U.S. Particle Accelerator School
Education in Beam Physics and Accelerator Technology

Simulations of Beam and Plasma Systems

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Special Topics

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U.S. DEPARTMENT OF ENERGY Office of Science

ECP EXASCALE COMPUTING PROJECT

NERSC

BERKELEY LAB Lawrence Berkeley National Laboratory

Outline

- Particle pushers
  - Relativistic Boris pusher
  - Lorentz invariant pusher
  - Application to the modeling of electron cloud instability
- Quasistatic method
  - Concept
  - Application to the modeling of electron cloud instability
- Optimal Lorentz boosted frame
  - Concept
  - Application to the modeling of electron cloud instability
  - Generalization
  - Application to the modeling of laser-plasma accelerators
    - Numerical Cherenkov instability and mitigation
    - Pseudo-spectral Maxwell solvers

Relativistic Boris pusher

For the velocity component, the Boris pusher writes

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

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

Relativistic Boris pusher: problem with E+v × B≈0

Assuming E and B such that E+v × B=0:

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

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

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

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.

Lorentz invariant particle pusher

Replace Boris velocity pusher

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

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

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

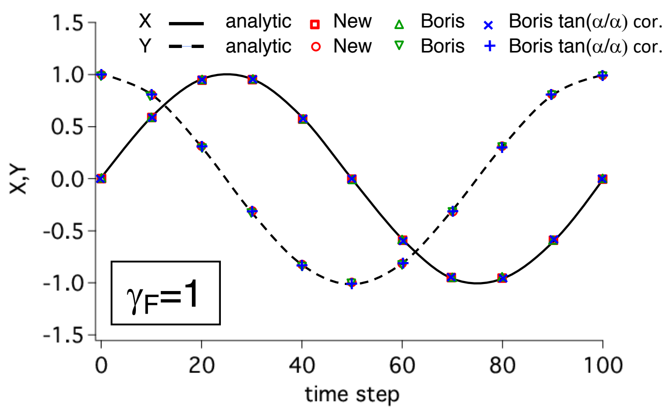
with

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

Lorentz invariant particle pusher: test w/ 1 particle

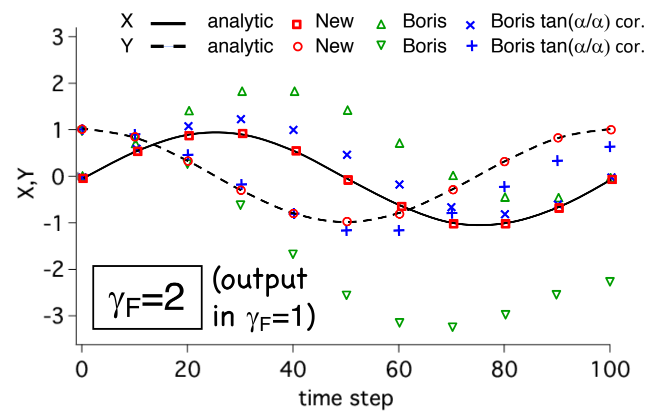
Lab frame

particle cycling in constant B field



Boosted frame γ=2

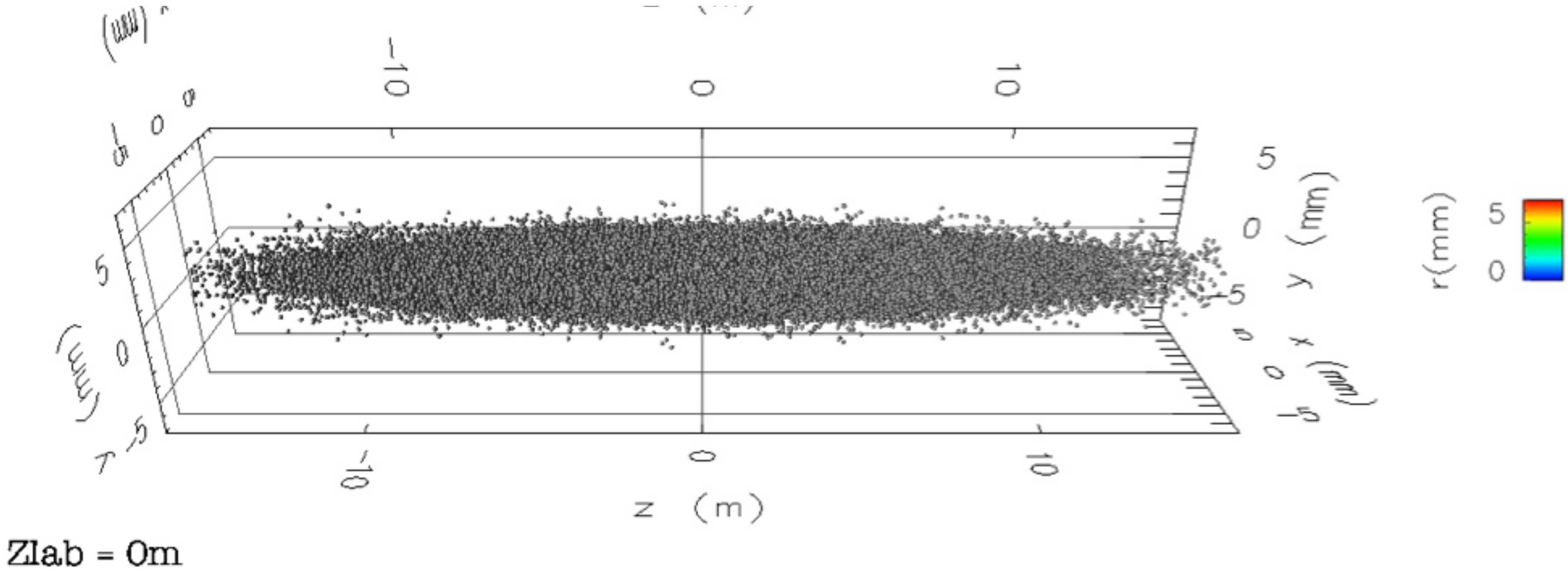
ExB drift adds to gyration



Application to modeling of two-stream instability

Calculation of e-cloud induced instability of a proton bunch

- Proton beam (γ=500, σ_z=13 cm), Propagation distance (~9.3 km), Continuous focusing, e- cloud after 2 km<z<8 km.



With Boris pusher: proton beam exploded transversely after a few betatron periods.
With new pusher: stable betatron oscillations.

