NORDITA

Exascale Thinking of Particle Energization Problems

from 28 August 2017 to 01 September 2017 | Nordita, Stockholm

Numerical methods in WarpX and PICSAR:
new tools toward exascale AMR-PIC modeling of relativistic plasmas

Jean-Luc Vay - Lawrence Berkeley National Laboratory

with A. Almgren[1], J. Bell[1], G. Blaclard[5,1], L. Ge[3], B. Godfrey[4,1], D. Grote[2], M. Kirchen[6], O. Kononenko[3], M. Hogan[3], R. Lehe[1], M. Lobet[5], A. Myers[1], C. Ng[3], J. Park[1], R. Ryne[1], O. Shapoval[1], M. Thevenet[1], H. Vincenti[5,1], W. Zhang[1]

[1]Lawrence Berkeley National Laboratory
[2]Lawrence Livermore National Laboratory
[3]SLAC Accelerator National Laboratory
[4]U. Maryland
[5]CEA Saclay, France
[6]U. Hamburg, Germany

EXASCALE COMPUTING PROJECT

National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY | Office of Science

Outline

- Context & overview of the project
- Code structure, libraries & optimization on Intel KNL
- Advanced algorithms
- Progress
- Next steps & Summary

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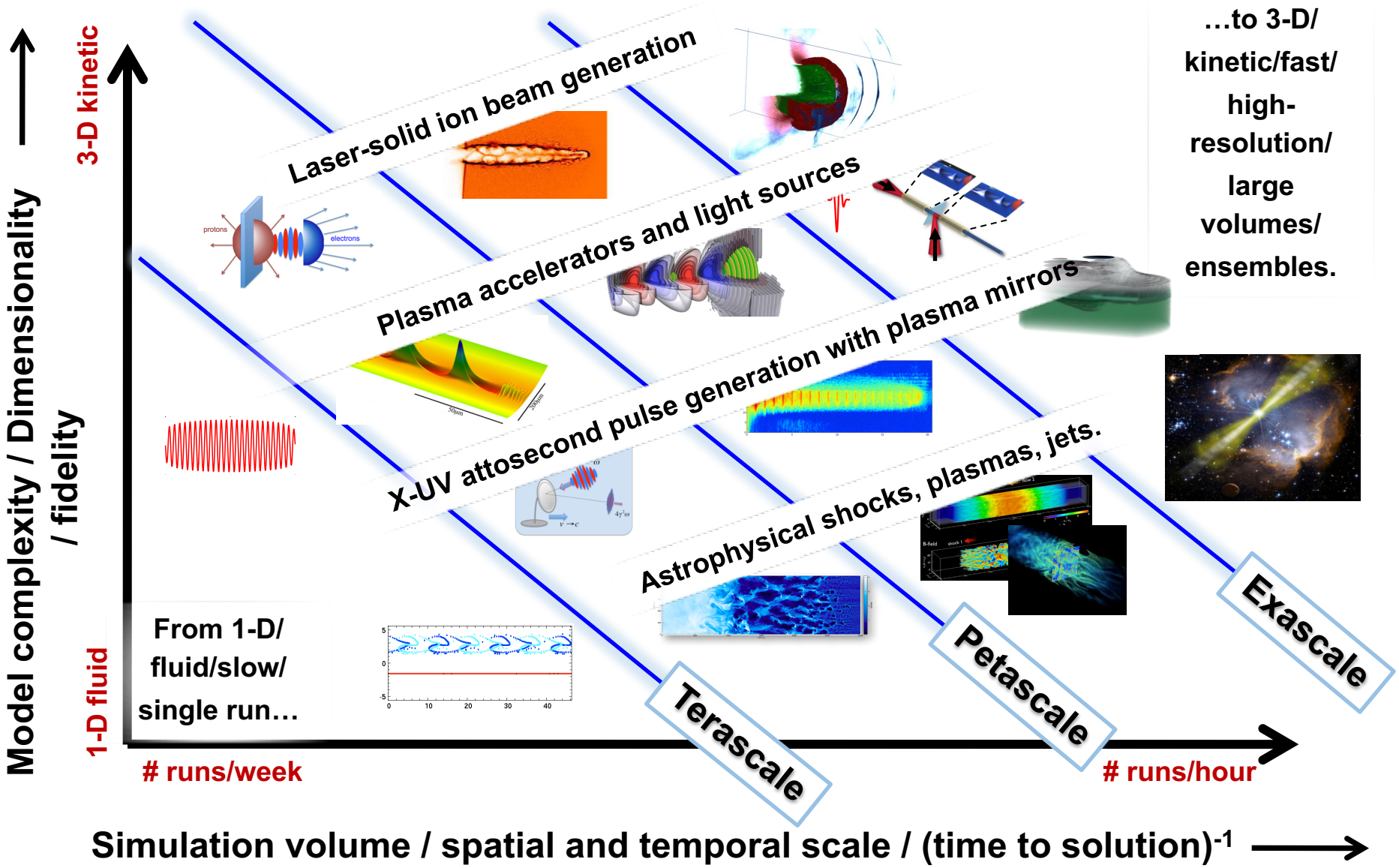
Plasma physics modeling is complex

- Rich physics, full of real instabilities, and even more spurious numerical instabilities
- Large range of space and time scales
- Field has fostered the development of better algorithms and pushed toward use of supercomputers
- The trend continues ➔ need for more accurate, stable algorithms with implementations that take advantage of emerging architectures and scale to future exascale machines

Plasma applications need more accurate, faster codes



U.S. DOE Exascale Computing Project (ECP)

- 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.
  - DOE is a lead agency within NSCI, along with DoD and NSF
  - Deployment agencies: NASA, FBI, NIH, DHS, NOAA
- ECP's work encompasses
  - applications,
  - system software,
  - hardware technologies and architectures, and
  - workforce development to meet scientific and national security mission needs.

EXASCALE COMPUTING PROJECT

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

Particle accelerators are essential tools in modern life

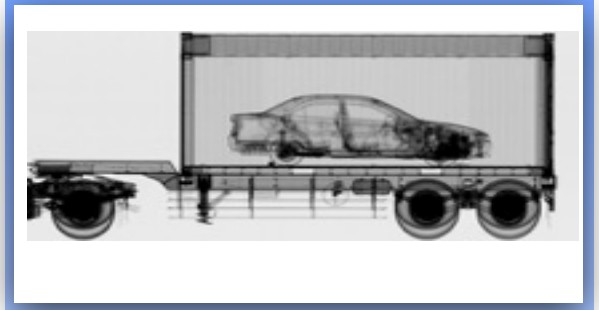
Medicine

- ~9000 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

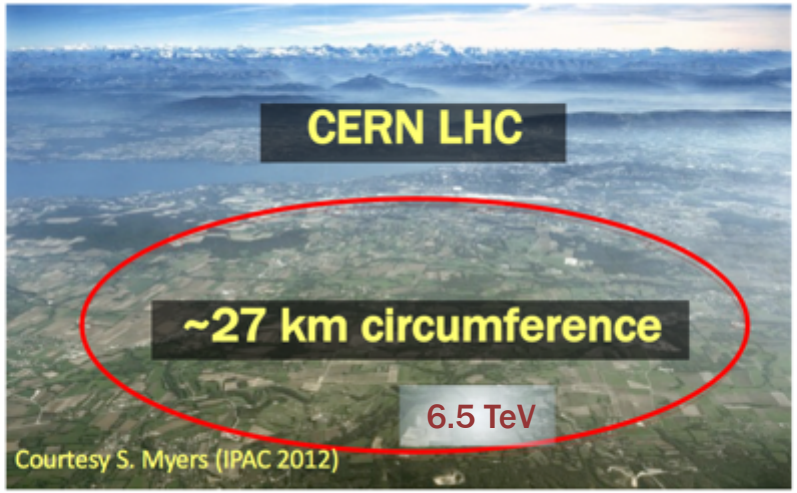
Opportunity for much bigger impact by reducing size and cost.

Plasma-based acceleration has the potential to make accelerators small (again), and cut cost dramatically

E. O. Lawrence

First cyclotron ~0.1 MeV

1930



W. Leemans

Plasma accelerator 1 GeV

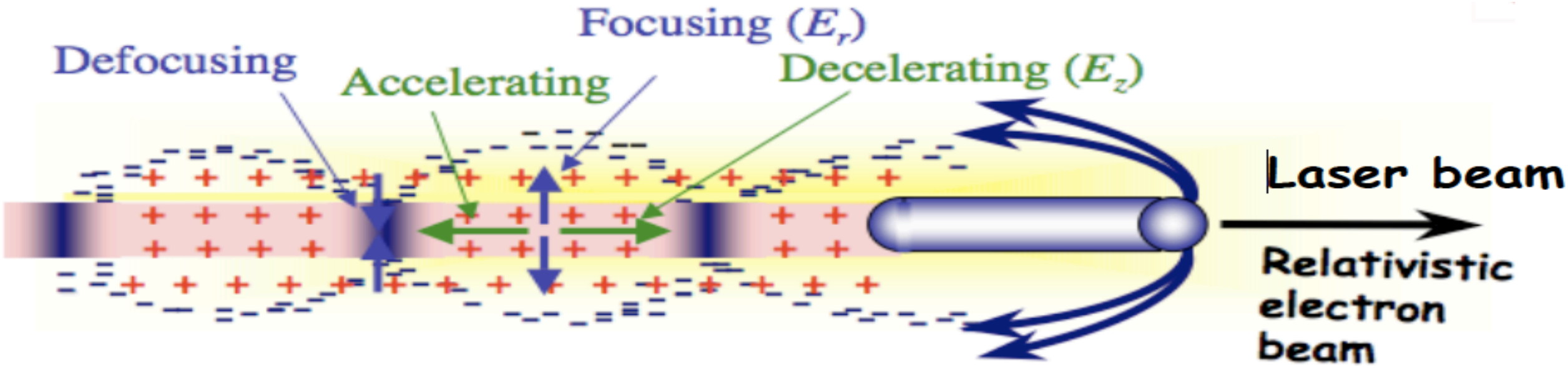
2009

Tens of plasma accelerator stages needed for a 1 TeV e^-e^+ collider.

BUT: simulations in 2-D can take days for 1 stage (even at insufficient resolution for collider beam quality).

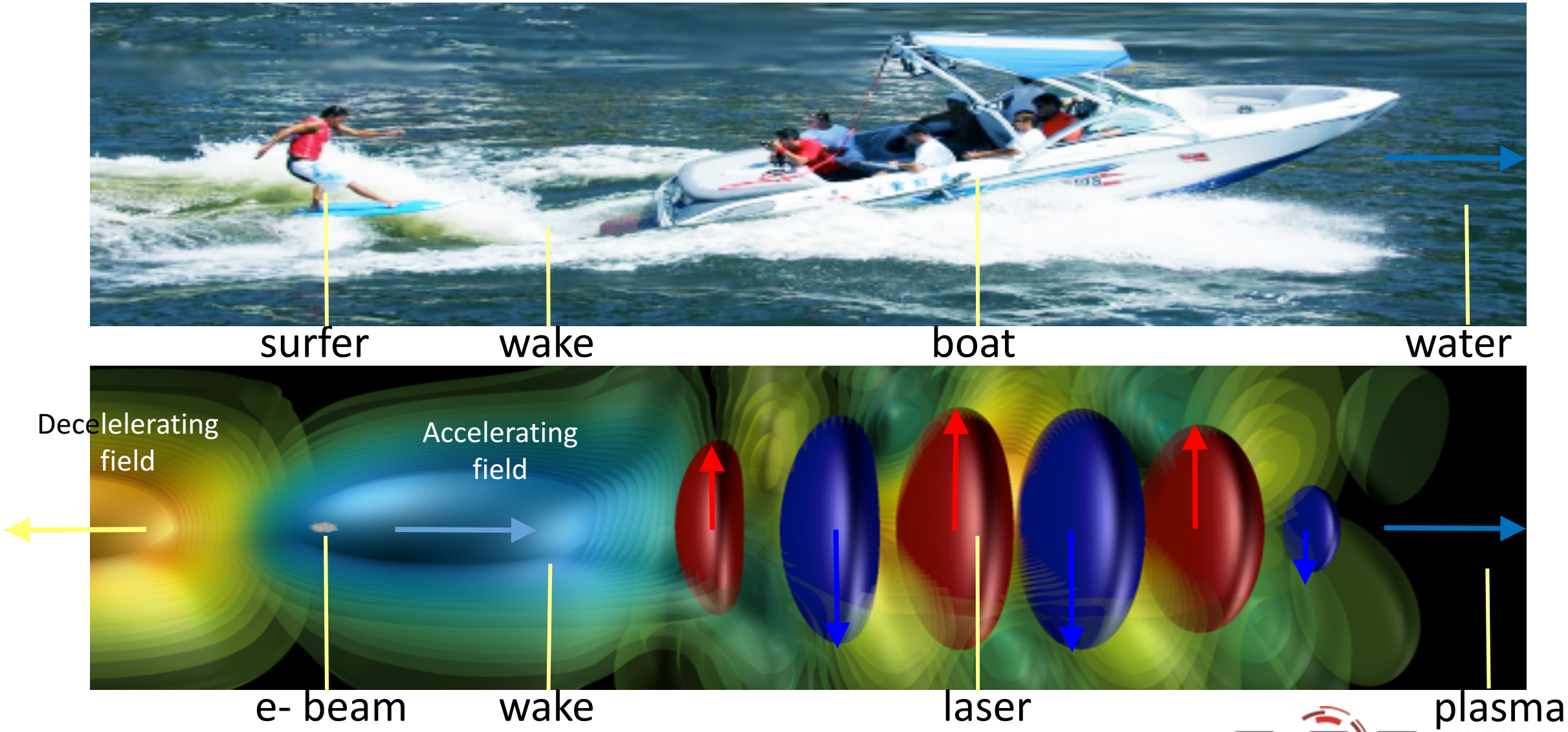
➔ ***Full 3-D modeling of tens of stages intractable without Exascale computing.***

Plasma accelerators “surf” electrons on plasma waves for *acceleration on ultra short distances*

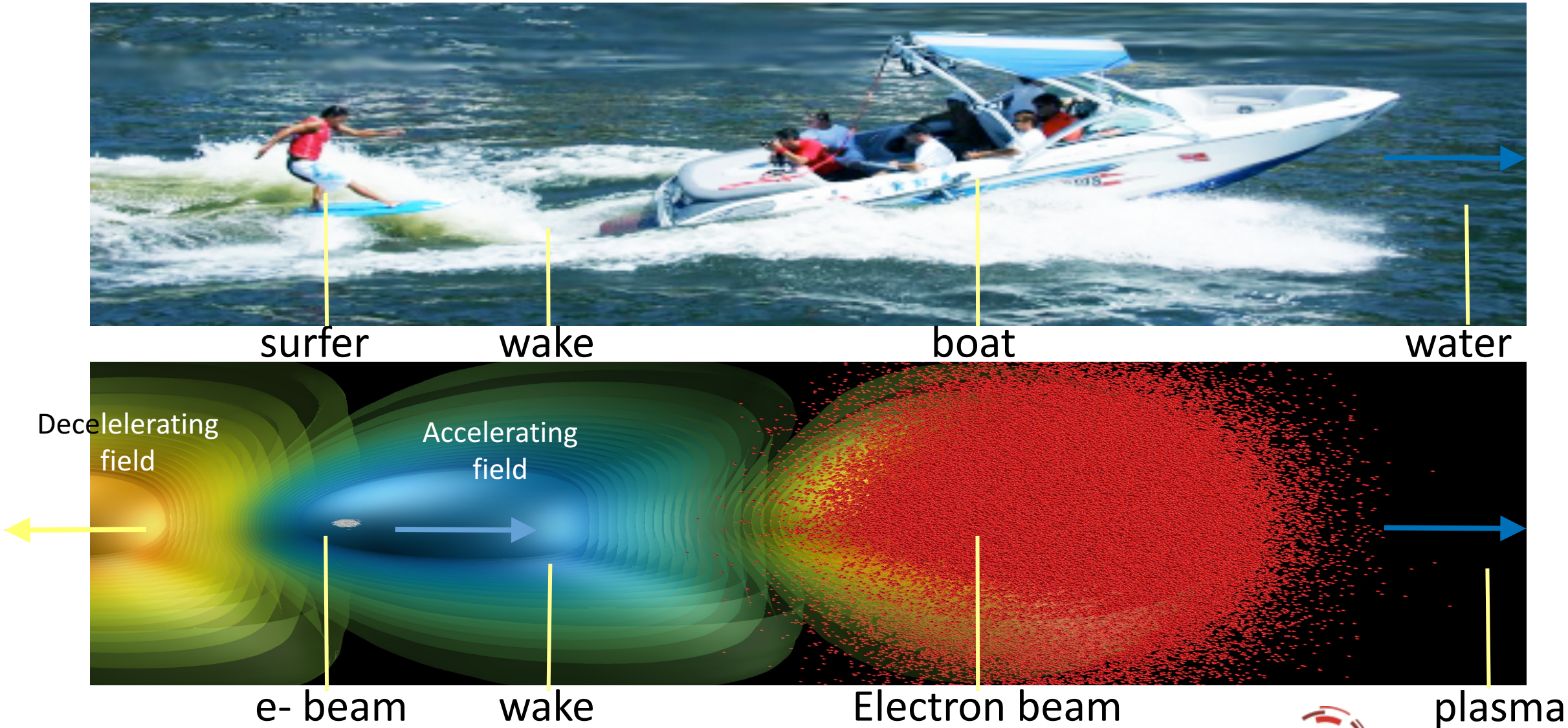


- Esarey, Schroeder, Leemans, Rev. Mod. Phys. 2009

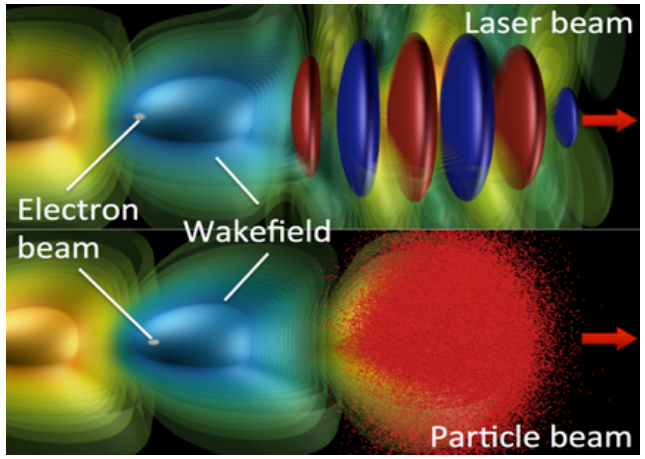
Example from simulation of laser-driven plasma accelerator



Example from simulation of particle beam-driven plasma accelerator



Plasma accelerators are challenging to model



Short driver/wake propagates through long plasma

➔ Many time steps.

For a 10 GeV LPA scale stage:

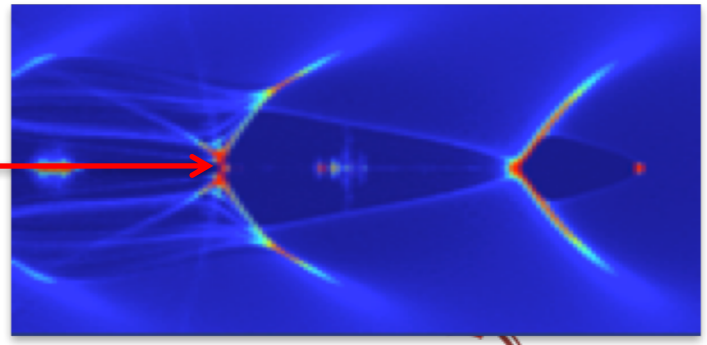
~**1μm** wavelength laser propagates into ~**1m** plasma

➔ millions of time steps needed

Non-linear regime:

very small features

➔ small grid cells

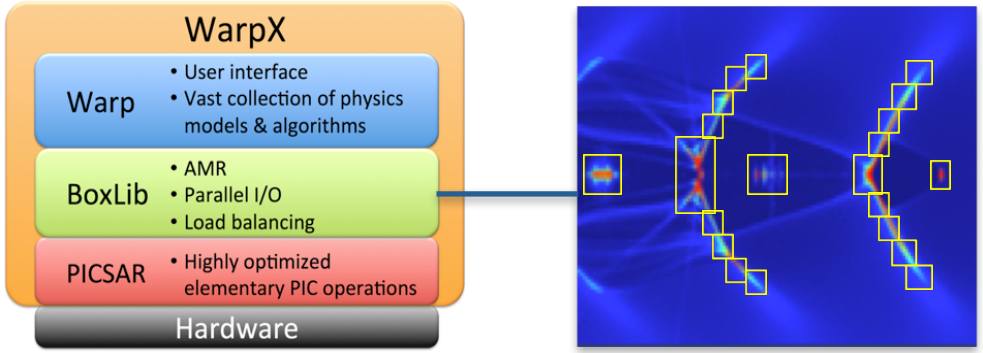


ECP Project WarpX: Exascale Modeling of Advanced Particle Accelerators

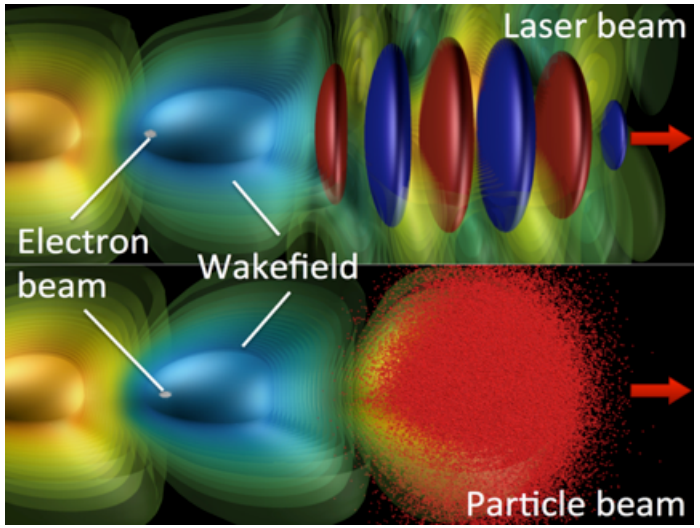
Goal (4 years): Convergence study in 3-D of 10 consecutive multi-GeV stages in linear and bubble regime, for laser- & beam-driven plasma accelerators.

How: ➔ Combination of most advanced algorithms

➔ Coupling of Warp+BoxLib/AMReX+PICSAR



➔ Port to emerging architectures (Xeon Phi, 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!

