.







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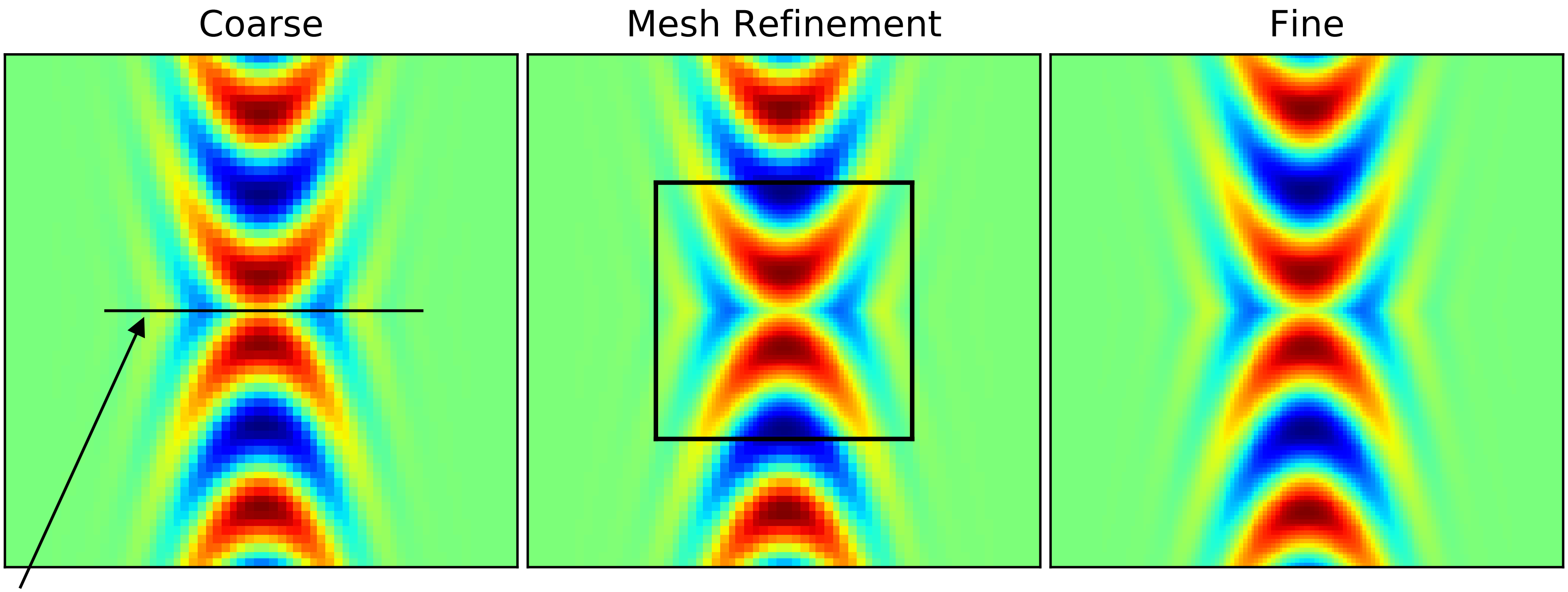
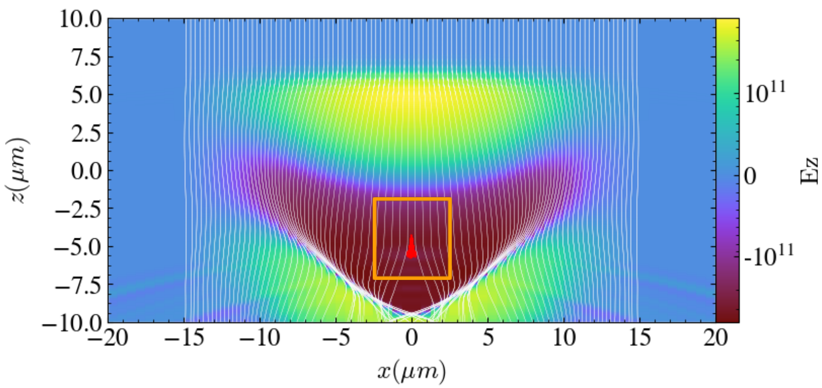
Laser injection with mesh refinement was validated

