UC SANTA BARBARA
Kavli Institute for
Theoretical Physics

Connecting Micro and Macro Scales:
Acceleration, Reconnection, and
Dissipation in Astrophysical Plasmas

Santa Barbara, CA, USA – Sept. 9-12, 2019

Novel Numerical Methods for Particle-in-Cell Modeling of Plasmas

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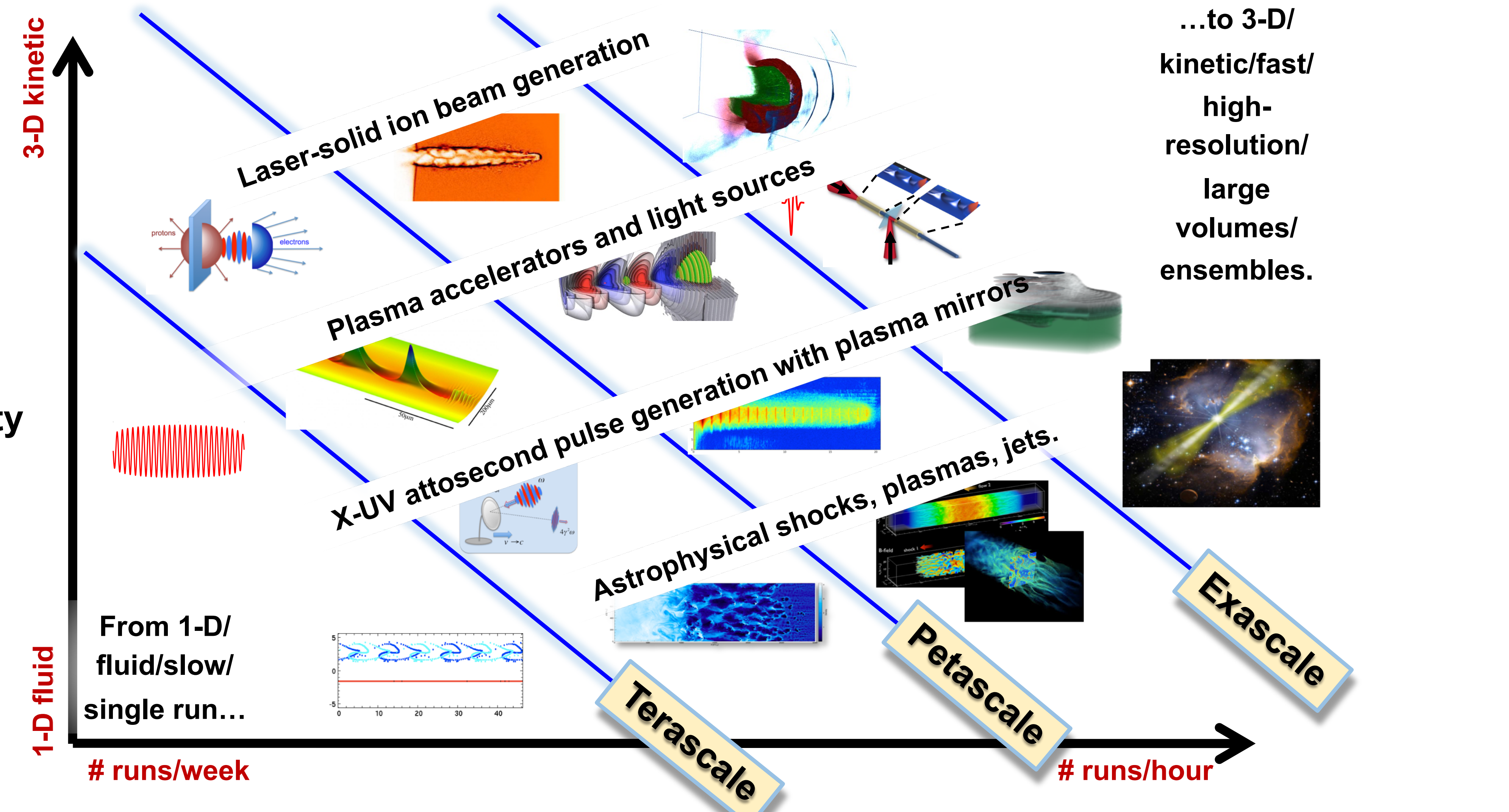
BERKELEY LAB
U.S. DEPARTMENT OF ENERGY | Office of Science
ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION ATAP
ECP EXASCALE COMPUTING PROJECT
BLAST BERKELEY LAB ACCELERATOR SIMULATION TOOLKIT

Outline

- Introduction
- Issues and some solutions
  - Particle pusher
  - Field solver
  - Numerical Cherenkov Instability
  - Mesh refinement
  - Optimal Lorentz boosted frame
- Conclusion

Theory & Modeling of Plasmas involve complex physics with a wide range of space & time scales

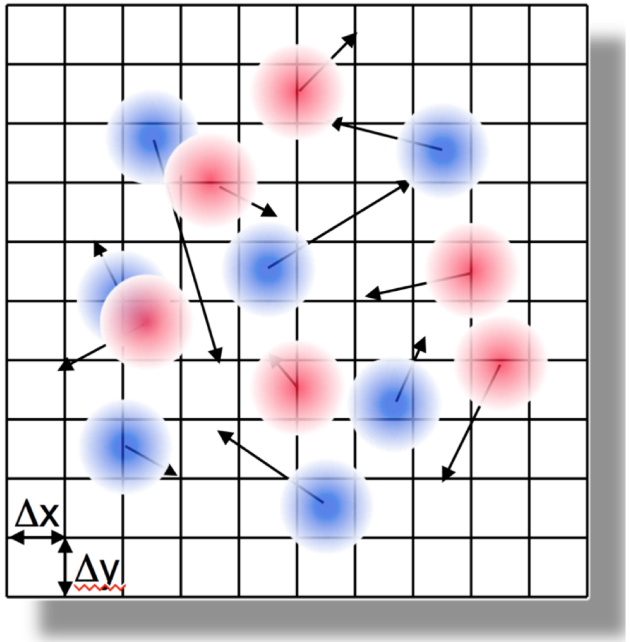
Increase complexity, dimensionality & fidelity.



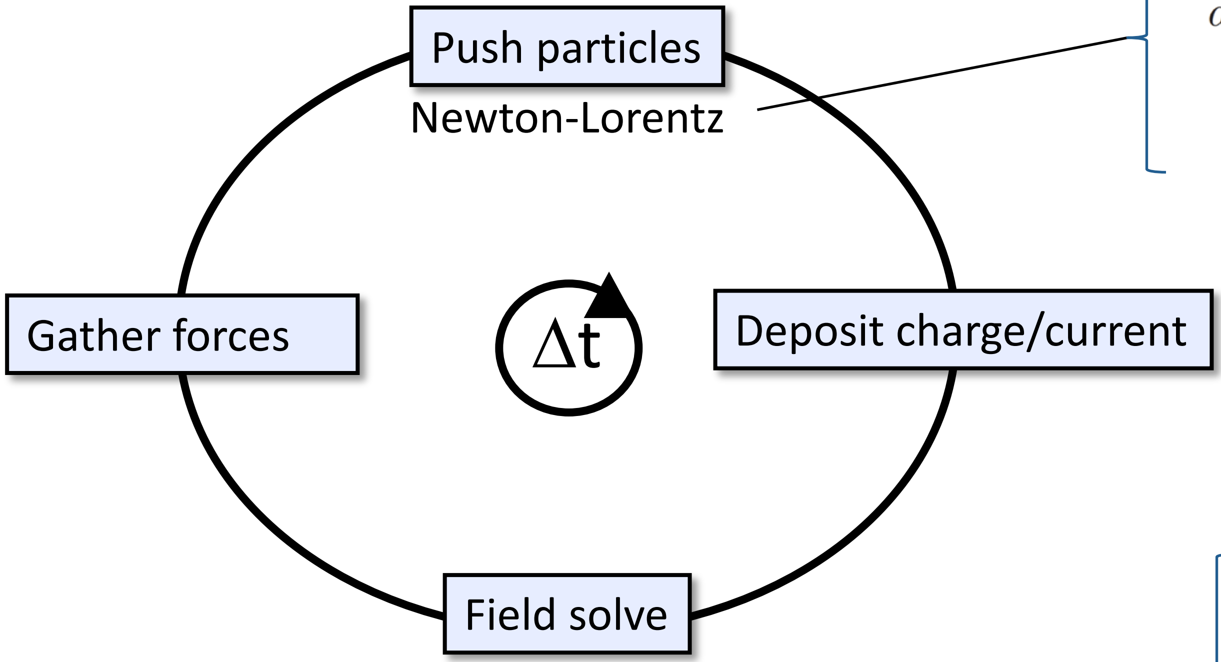
Increase simulation volume & spatiotemporal scale range; decrease time to solution.

The Particle-In-Cell method is very widely used

Lagrangian macro-particles



Eulerian fields on grids
(usually Cartesian)



$$\frac{d(\gamma \mathbf{v})}{dt} = \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}),$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{v},$$

$$\Delta \phi = \rho$$

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

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

usually: second-order staggered finite-differences (leapfrog) discretization

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Integration of Newton-Lorentz: Leapfrog Boris pusher

Position update $\frac{d\mathbf{x}}{dt} = \mathbf{v}$ ⇒ $x^{n+1/2} = x^{n-1/2} + \Delta t\ v^n$

For the velocity component, the Boris pusher writes

$$\frac{d(\gamma\mathbf{v})}{dt} = \frac{q}{m}(\mathbf{E} + \mathbf{v}\times\mathbf{B}) \Rightarrow u^{n+1} = u^n + \frac{q\Delta t}{m}\left(E^{n+1/2} + \frac{u^{n+1}+u^n}{2\gamma^{n+1/2}} \times B^{n+1/2}\right)$$

with $u = \gamma v$

Note choice for v

which decomposes into

one acceleration **+** ***one rotation*** **+** ***one acceleration***

$$u^- = u^n + \frac{q\Delta t}{2m}E^{n+1/2} \Rightarrow u^+ - u^- = \frac{q\Delta t}{2m\gamma^{n+1/2}}\left(u^+ + u^-\right)\times B^{n+1/2} \Rightarrow u^{n+1} = u^+ + \frac{q\Delta t}{2m}E^{n+1/2}$$

with $$\gamma^{n+1/2} = \sqrt{1+\left(u^n + \frac{q\Delta t}{2m}E^{n+1/2}\right)^2 / c^2} = \sqrt{1+\left(u^{n+1} - \frac{q\Delta t}{2m}E^{n+1/2}\right)^2 / c^2}$$

However Boris pusher fails for ultra-relativistic beams

Assuming E and B such that E+v×B=0:

$$\Rightarrow \quad u^{n+1} = u^n \qquad \Rightarrow \quad \gamma^{n+1/2} = \gamma^n = \gamma^{n+1}$$

$$\Rightarrow \quad \gamma^{n+1/2} = \sqrt{1 + \left(u^n + \frac{q\Delta t}{2m} E^{n+1/2}\right)^2 / c^2} = \sqrt{1 + \left(u^n - \frac{q\Delta t}{2m} E^{n+1/2}\right)^2 / c^2}$$

$$\Rightarrow \quad E^{n+1/2} = -E^{n+1/2} = 0 \qquad \Rightarrow \quad B^{n+1/2} = 0$$

meaning that pusher is consistent with (E+v×B=0) only if E=B=0, and is thus inaccurate for e.g. ultra-relativistic beams.

J.-L. Vay, "Simulation of beams or plasmas crossing at relativistic velocity", *Phys. Plasmas* **15** 056701 (2008)

This can be fixed by choosing a different velocity for v x B

Replace Boris velocity pusher

- Velocity push: $$u^{n+1} = u^n + \frac{q\Delta t}{m}\left(E^{n+1/2} + \boxed{\frac{u^{n+1} + u^n}{2\gamma^{n+1/2}}} \times B^{n+1/2}\right)$$ $u = \gamma v$

with

- Velocity push: $$u^{n+1} = u^n + \frac{q\Delta t}{m}\left(E^{n+1/2} + \boxed{\frac{v^{n+1} + v^n}{2}} \times B^{n+1/2}\right)$$

Looks implicit but solvable analytically*

$$\begin{cases} \gamma^{i+1} = \sqrt{\dfrac{\sigma + \sqrt{\sigma^2 + 4(\tau^2 + u^{*2})}}{2}} \\ \mathbf{u}^{i+1} = [\mathbf{u}' + (\mathbf{u}' \cdot \mathbf{t})\mathbf{t} + \mathbf{u}' \times \mathbf{t}]/(1+t^2) \end{cases}$$

with

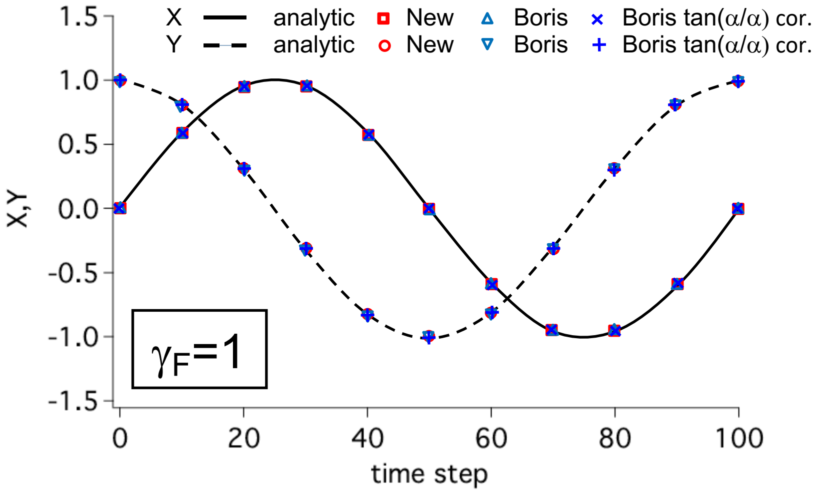
$$\begin{cases} \mathbf{u}' = \mathbf{u}^{\mathbf{i}} + \dfrac{q\Delta t}{m}\left(\mathbf{E}^{i+1/2} + \dfrac{\mathbf{v}^i}{2} \times \mathbf{B}^{i+1/2}\right) \\ \boldsymbol{\tau} = (q\Delta t/2m)\mathbf{B}^{i+1/2} \\ u^* = \mathbf{u}' \cdot \boldsymbol{\tau}/c \\ \sigma = \gamma'^2 - \tau^2 \\ \gamma' = \sqrt{1 + u'^2/c^2} \\ \mathbf{t} = \boldsymbol{\tau}/\gamma^{i+1} \end{cases}$$

J.-L. Vay, "Simulation of beams or plasmas crossing at relativistic velocity", *Phys. Plasmas* **15** 056701 (2008)