PI: Jean-Luc Vay (LBNL)

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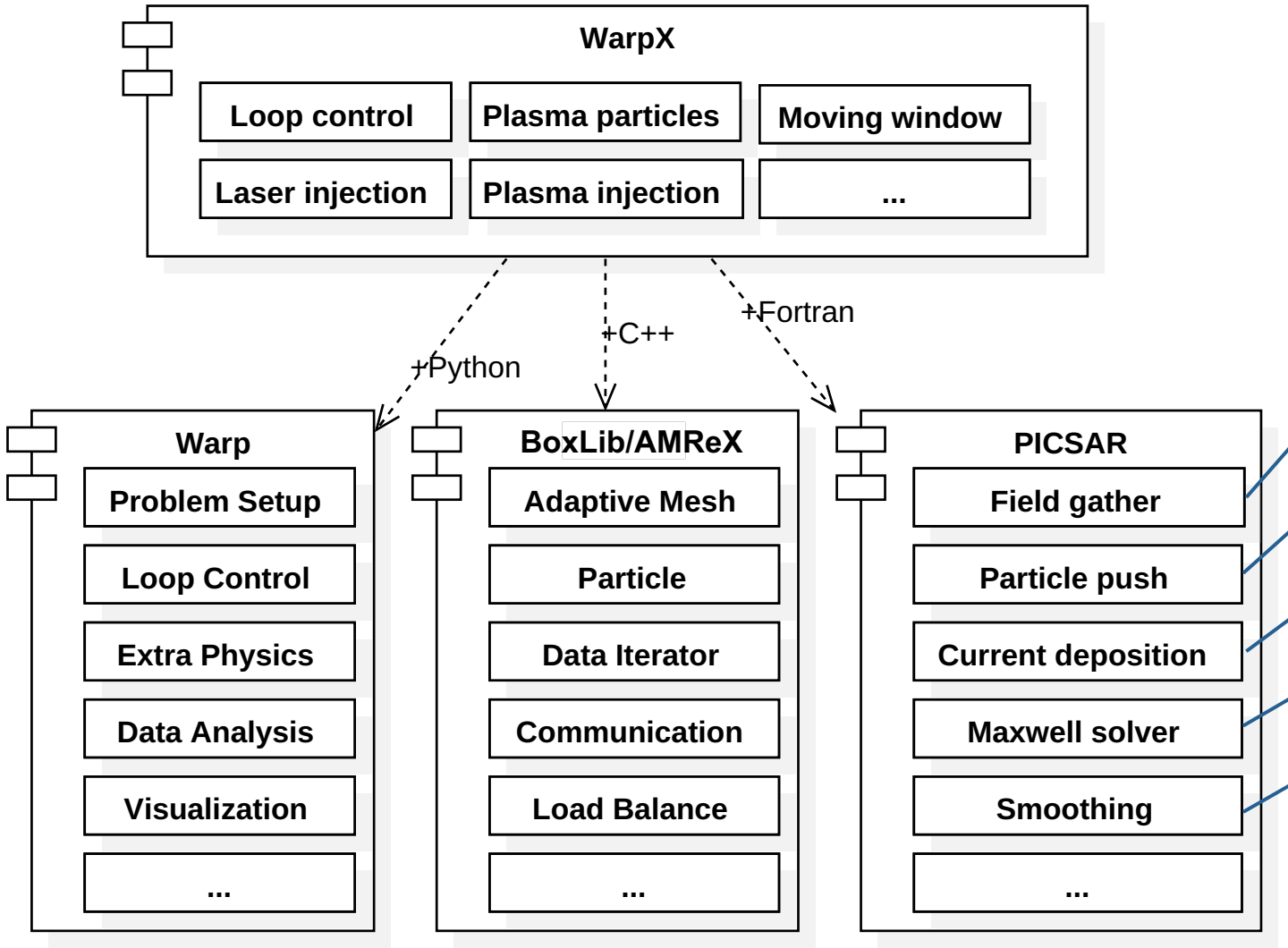
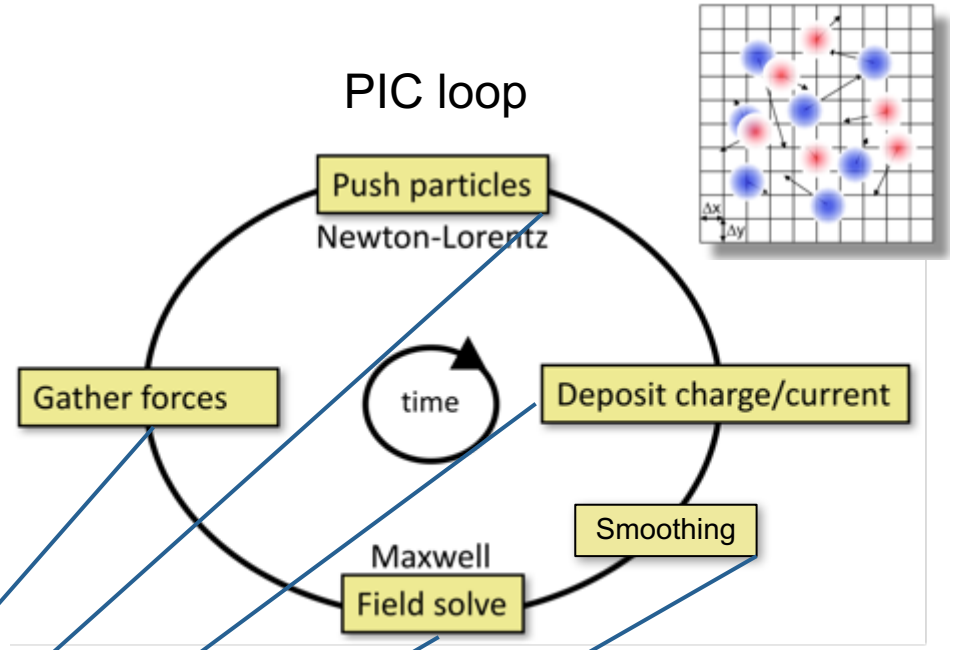
UML Diagram of WarpX details code structure





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

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

NESAP Codes

NERSC

Advanced Scientific Computing Research
Almgren (LBNL) **BoxLib AMR Framework**
Trebotich (LBNL) **Chombo-crunch**

High Energy Physics
Vay (LBNL) **WARP & IMPACT**
Toussaint(Arizona) **MILC**
Habib (ANL) **HACC**

Nuclear Ph
Maris (Iowa
Joo (JLAB)
Christ/Kars
(Columbia/

Basic Energy Sciences
Kent (ORNL) **Quantum Espresso**
Deslippe (NERSC) **BerkeleyGW**
Chelikowsky (UT) **PARSEC**
Bylaska (PNNL) **NWChem**
Newman (LBNL) **EMGeo**

Biological and Environmental Research
Smith (ORNL) **Gromacs**
Yelick (LBNL) **Meraculous**
Ringler (LANL) **MPAS-O**
Johansen (LBNL) **ACME**
Dennis (NCAR) **CESM**

U.S. DEPARTMENT OF ENERGY | Office of Science

Mathieu Lobet

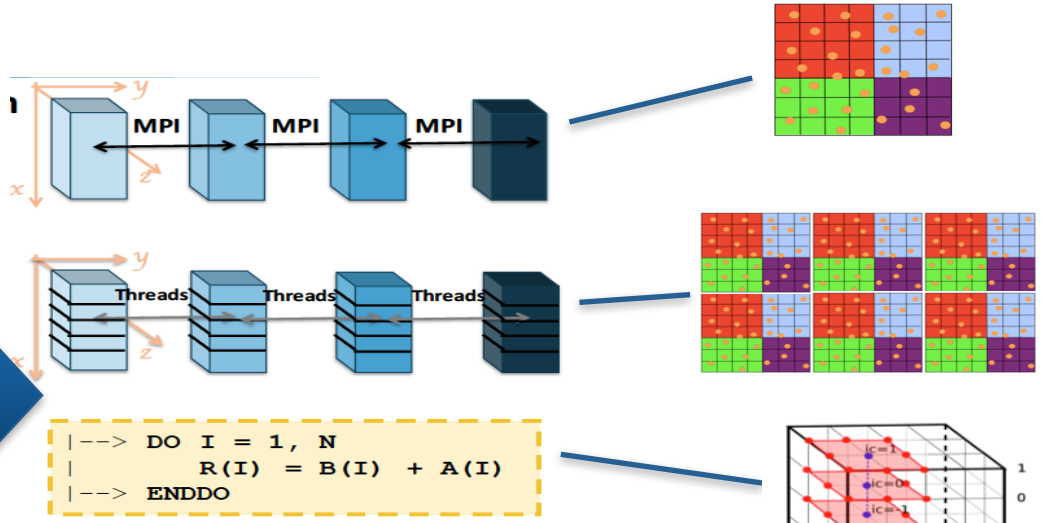
Ex-NESAP postdoc
(now at CEA, Saclay, France)

Collaboration with Henri Vincenti

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

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

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

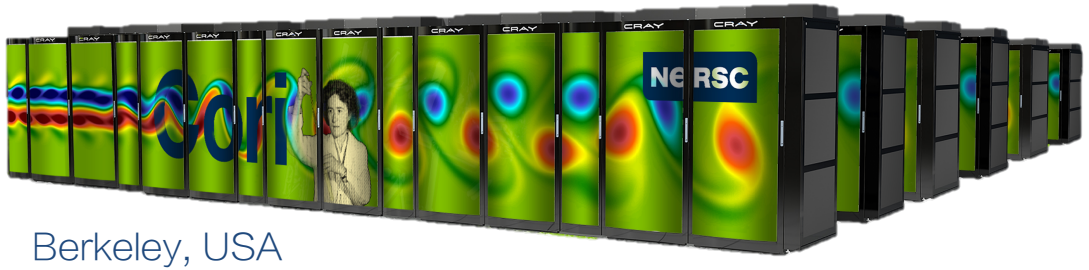


*H. Vincenti, R. Lehe, R. Sasanka and J.-L. Vay, *Comp. Phys. Comm.* , 210, 145-154 (2017).

PICSAR website: https://picsar.net – to be open source access soon.

EXASCALE COMPUTING PROJECT

Newest NERSC supercomputer based on Intel KNL

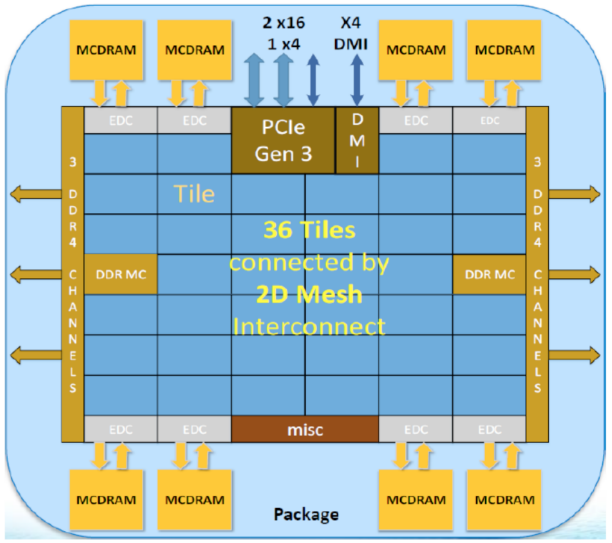


Berkeley, USA

Cori*:

- 9,688 Intel KNL nodes (658,784 cores)
- 29.1 PFlops total (theoretical peak)
- # 6 on top500 list

Intel KNL



Peak performance: 3 TfFops per socket:

- 68 cores at 1.4–1.6 Ghz for energy performance
- 4 threads/core
- 2 VPU AVX-512 vector register per core (up to 16 DP floats)
- 34 Mb L2 cache per node but no L3

KNL does not forgive optimization laziness anymore

- Frequency divided by 2 per core
- No low latency L3 cache

[1] www.nersc.gov

Courtesy J. Deslippe, M. Lobet

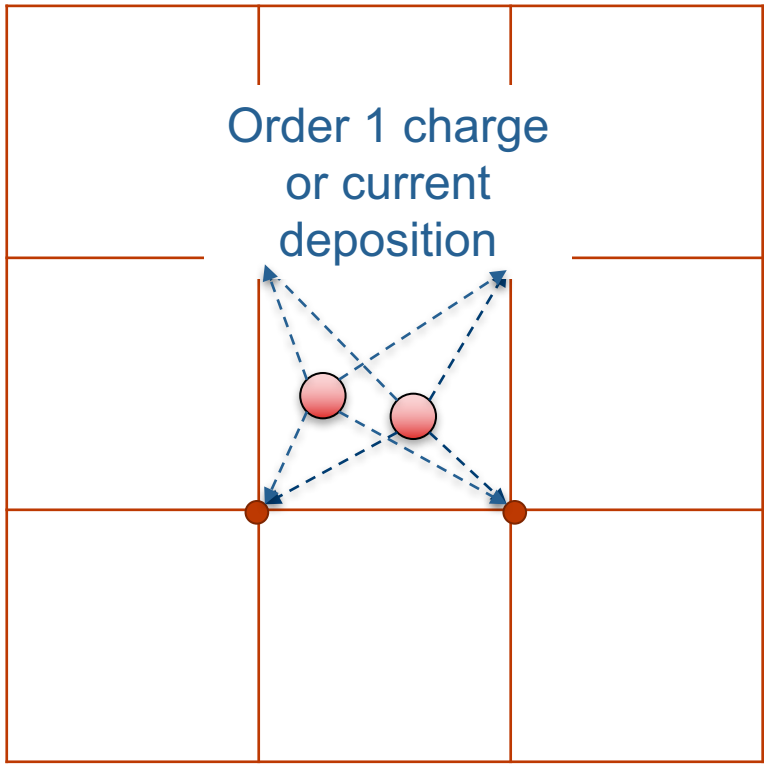
Charge/current deposition leads to Vectorization bottleneck

Data is also not contiguous in memory

```
! Charge deposition simplified algorithm

For each particle in a tile:

   1) Determine nearby nodes on the charge grid

   2) Compute current/charge of the particle

   3) Deposit contributions to the charge grid
```

- Step 1) & 2) can be vectorized
- Step 3) prevents vectorization due to memory races when 2 particles are in the same cell
- Grid nodes not aligned in memory: gather/scatter

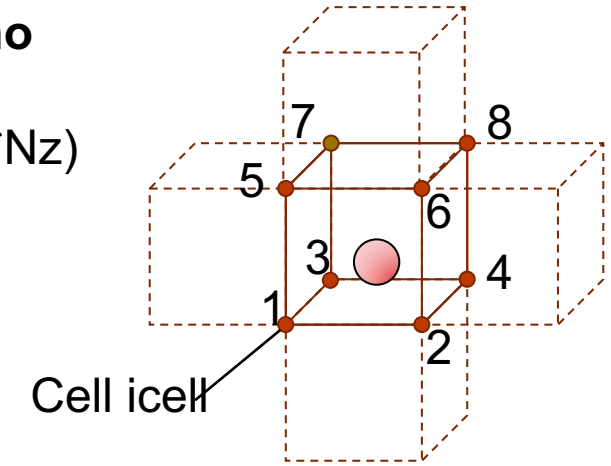
- Charge rho(NCELLS)
- Current grids Jx(NCELLS), Jy(NCELLS), Jz(NCELLS)



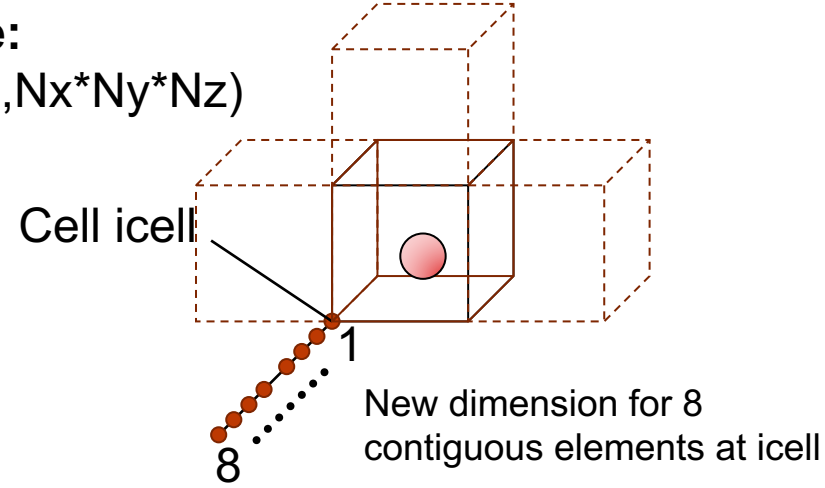
Revised data structure enables vectorization*

And contiguous data in memory

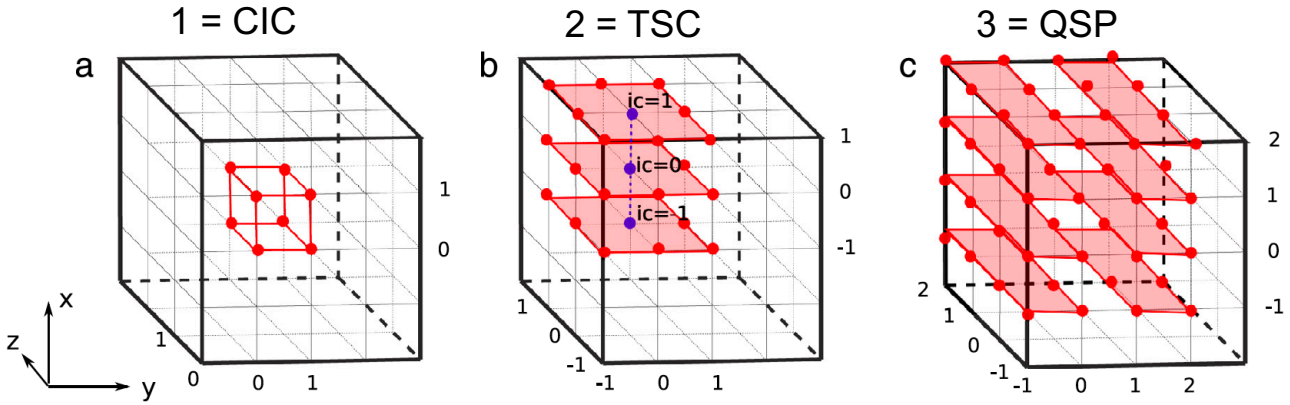
Original Rho structure:
Rho(Nx*Ny*Nz)



New Rhocell structure:
Rhocell(8,Nx*Ny*Nz)



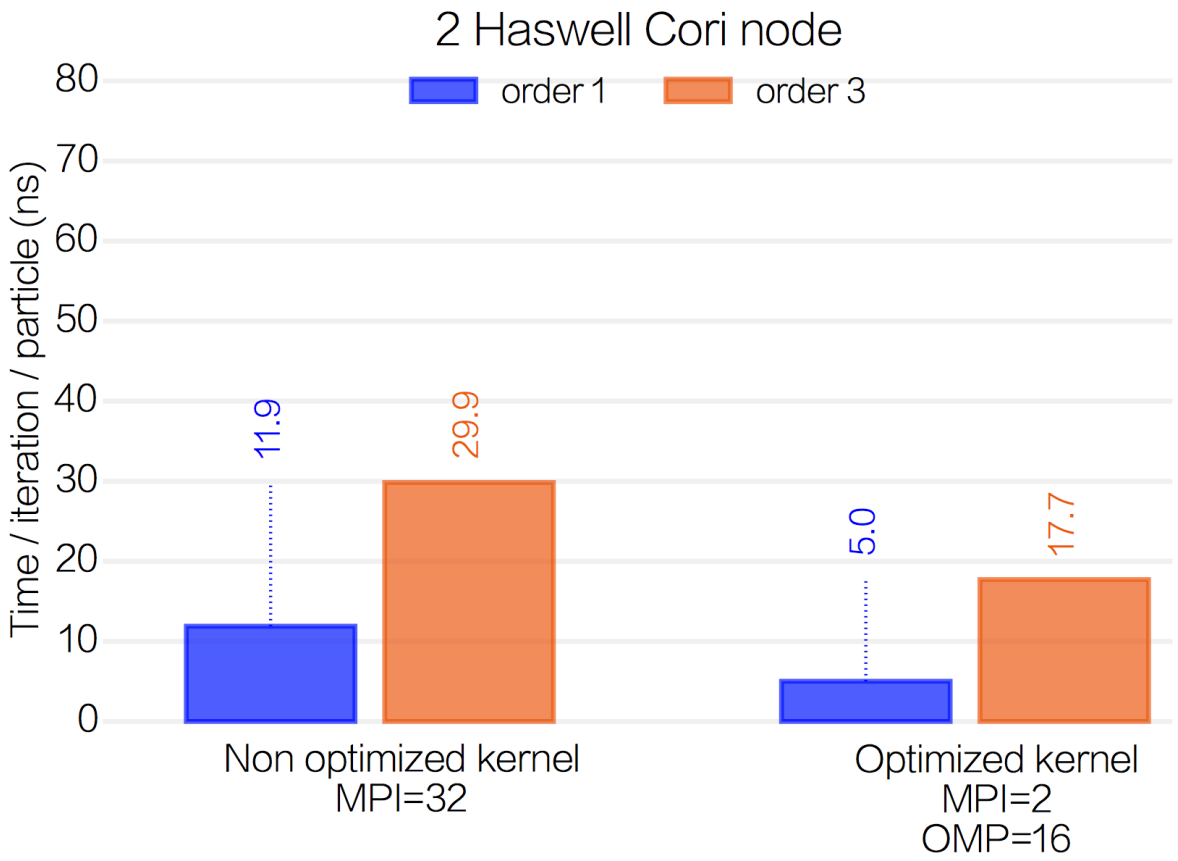
Order of deposition

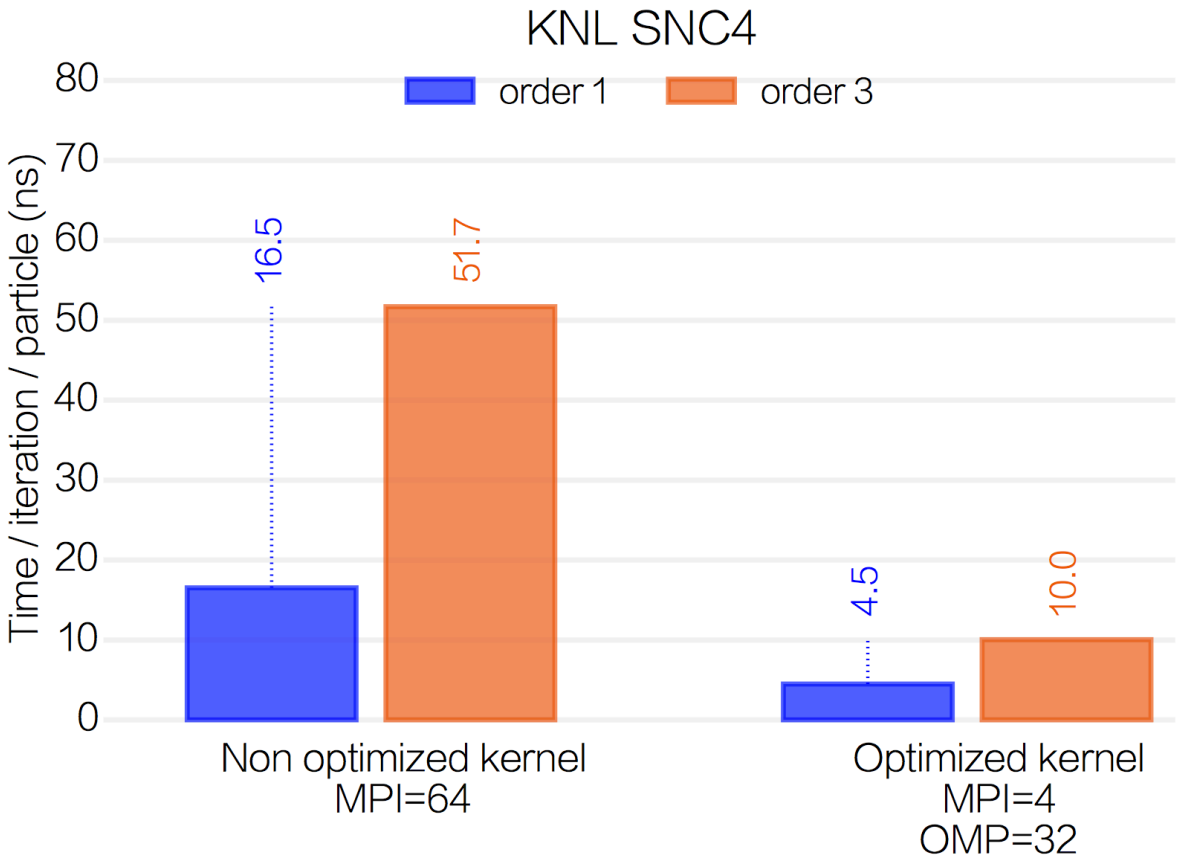


- New dimension in the current and charge array to access vertices of a cell in a contiguous way
- Enable vectorization of the deposition with no memory races, no gather/scatter
- Reduction at the end in the original structure: Non-efficient vectorization but in O(Ncells) with Ncells << Nparticles