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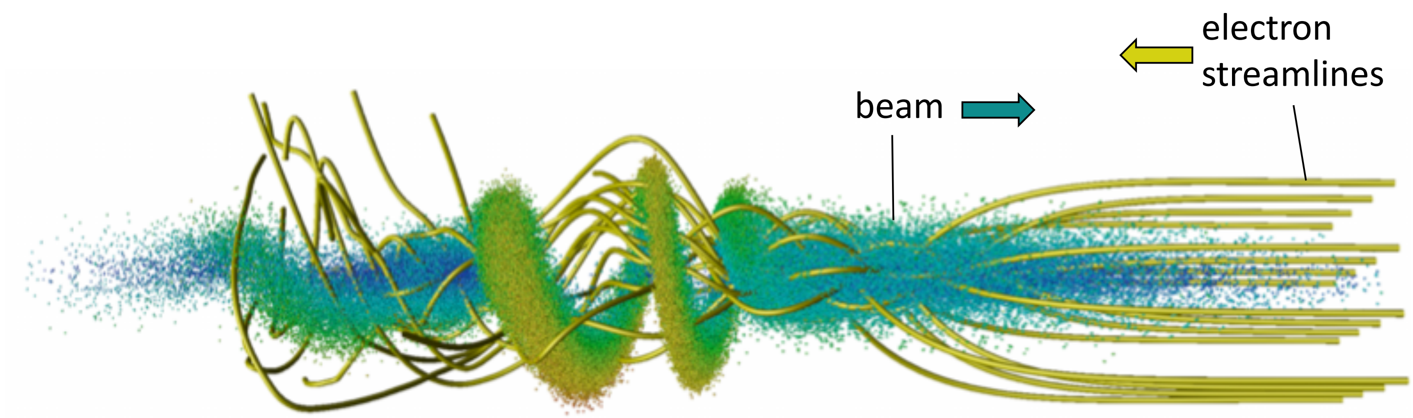
Modeling of two-stream instability is expensive

Need to follow short (σ_z=13 cm) and stiff (γ=500) proton beam for kilometers:

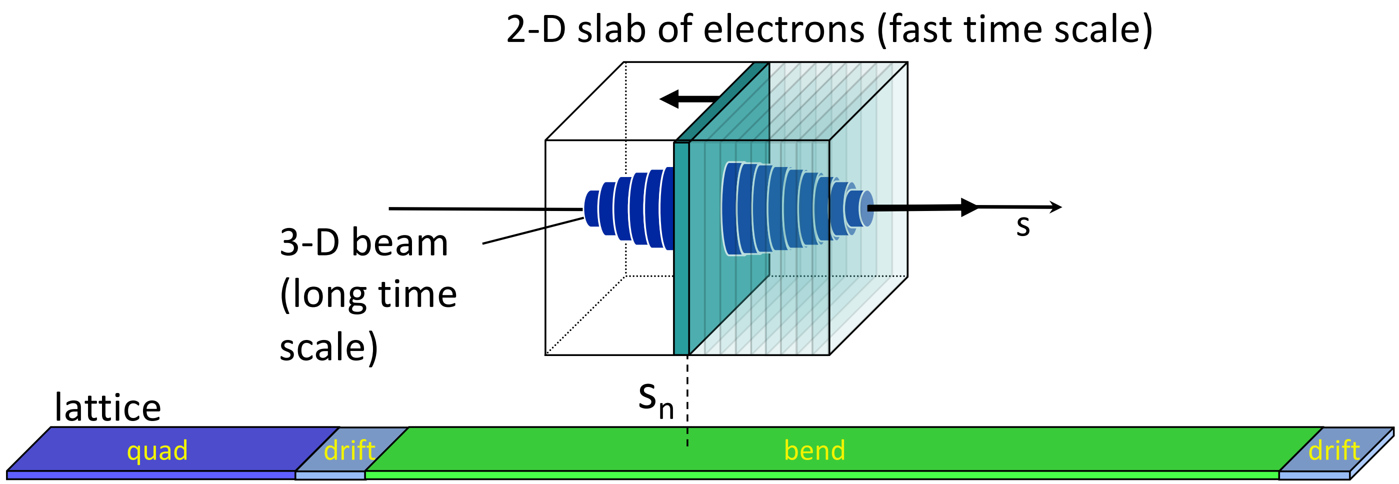
- mobile background electrons react in fraction of beam ➔ small time steps



Two solutions:

- separate treatment of slow (beam) and fast (electrons) components ➔ quasistatic approx.
- solve in a Lorentz boosted frame which matches beam & electrons time scales

Quasistatic approximation



repeat

1. 2-D slab of electrons is stepped backward (with small time steps) through the beam field and its self-field (solving 2-D Poisson at each step),
2. 2-D electron fields are stacked in a 3-D array and added to beam self-field,
3. 3-D field is used to kick the 3-D beam,
4. 3-D beam is pushed to next station with large time steps,
5. Solve Poisson for 3-D beam self-field.

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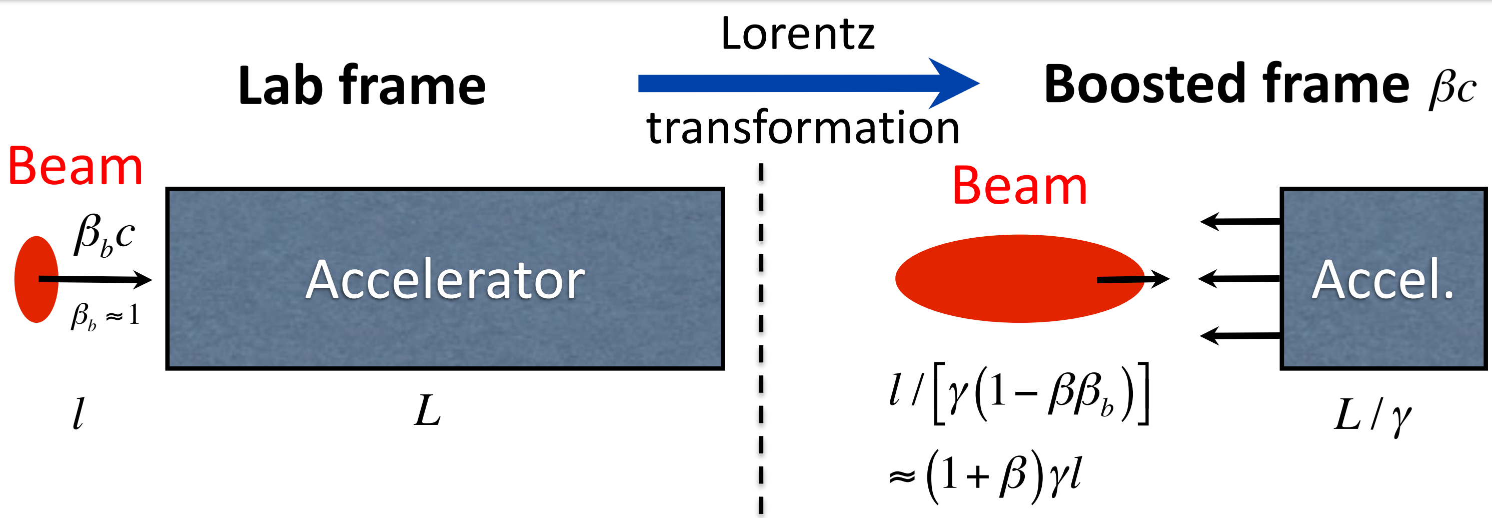
Optimal Lorentz boosted frame



Many time steps needed to follow short stiff high-energy beam into long accelerator filled with fast reacting electron clouds.

Much less time steps needed to follow long low-energy beam into shorter accelerator filled with stiffer electron clouds.