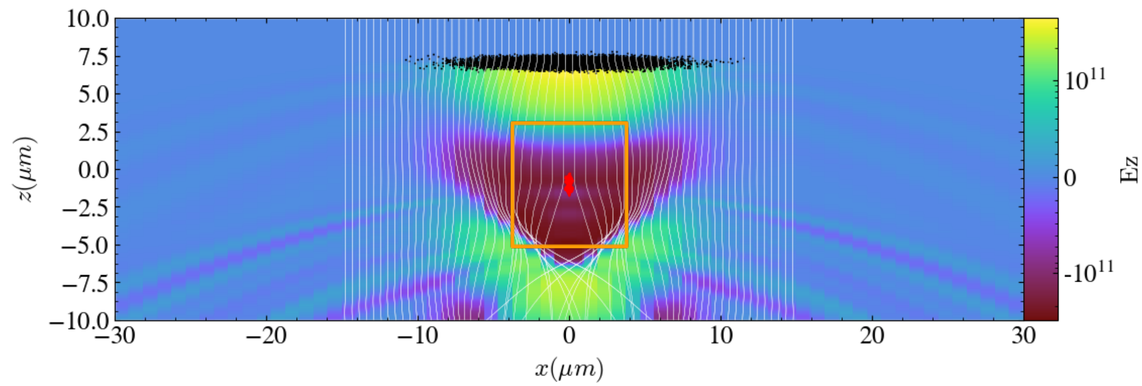


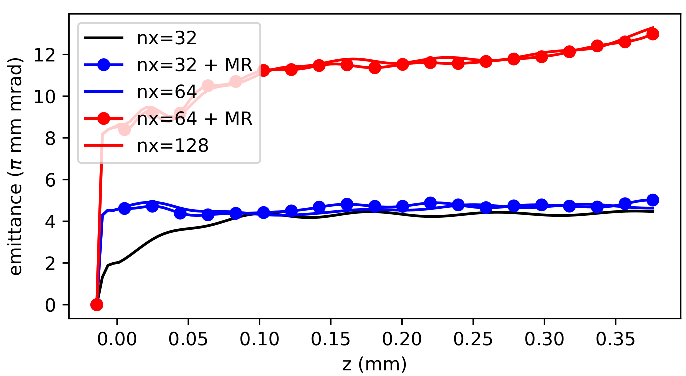
Laser generated with antenna.

First simulations of plasma accelerators with MR patch (09/17)

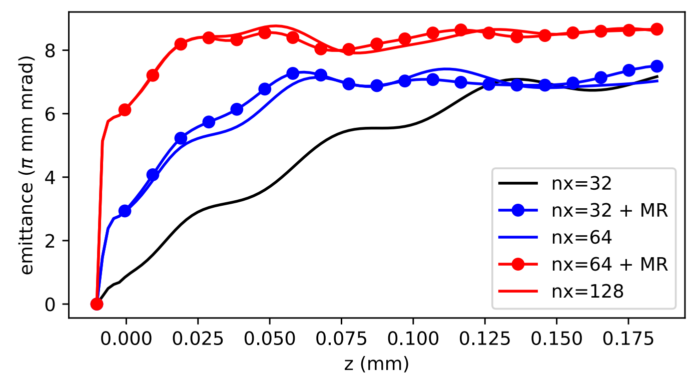
Laser driven **2-D** **Particle beam driven**







Simulations with small MR patch recover results using finer grid over the entire box.



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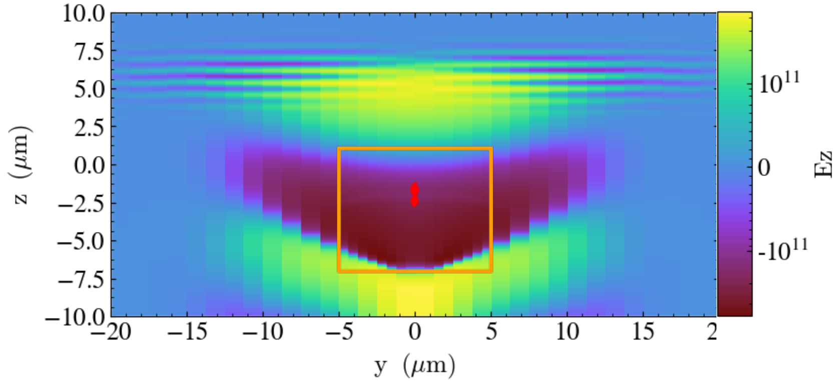
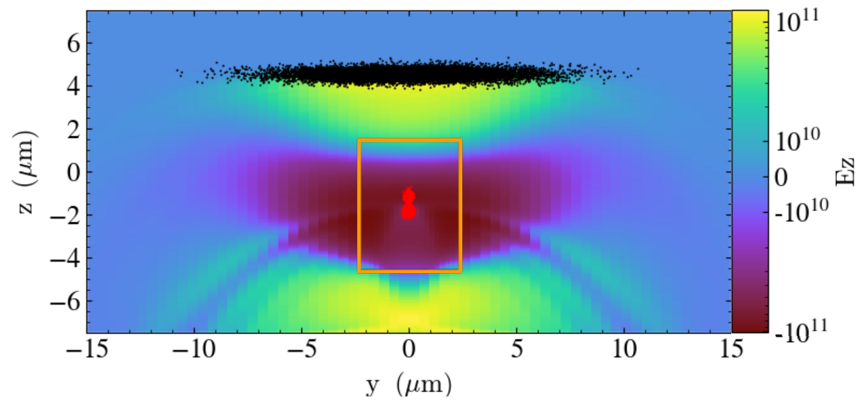
First simulations of plasma accelerators with MR patch (09/17)