New choice leads to better accuracy with ExB drifts

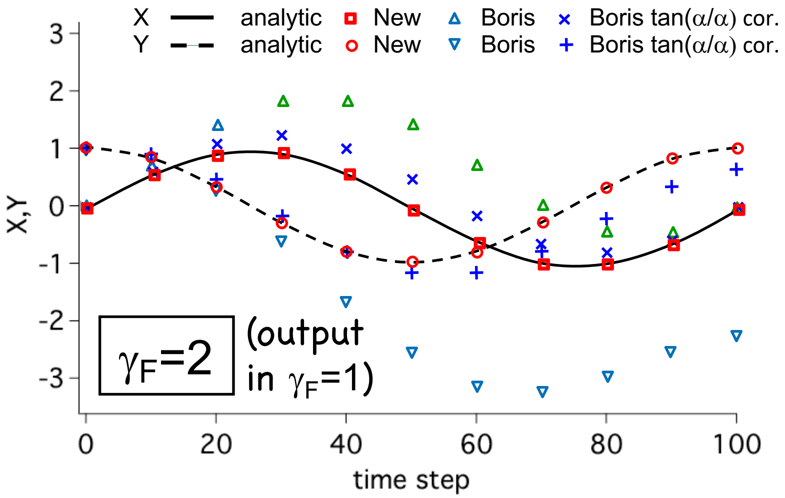
Lab frame

particle cycling in constant B field



Boosted frame γ=2

ExB drift adds to gyration



Other variations have been proposed, e.g. Higuera-Cary

Boris

- Velocity push: $u^{n+1} = u^n + \frac{q\Delta t}{m}\left(E^{n+1/2} + \frac{u^{n+1}+u^n}{2\gamma^{n+1/2}} \times B^{n+1/2}\right)$

$u = \gamma v$

Vay

- Velocity push: $u^{n+1} = u^n + \frac{q\Delta t}{m}\left(E^{n+1/2} + \frac{v^{n+1}+v^n}{2} \times B^{n+1/2}\right)$

Higuera-Cary

- Velocity push: $u^{n+1} = u^n + \frac{q\Delta t}{m}\left(E^{n+1/2} + \frac{u^{n+1}+u^n}{2\bar{\gamma}} \times B^{n+1/2}\right)$

A. V. Higuera, J. R. Cary, "**Structure-preserving** second-order integration of relativistic charged particle trajectories in electromagnetic fields", *Phys. Plasmas* **24**, 052104 (2017)

with $\bar{\gamma} = \sqrt{1 + \frac{u^{n+1}+u^n}{2c}}$

Many other particle pushers exist (RK, Pétri, Ripperda, etc.), each with pros & cons.

Choice depends on physics to be studied. Some comparisons exist but more needed.

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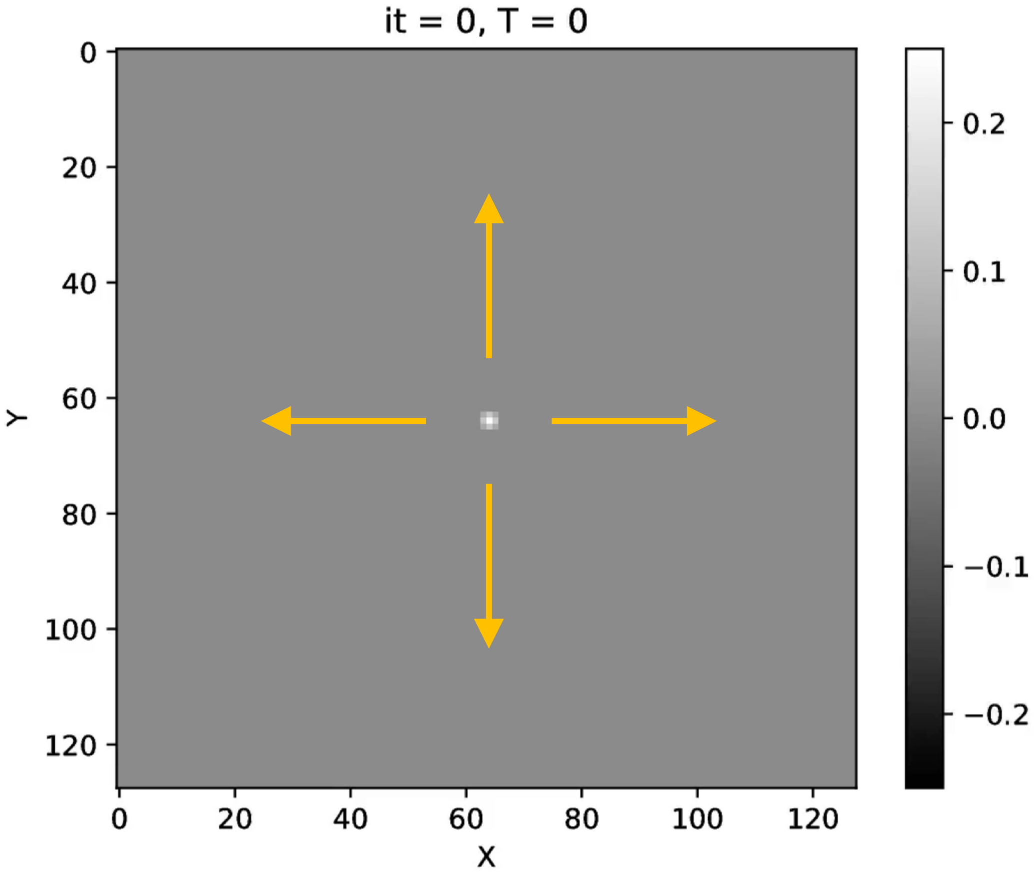
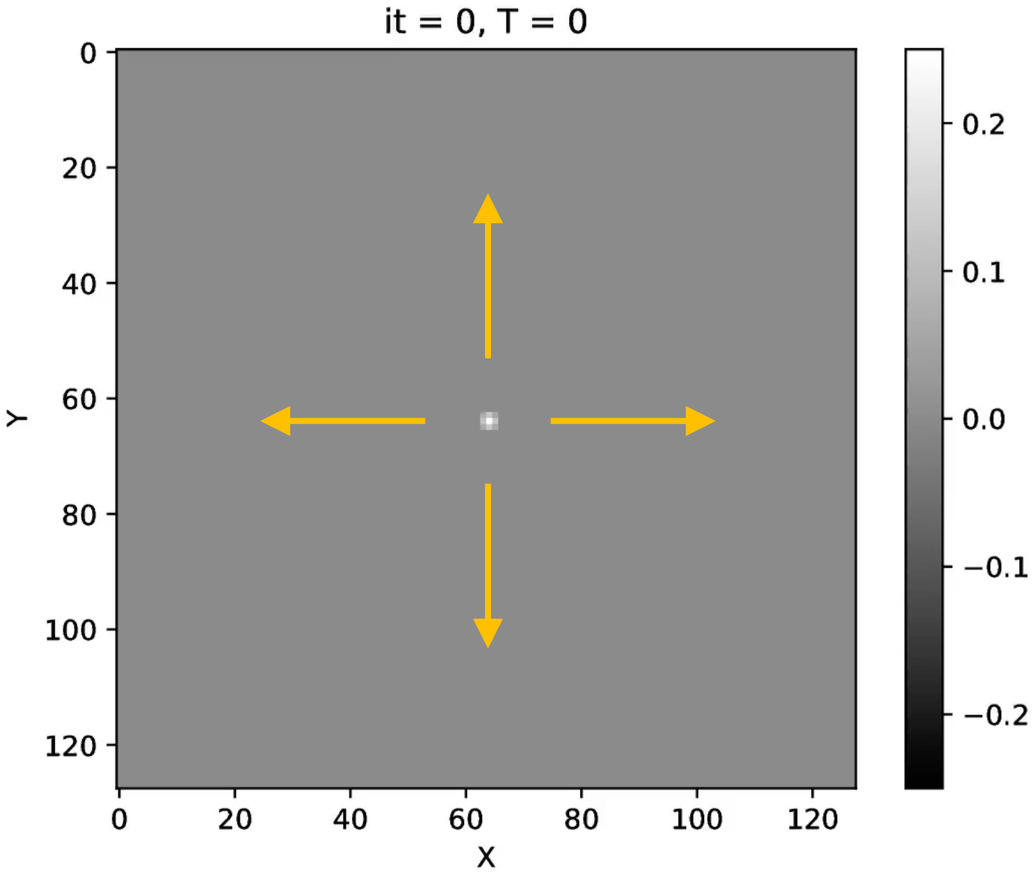
FDTD numerical dispersion: expanding electromagnetic pulse test

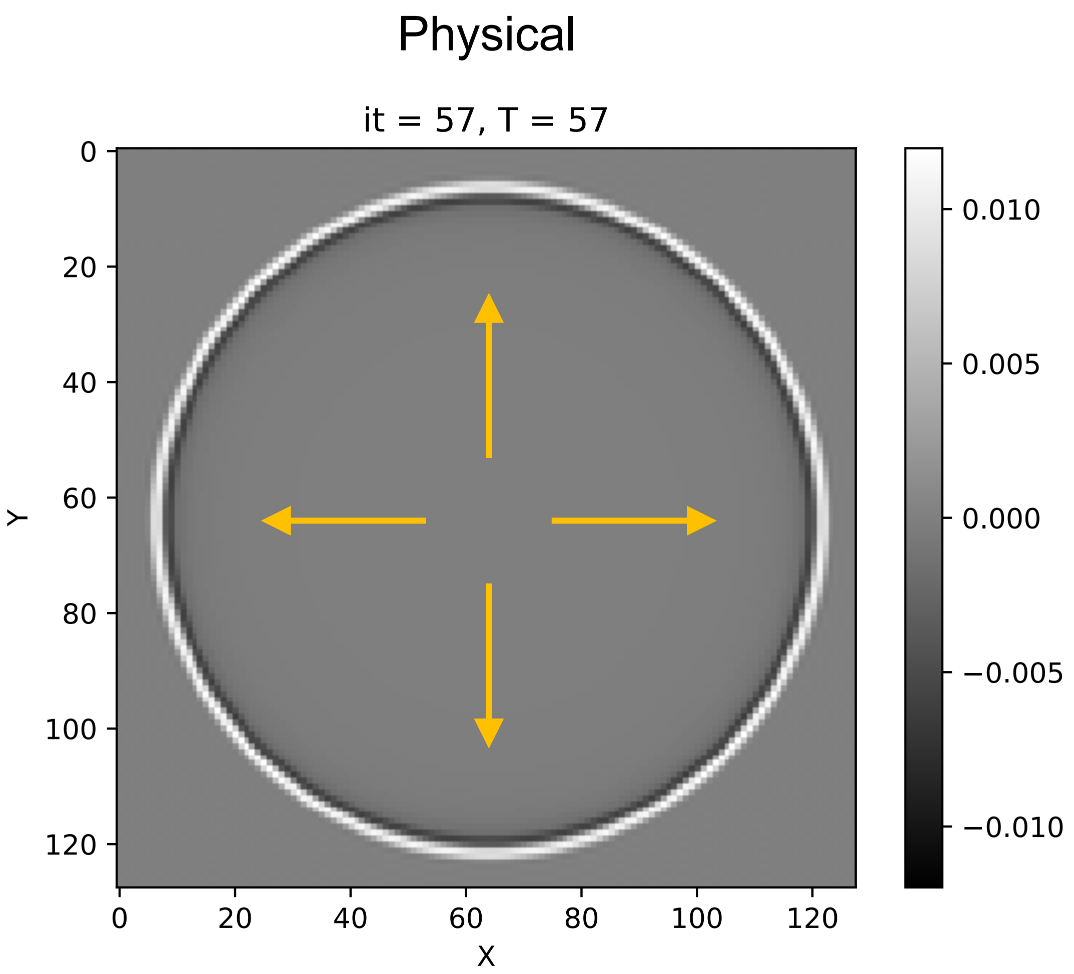
Physical

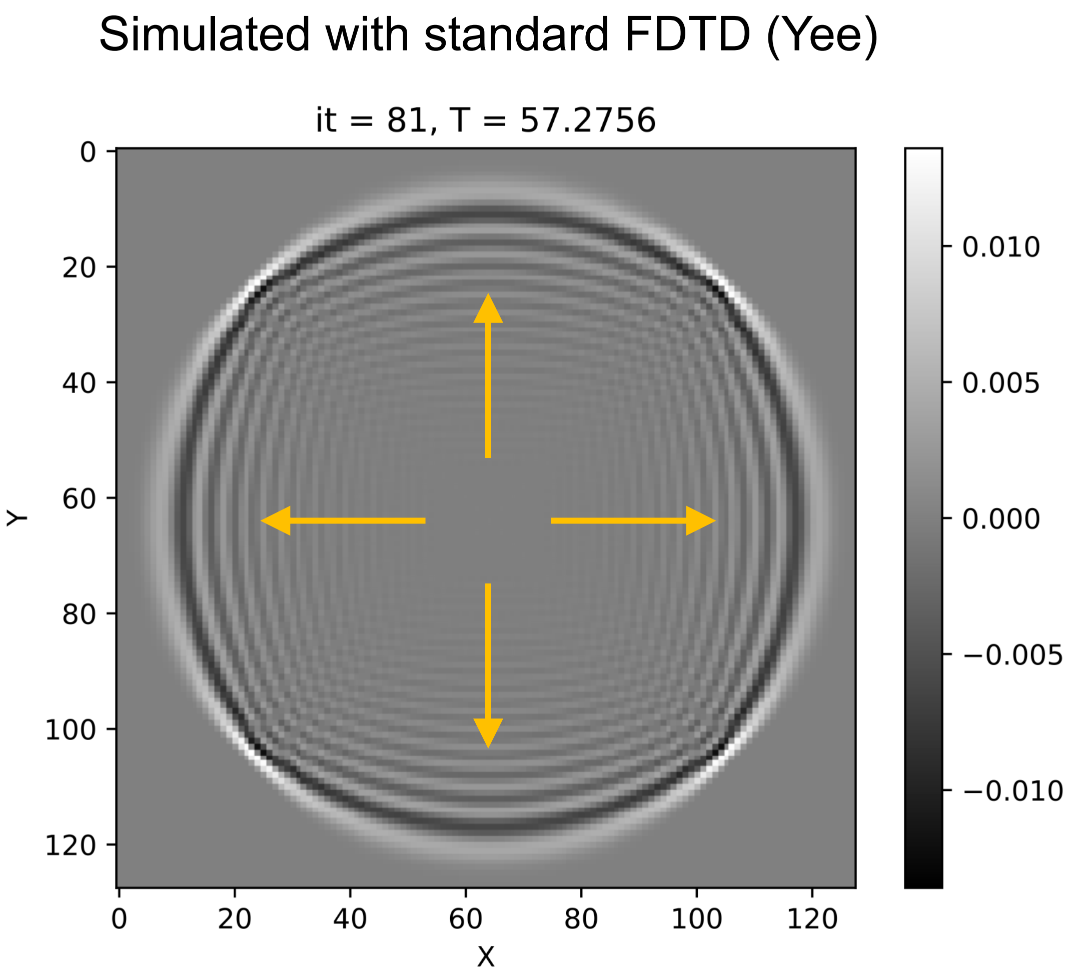


Simulated with standard FDTD (Yee)



Example: expanding electromagnetic pulse

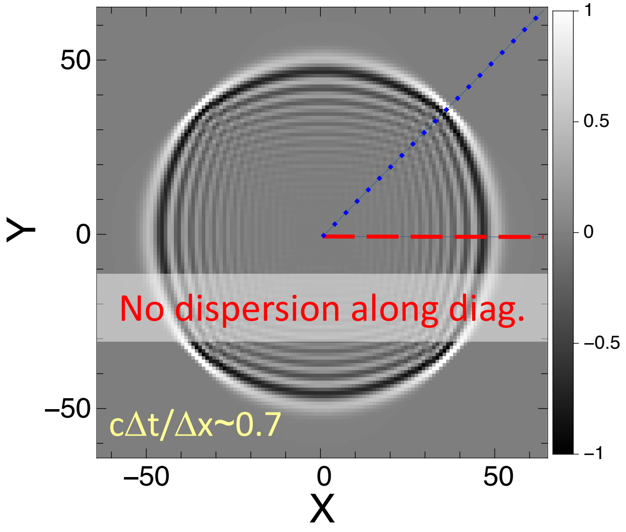


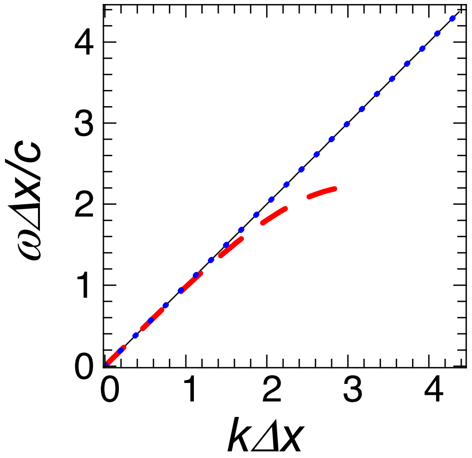


Numerical dispersion depends on time step, wavelength & angle.