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

PICSAR single-node performance on Haswell and KNL





Speed-up of 2 on Haswell node

Speed-up of 5 on KNL node

With optimizations, KNL is 1.8 times faster than Haswell node at order 3

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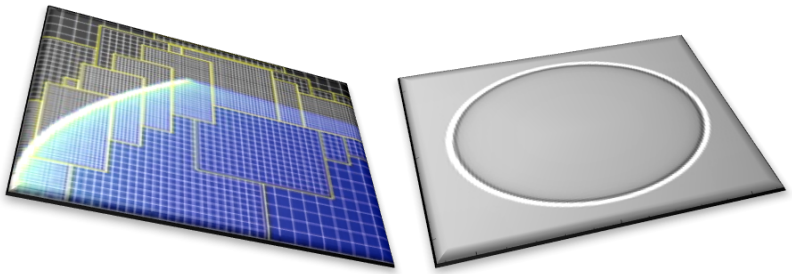
We will combine advanced algorithms

Lower # time steps:

- optimal Lorentz boosted frame

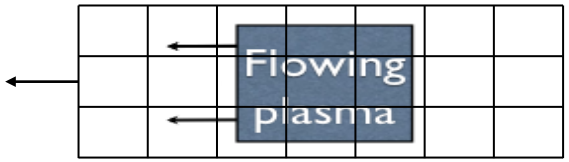
Higher accuracy:

- AMR
- Pseudo-spectral Analytical Maxwell solvers



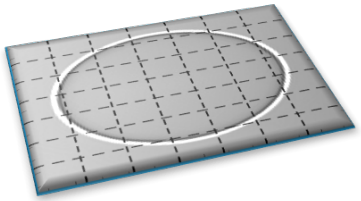
Higher stability

- Galilean T. to suppress Numerical Cherenkov Instability



Higher scalability

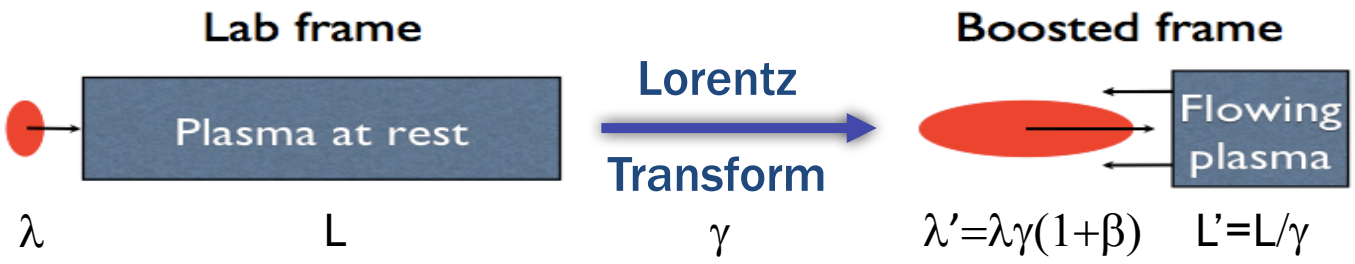
- FFT Maxwell solvers on local domains + domain decomposition



We are combining advanced algorithms

Lower # time steps:

- optimal Lorentz boosted frame



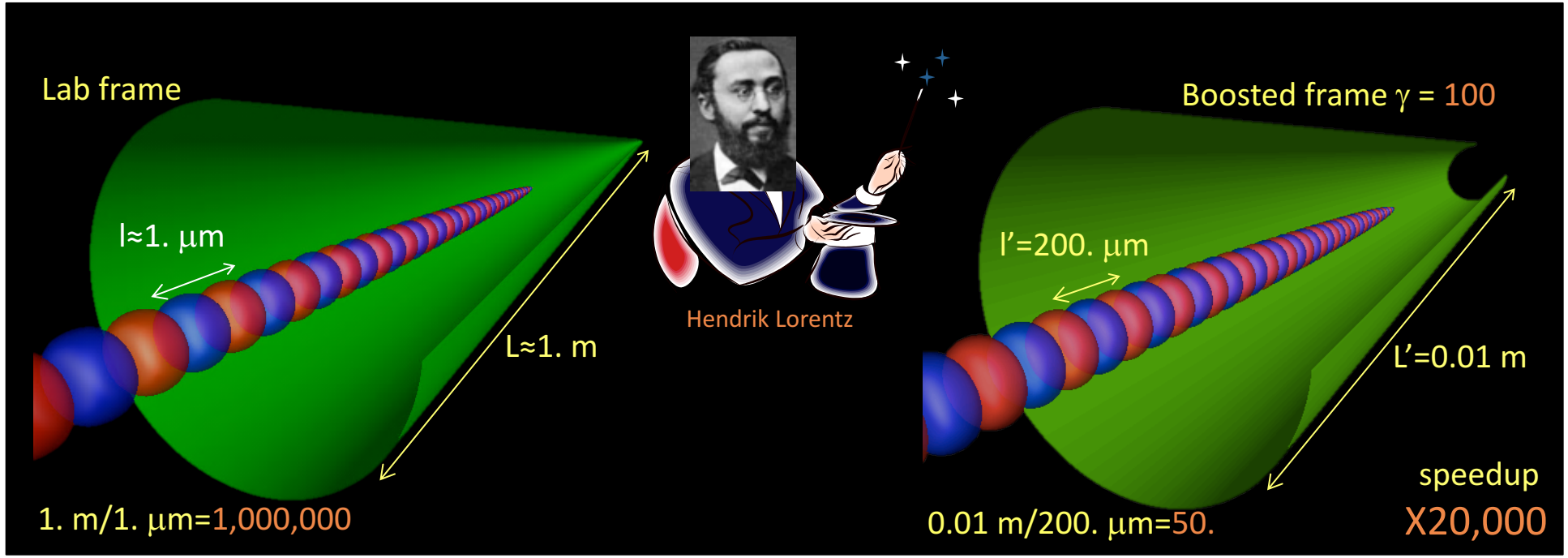
λ L γ $\lambda'=\lambda\gamma(1+\beta)$ $L'=L/\gamma$

time steps α L/λ

time steps α L'/λ'

➔ Speedup = $(L'/\lambda')/(L/\lambda) = \gamma^2(1+\beta)$

Example: 10 GeV scale laser-plasma accelerator stage

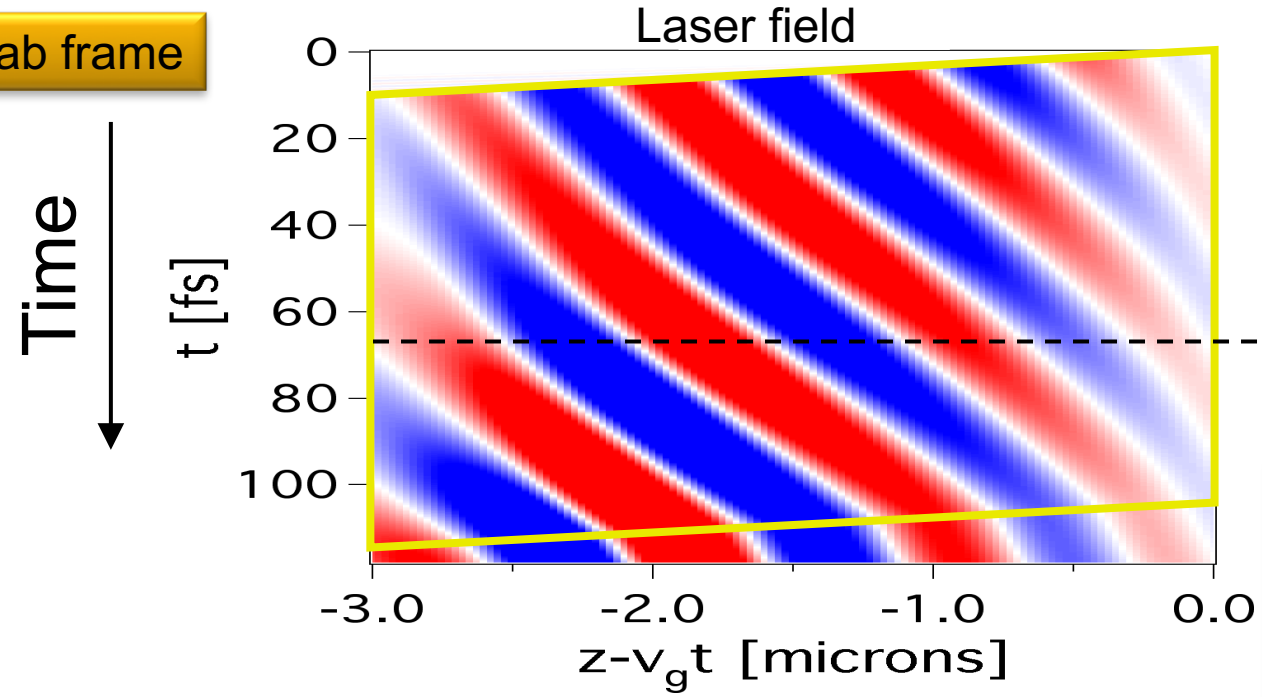


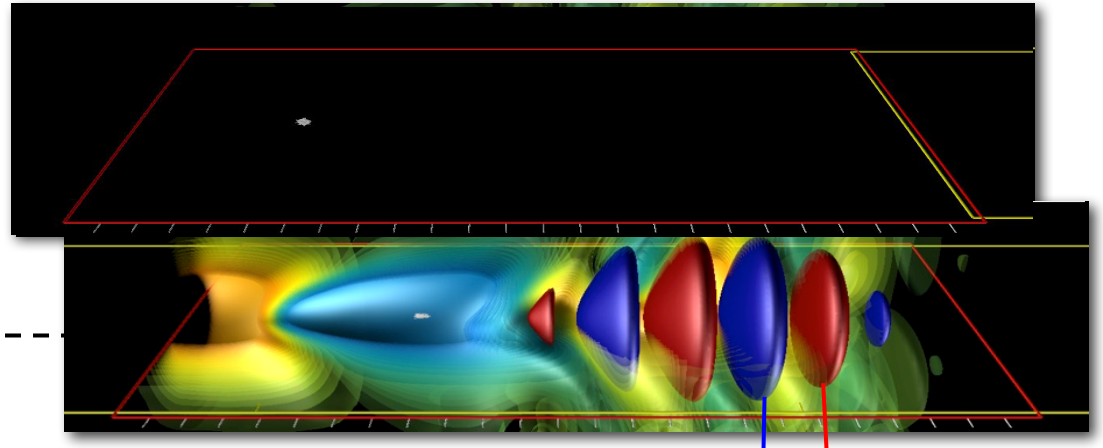
Faster, but:

- plasma with relativistic drift is sensitive to numerical Cherenkov instability (NCI)
- physics in boosted frame looks different from physics in lab frame

  ➔ need to transform data back to lab. Frame.

Lab frame

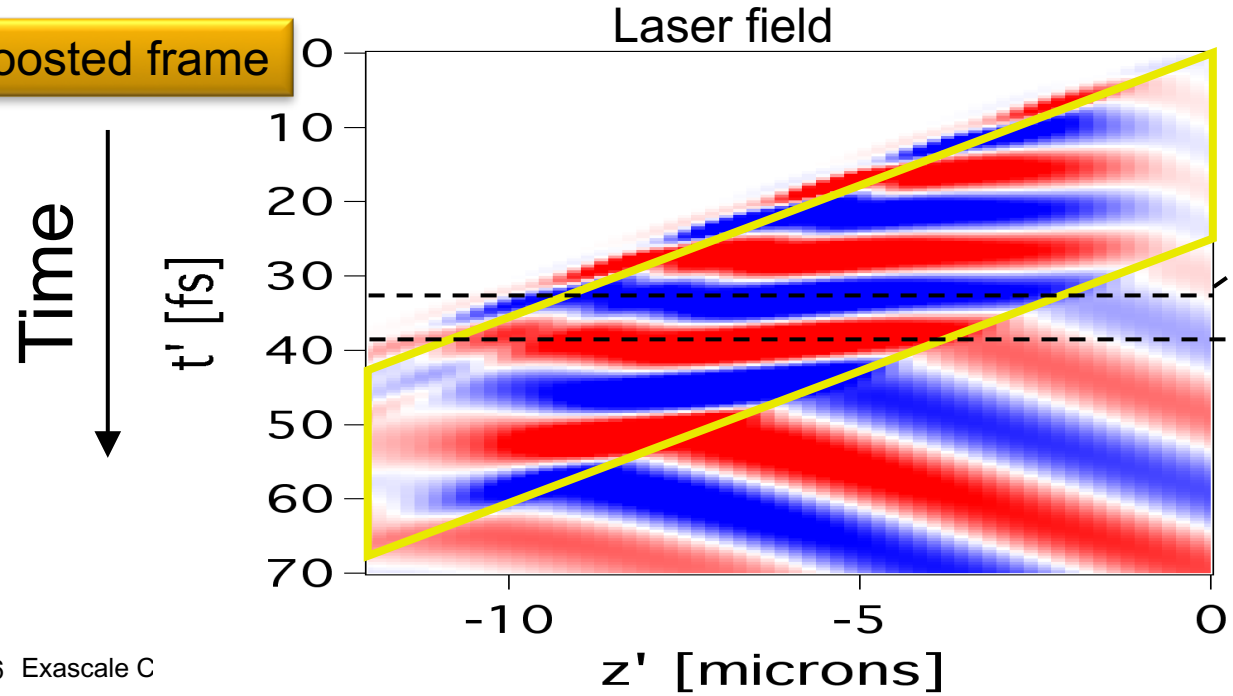


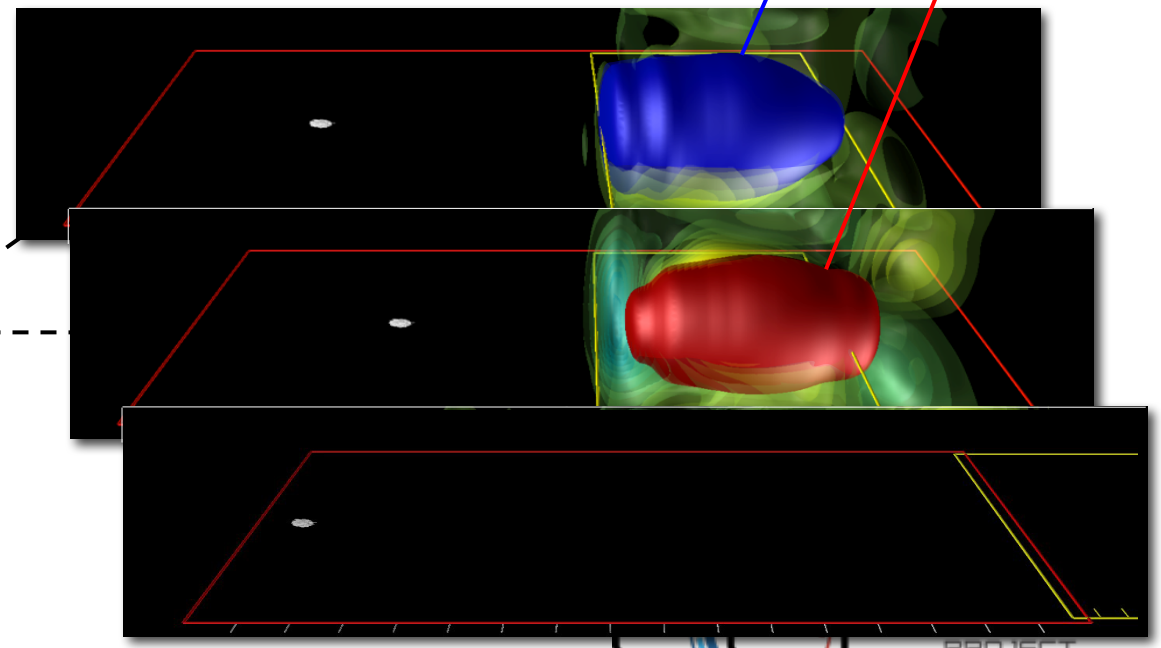


Hyperbolic rotation from Lorentz Transformation converts laser…

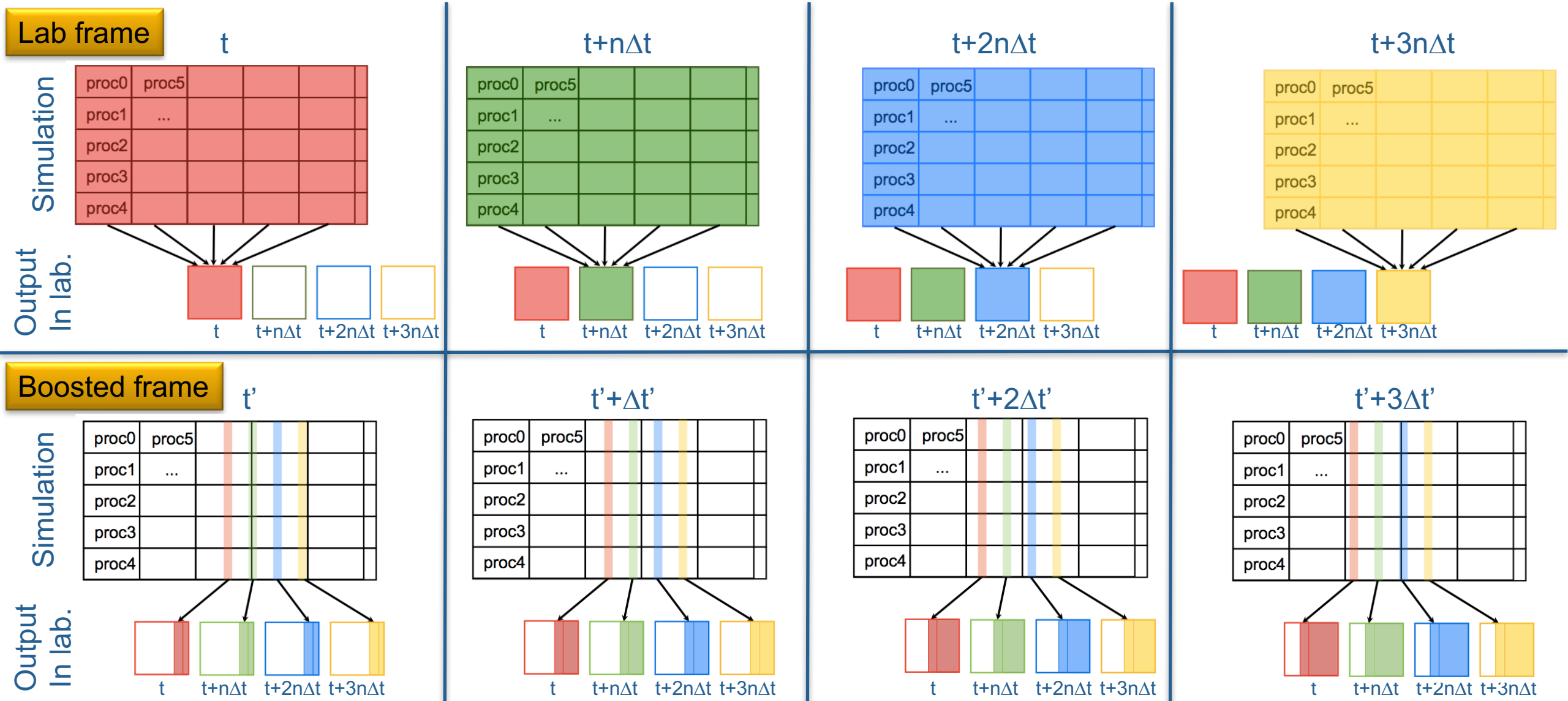
…*spatial oscillations* into *time beating*

Boosted frame





Specialized output needed to reconstruct data in lab frame



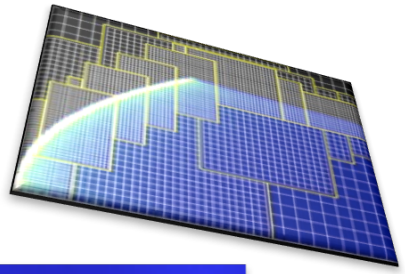
We are combining advanced algorithms

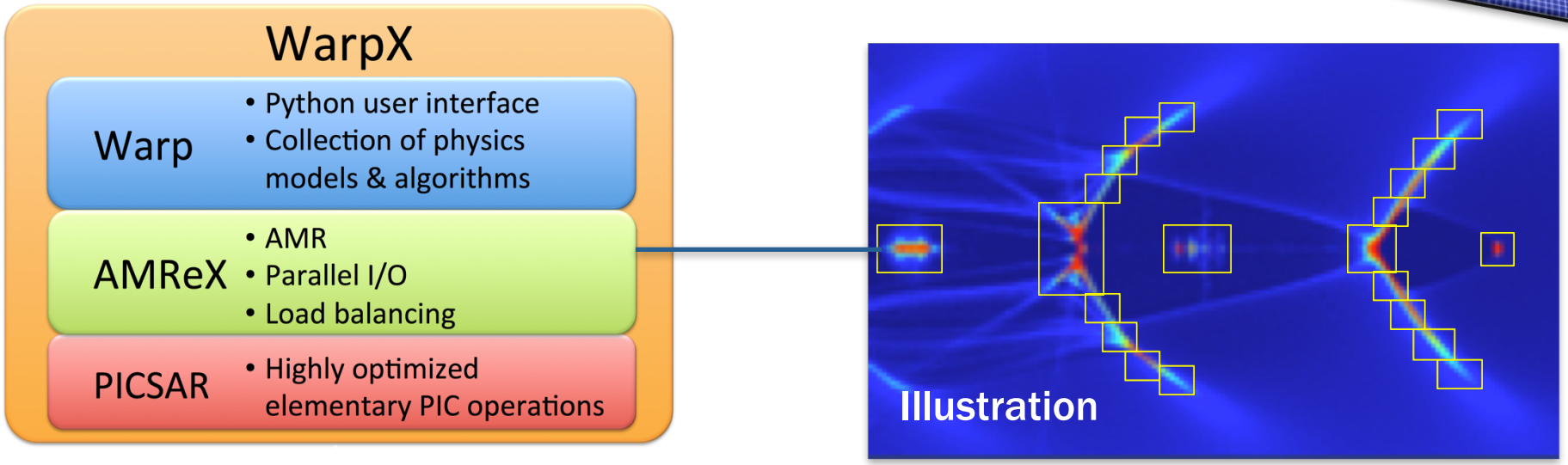
Lower # time steps:

- optimal Lorentz boosted frame

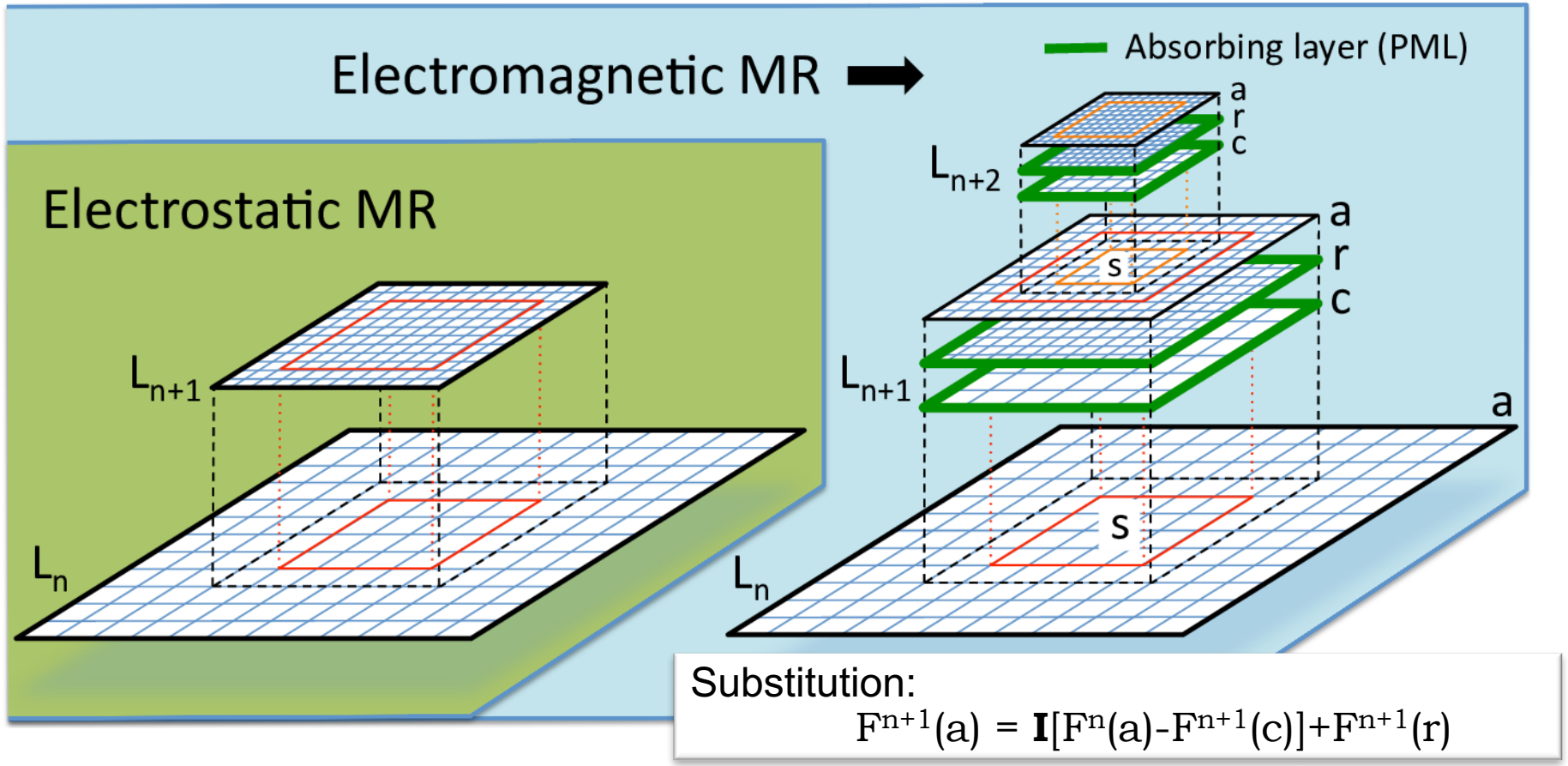
Higher accuracy:

- 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

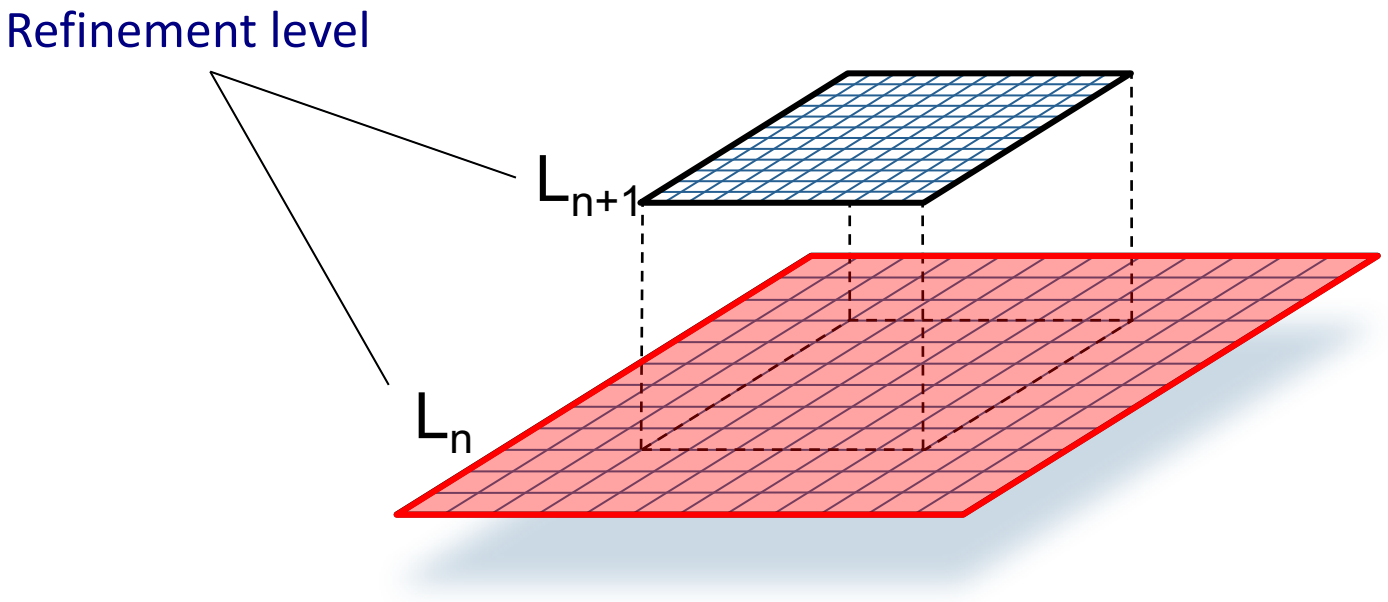
$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

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

$$\frac{\partial F}{\partial t} = \nabla \cdot \mathbf{E} - \rho$$

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).

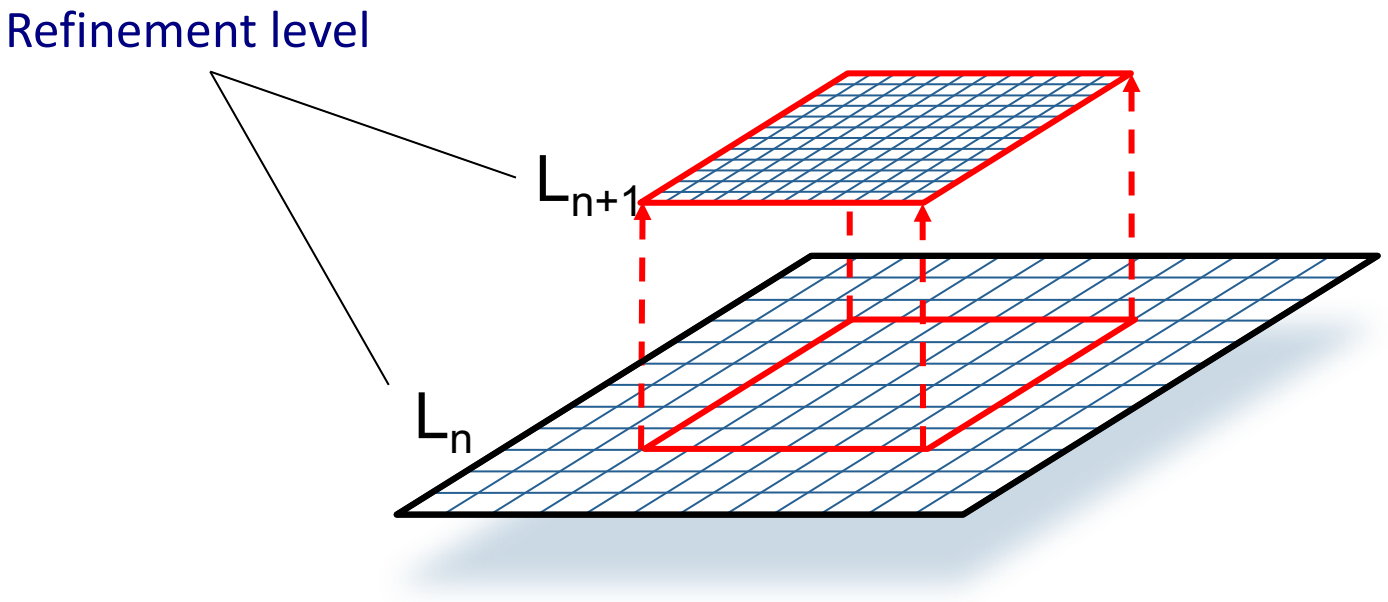
Electrostatic mesh refinement algorithm is straightforward



Solving boundary value problem on successive levels:

1. **Solve on coarse grid.**
2. Interpolate on fine grid boundaries.
3. Solve on fine grid.

Electrostatic mesh refinement algorithm is straightforward



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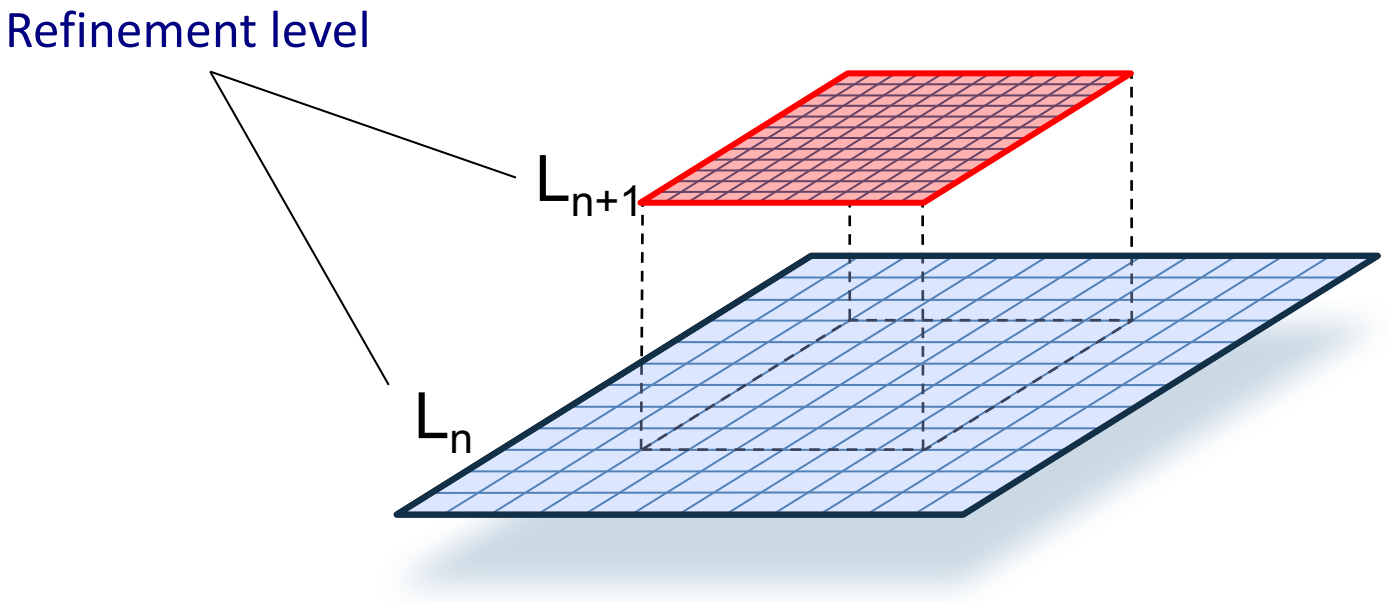
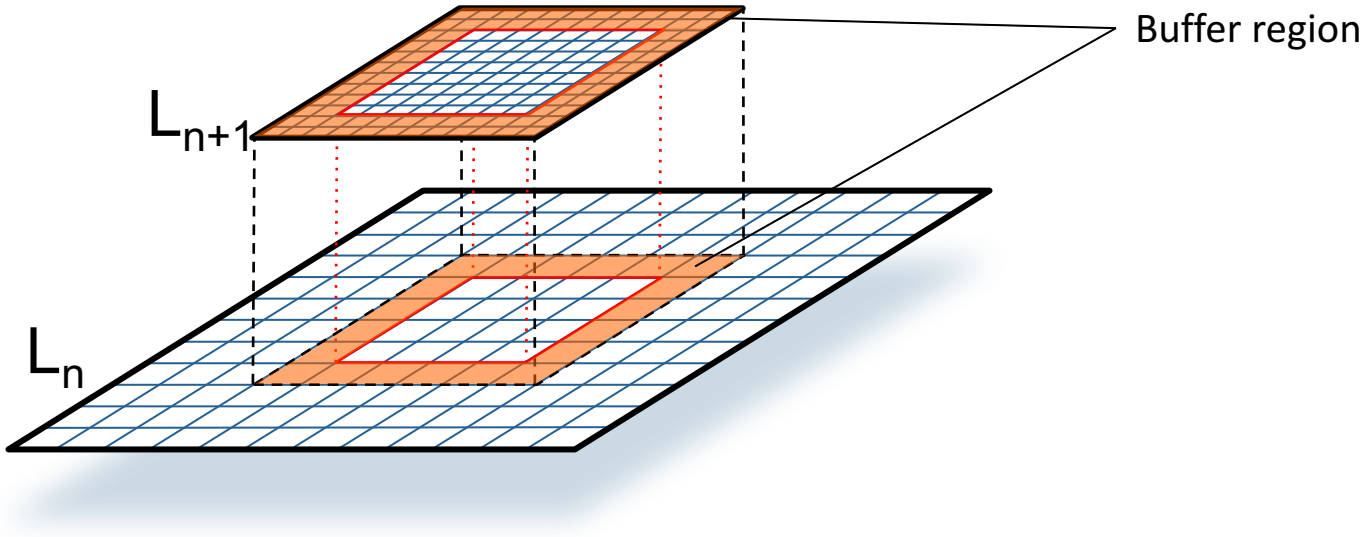


Solving boundary value problem on successive levels:

1. Solve on coarse grid.
2. Interpolate on fine grid boundaries.
3. **Solve on fine grid.**

Addition of buffer zone to control spurious “self-force”



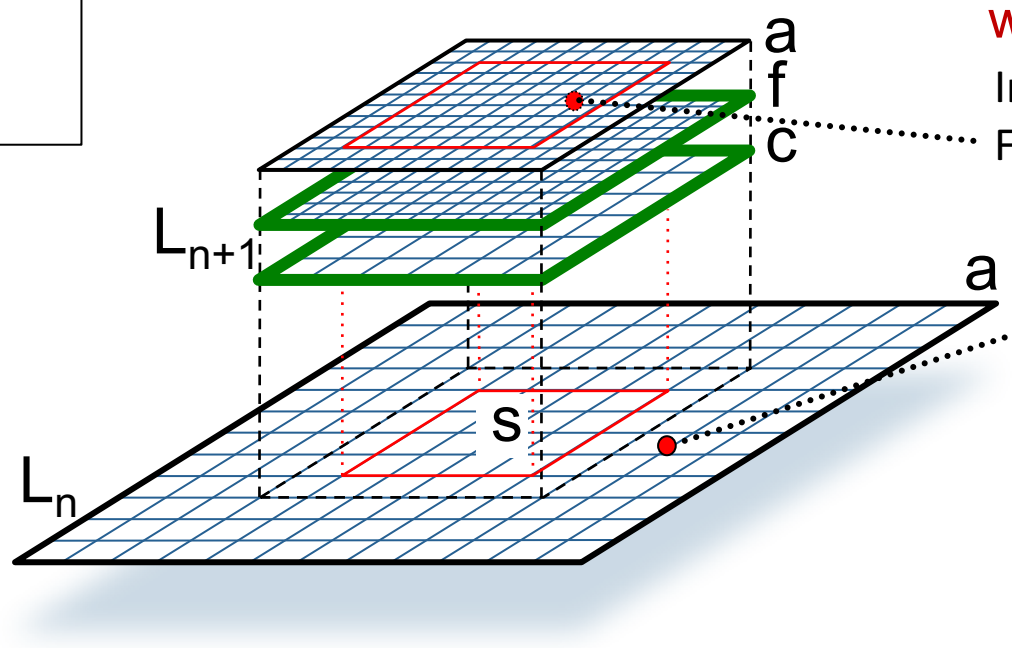
Solving boundary value problem on successive levels:

1. Solve on coarse grid.
2. Interpolate on fine grid boundaries.
3. Solve on fine grid.
4. **Disregard fine grid solution close to edge when gathering force onto particles.**

Electromagnetic MR algorithm is more complex

Interpolation between levels induces reflection of EM waves
➔ decoupling of levels with termination of regions with PMLs

absorbing layer (PML)
a = auxilliary
f = fine
c = coarse



Substitution of coarse solution with refined solution.

Inside patch at L_{n+1}:
$F_{n+1}(a) = I[F_n(s)-F_{n+1}(c)]+F_{n+1}(f)$

Main grid: $F_n(a)$

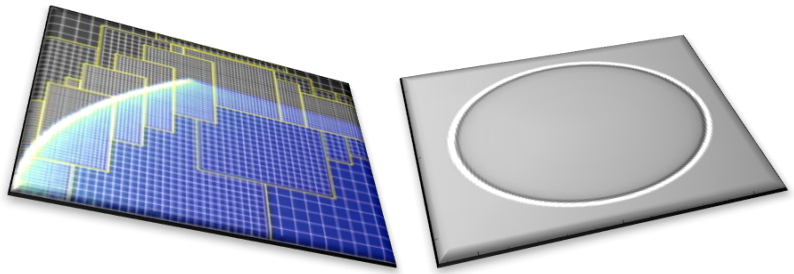
We are combining advanced algorithms

Lower # time steps:

- optimal Lorentz boosted frame

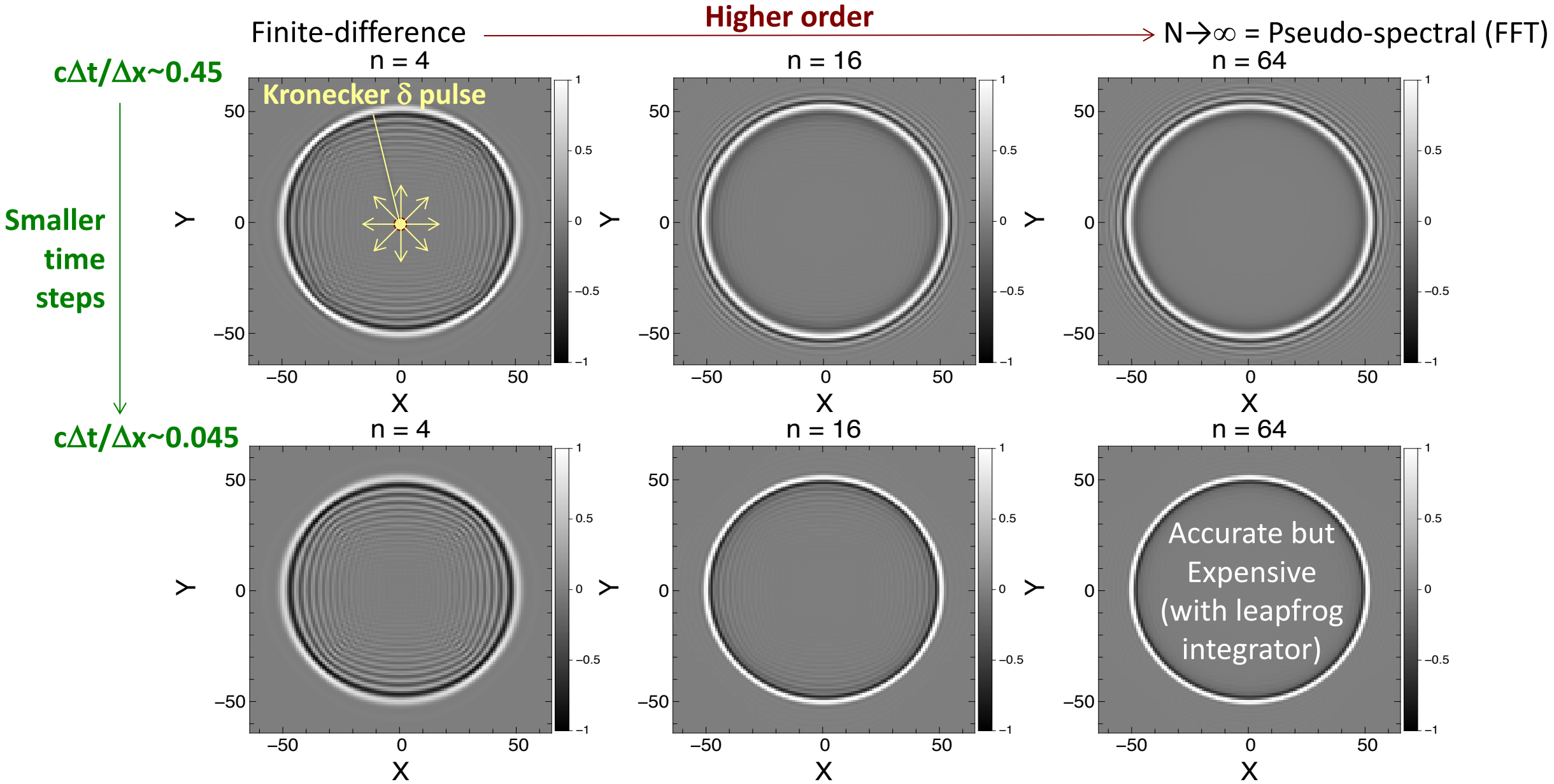
Higher accuracy:

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



Arbitrary-order Maxwell solver offers flexibility in accuracy

(on centered or staggered grids)

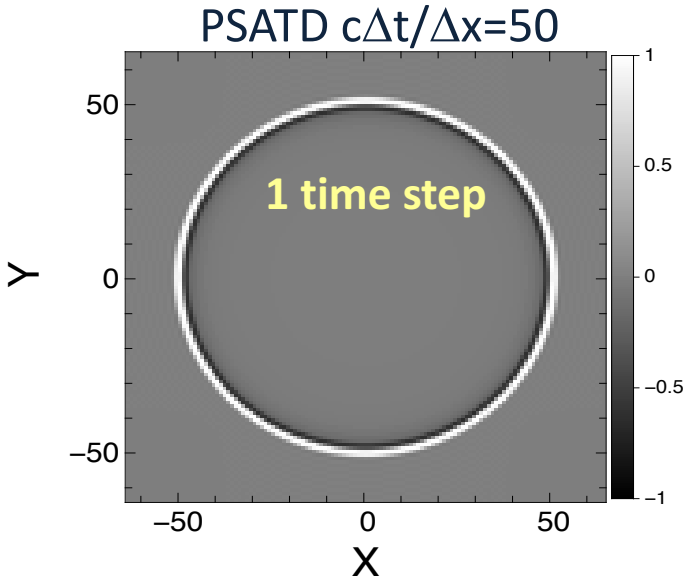


Analytical integration in Fourier space offers infinite order

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 ($k=k^{oo} \rightarrow k^n$).