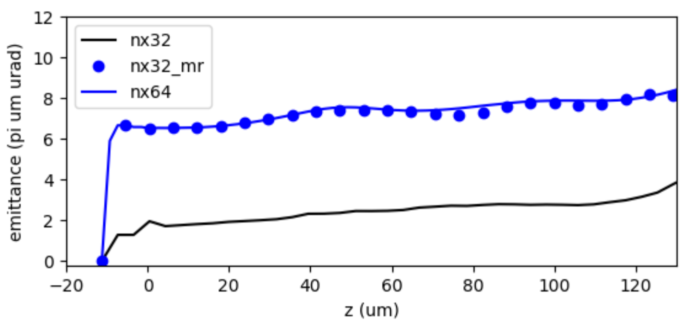
Laser driven

3-D

Particle beam driven







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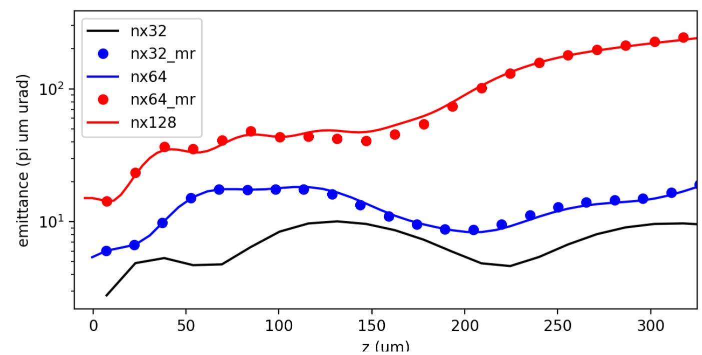

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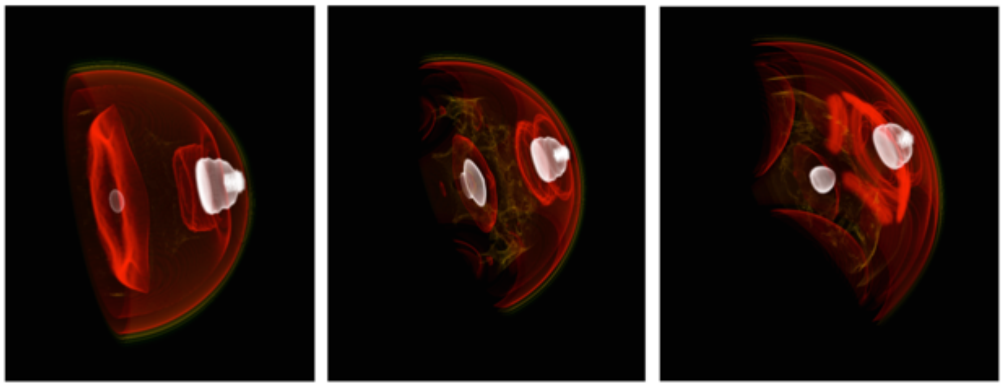
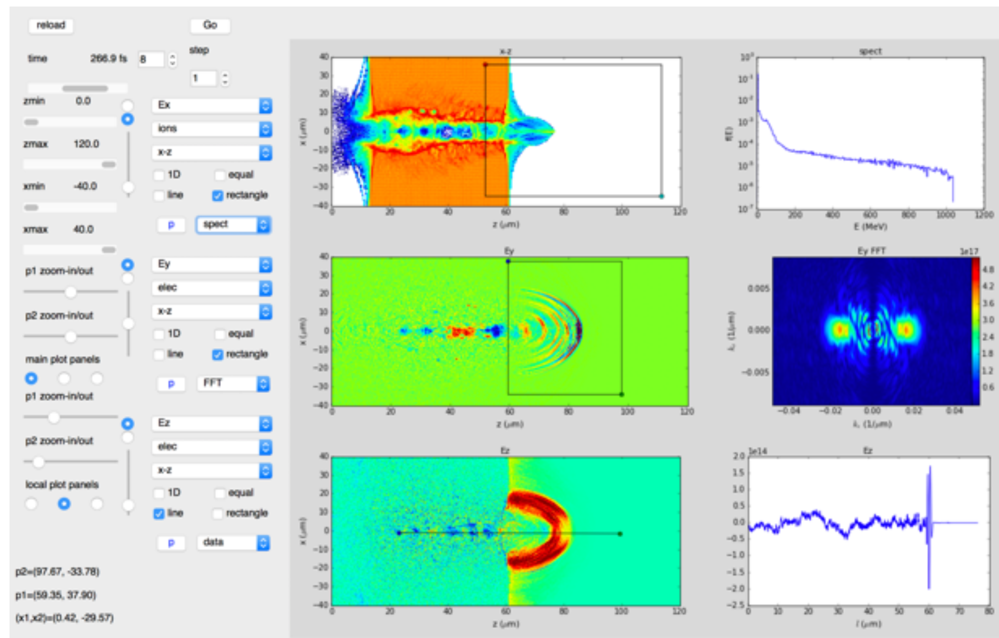
WarpX visualization tools are being developed