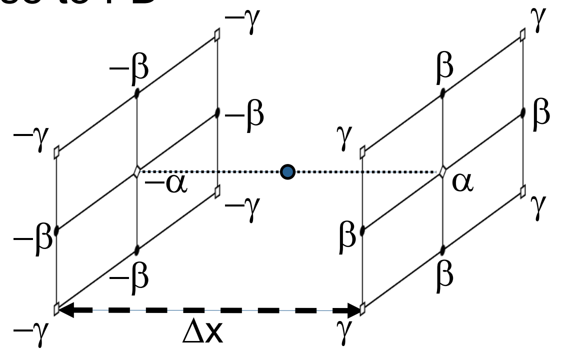
Non-Standard FD solvers offer some tunability

FDTD (Yee)



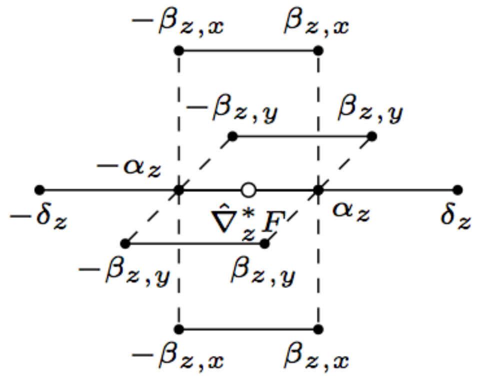


NSFD[1,2]: weighted average of quantities transverse to FD

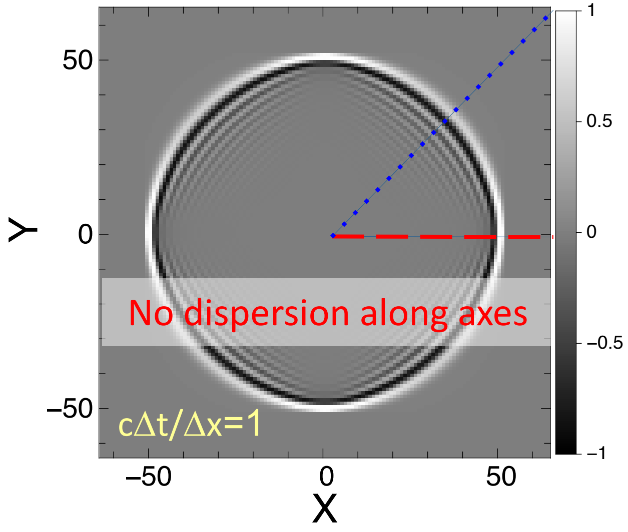


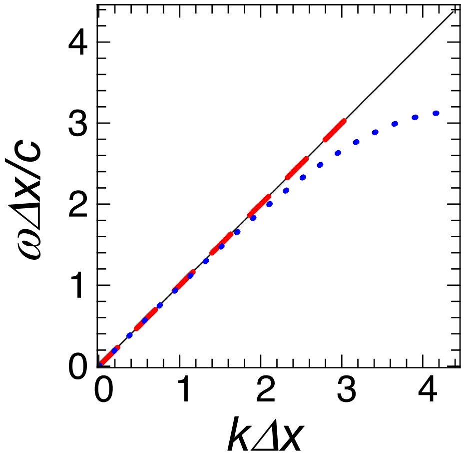
- Adaptations to PIC[3,4,5]

Lehe[6] algorithm:



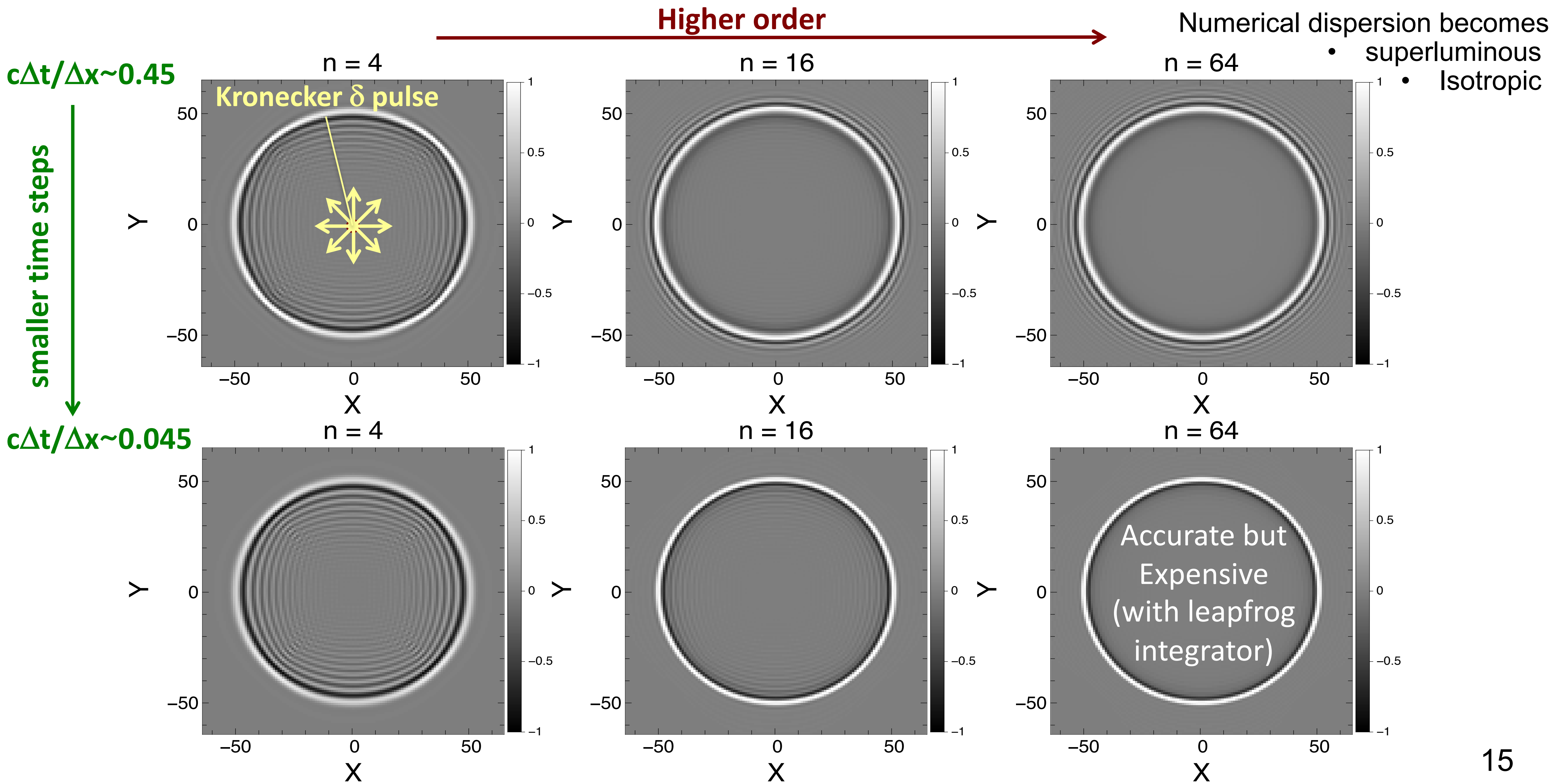
NS-FDTD (Karkkainen/Lehe)





[1]J. B. Cole, IEEE Trans. Microw. Theory Tech. **45** (1997).
[2]M. Karkkainen et al., Proc. ICAP, Chamonix, France (2006).
[3]A. Pukhov, J. Plasma Physics **61** (1999) 425.
[4]J.-L. Vay et al, J. Comput. Phys. **230** (2011) 5908.
[5]B. Cowan et al, PRST-AB **16** (2013) 041303.
[6]R. Lehe et al, PRST-AB **16** (2013) 021301.

Arbitrary-order Maxwell solver offers higher flexibility in accuracy



Pseudo-spectral solvers offer infinite order spatial derivatives

Finite-Difference Time-Domain (FDTD)

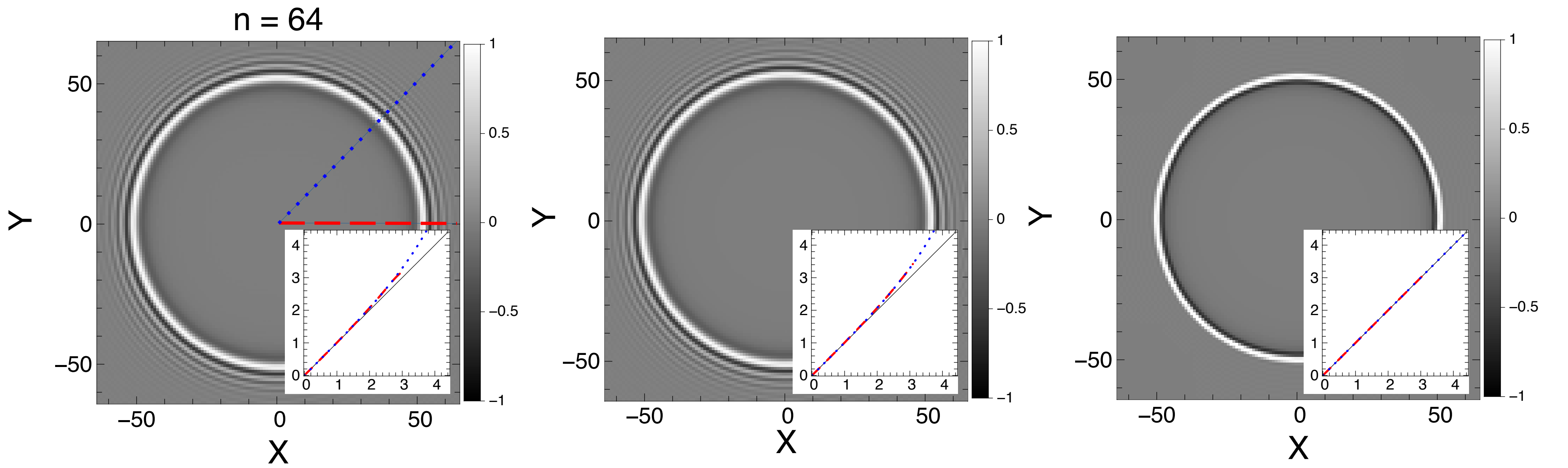
$$B_z^{n+1} = B_z^n + \Delta t\left(\frac{\Delta E_x}{\Delta y} - \frac{\Delta E_y}{\Delta x}\right)$$

Pseudo-Spectral Time-Domain (PSTD)

$\mathcal{F}$=FFT

$$B_z^{n+1} = B_z^n + \Delta t\left[\mathcal{F}^{-1}\left(ik_y\,\mathcal{F}\left(E_x\right)\right) - \mathcal{F}^{-1}\left(ik_x\,\mathcal{F}\left(E_y\right)\right)\right]$$

FDTD cΔt/Δx~0.45 | PSTD cΔt/Δx~0.45 | PSTD cΔt/Δx~0.045



PSTD is limit of high-order FDTD when n→infinity.

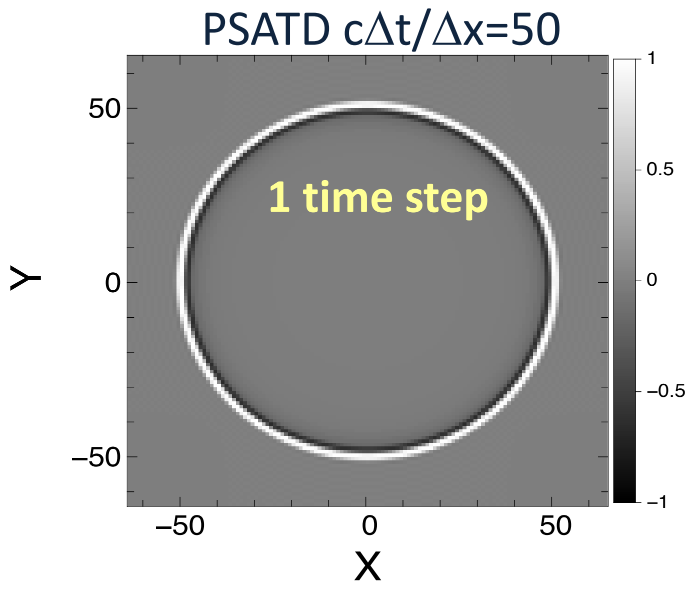
PSTD converges to exact solution (on grid) for Δt→0.

Analytical time integration in Fourier space offers exact solution

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*$^{\infty}$→ *k*^{n}).

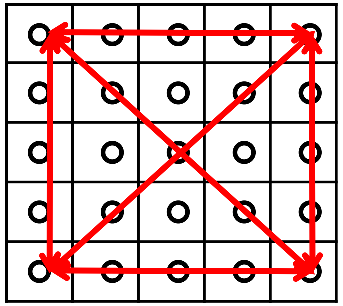
But what about scalability?