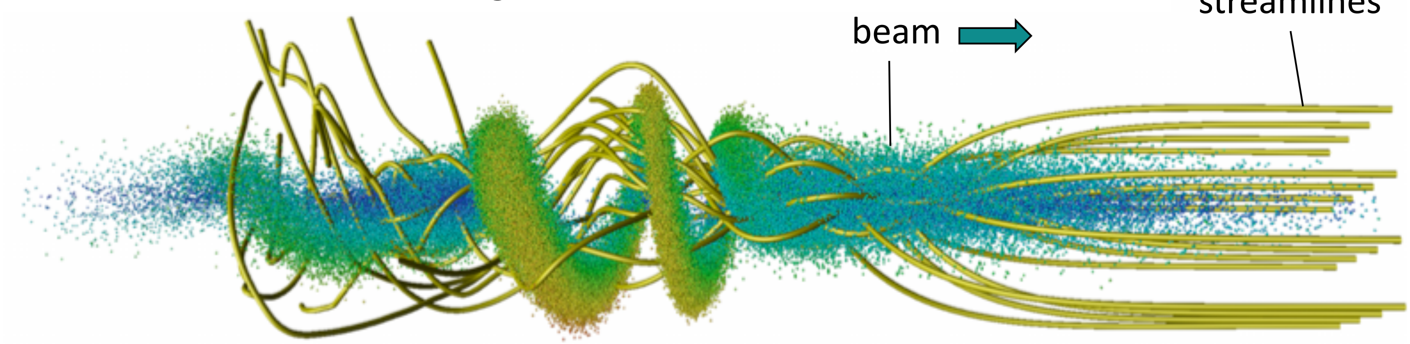
Number of time steps divided by $(1+\beta)\gamma^2$

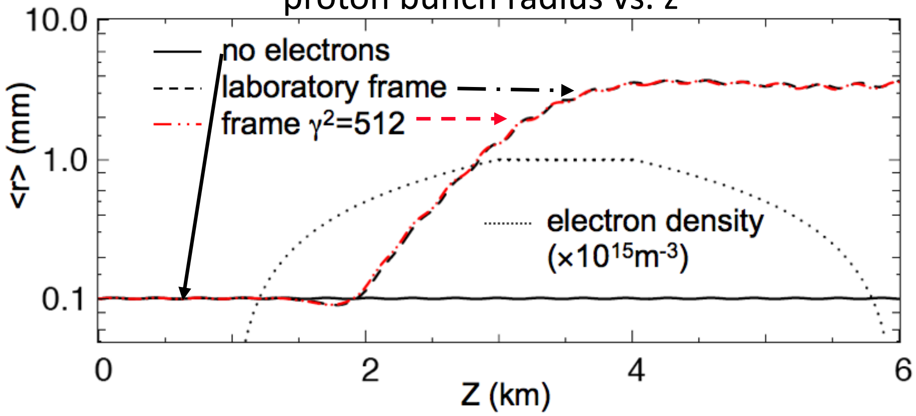
With high γ, orders of magnitude speedups are possible.

Application to modeling of two-stream instability

Calculation of e-cloud induced instability of a proton bunch

- Proton beam: γ=500, σ_z=13 cm
- L=6 km, continuous focusing





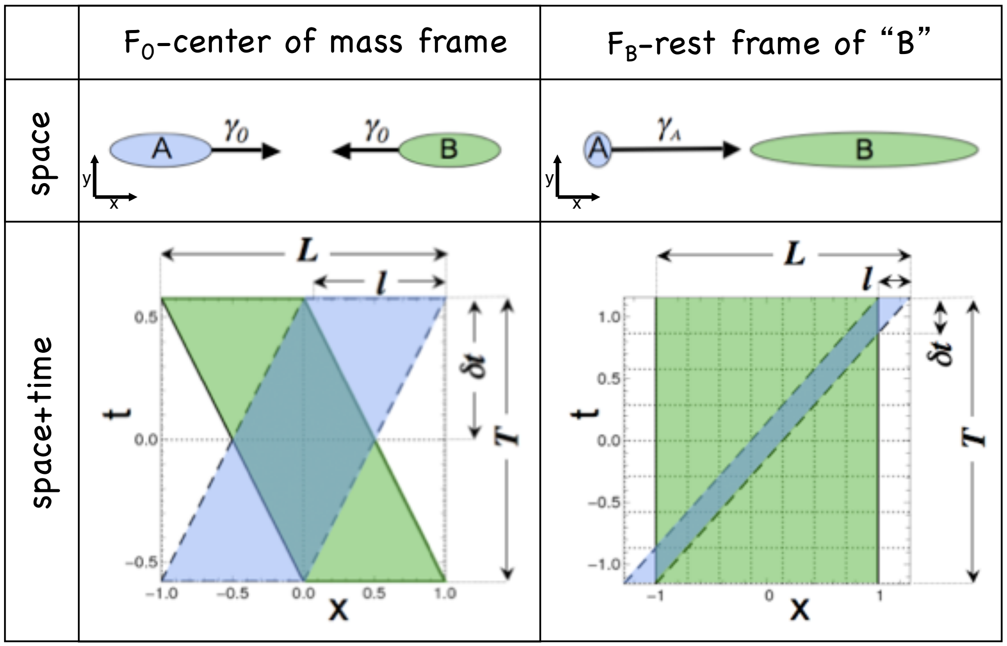
CPU time (on 8 cores in 2006):
- **lab frame: >2 weeks**
- **frame with γ^2=512: <30 min**

Speedup x1000

Generalization of optimal boosted frame approach

General formulation:

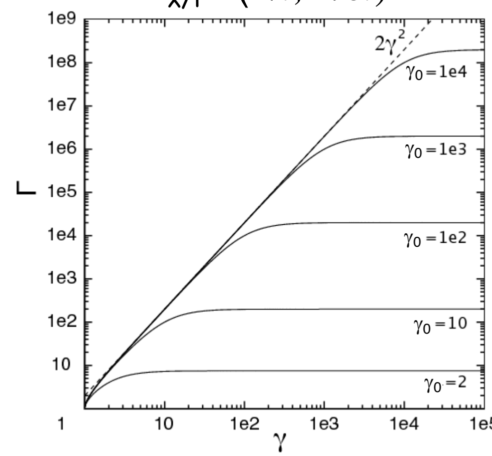
crossing of 2 relativistic objects



Range of space/time scales

$\Gamma_{x/t} \propto \gamma^{2}$□

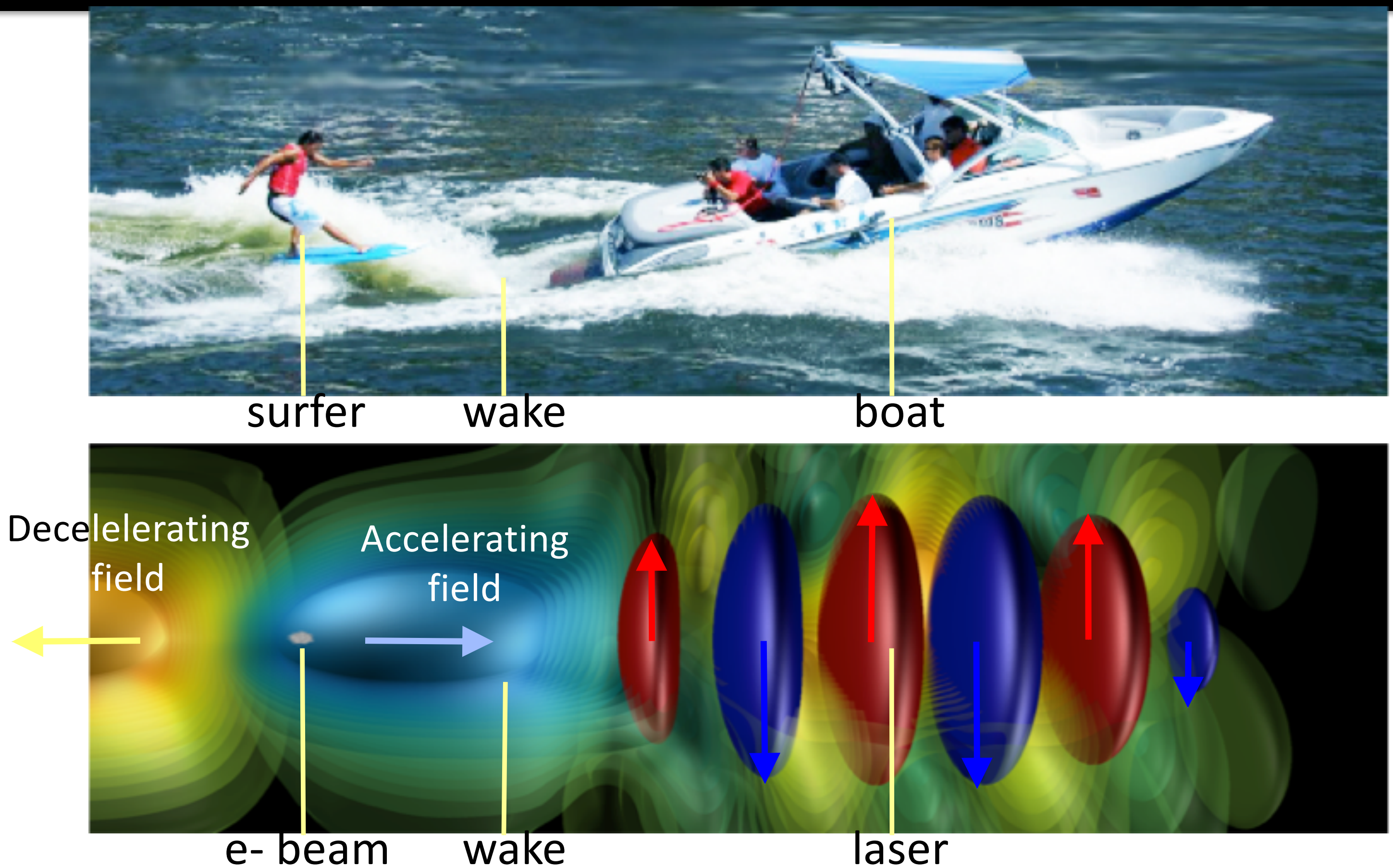
$\Gamma_{x/t} = (L/l,\ T/\delta t)^*$



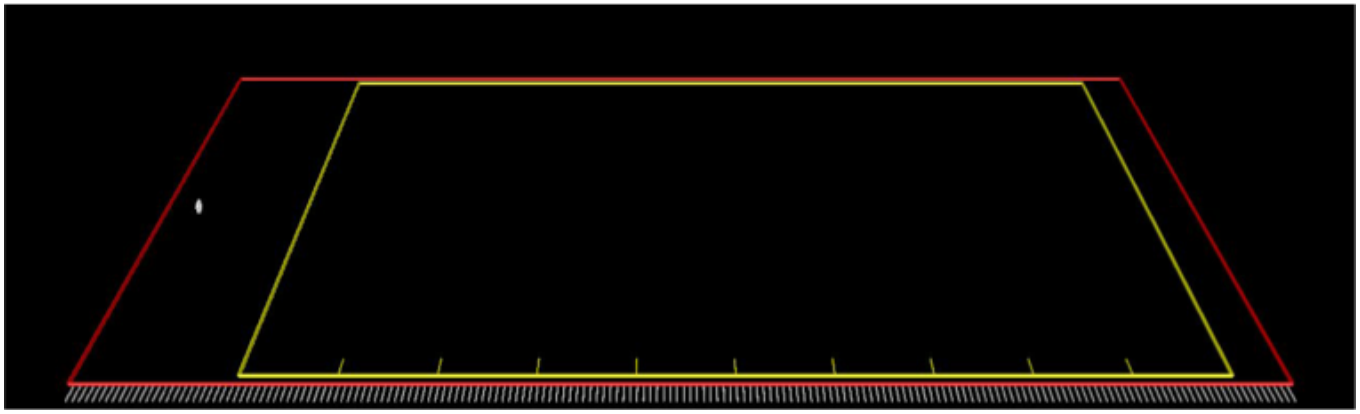
The range of space and time scales is not a Lorentz invariant and scales as γ^2 for the crossing of two relativistic objects (matter of photons).

Applicable to study of electron cloud effects, plasma accelerators, free electron lasers, etc.

Laser plasma accelerators "surf" electrons on plasma waves
for acceleration on ultra short distances



Modeling from first principle is very challenging



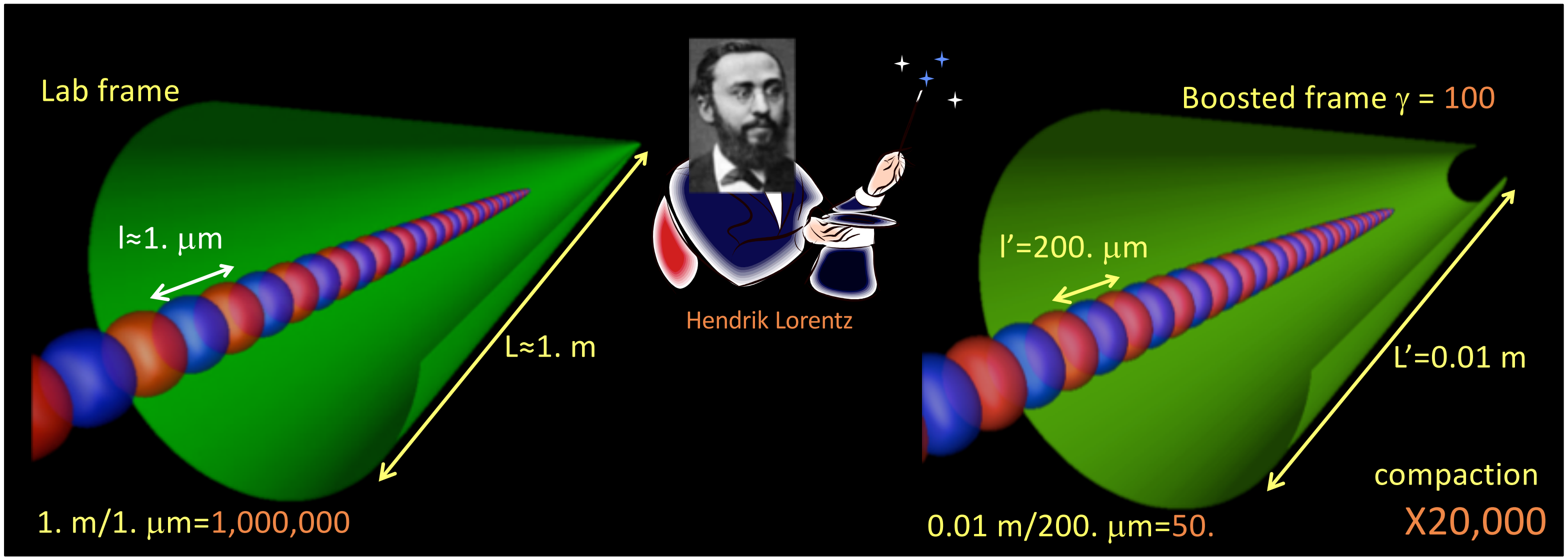
For a 10 GeV scale stage:

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

➔ millions of time steps needed

(similar to modeling **5m** boat crossing ~**5000** km Atlantic Ocean)

Optimal boosted frame enables large speedup



But does not come completely for free:

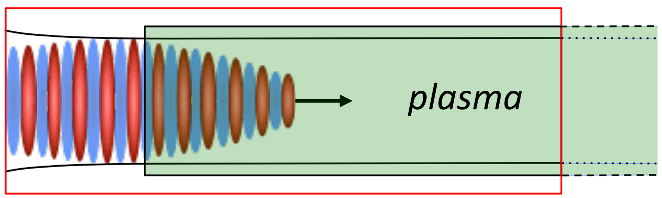
- **Laser injection.**
- **Numerical Cherenkov instability.**
- **Diagnostics.**

Laser injection through moving plane solves initialization issue in BF

Problem

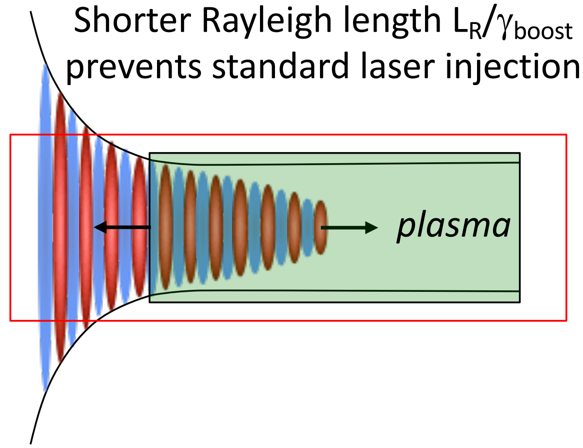
Lab frame

Standard laser injection
from left boundary or all at once



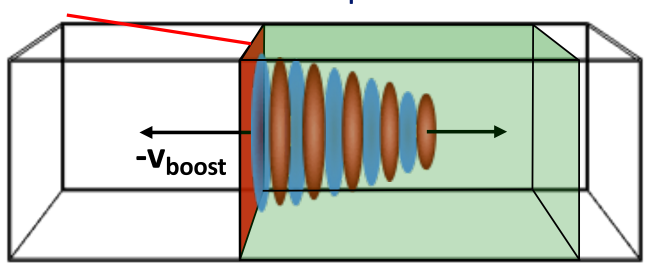
Boosted frame

Shorter Rayleigh length L_R/γ_{boost}
prevents standard laser injection



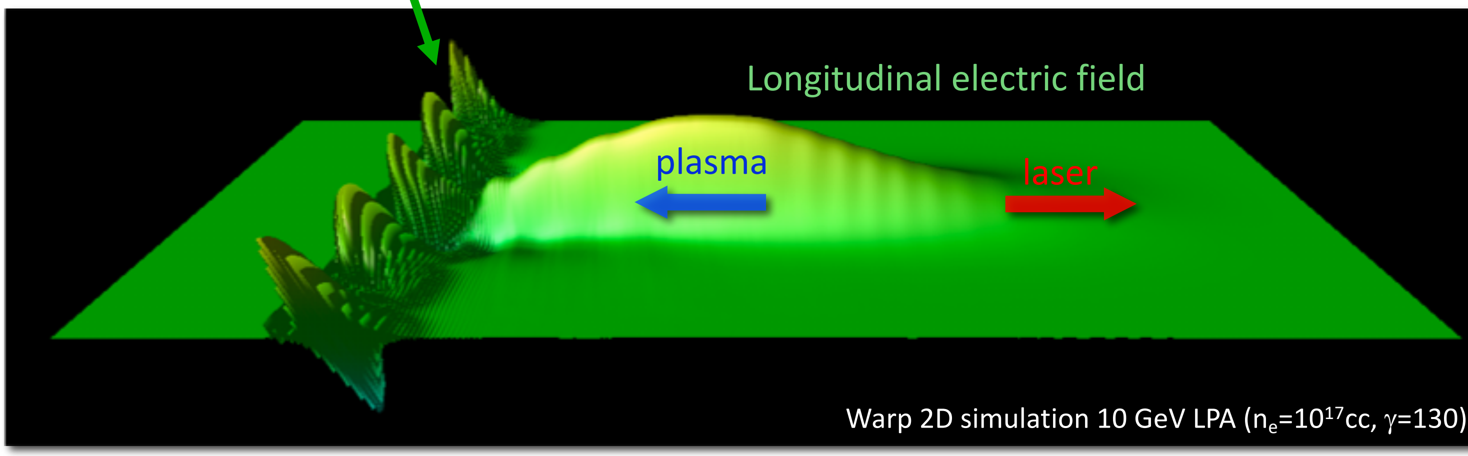
Solution

injection through a **moving planar antenna** in front of plasma



- Laser injected using macroparticles using Esirkepov current deposition ==> verifies Gauss' Law.
- For high γ_{boost}, backward radiation is blue shifted and unresolved.