3D rendering of WarpX plasma accelerator simulation with yt



Prototype WarpX data analysis GUI



- 2D/3D visualization with matplotlib, yt, VisIt
  - Supports AMReX & OpenPMD data structures
- Interface using Python, Jupyter notebooks or GUI.

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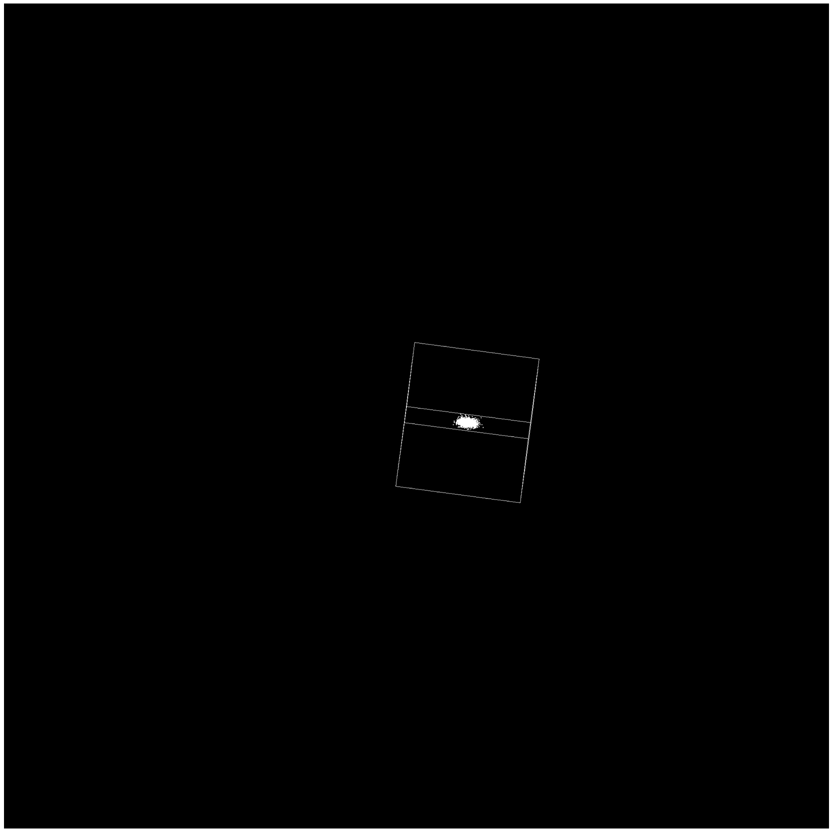
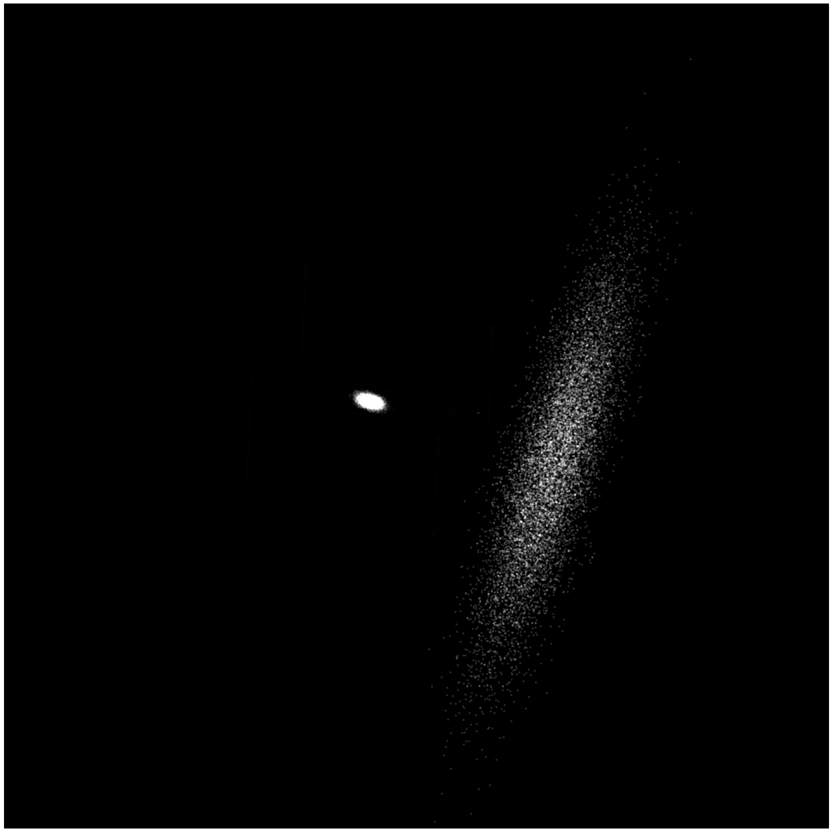
Examples of movies using Yt