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

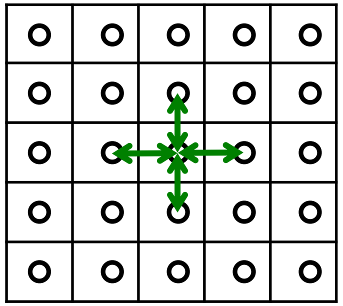
FFTs are global → harder to scale to large # of computer nodes

Spectral | **Finite Difference (FDTD)**

global "costly" communications vs local "cheap" communications

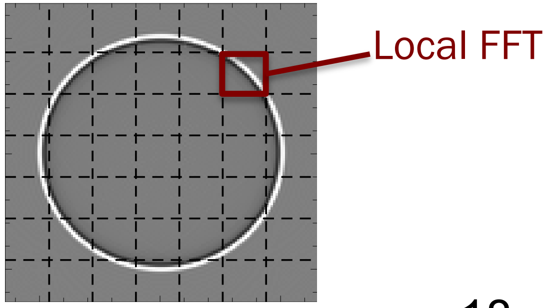


vs



Harder to scale | Easier to scale

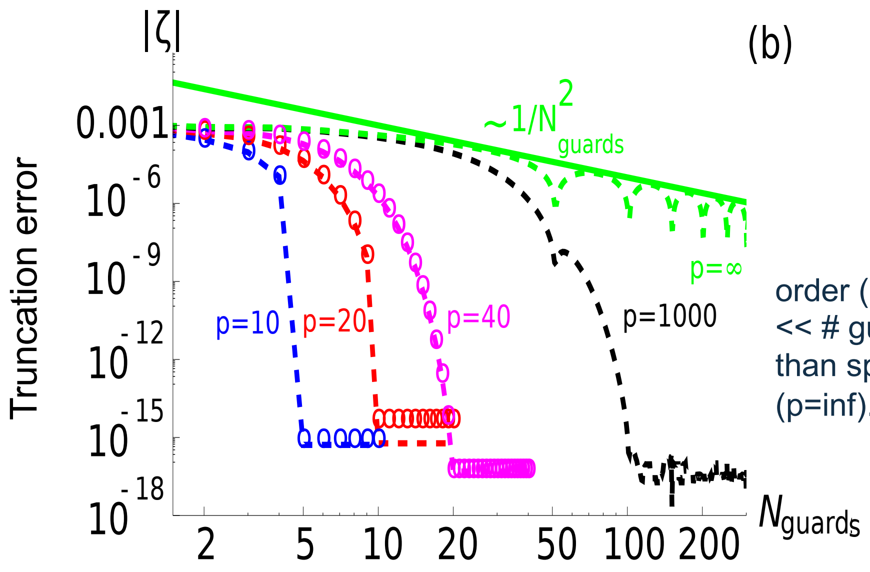
Finite speed of light → local FFTs → spectral accuracy+FDTD scaling!



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

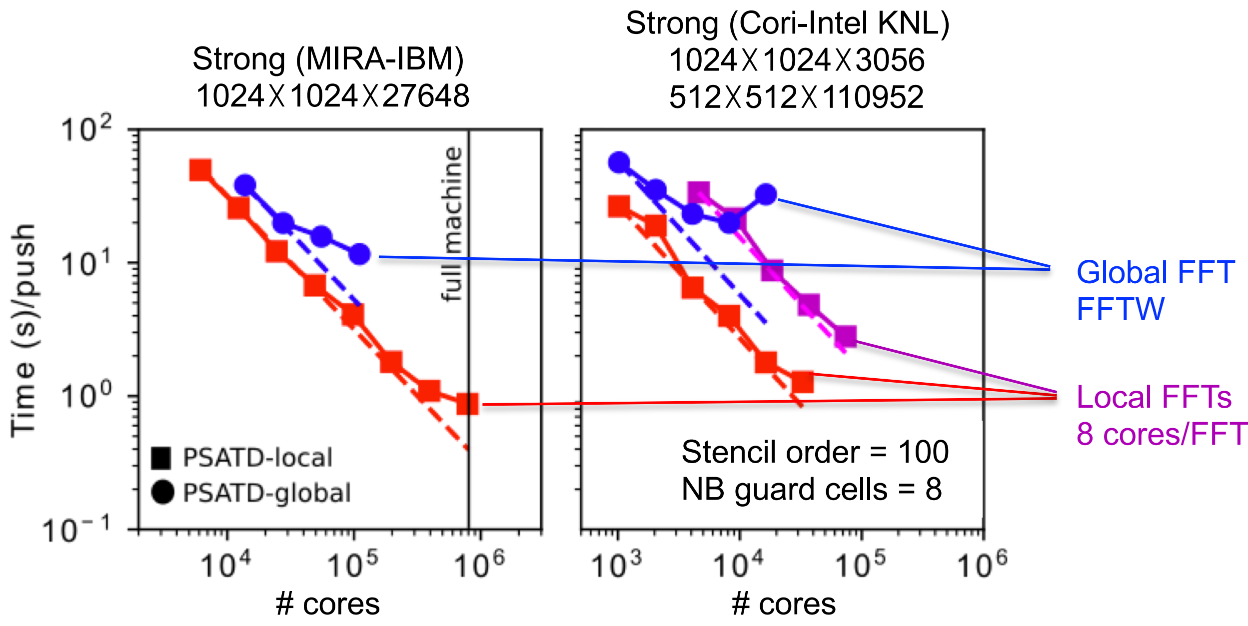
Truncation error analysis ➔ ultra-high order possible with much improved stability



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

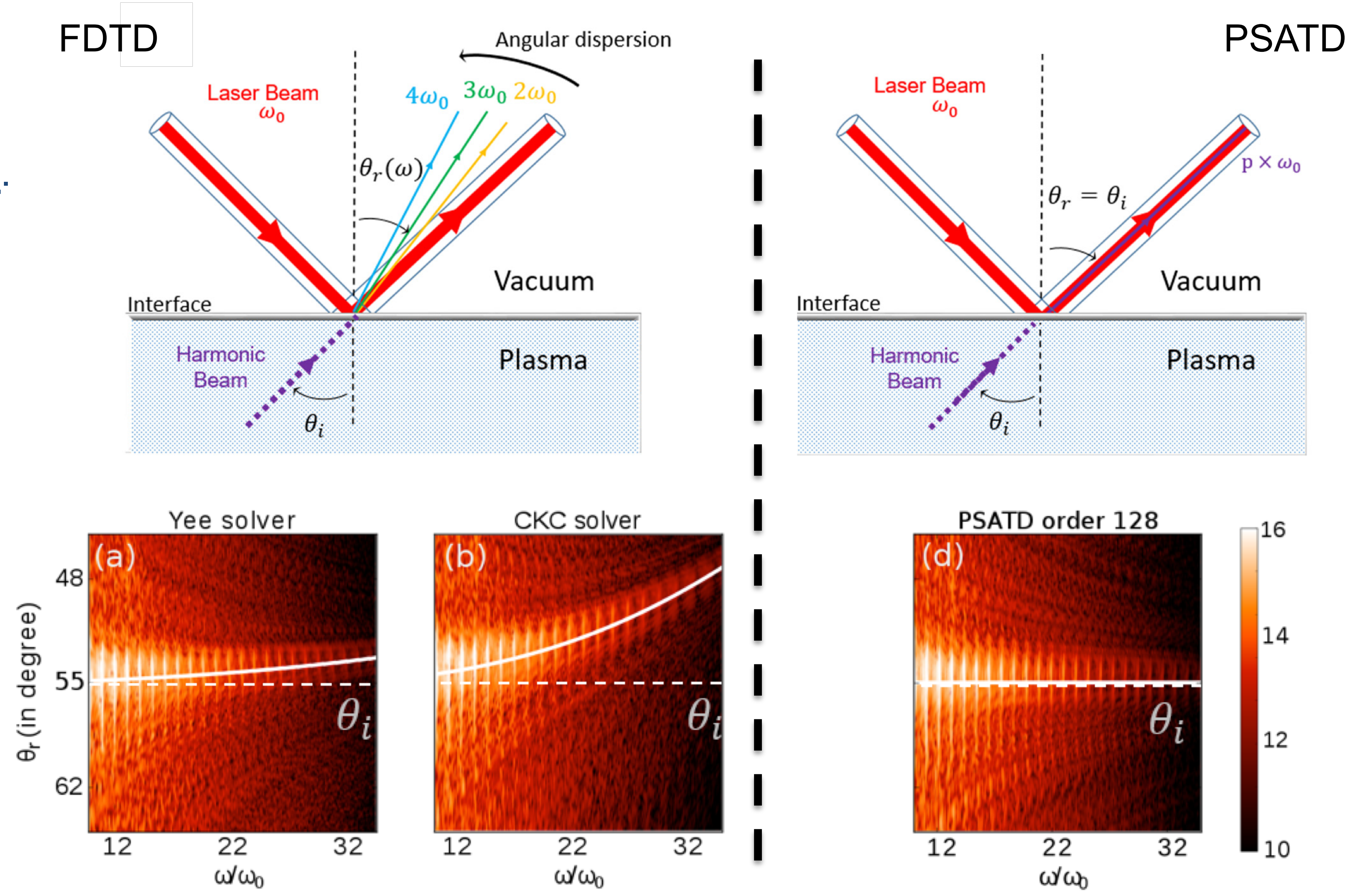


H. Vincenti, J.-L. Vay, *Comput. Phys. Comm.* **228**, 22-29 (2018)

PSATD solver enables accurate modeling of plasma mirrors

Problem: Standard second-order Maxwell solvers lead to **numerical angular dispersion**.

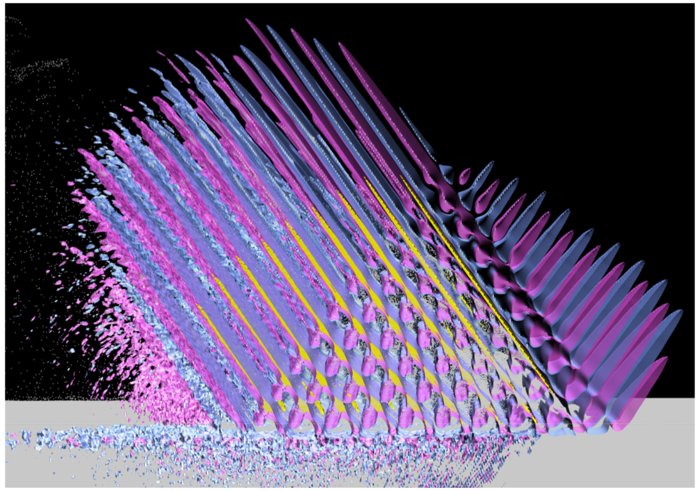
Solution: PSATD solver gives correct reflection angle at all wavelength.

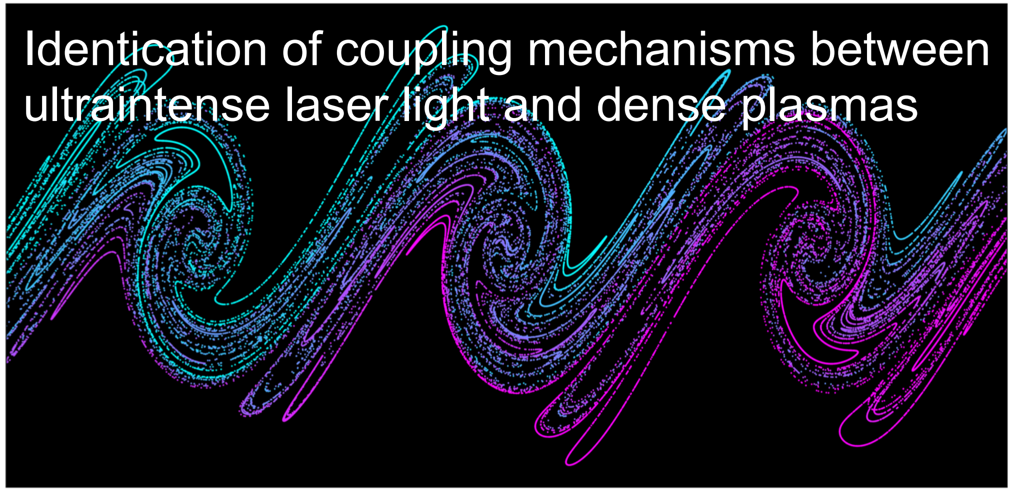


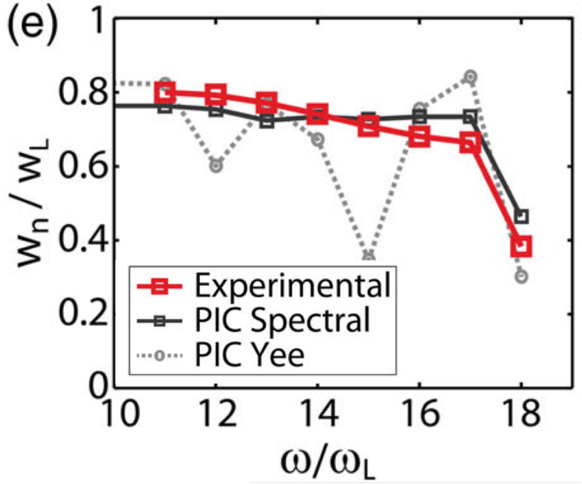
G. Blaclard, H. Vincenti, R. Lehe and J-L Vay, PRE **96**, 033305 (2017)

This led to unprecedented 3D modeling of plasma mirrors

Spatial Properties of High-Order Harmonic Beams from Plasma Mirrors







PSATD enable correct prediction of source size

Comprehensive experimental and numerical study

➔ reveals a clear transition from the temporally-periodic Brunel mechanism to a chaotic dynamic associated to stochastic heating.