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)

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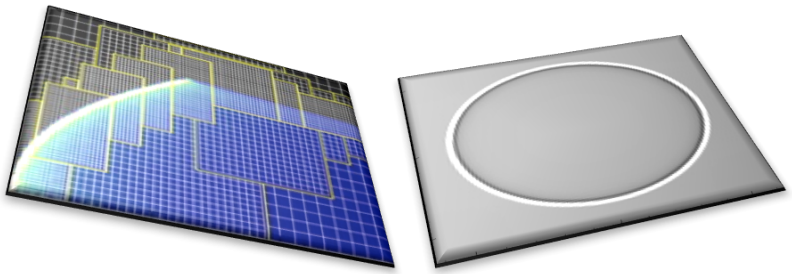
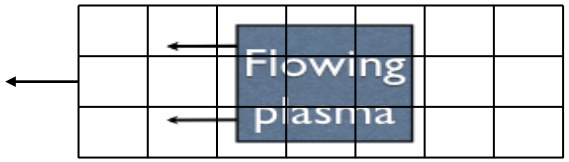


Higher stability

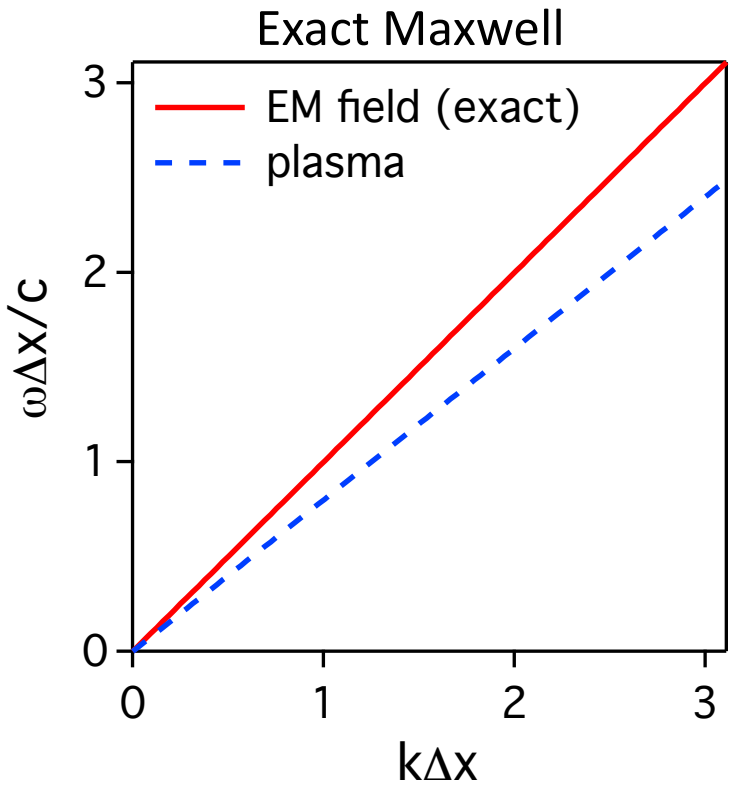
- Galilean T. to suppress Numerical Cherenkov Instability

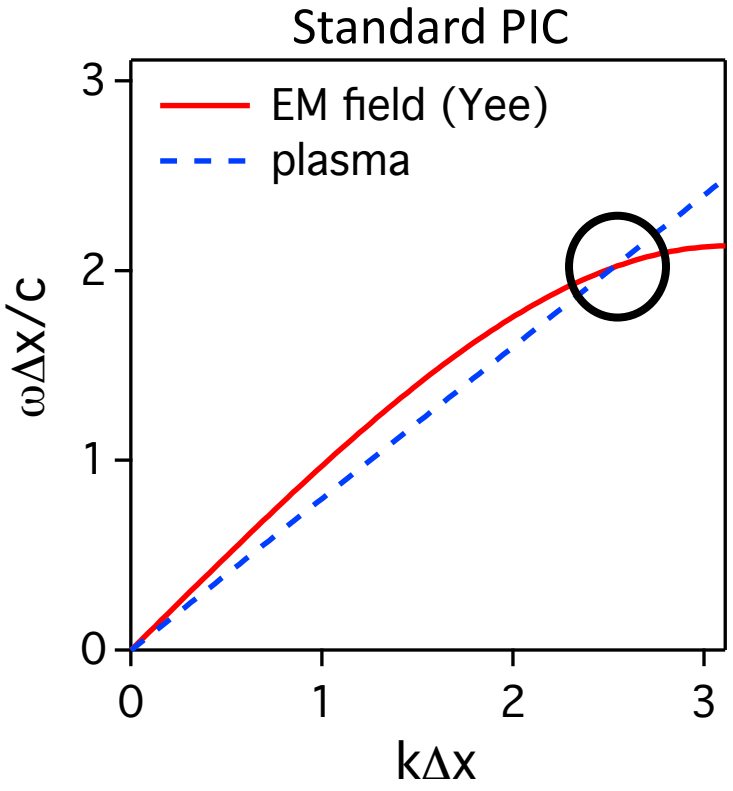


Relativistic plasmas PIC subject to “numerical Cherenkov”

B. B. Godfrey, “Numerical Cherenkov instabilities in electromagnetic particle codes”, *J. Comput. Phys.* **15** (1974)

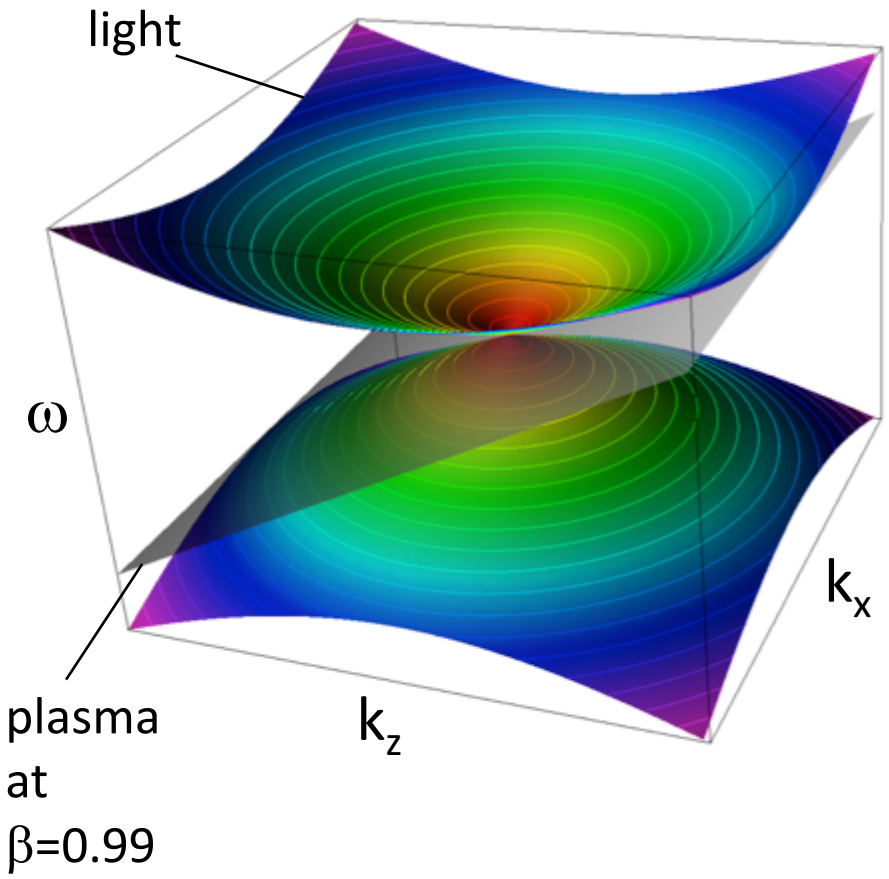
Numerical dispersion leads to crossing of EM field and plasma modes -> instability.



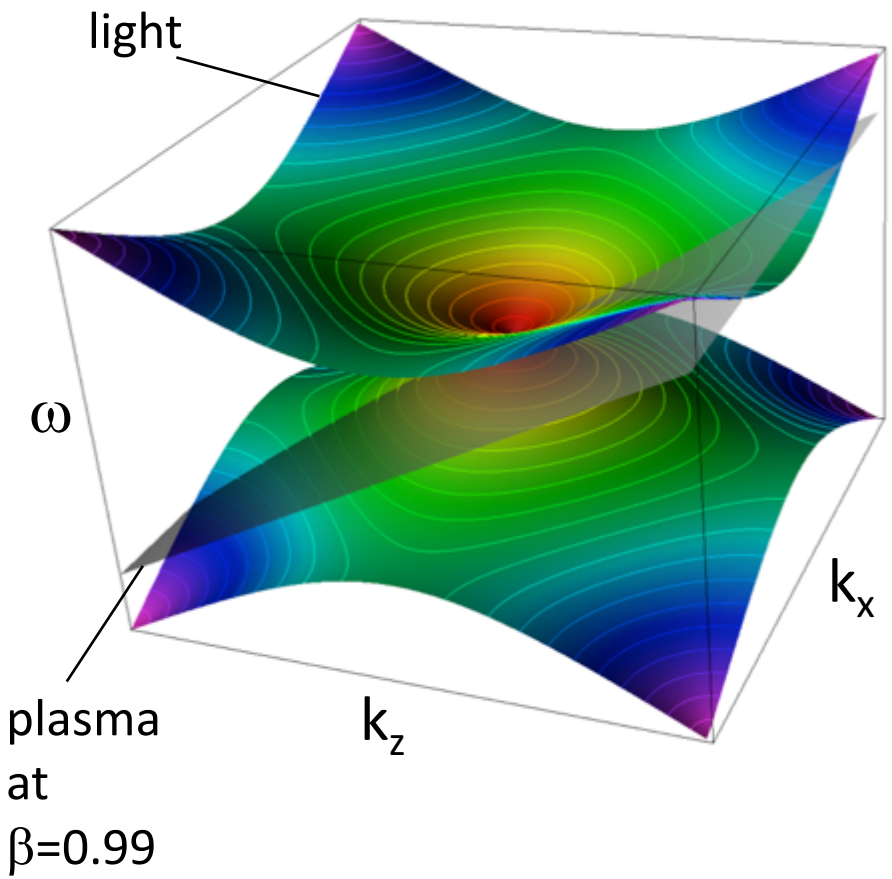


Space/time discretization aliases ➔ more crossings in 2/3-D

Exact Maxwell



Standard PIC



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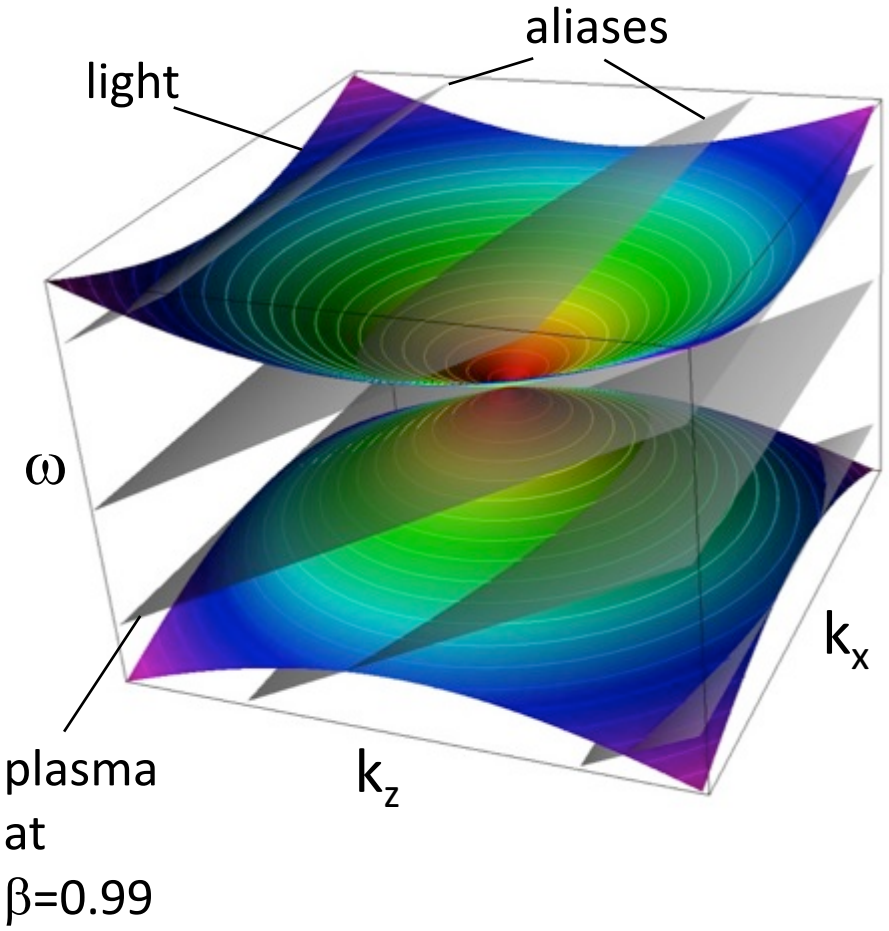
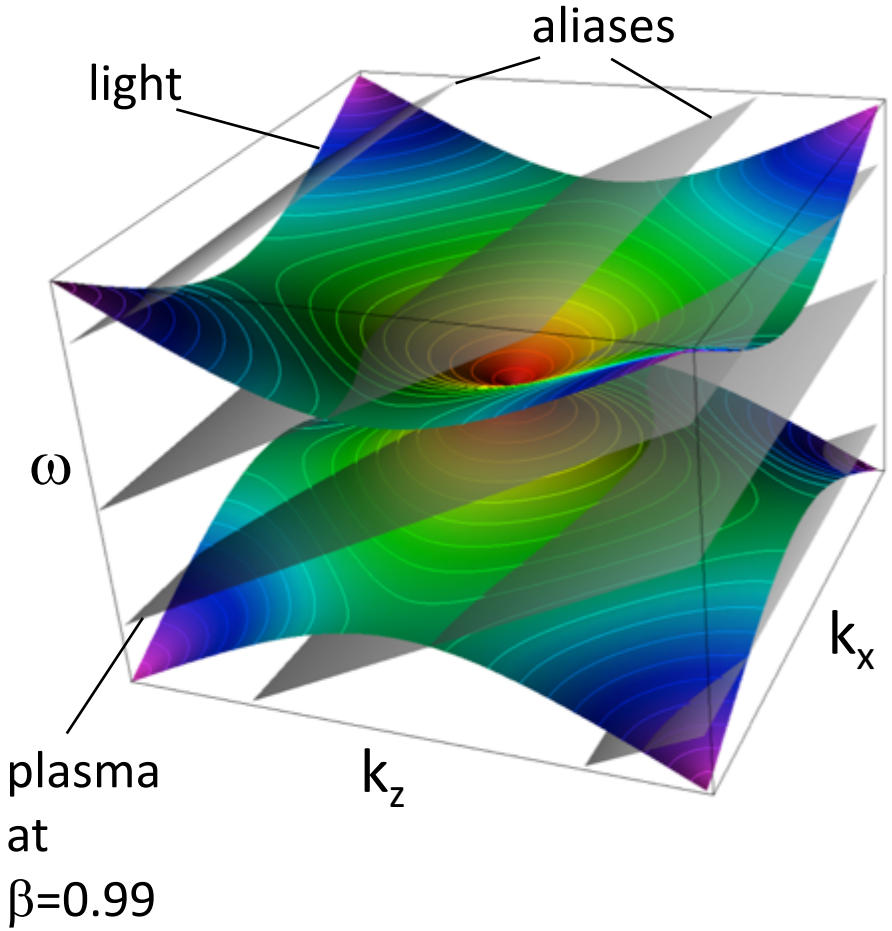


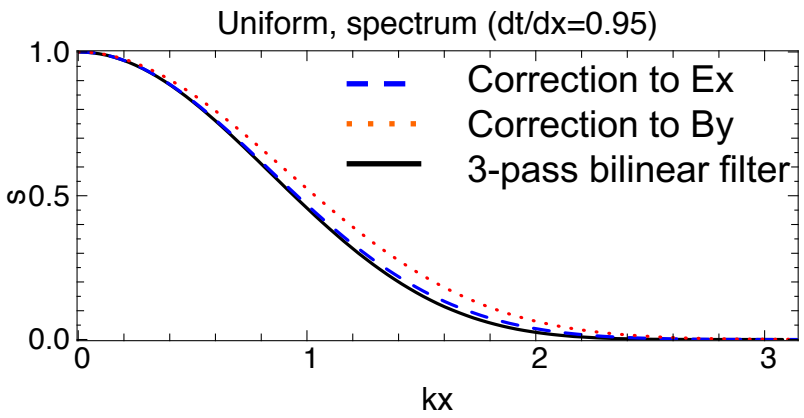
Standard PIC



Need to consider at least first aliases m_x={-3…+3} to study stability.

Local special filter efficiently suppresses instability

Filters fields seen by particles using 9-points linear smoothing in direction of plasma drift;



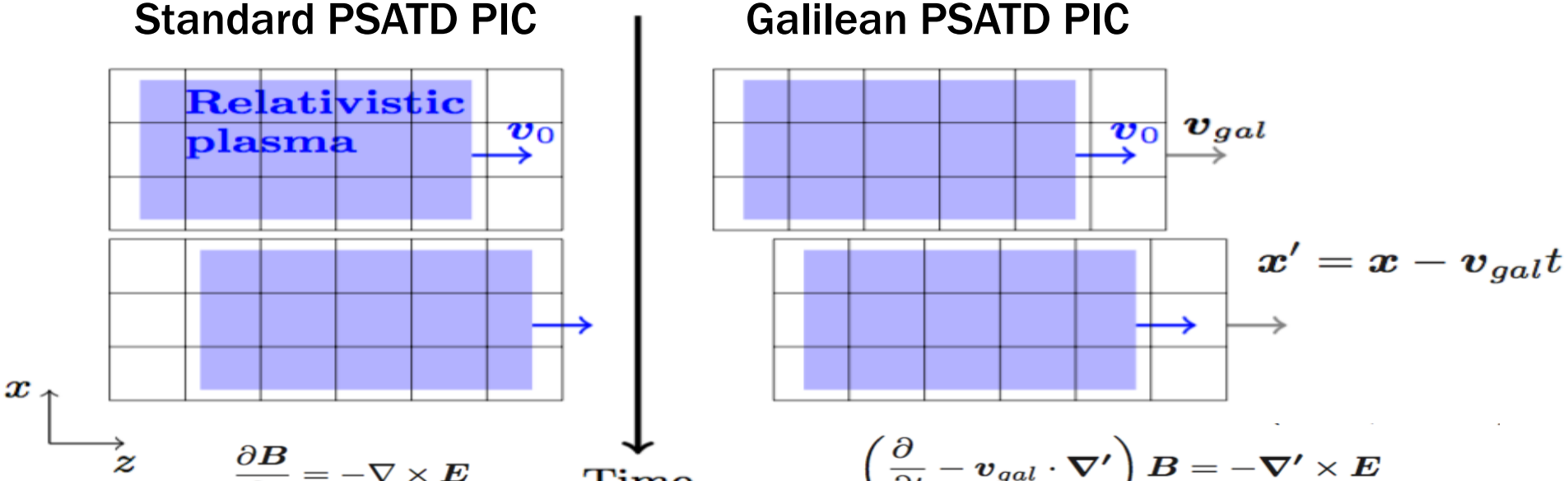
- key feature:
  - slightly different smoothing for Ex and By
- inexpensive and easy to implement
- local: amount of smoothing similar to standard 3-pass bilinear filter

*B. Godfrey & J.-L. Vay, *J. Comput. Phys.* **267** (2014)

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 $\boxed{\boldsymbol{j}(\boldsymbol{x},t)}$ $\boxed{\boldsymbol{j}(\boldsymbol{x}',t)}$ 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)*