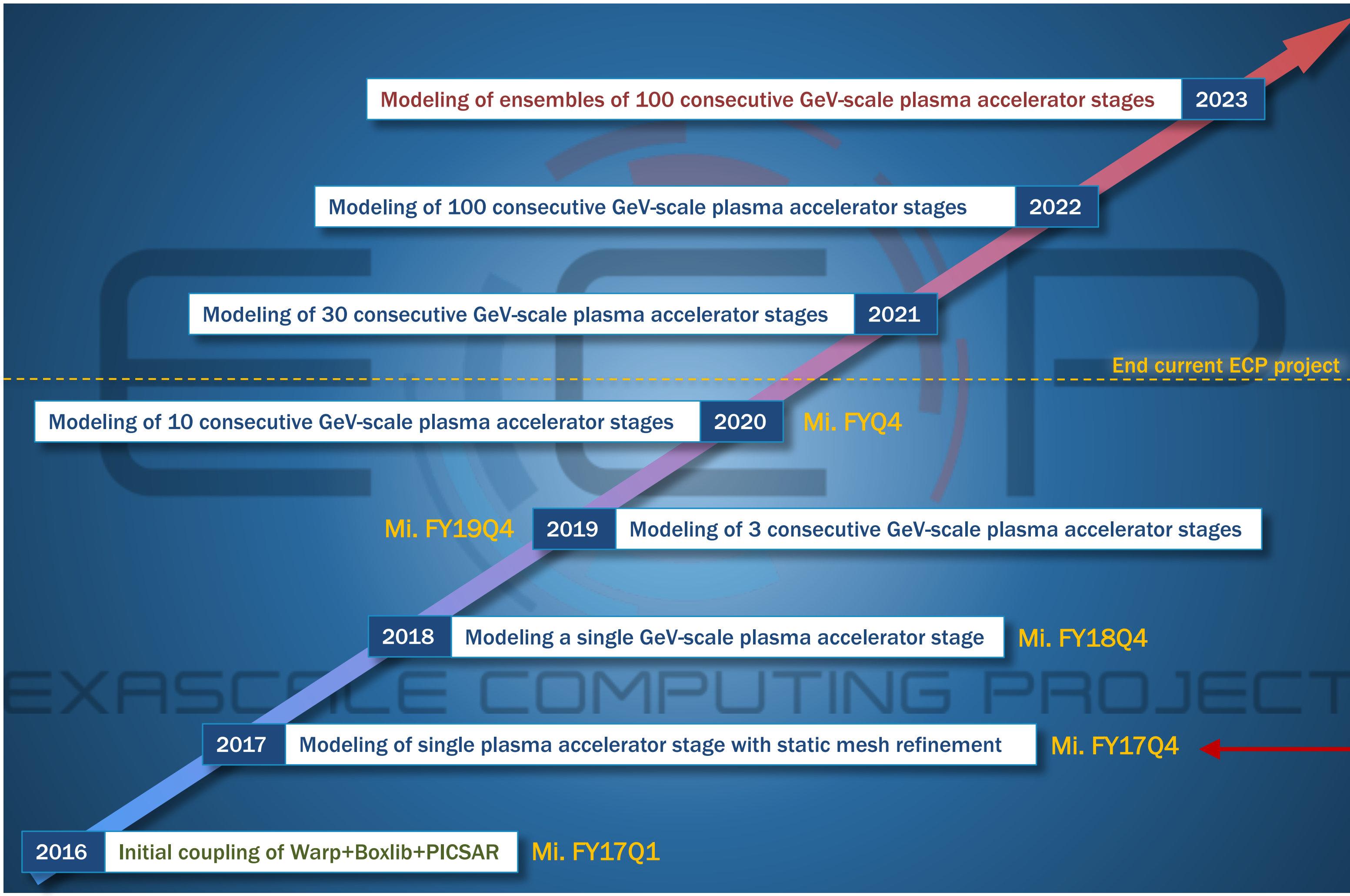
Movies by Maxence Thevenet

Outline

- Context & overview of the project
- Code structure
- Advanced algorithms
- Progress
- **Next steps**

7-year plan for Exascale project WarpX

From initial code coupling to ensemble of 100 GeV-scale stages