A. Leblanc, S. Monchocé, H. Vincenti, S. Kahaly, J.-L. Vay, F. Quéré, *Phys. Rev. Lett.* **119**, 155001 (2017)

L. Chopineau, A. Leblanc, G. Blaclard, A. Denoeud, M. Thévenet, J-L. Vay, G. Bonnaud, P. Martin, H. Vincenti, and F. Quéré, *Phys. Rev. X* **9**, 011050 (2019)

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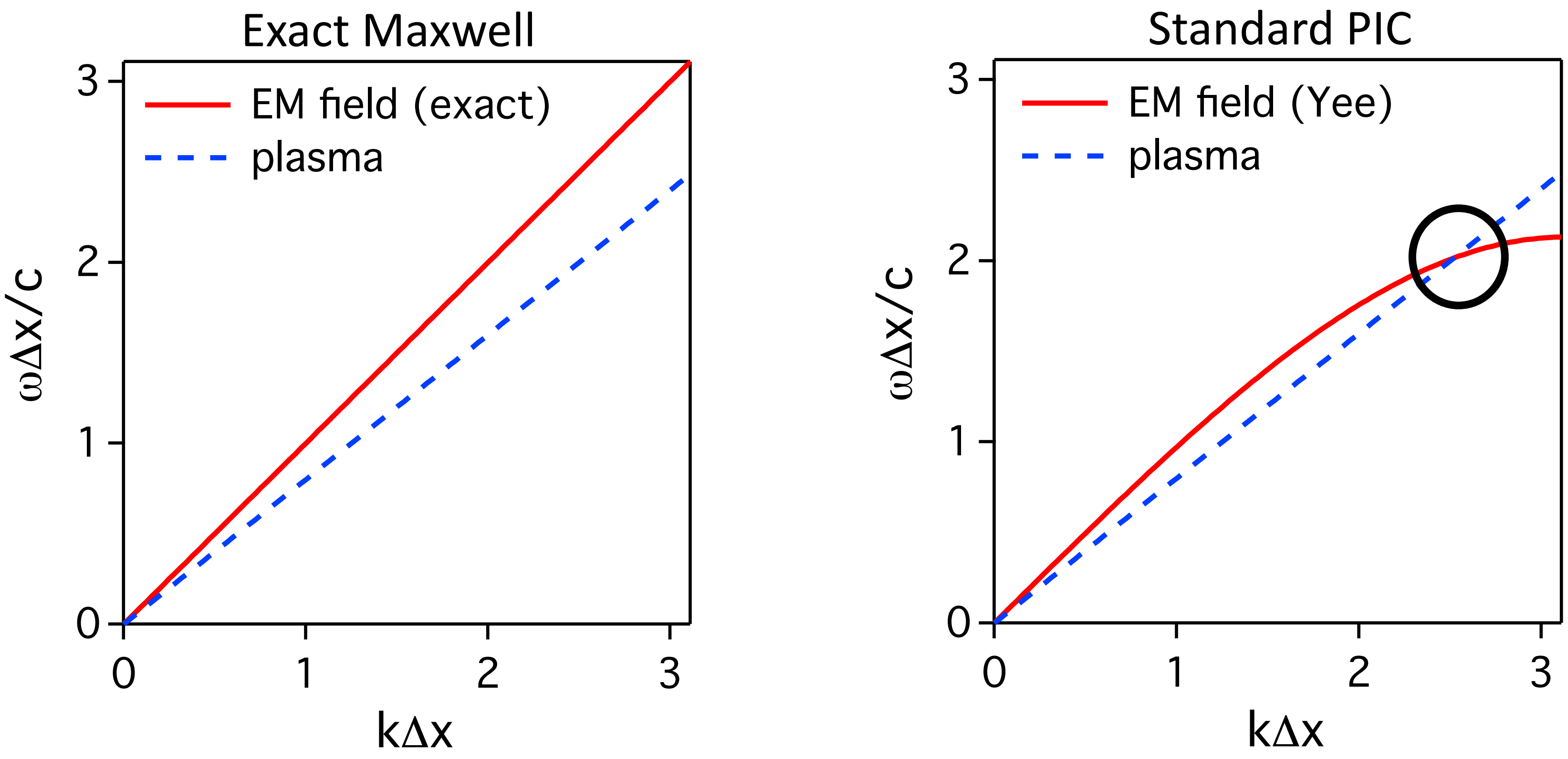
Relativistic plasmas PIC subject to “numerical Cherenkov instability” (NCI)

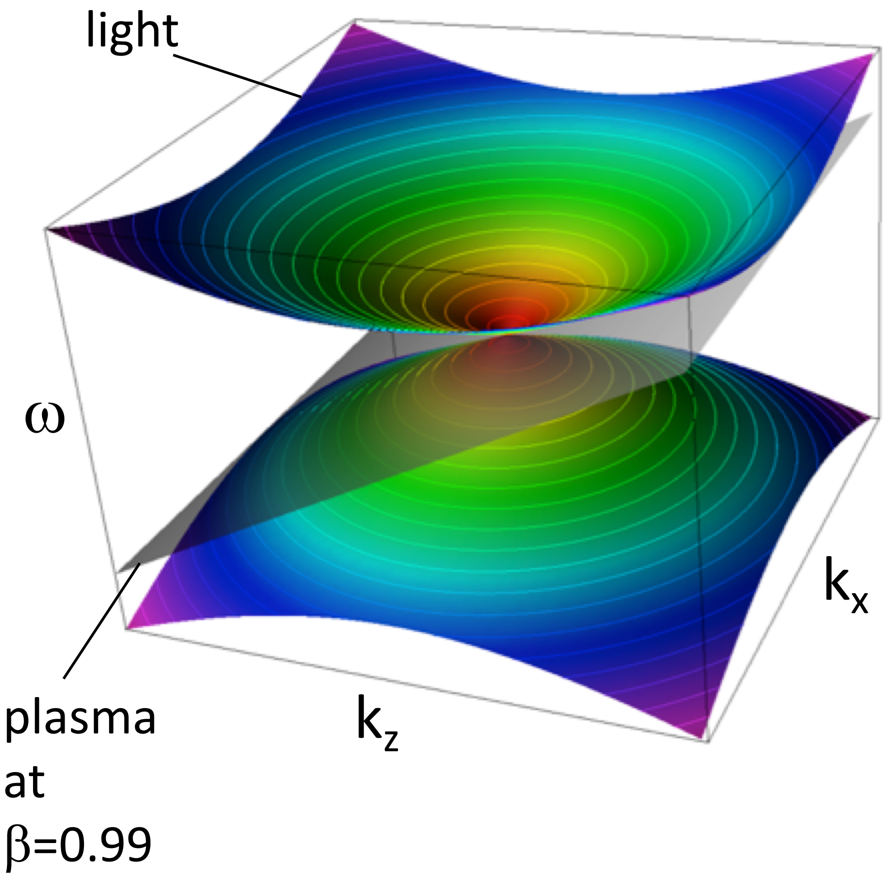
Numerical dispersion leads to crossing of EM field and plasma modes -> instability.



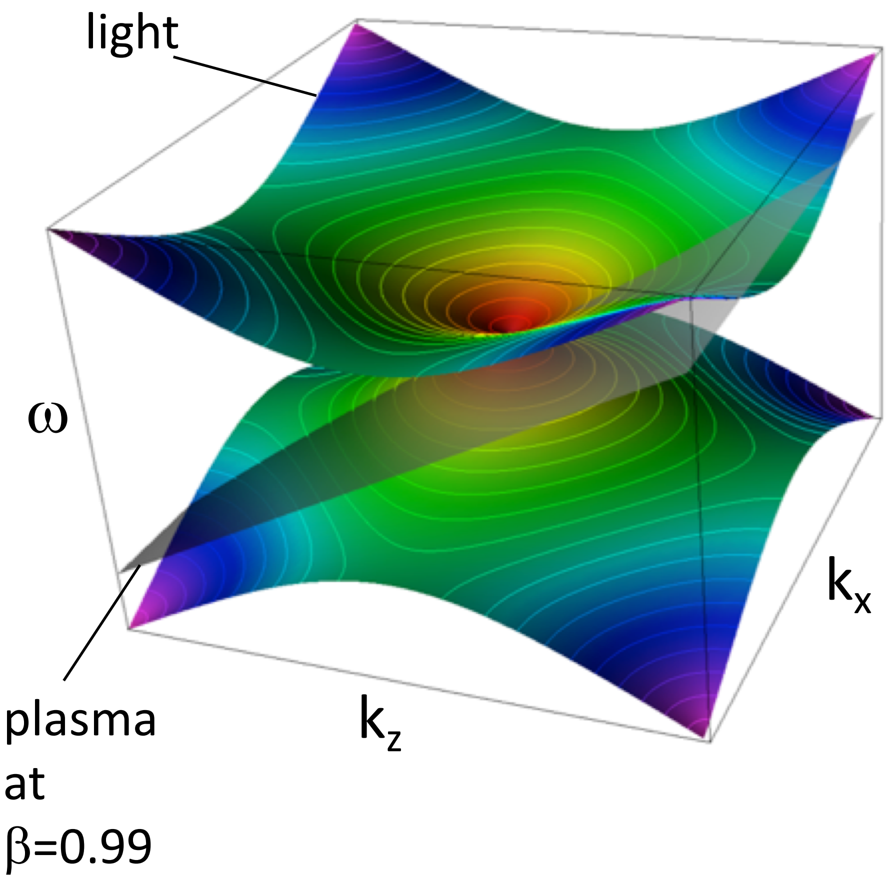
B. B. Godfrey, “Numerical Cherenkov instabilities in electromagnetic particle codes”, *J. Comput. Phys.* **15** (1974)

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

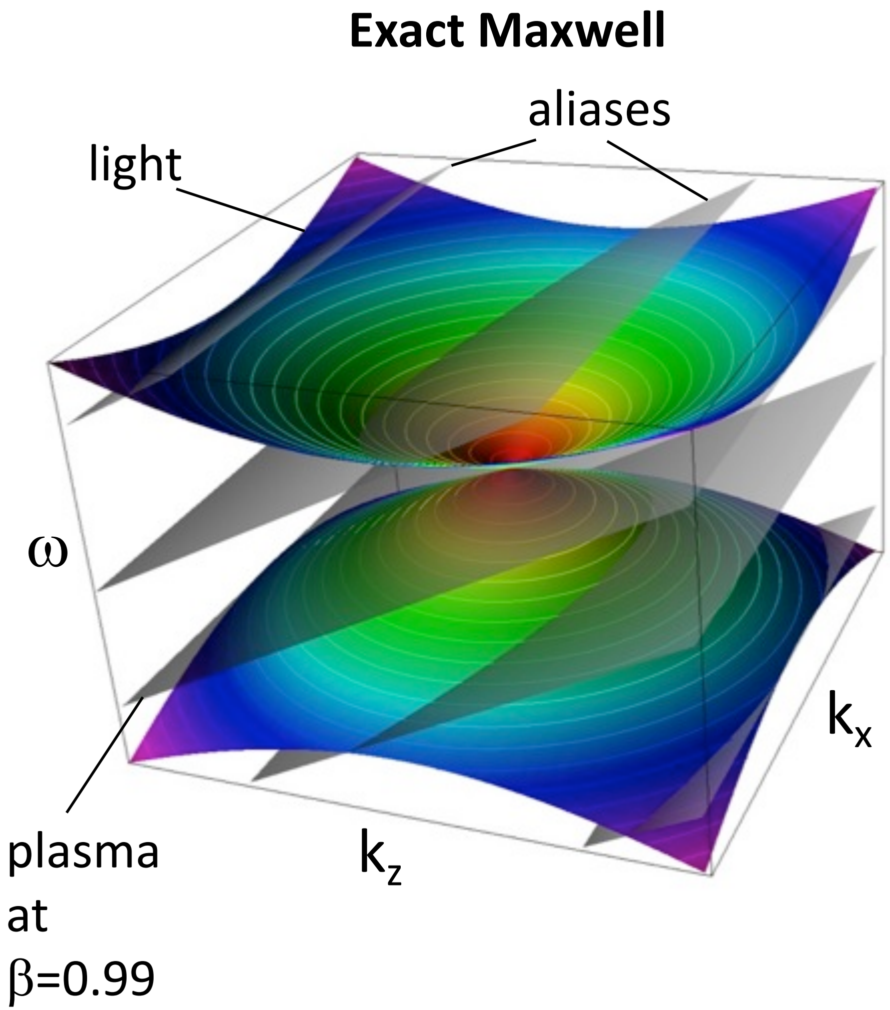
Exact Maxwell

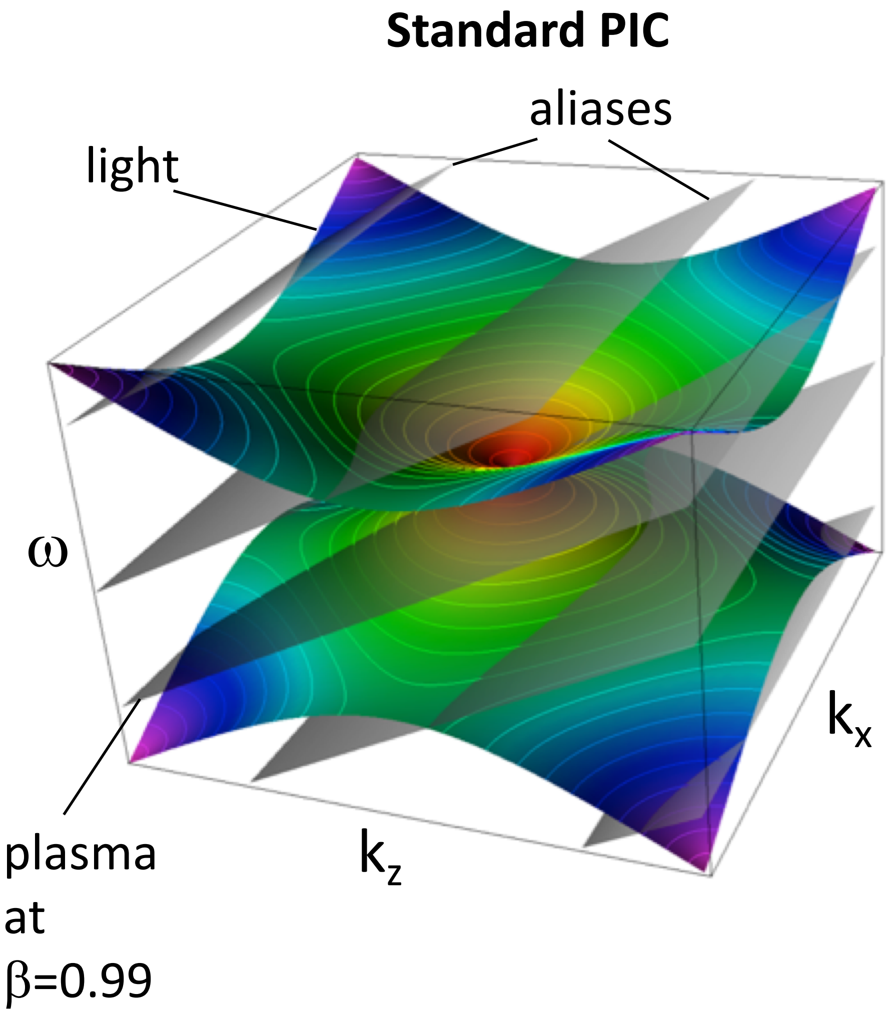


Standard PIC



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





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

Analysis and mitigation of NCI has had renewed interest

Analysis of NCI has been generalized:

- **to finite-difference PIC codes (“Magical” time step explained):**
  - B. B. Godfrey and J.-L. Vay, *J. Comp. Phys.* **248**, 33 (2013).
  - X. Xu, et. al., *Comp. Phys. Comm.* **184**, 2503 (2013).
- **to pseudo-spectral PIC codes:**
  - B. B. Godfrey, J. -L. Vay, I. Haber, *J. Comp. Phys.* **258**, 689 (2014).
  - P. Yu et. al, *J. Comp. Phys.* **266**, 124 (2014).