Short wavelength instability observed at entrance of plasma for large γ (≥100)

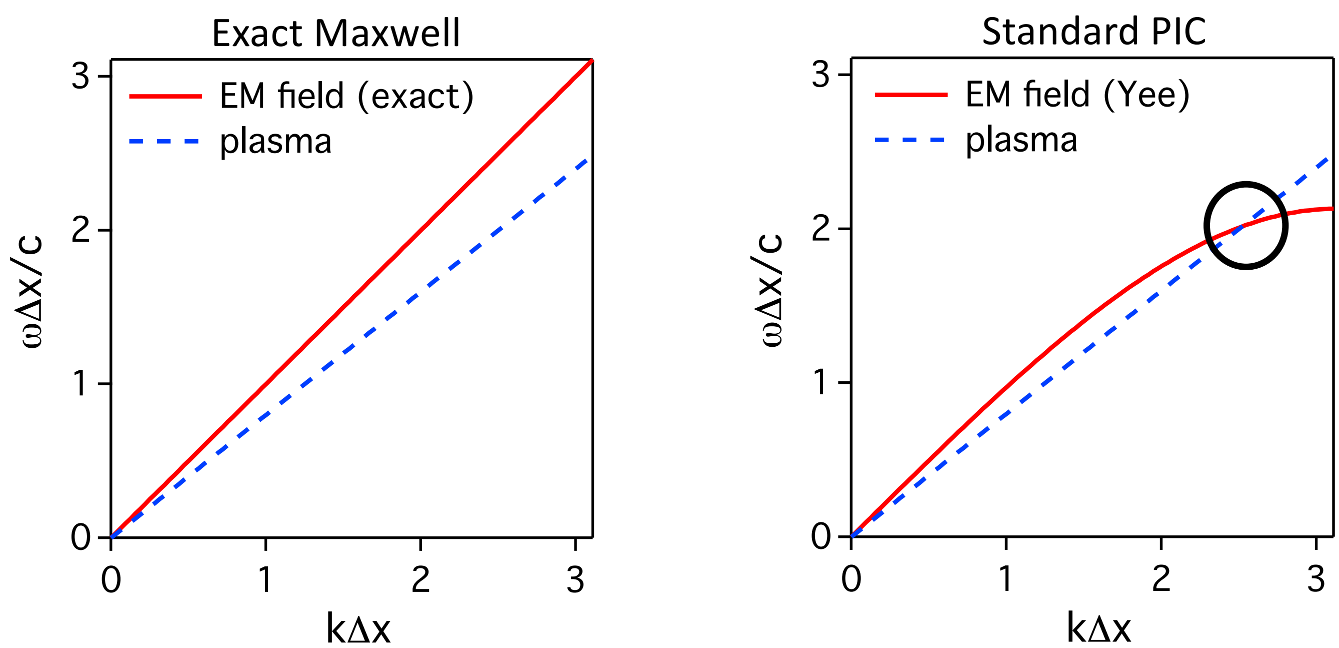


Due to “numerical Cherenkov instability”.

Relativistic plasmas PIC subject to “numerical Cherenkov”

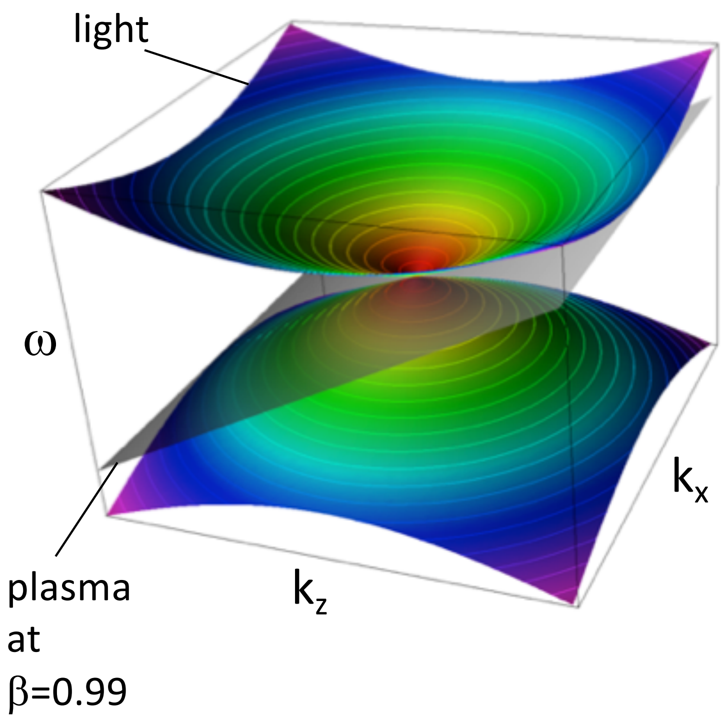
B. B. Godfrey, “Numerical Cherenkov instabilities in electromagnetic particle codes”, *J. Comput. Phys.* **15** (1974)