2nd ECP ExaFlop system

Aurora – 1 ExaFlops

Code to be released open source to community.

Now

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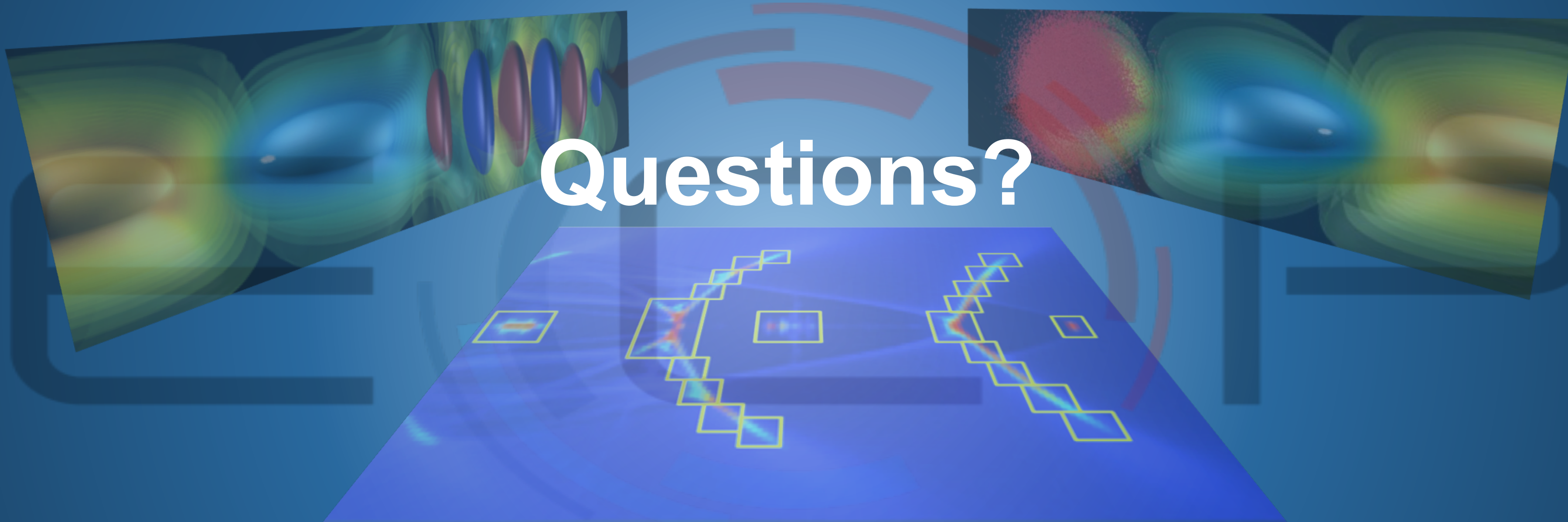
Thank you!

Questions?



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