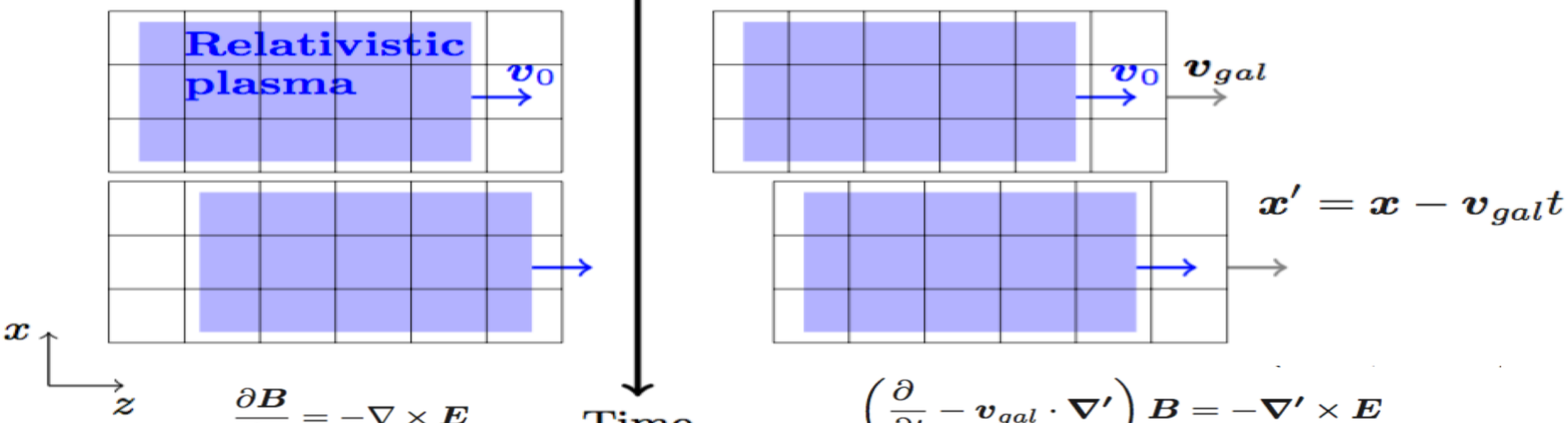
Efficient suppression techniques were recently developed:

- **for finite-difference PIC codes:**
  - B. B. Godfrey and J.-L. Vay, *J. Comp. Phys.* **267**, 1 (2014).
- **for pseudo-spectral PIC codes:**
  - B. B. Godfrey, J.-L. Vay, I. Haber, *IEEE Trans. Plas. Sci.* **42**, 1339 (2014).
  - P. Yu, et. al., *Comp. Phys. Comm.*, **192**, 32 (2015).
  - B. B. Godfrey and J.-L. Vay, *Comp. Phys. Comm.*, **196**, 221 (2015).

PSATD enables time 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

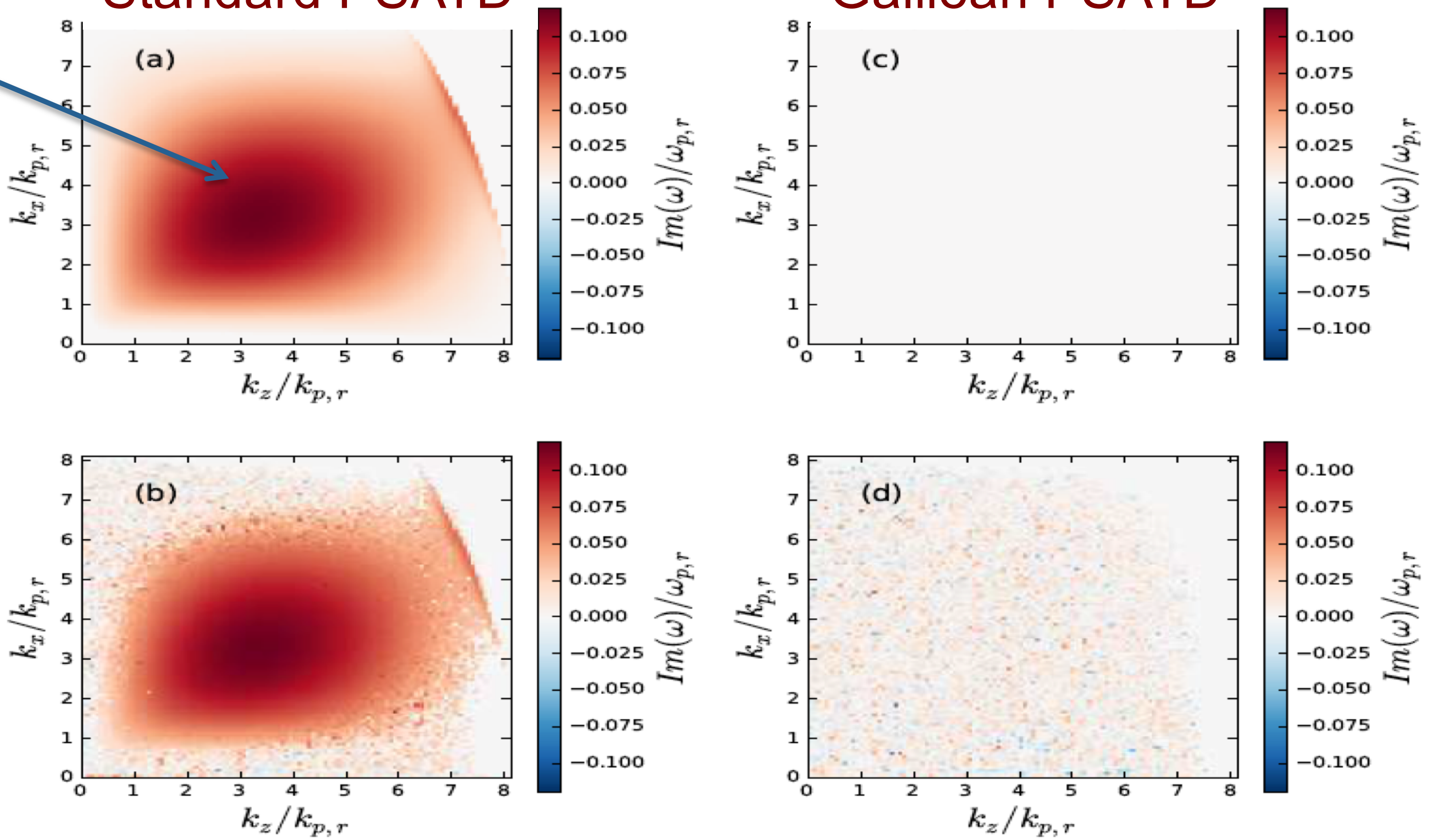
Uniform plasma streaming in 2D periodic box

Instability growth rate

Standard PSATD | Galilean PSATD

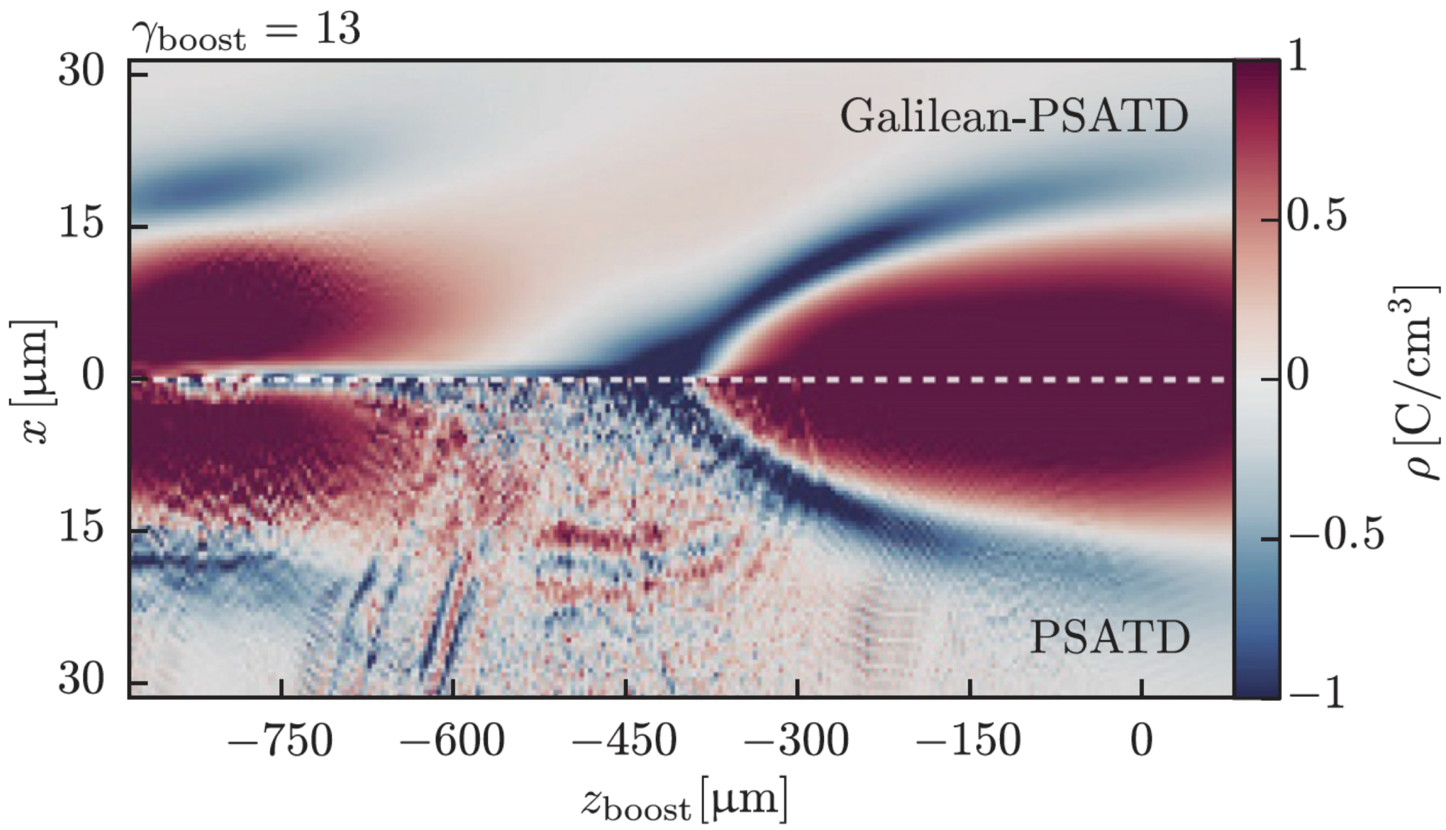
Analysis

Simulation



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

And is also the most stable algo. for plasma acceleration simulations



Axisymmetric simulation

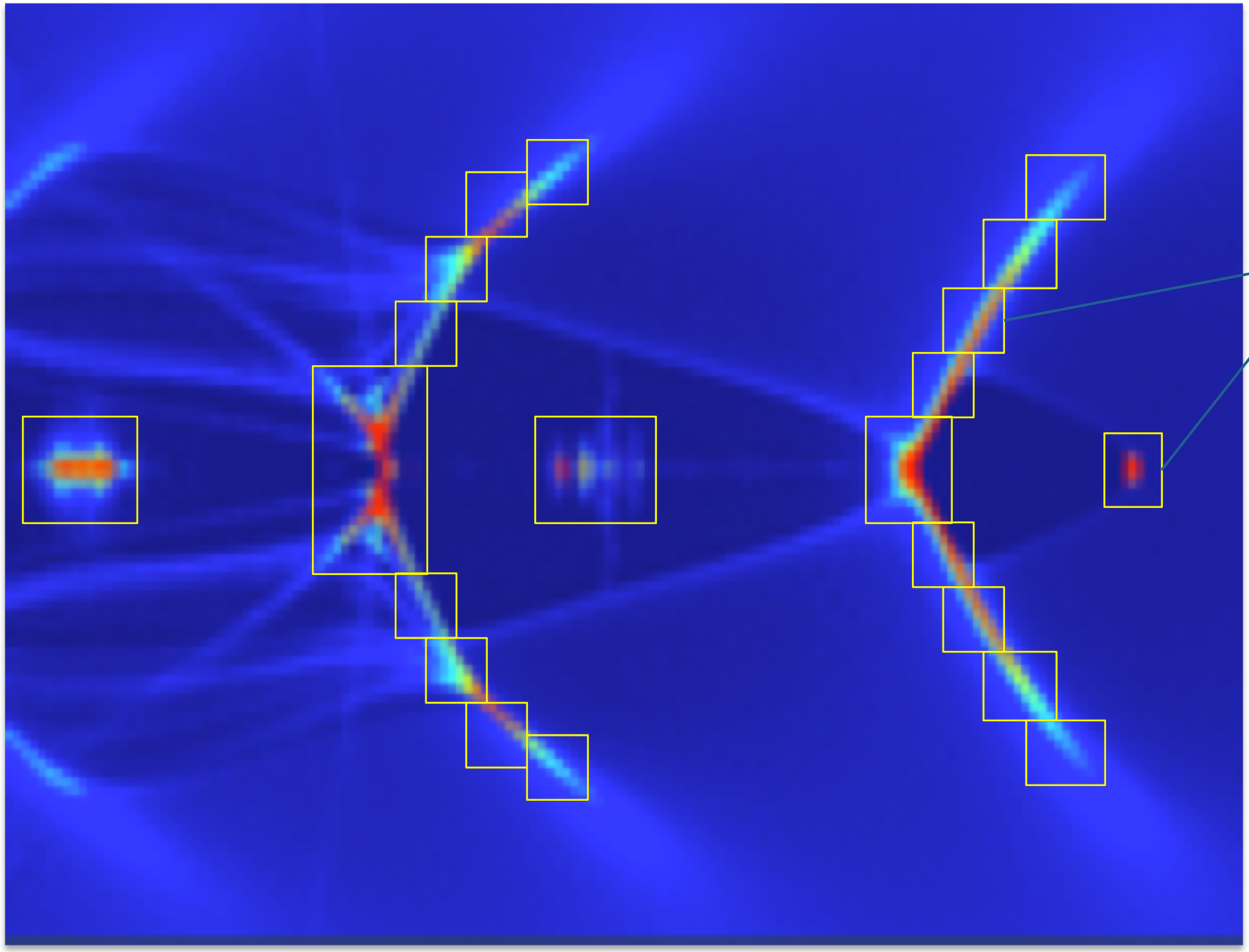
code FBPIC (2016)

The method has been successfully tested on 2-grid systems for astrophysical relativistic shocks (unpublished).