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

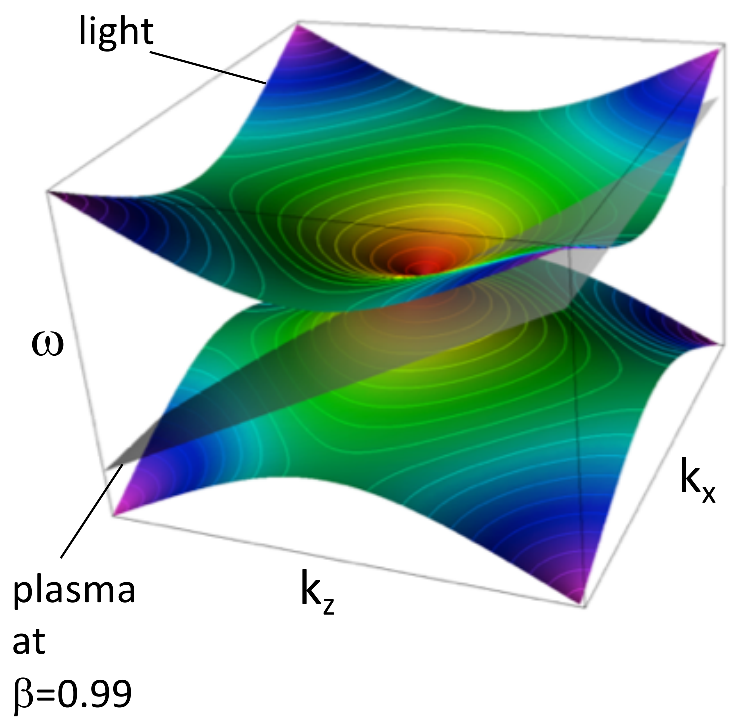


Space/time discretization aliases ➔ more crossings in 2/3-D

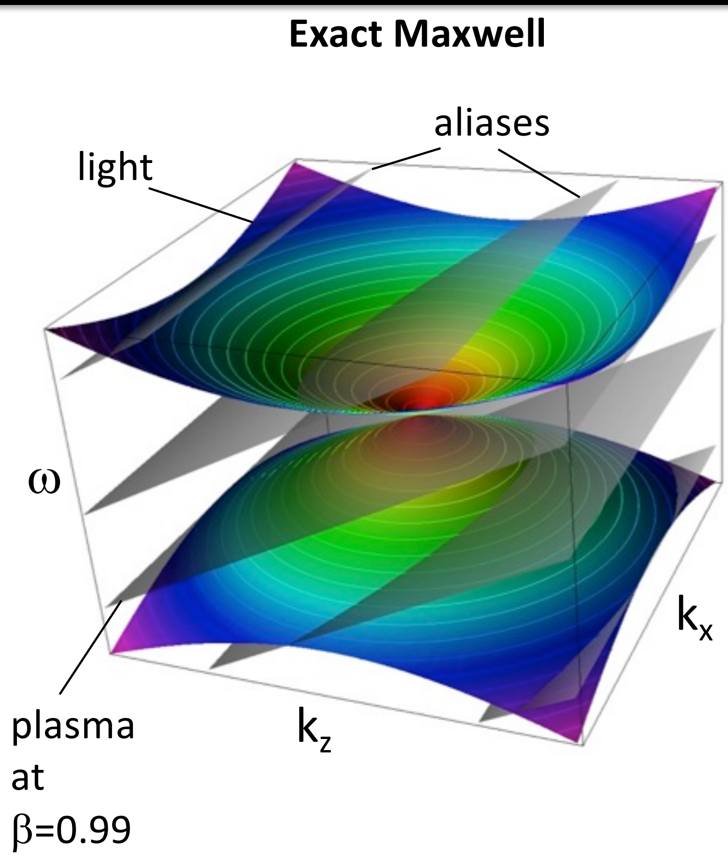
Exact Maxwell

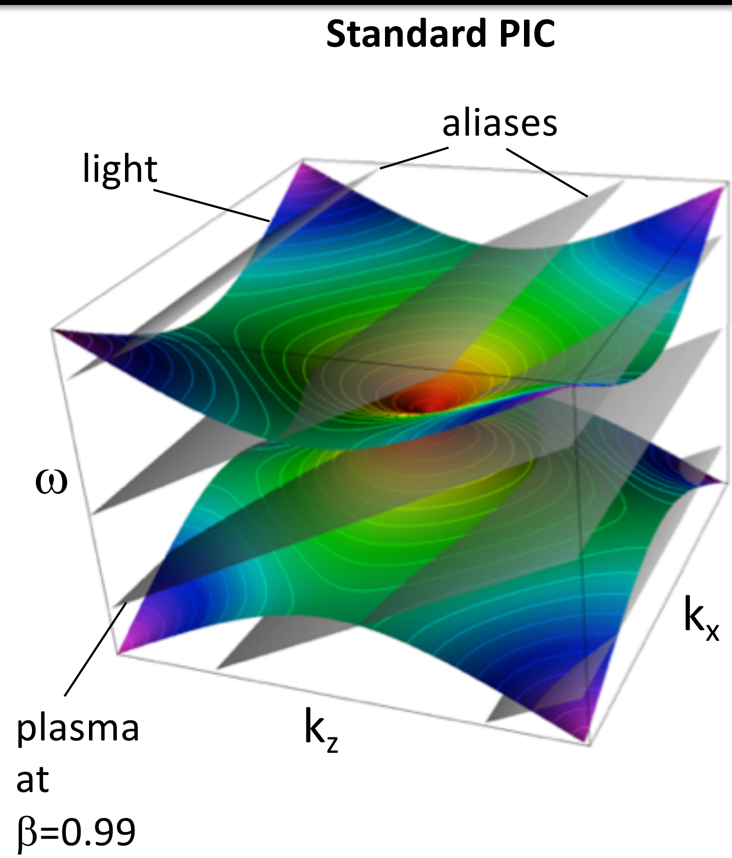


Standard PIC



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

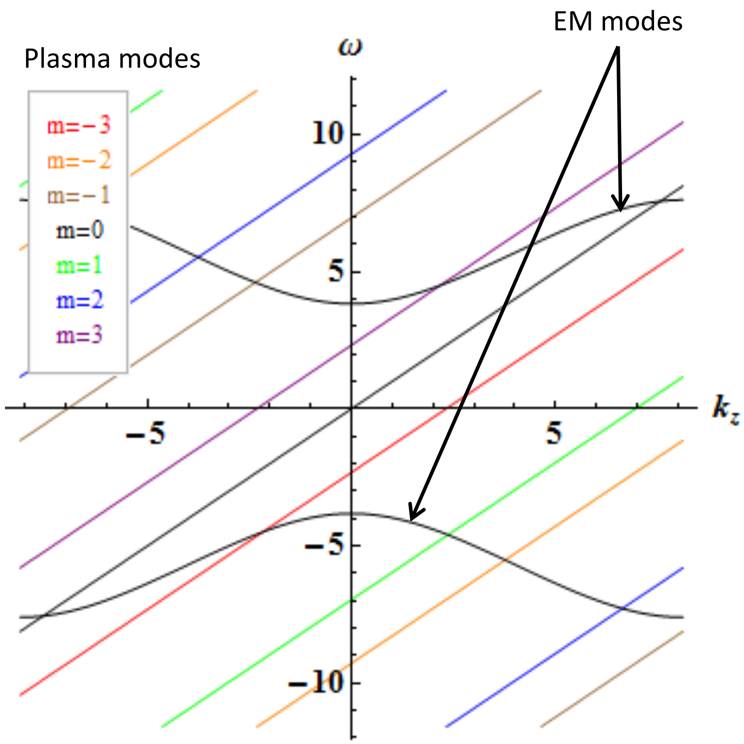




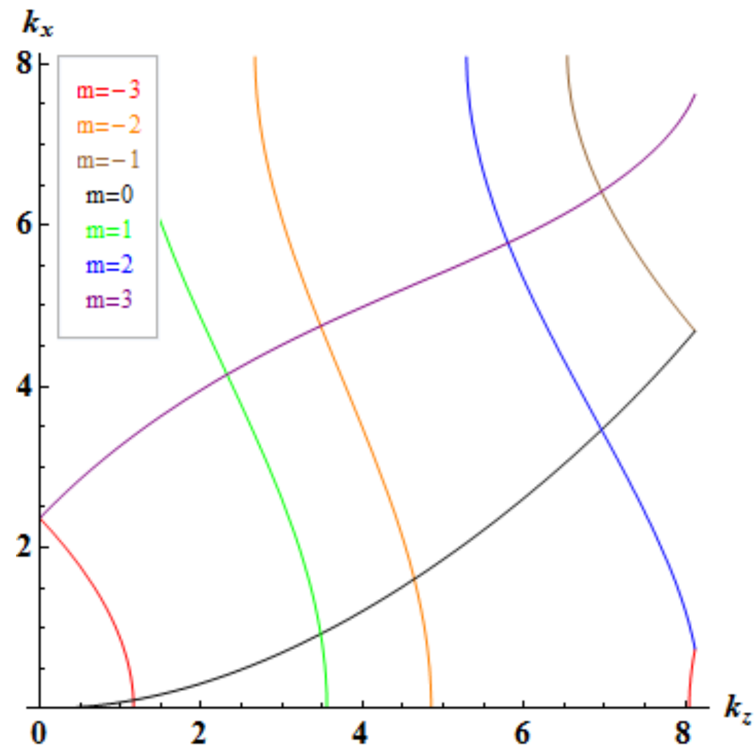
Analysis calls for full PIC numerical dispersion relation