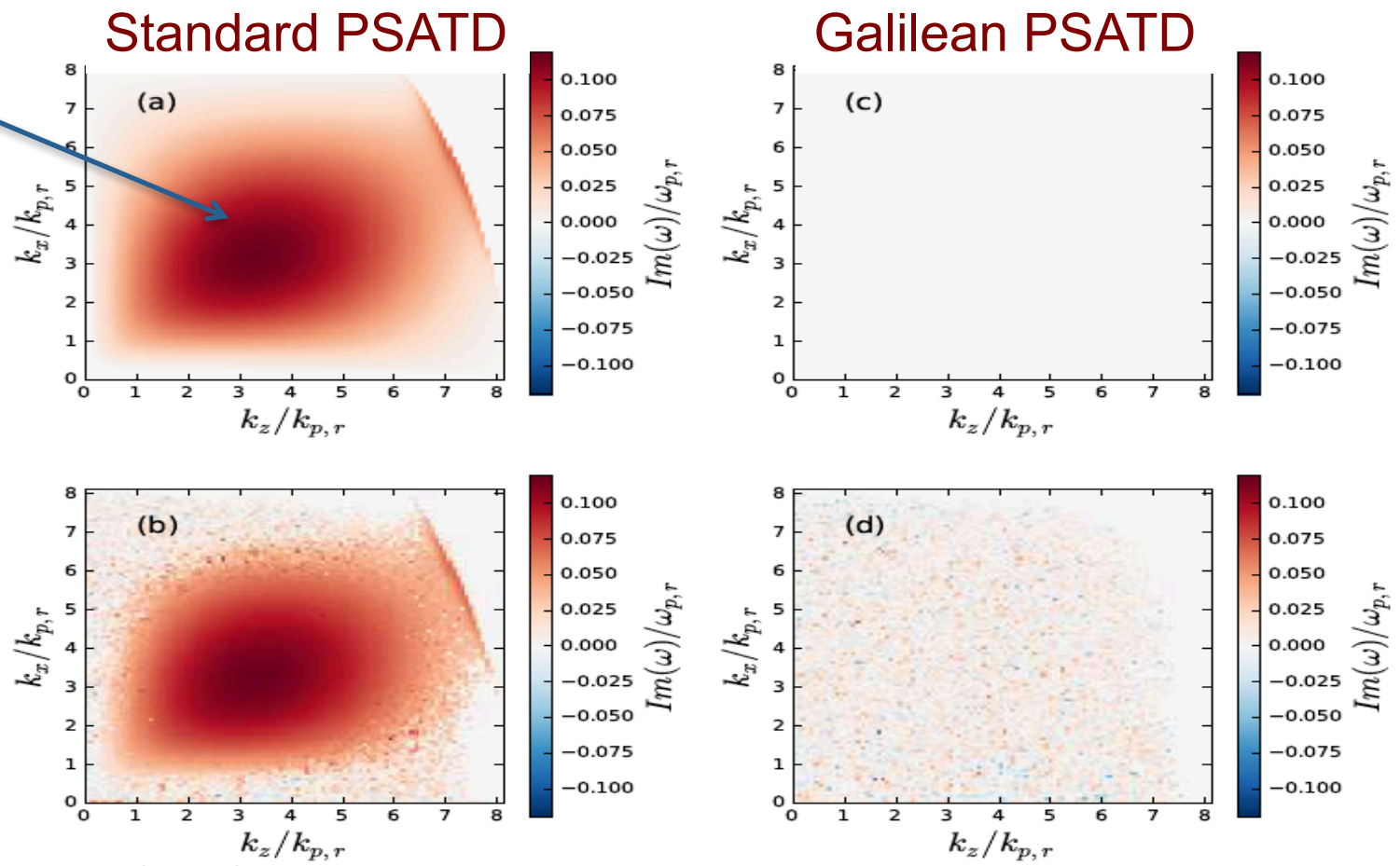
Galilean PSATD is stable for uniform relativistic flow

Uniform plasma streaming in 2D periodic box

Instability growth rate

Analysis

Simulation



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

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Higher accuracy:

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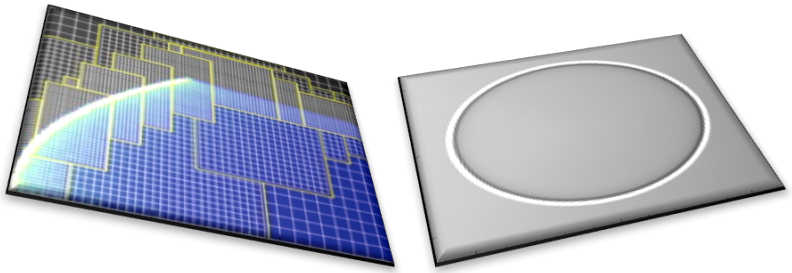
- Pseudo-spectral Analytical Maxwell solvers



Higher stability

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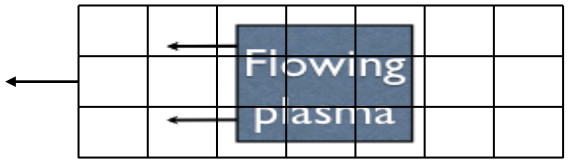
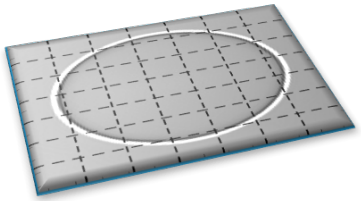


Higher scalability

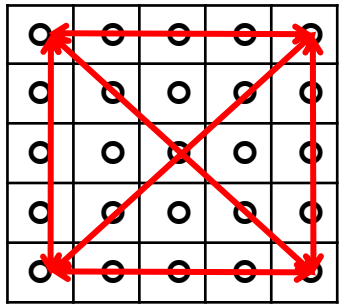
- FFT Maxwell solvers on local domains + domain decomposition



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

Spectral

global "costly" communications

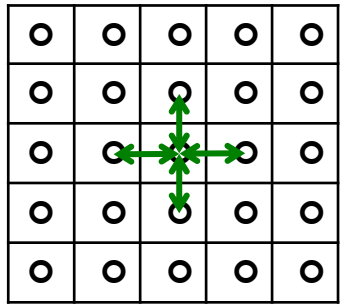


Harder to scale

vs

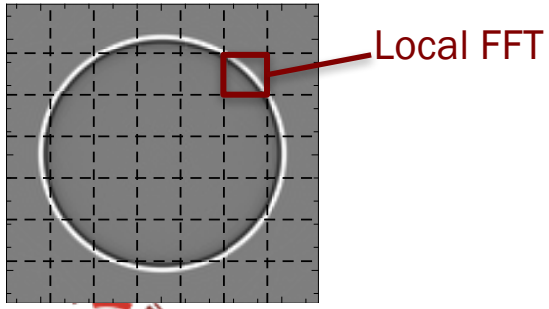
Finite Difference (FDTD)

local "cheap" communications



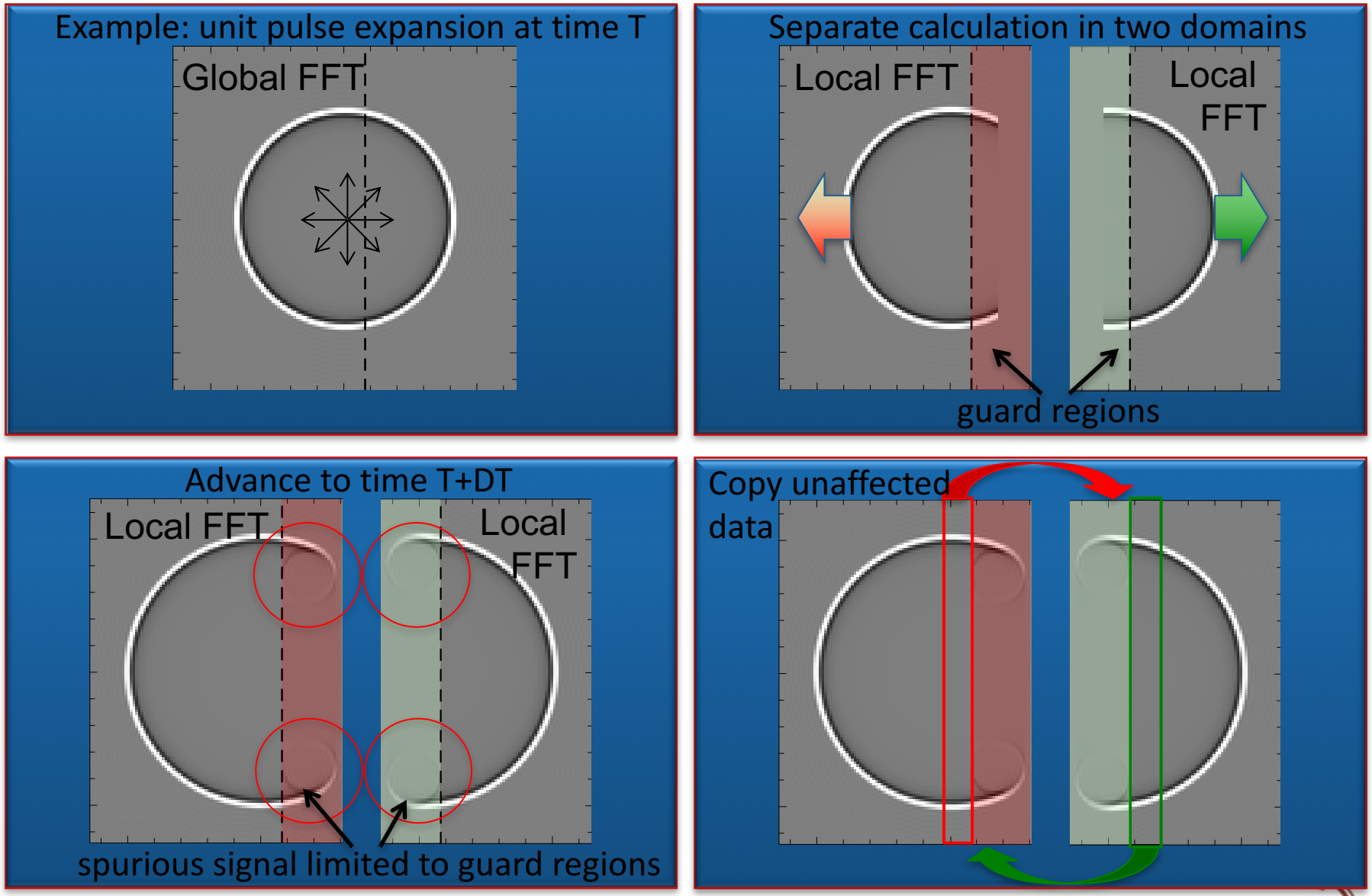
Easier to scale

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



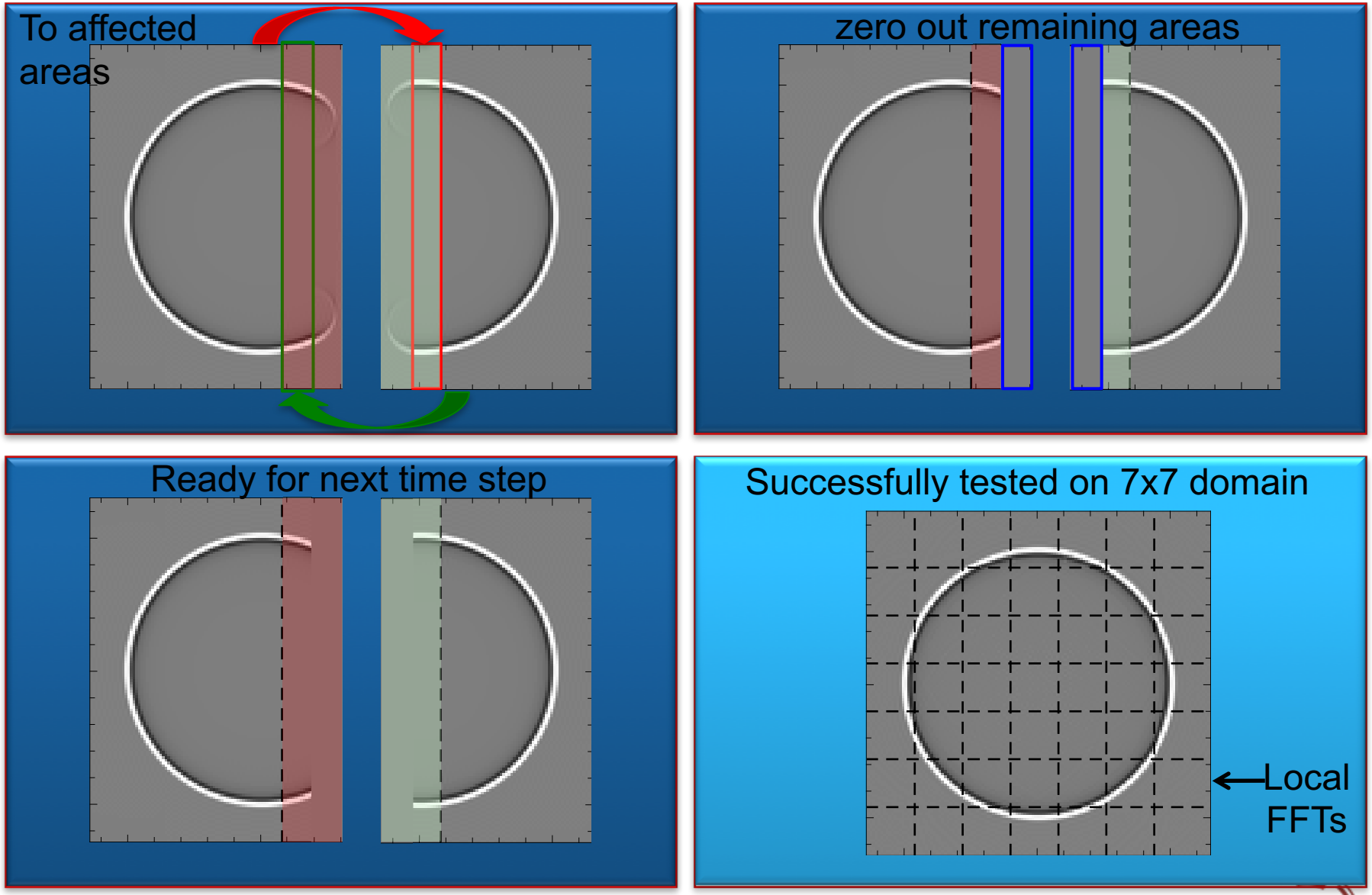
J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260 (2013)
H. Vincenti, J.-L. Vay, *Comput. Phys. Comm.* **200**, 147 (2016)

Local FFT example on single pulse – part 1



*J.-L. Vay, I. Haber, B. Godfrey, *J. Comput. Phys.* **243**, 260-268 (2013)

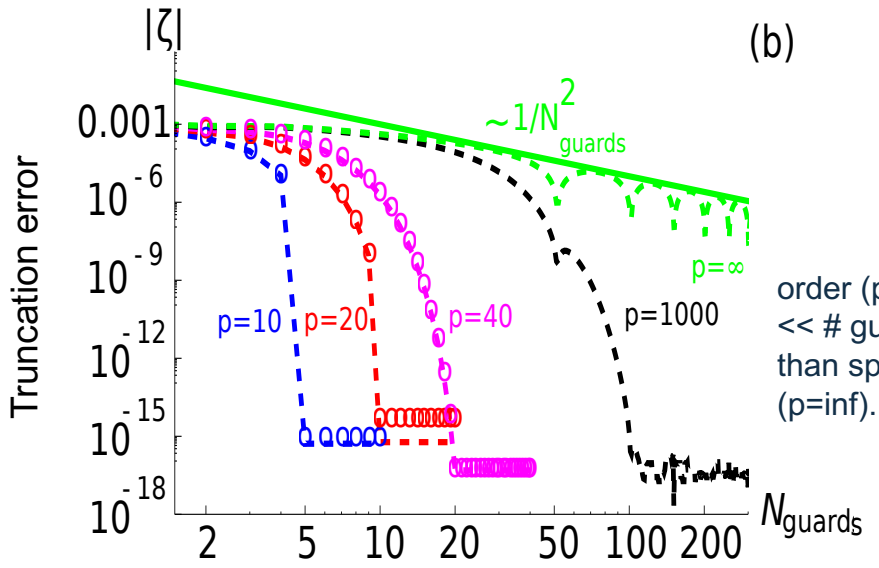
Local FFT example on single pulse – part 2



Truncation errors may lead to instabilities that needed to be studied.

Finite-order stencil offers scalable ultra-high order solver

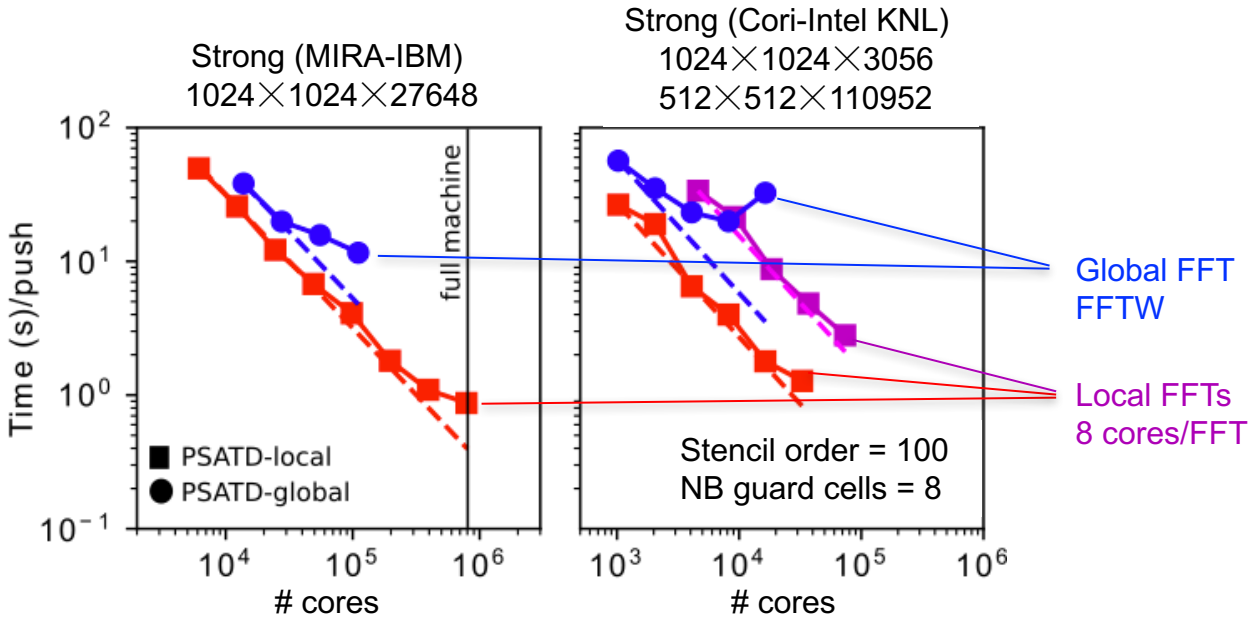
Truncation error analysis ➔ ultra-high order possible with much improved stability



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



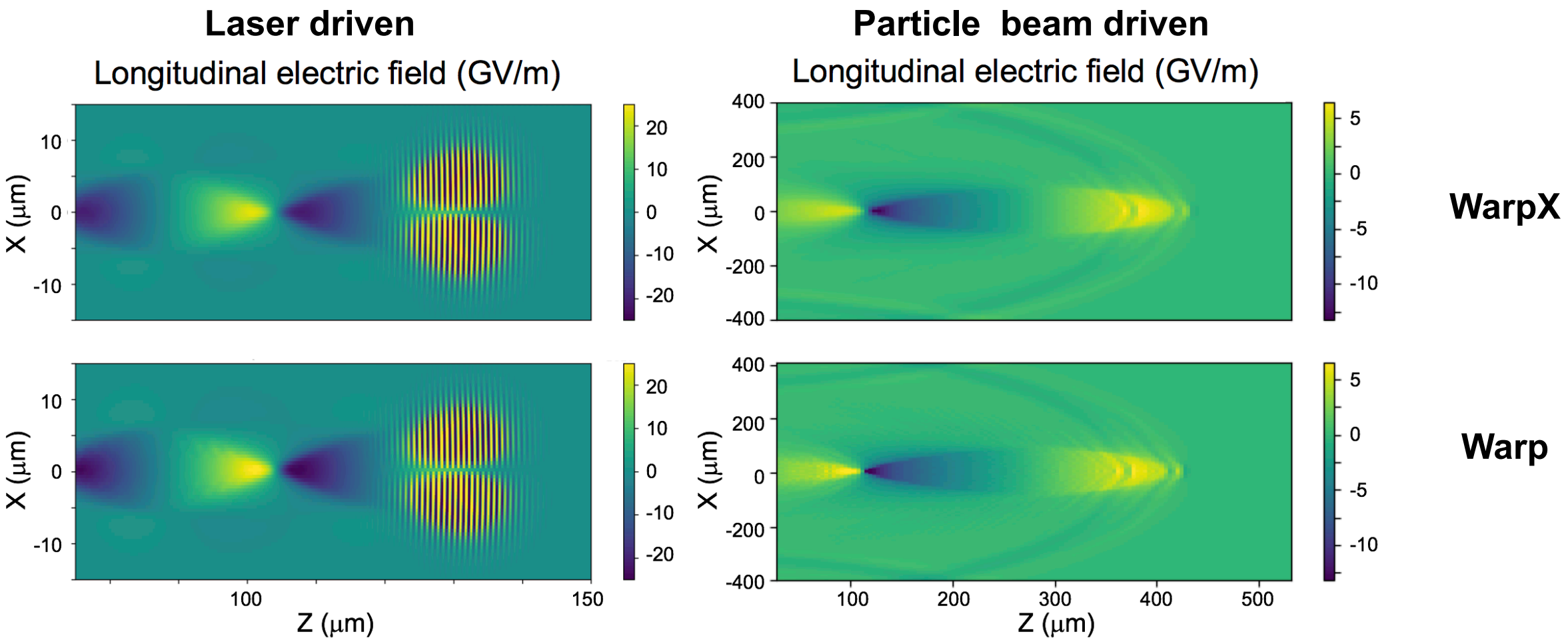
H. Vincenti, J.-L. Vay, "Ultrahigh-order Maxwell solver with extreme scalability for electromagnetic PIC simulations of plasmas.", http://arxiv.org/abs/1707.08500.

Applied successfully to modeling of laser-plasma experiments at CEA Saclay in cases where standard second-order FDTD solvers fail (PRL in press, other papers in preparation).