Outline

- Introduction
- Issues and some solutions
  - Particle pusher
  - Field solver
  - Numerical Cherenkov Instability
  - **Mesh refinement**
  - Optimal Lorentz boosted frame
- Conclusion

Mesh refinement enables "zooming" on regions of interest



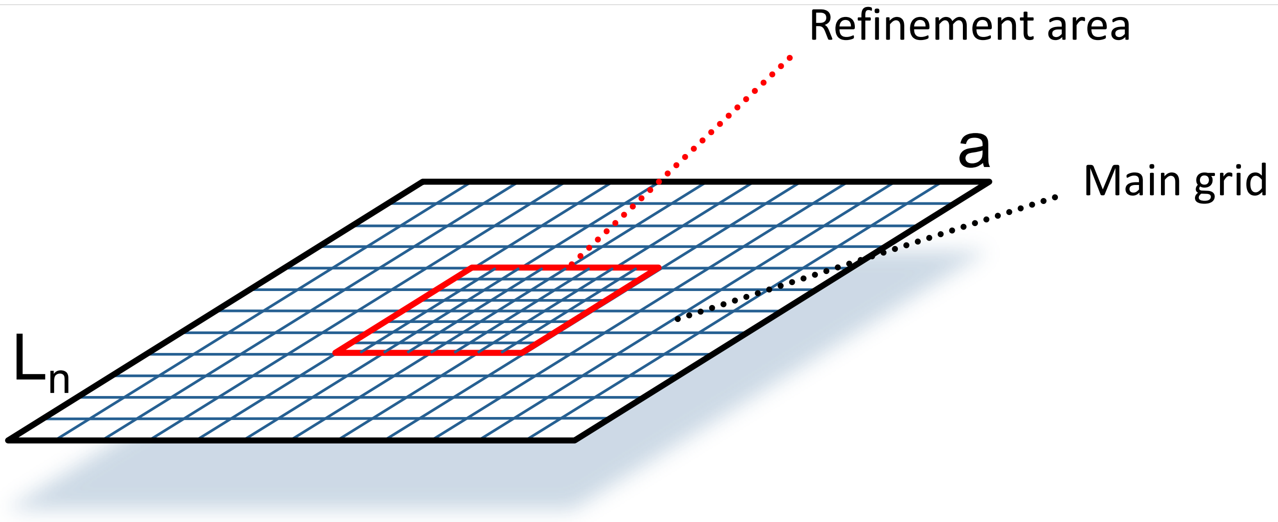
e.g. around small features and/or sharp gradients

But mesh refinement (MR) requires special care with PIC, especially EM-PIC!

Mesh refinement requires special algorithm[1,2]

Need to avoid spurious:

1. self-forces
2. wave reflections
3. dispersion mismatch



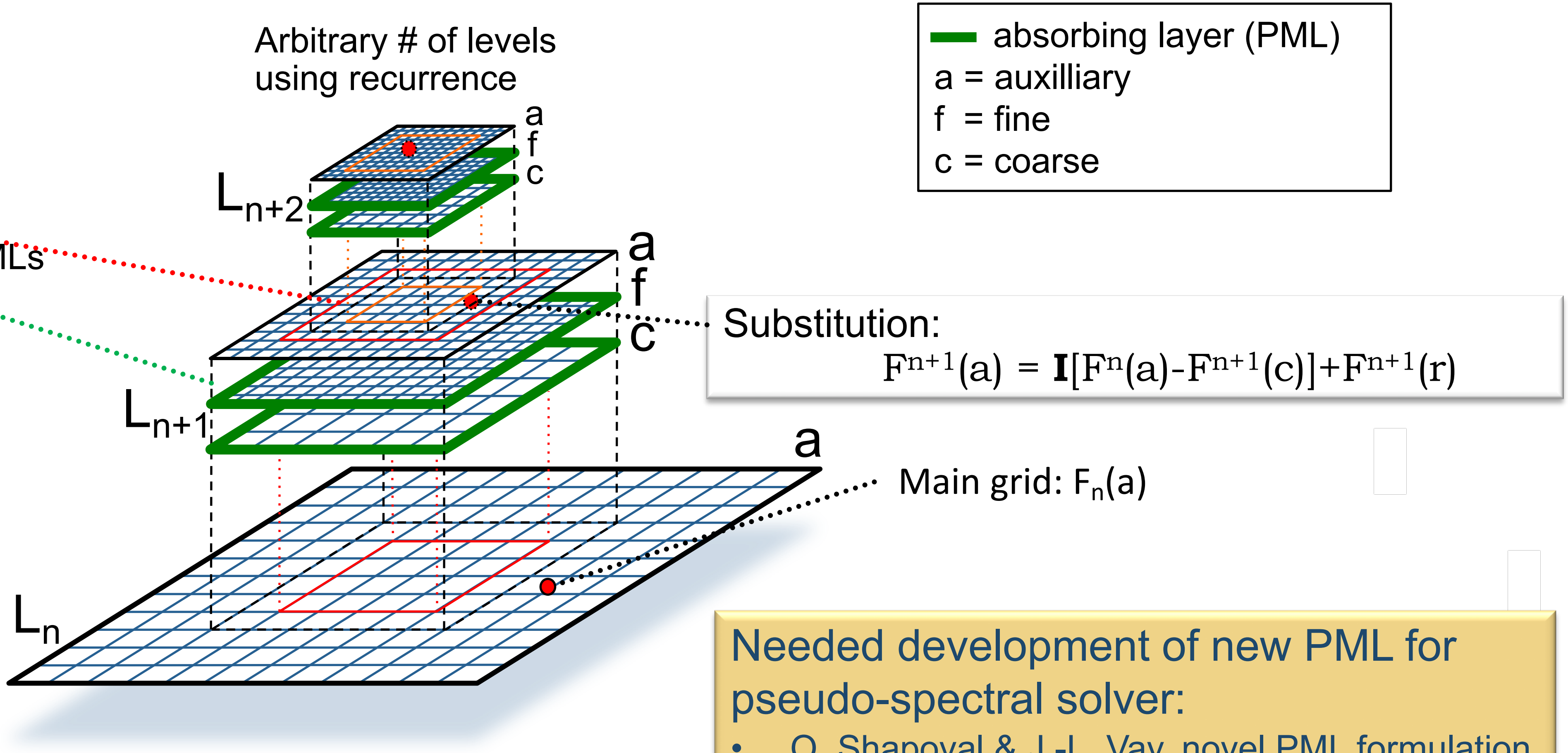
Mesh refinement requires special algorithm[1,2]

Need to avoid spurious:

1. self-forces
2. wave reflections
3. dispersion mismatch

➔

1. buffer regions
2. multiple grids with PMLs around patches
3. subcycling/pseudo-spectral solvers



Needed development of new PML for pseudo-spectral solver:

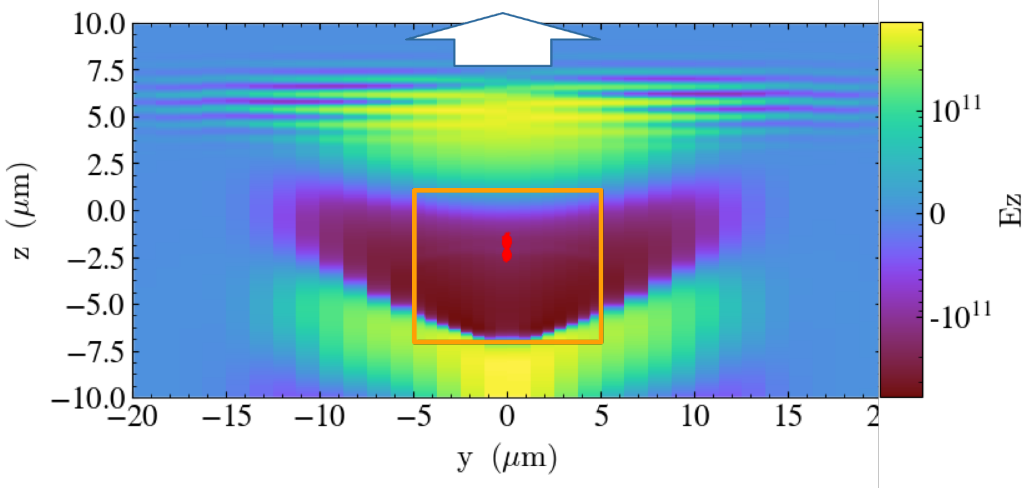
- O. Shapoval & J.-L. Vay, novel PML formulation published in Comput. Phys. Comm. 235 (2018)

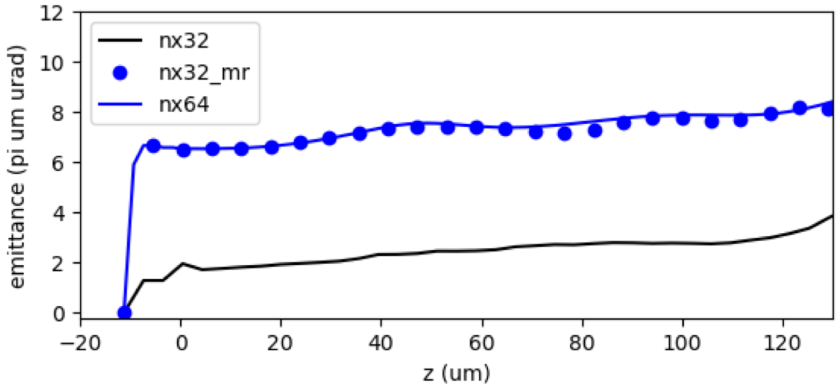
[1]J.-L. Vay, J.-C. Adam, A. Héron, *Computer Physics Comm.* **164**, 171-177 (2004).
[2]J.-L. Vay, D. P. Grote, R. H. Cohen, & A. Friedman, *Computational Science & Discovery* **5**, 014019 (2012).

Example: simulations of plasma accelerators with mesh refinement

(09/17)

Laser driven

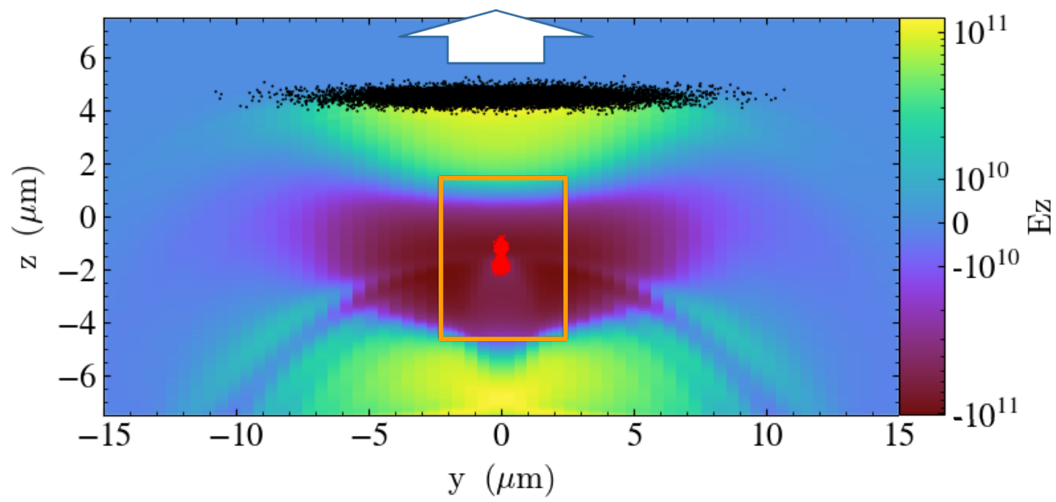


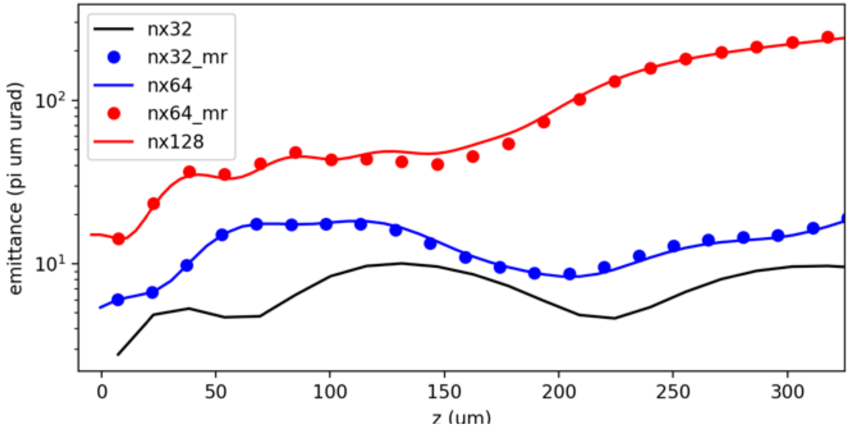


3-D WarpX

Mesh refinement focuses resolution only where needed

Particle beam driven

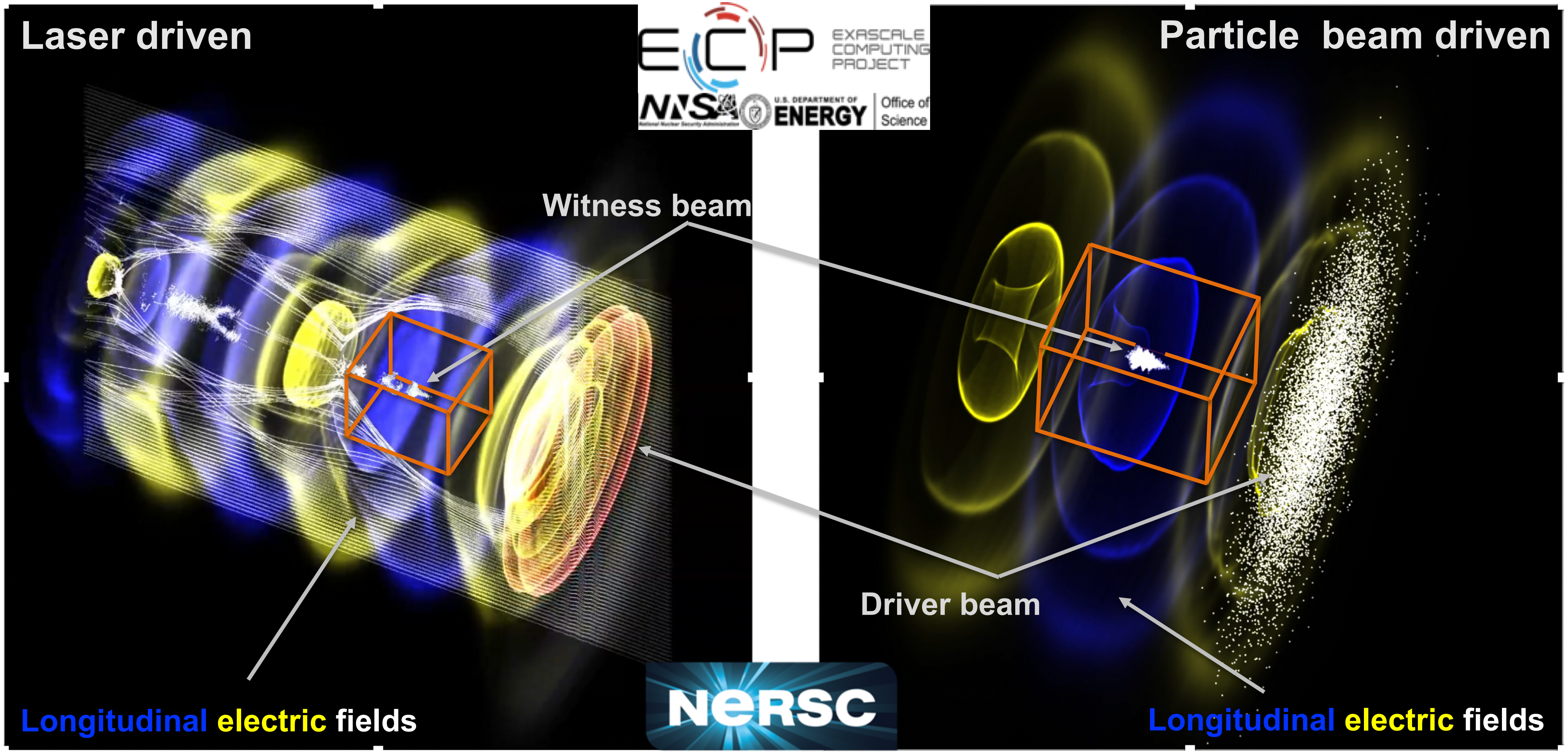




$n_e = 10^{19}$/cc, acceleration~100 MeV

Details of simulations: J.-L. Vay et al, *NIM A* **909**, 486-479 (2018) https://doi.org/10.1016/j.nima.2018.01.035

Movies from 3-D WarpX simulations with mesh refinement



Movies by Maxence Thevenet

$n_e=10^{19}$/cc, acceleration~100 MeV
Details of simulations: J.-L. Vay et al, NIM A, 909, 486-479 (2018) https://doi.org/10.1016/j.nima.2018.01.035

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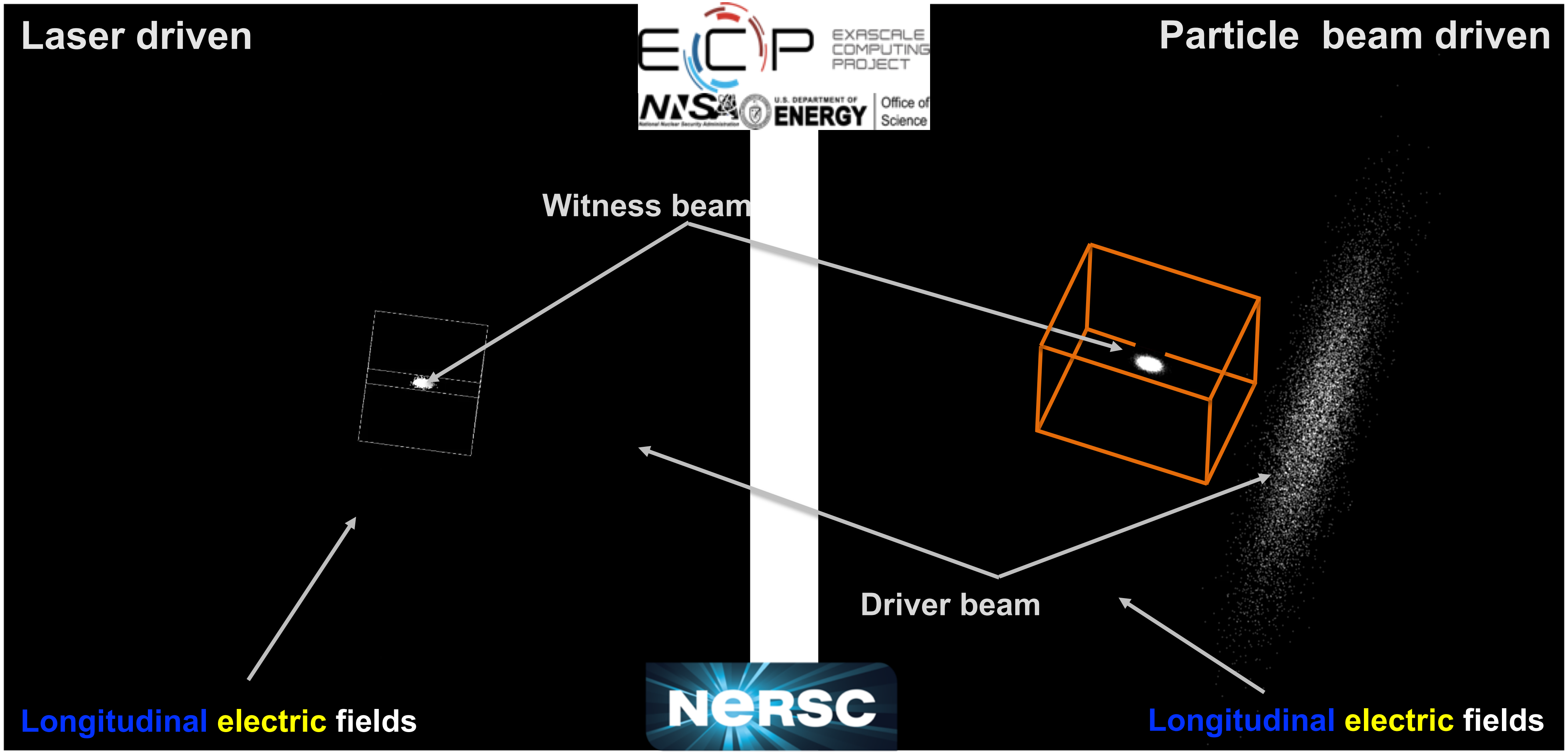

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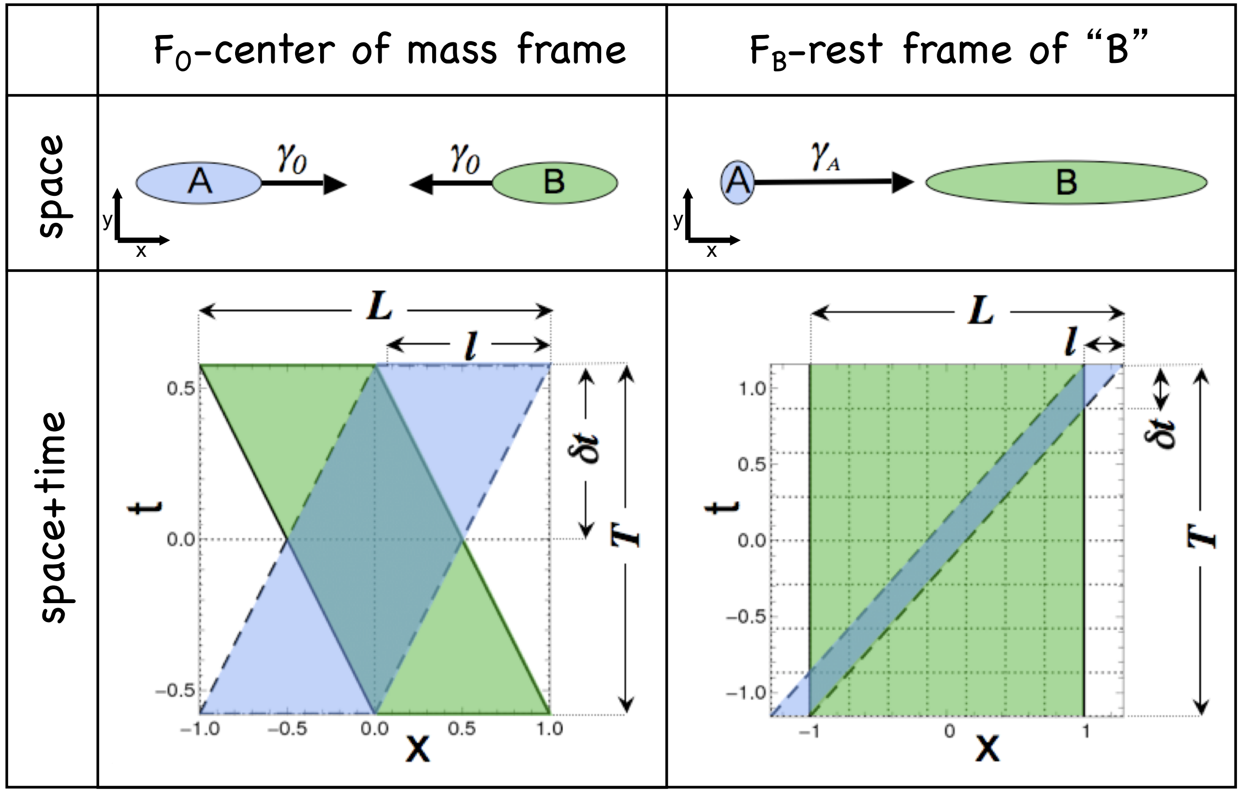
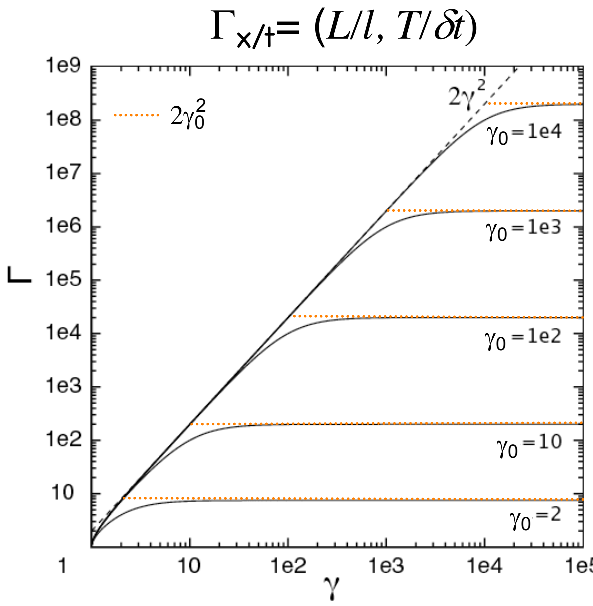
Range of space & time scales is not a relativistic invariant

crossing of 2 relativistic objects





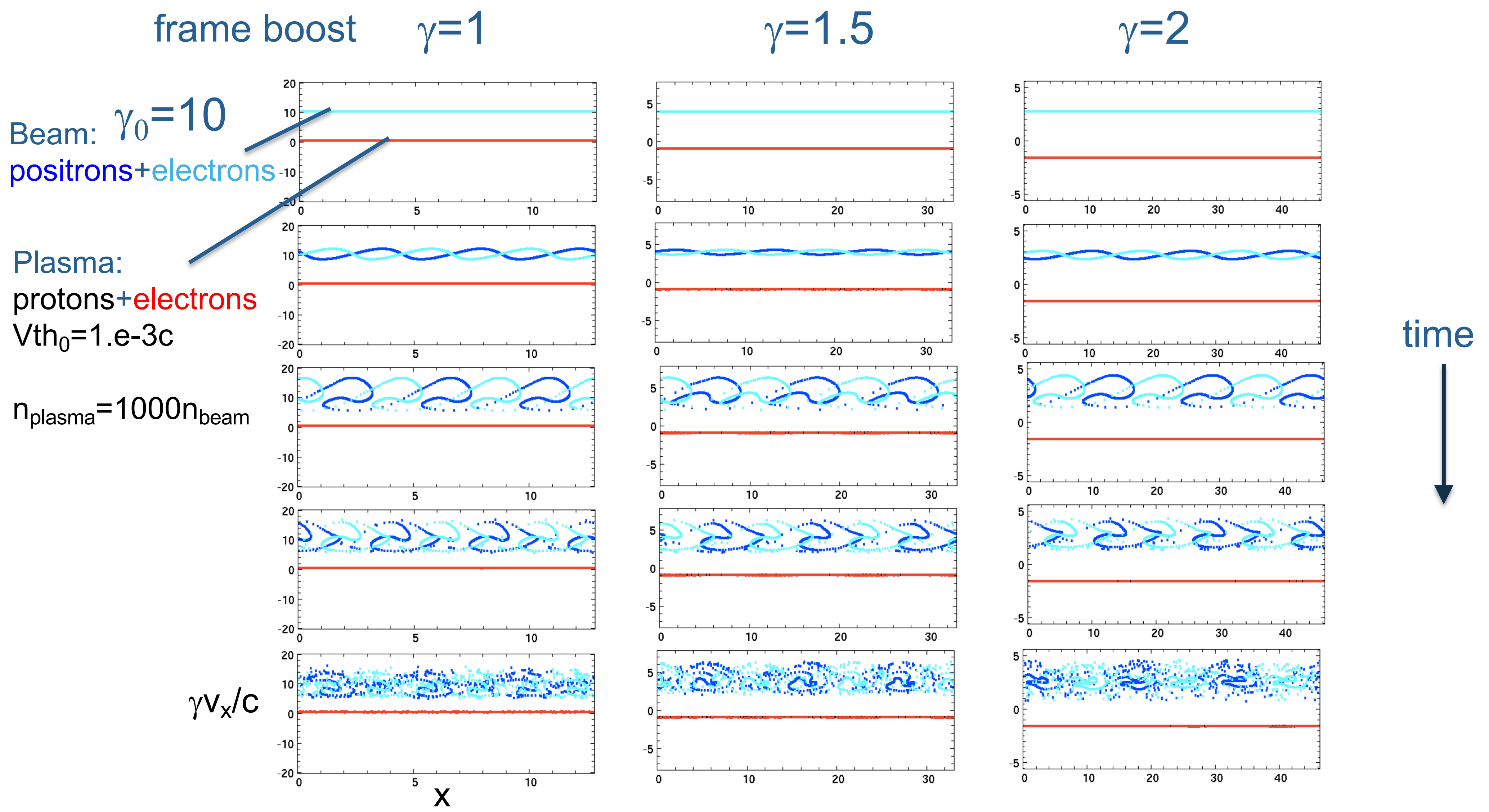
Γ is not invariant under a Lorentz transformation: $\Gamma_{x/t} \propto \gamma^2$.

γ^2 speedup demonstrated for 2-stream insta., plasma accelerators, FEL, …

Can it apply to 2-stream insta of relevance to astro plasmas, e.g. blazar studies?

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

Test beam-plasma two-stream instability in various frames



~4x faster **~7.5x faster**

The algorithms are being implemented in the code WarpX

- Open source code **WarpX**
  - https://github.com/ECP-WarpX
  - Developed as part of DOE Exascale Computing Project
  - Runs on CPUs and GPUs; built on AMReX (https://github.com/AMReX-Codes)
  - Still in development
    - Implemented (partial list):
      - **Maxwell:** FDTD (3D, 2D-XY and 2D-RZ^{++}), PSATD (3D, 2D-XY); **Particle pushers:** Boris and Vay; Dynamic load balancing; **Lorentz boosted frame**; **NCI:** Godfrey filter (3D, 2D-XY); **Ionization:** ADK; **BC:** periodic and PML, etc.
    - Under implementation or not yet ready for production or planned (partial list):
      - **Mesh refinement**; **Maxwell:** PSATD (2D-RZ^{++}); **Particle splitting**; **NCI:** Galilean (3D, 2D XY); **Particle pushers:** Higuera-Cary, etc.
  - First astro application
    - see poster from Revathi Jambunathan on “Fully-kinetic Particle-In-Cell Simulations of Pulsar Magnetospheres”

Summary

- Plasmas modeling involves wide range of space/time scales

- Standard PIC algorithm is not always sufficient

- Recent advances offer new solutions
  - Particle pushers
  - Pseudo Spectral Analytical Time Domain Field solver
  - Numerical Cherenkov Instability mitigation (filter, Galilean method, …)
  - Mesh refinement
  - Optimal Lorentz boosted frame

- Algorithms being implemented in open source code WarpX