Outline

- Context & overview of the project
- Code structure, libraries & optimization on Intel KNL
- Advanced algorithms
- **Progress**
- Next steps & Summary

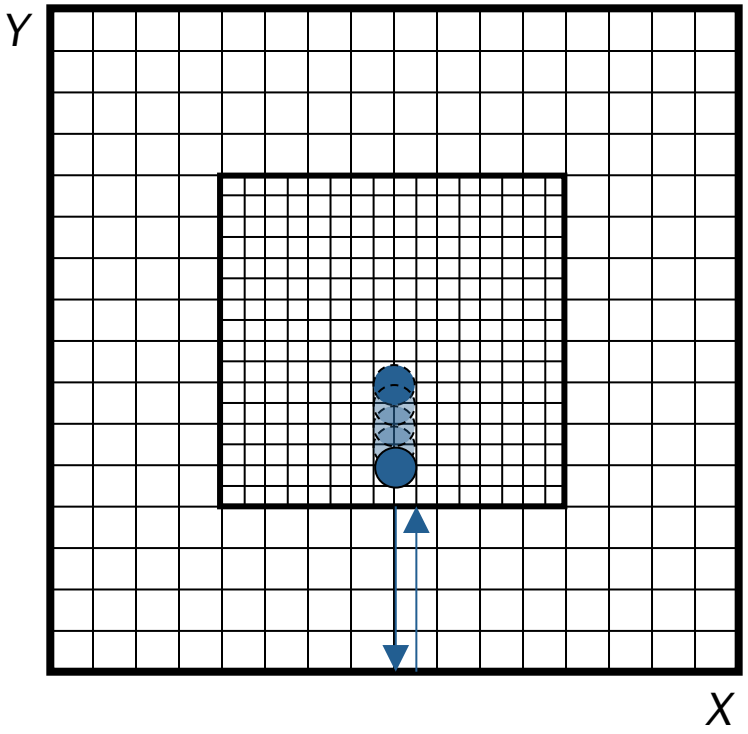
First simulations of plasma-based accelerators with WarpX (03/17)

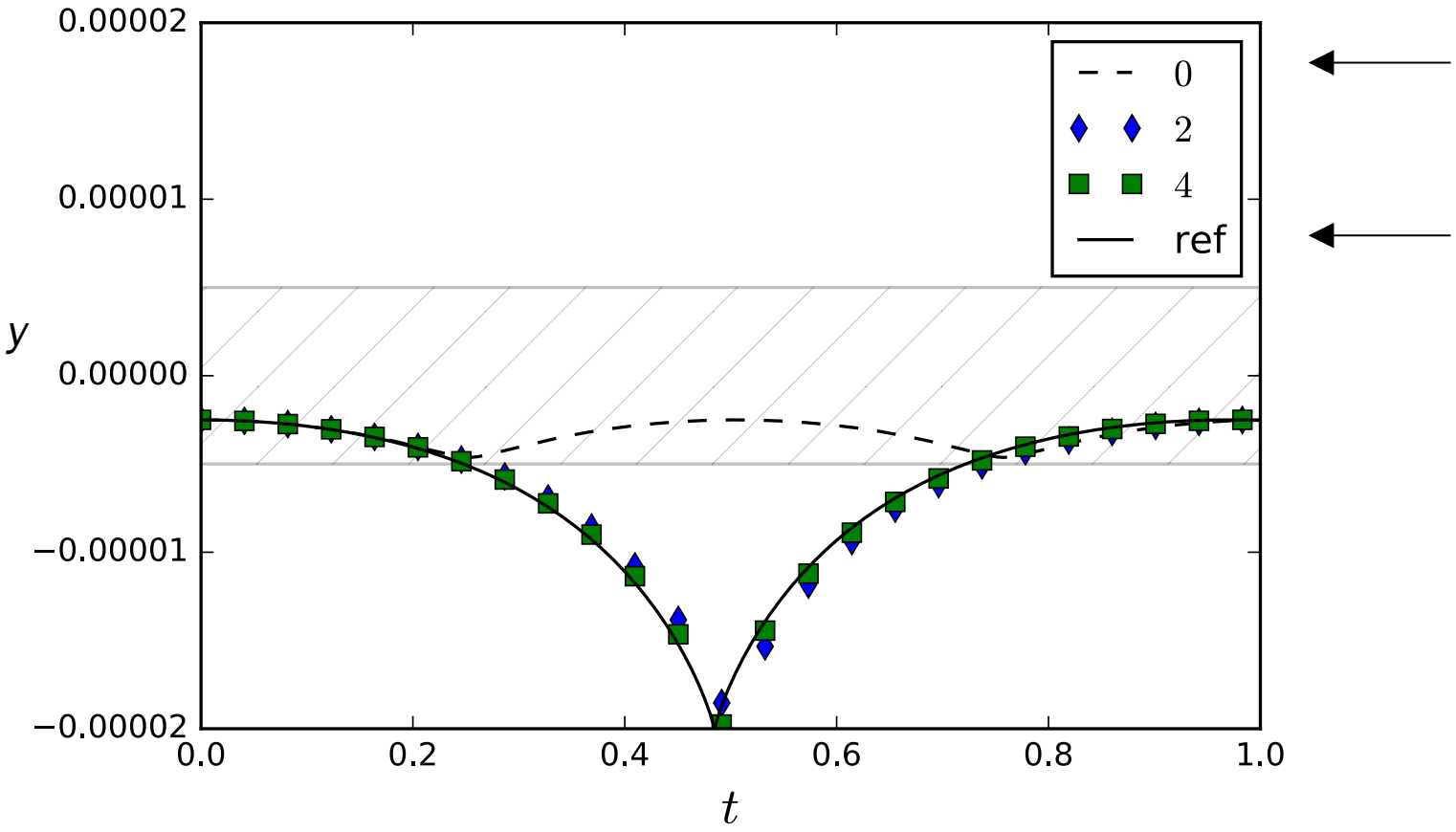


WarpX successfully benchmarked against Warp.

Electrostatic MR was implemented and tested

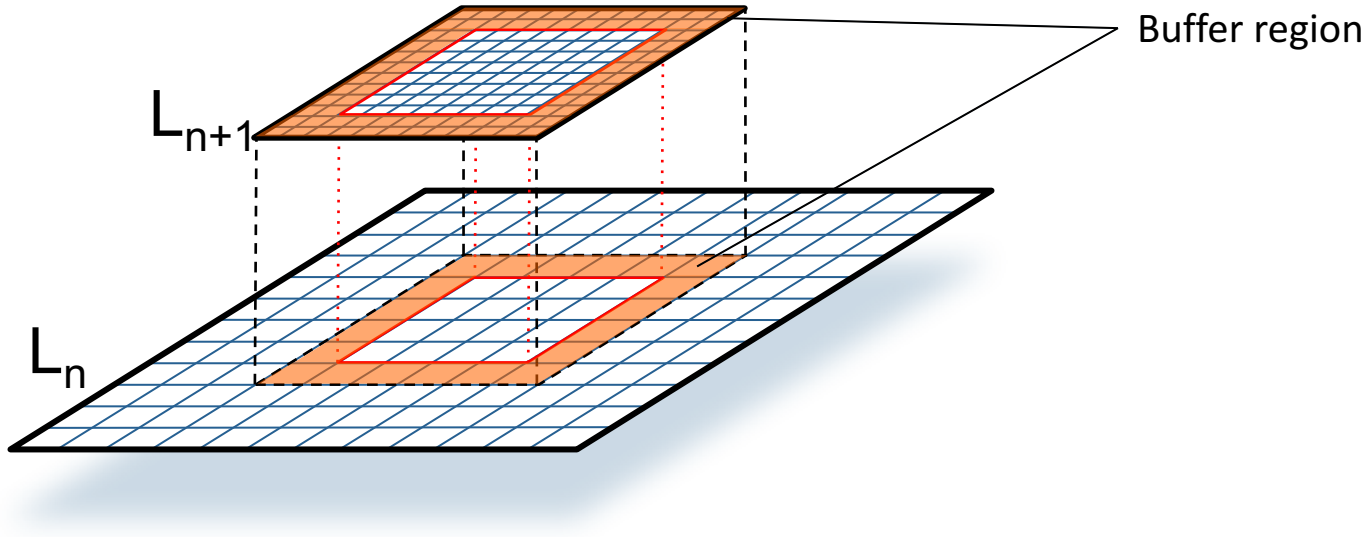
Test: Single particle attracted by image in conducting wall





Mesh refinement induces spurious “self-force” at interface.

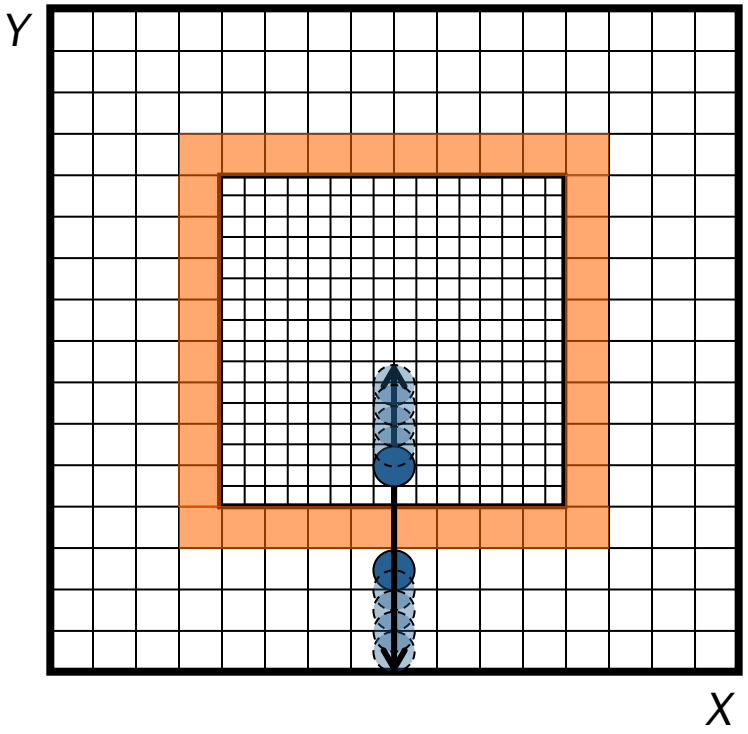
Addition of buffer zone to control spurious “self-force”

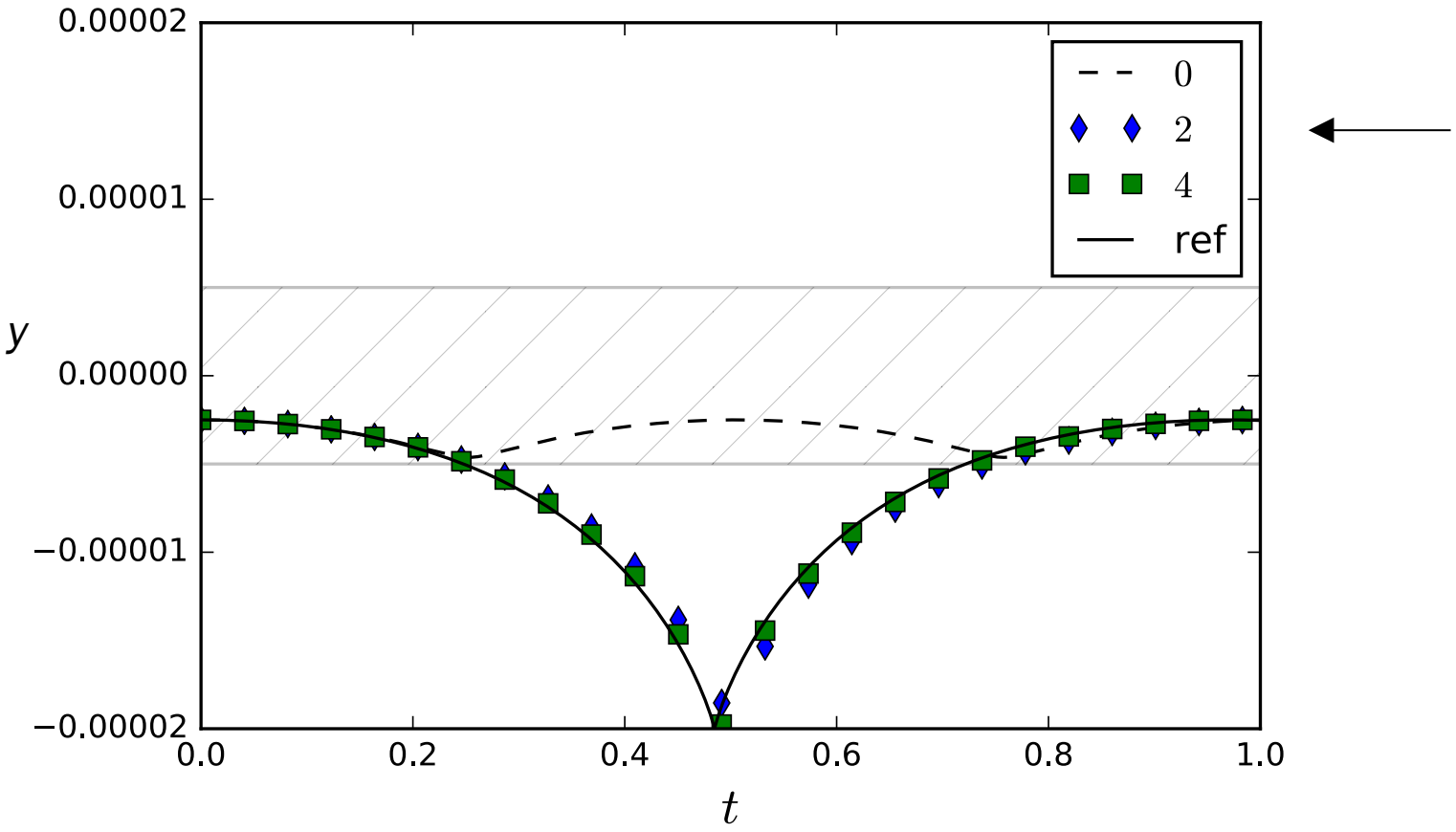


Solving boundary value problem on successive levels:

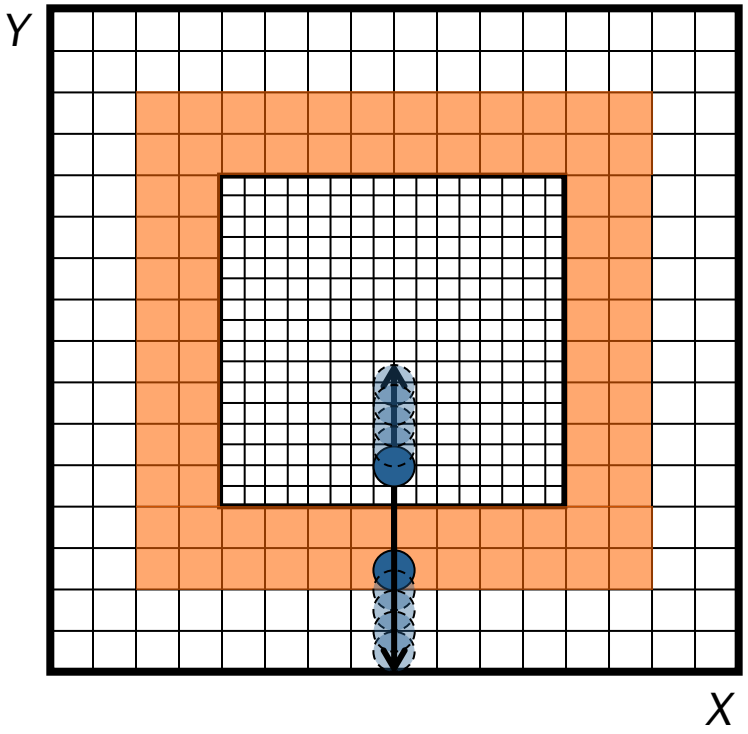
1. Solve on coarse grid.
2. Interpolate on fine grid boundaries.
3. Solve on fine grid.
4. **Disregard fine grid solution close to edge when gathering force onto particles.**

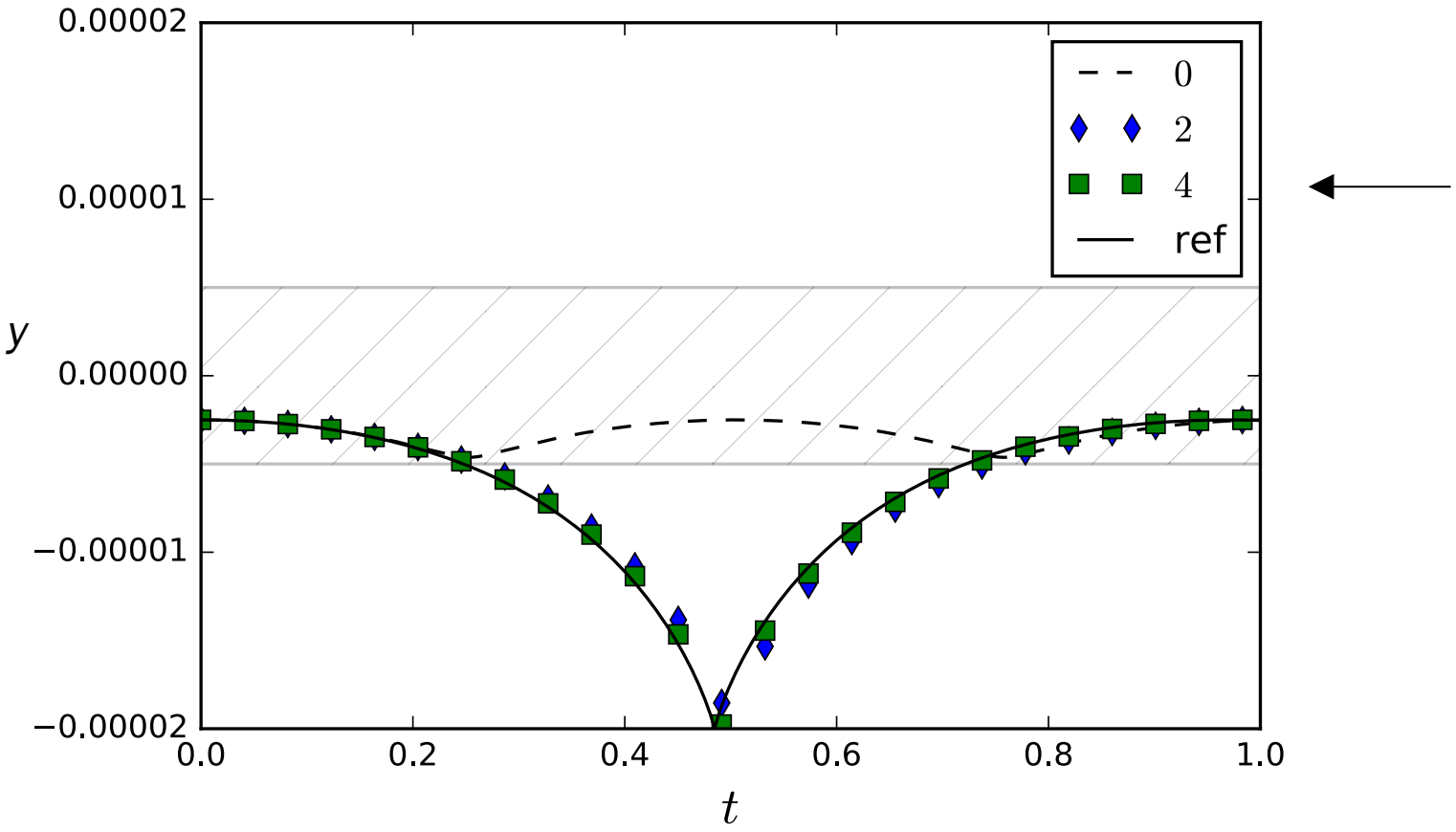
Adding a buffer region removes spurious trapping





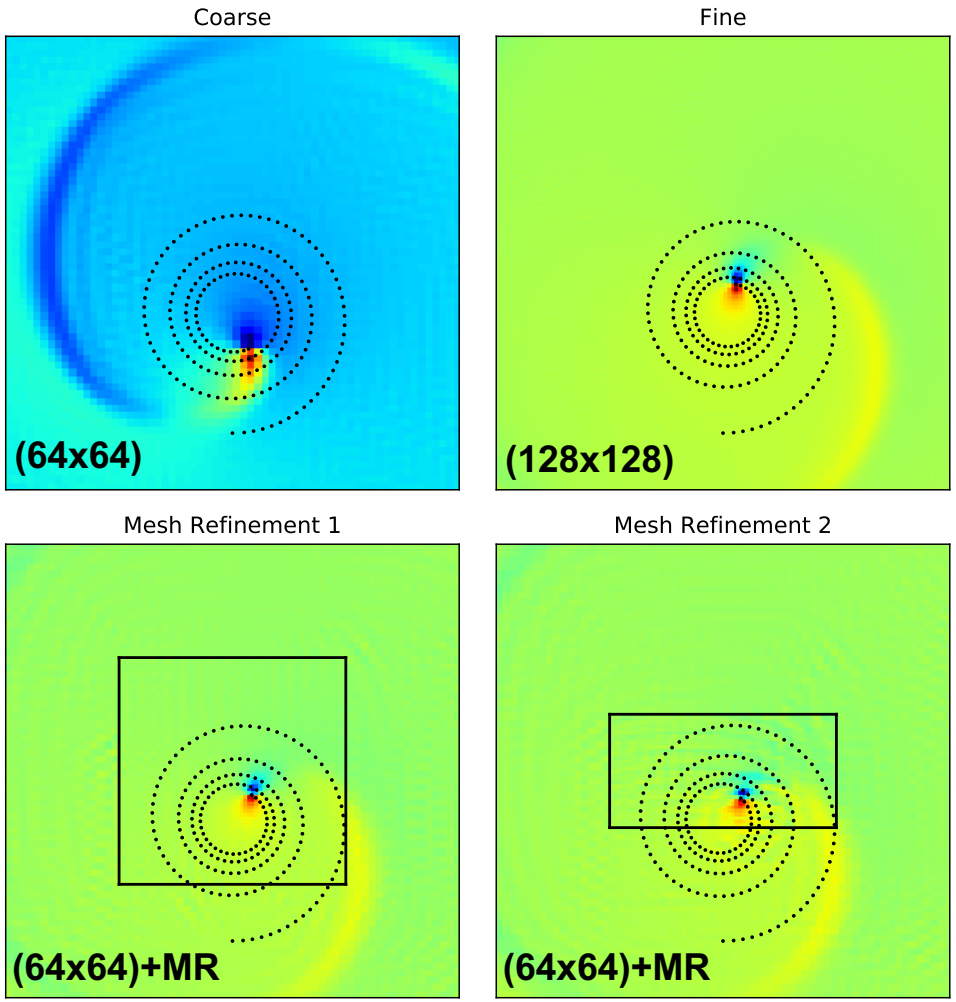
Wider buffer region enables accurate result

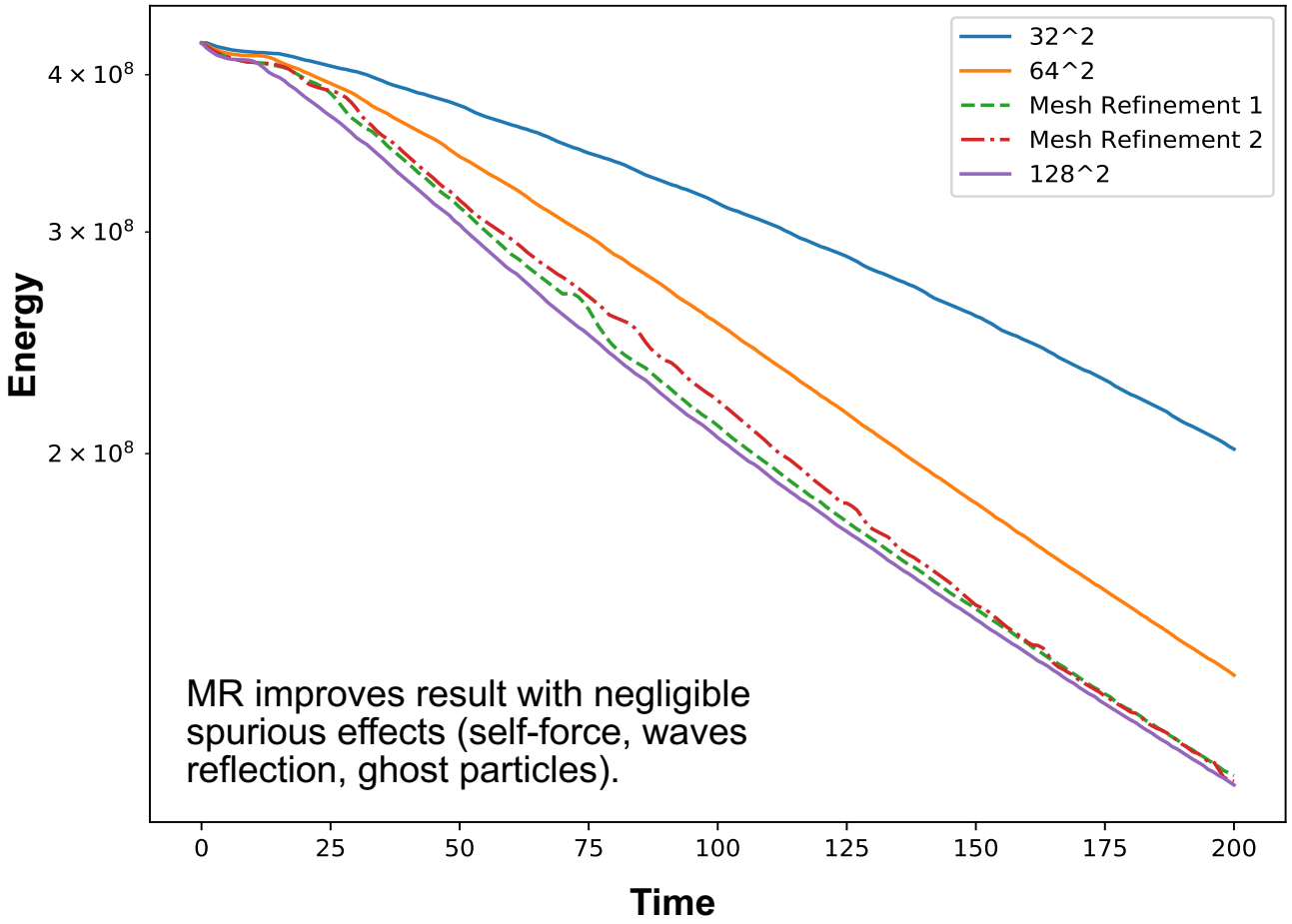




Electromagnetic MR was implemented and tested

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





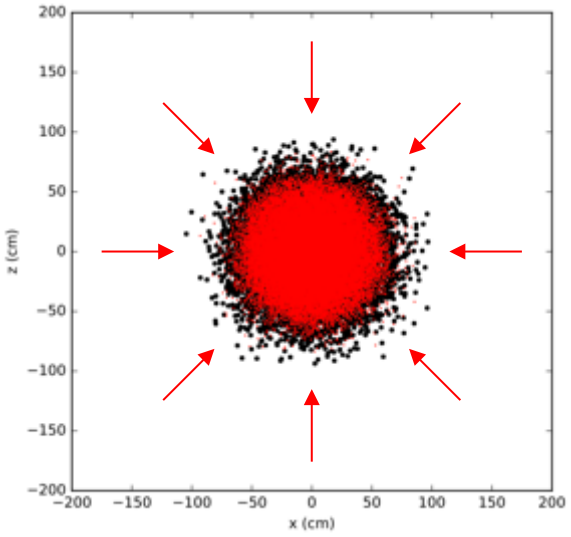
Note: buffer region not implemented yet; expected to improve results once implemented.

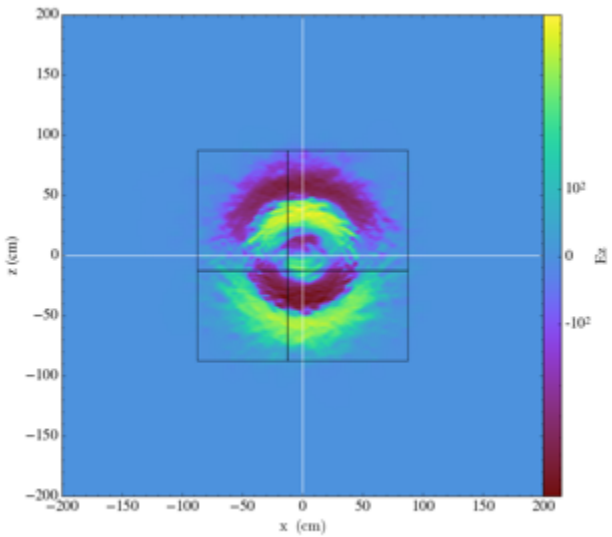
Validation on many particles `beam breathing' test

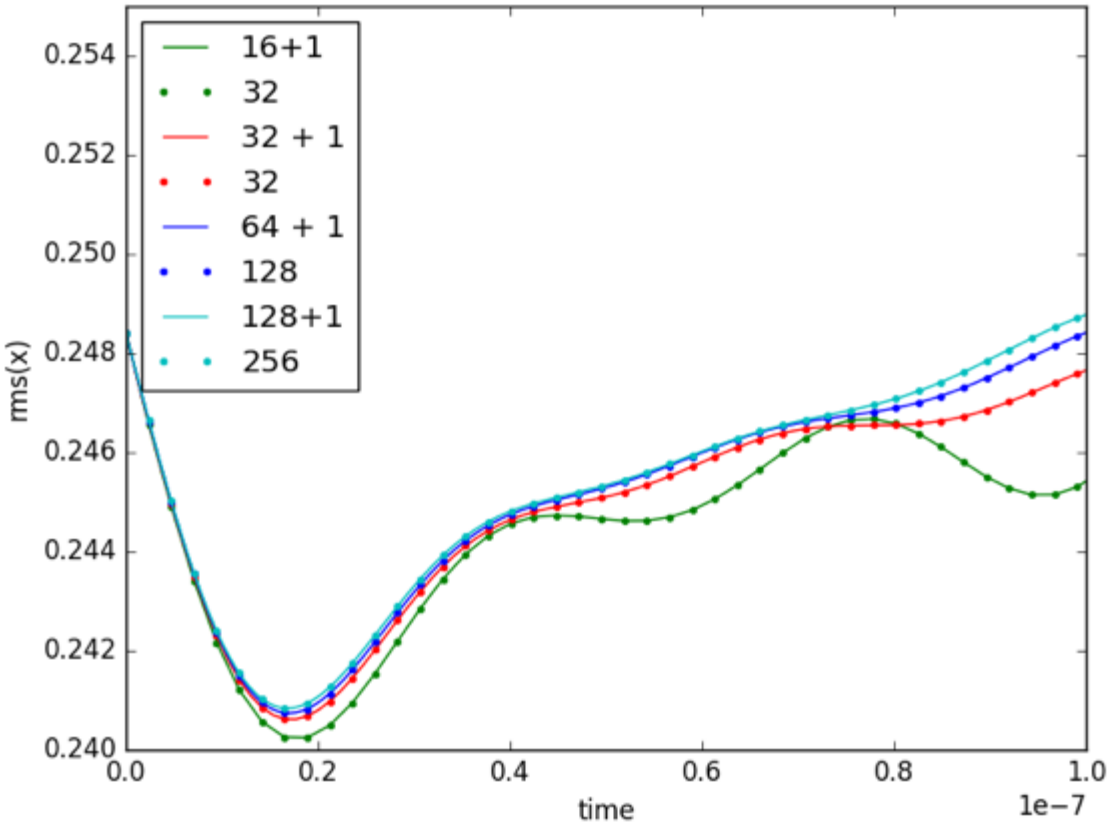
Electron Gaussian distribution with inward initial radial velocity on top of static proton dist.

Electron beam contraction/expansion depends on resolution.

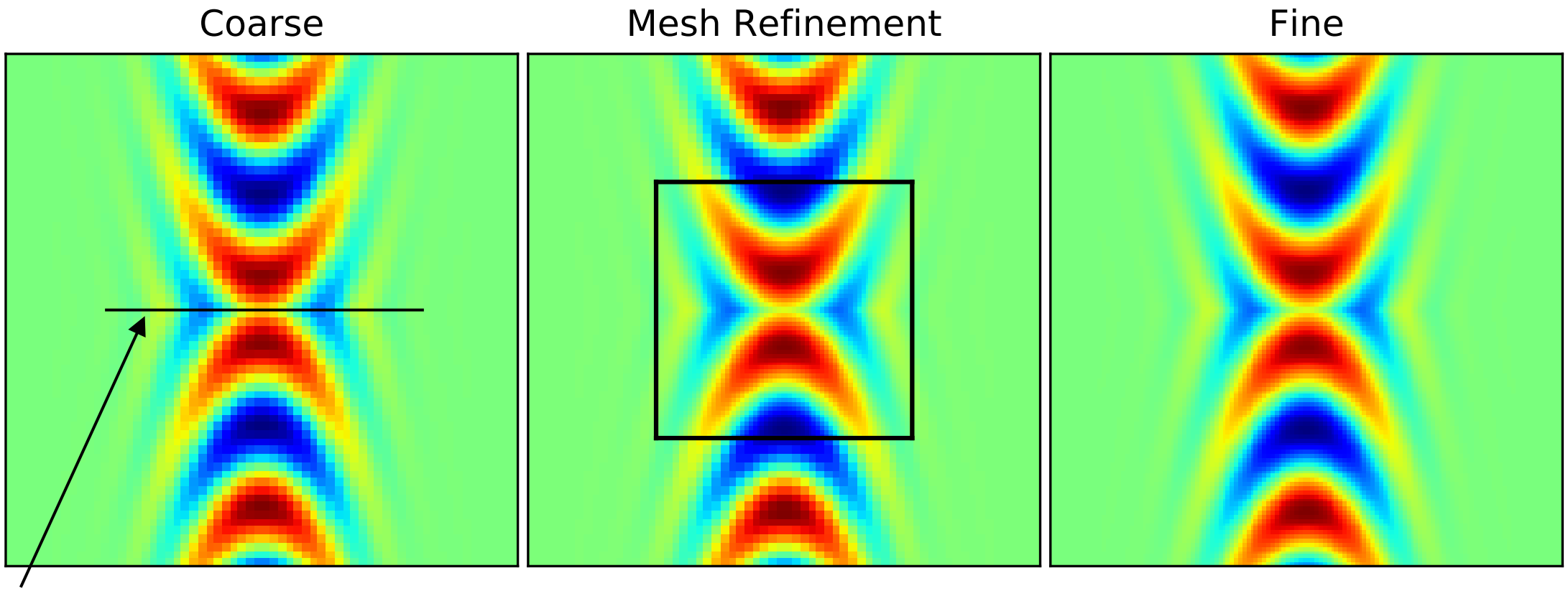
MR enables higher accuracy, covering fraction of box.





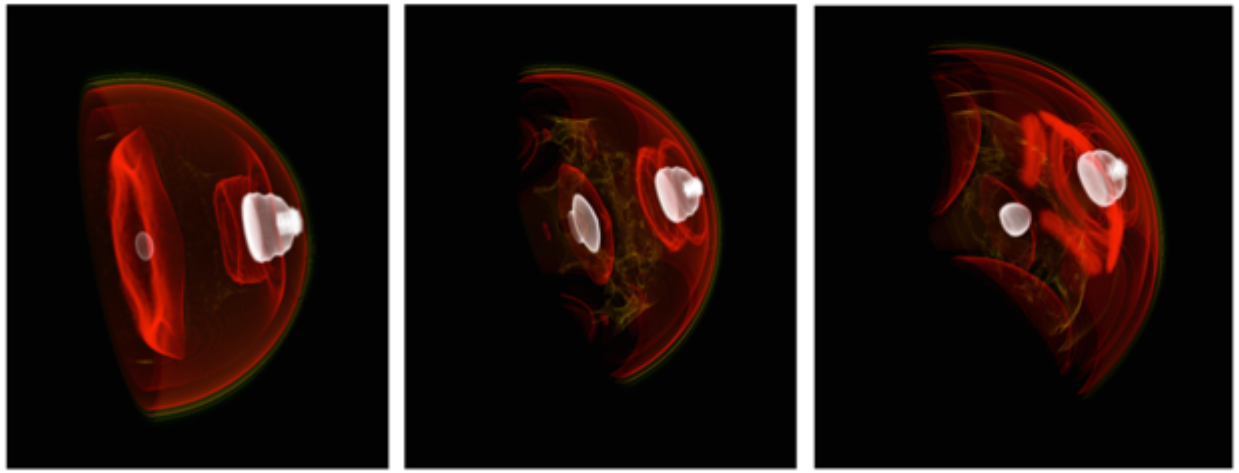


Laser injection with mesh refinement was validated

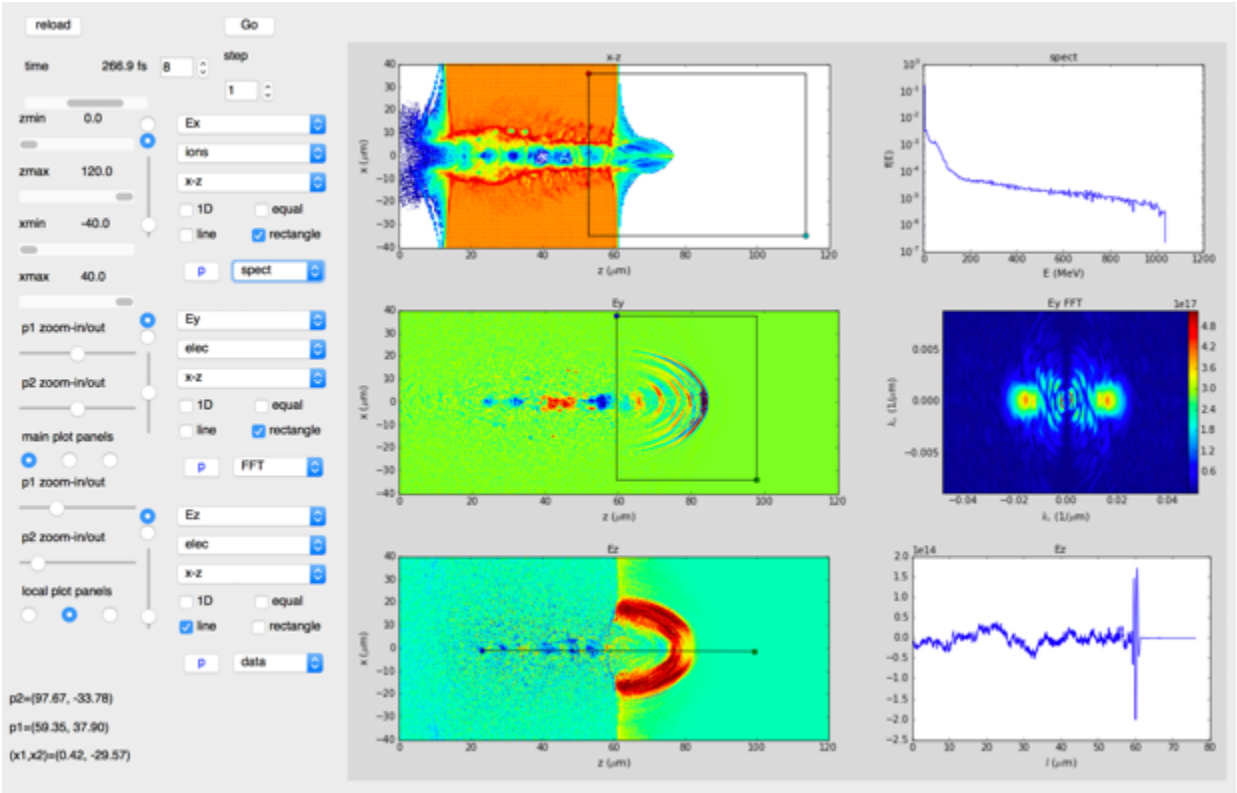


WarpX visualization tools are being developed

3D rendering of WarpX plasma accelerator simulation with yt



Prototype WarpX data analysis GUI



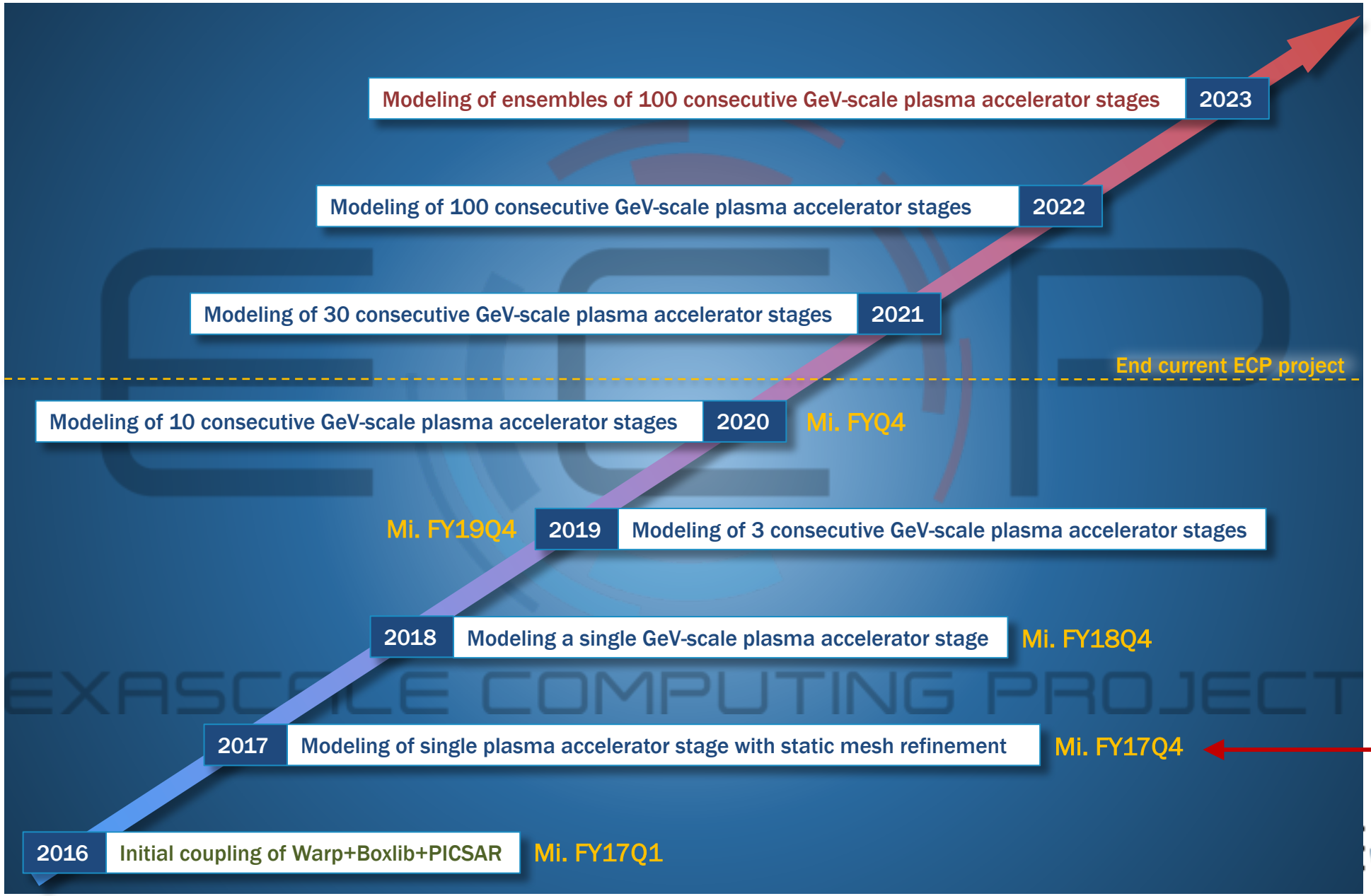
- 2D/3D visualization with matplotlib, yt, VisIt
  - Supports AMReX & OpenPMD data structures (OpenPMD dev. Synergistic with CAMPA)
- Interface using Python, Jupyter notebooks and/or GUI.

Outline

- Context & overview of the project
- Code structure, libraries & optimization on Intel KNL
- Advanced algorithms
- Progress
- **Next steps & Summary**

7-year plan for Exascale project WarpX

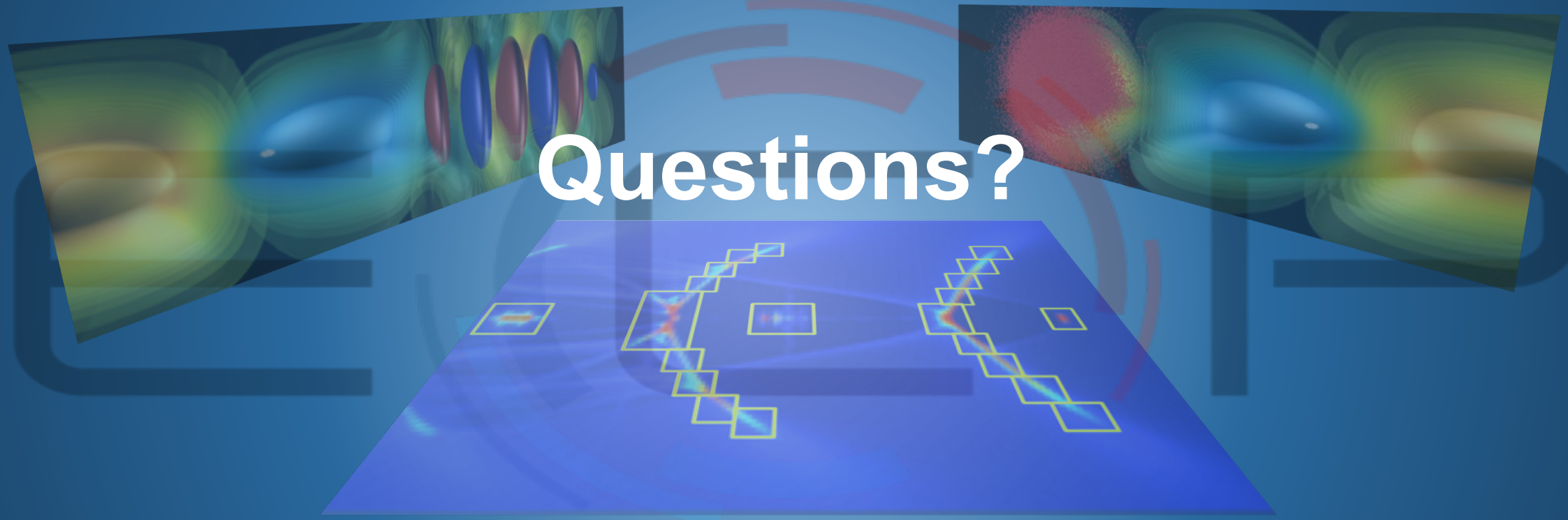
From initial code coupling to ensemble of 100 GeV-scale stages



Summary and outlook

- Modeling of plasmas is complex
  - Rich physics, instabilities, many time scales, …
  - Need to continue pushing the frontier with better algorithms and Exascale computing
- New generation processors (Manycore, GPU, …) need special care
- PICSAR provides open source community library for PIC kernel
- WarpX project is developing exascale-ready AMR-PIC code

Thank you!



Questions?