Maps of unstable modes

Normal modes
at $k_x=0.5\pi/\Delta x$ for $c\Delta t=0.7\Delta z$



Projection of normal modes intersection



Numerical dispersion relation of full-PIC algorithm

2-D relation (Fourier space):

$$\begin{pmatrix} \xi_{z,z} + [\omega] & \xi_{z,x} & \xi_{z,y} + [k_x] \\ \xi_{x,z} & \xi_{x,x} + [\omega] & \xi_{x,y} - [k_z] \\ [k_x] & -[k_z] & [\omega] \end{pmatrix} \begin{pmatrix} E_z \\ E_x \\ B_y \end{pmatrix} = 0.$$

$$[\omega] = \sin\left(\omega \frac{\Delta t}{2}\right) / \left(\frac{\Delta t}{2}\right) \quad [k_z] = k_z \sin\left(k \frac{\Delta t}{2}\right) / \left(k \frac{\Delta t}{2}\right) \quad [k_x] = k_x \sin\left(k \frac{\Delta t}{2}\right) / \left(k \frac{\Delta t}{2}\right)$$

$$S^J = \left[\sin\left(k_z' \frac{\Delta z}{2}\right) \Big/ \left(k_z' \frac{\Delta z}{2}\right)\right]^{\ell_z+1} \left[\sin\left(k_x' \frac{\Delta x}{2}\right) \Big/ \left(k_x' \frac{\Delta x}{2}\right)\right]^{\ell_x+1},$$

$$S^{E_z} = \left[\sin\left(k_z' \frac{\Delta z}{2}\right) \Big/ \left(k_z' \frac{\Delta z}{2}\right)\right]^{\ell_z} \left[\sin\left(k_x' \frac{\Delta x}{2}\right) \Big/ \left(k_x' \frac{\Delta x}{2}\right)\right]^{\ell_x+1} (-1)^{m_z},$$

$$S^{E_x} = \left[\sin\left(k_z' \frac{\Delta z}{2}\right) \Big/ \left(k_z' \frac{\Delta z}{2}\right)\right]^{\ell_z+1} \left[\sin\left(k_x' \frac{\Delta x}{2}\right) \Big/ \left(k_x' \frac{\Delta x}{2}\right)\right]^{\ell_x} (-1)^{m_x},$$

$$S^{B_y} = \cos\left(\omega \frac{\Delta t}{2}\right) \left[\sin\left(k_z' \frac{\Delta z}{2}\right) \Big/ \left(k_z' \frac{\Delta z}{2}\right)\right]^{\ell_z} \left[\sin\left(k_x' \frac{\Delta x}{2}\right) \Big/ \left(k_x' \frac{\Delta x}{2}\right)\right]^{\ell_x} (-1)^{m_z+m_x}.$$

*B. B. Godfrey, J. L. Vay, I. Haber, J. Comp. Phys. 248 (2013)

Numerical dispersion relation of full-PIC algorithm (II)

$$\xi_{z,z} = -n\gamma^{-2}\sum_m S^J S^{E_z} \csc^2\left[(\omega - k'_z v)\frac{\Delta t}{2}\right] \left(k k_z^2 \Delta t + \zeta_z k_x^2 \sin(k\Delta t)\right)\Delta t\,[\omega]\,k'_z/4k^3 k_z,$$

$$\xi_{z,x} = -n\sum_m S^J S^{E_x} \csc\left[(\omega - k'_z v)\frac{\Delta t}{2}\right]\eta_z k'_x/2k^3 k_z,$$

$$\xi_{z,y} = nv\sum_m S^J S^{B_y} \csc\left[(\omega - k'_z v)\frac{\Delta t}{2}\right]\eta_z k'_x/2k^3 k_z,$$

$$\xi_{x,z} = -n\gamma^{-2}\sum_m S^J S^{E_z} \csc^2\left[(\omega - k'_z v)\frac{\Delta t}{2}\right] \left(k\Delta t - \zeta_z \sin(k\Delta t)\right)\Delta t\,[\omega]\,k_x k'_z/4k^3,$$

$$\xi_{x,x} = -n\sum_m S^J S^{E_x} \csc\left[(\omega - k'_z v)\frac{\Delta t}{2}\right]\eta_x k'_x/2k^3 k_x,$$

$$\xi_{x,y} = nv\sum_m S^J S^{B_y} \csc\left[(\omega - k'_z v)\frac{\Delta t}{2}\right]\eta_x k'_x/2k^3 k_x,$$

*B. B. Godfrey, J. L. Vay, I. Haber, J. Comp. Phys. 248 (2013)

Numerical dispersion relation of full-PIC algorithm (III)

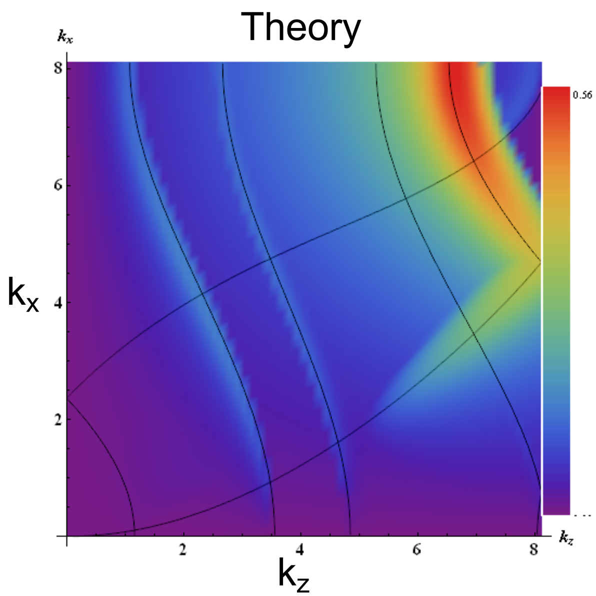
$$\eta_z = \cot\left[(\omega - k_z' v)\frac{\Delta t}{2}\right]\left(k k_z^2 \Delta t + \zeta_z k_x^2 \sin(k\Delta t)\right)\sin\left(k_z' v \frac{\Delta t}{2}\right) + \left(k\Delta t - \zeta_x \sin(k\Delta t)\right) k_z^2 \cos\left(k_z' v \frac{\Delta t}{2}\right),$$

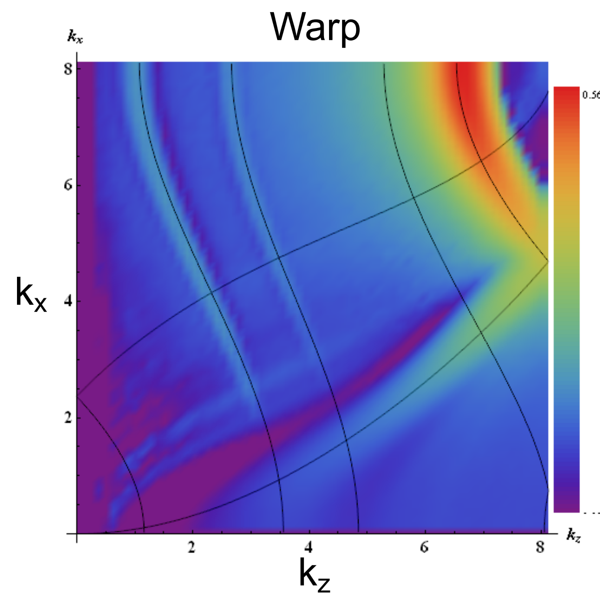
$$\eta_x = \cot\left[(\omega - k_z' v)\frac{\Delta t}{2}\right]\left(k\Delta t - \zeta_z \sin(k\Delta t)\right) k_x^2 \sin\left(k_z' v \frac{\Delta t}{2}\right) + \left(k k_x^2 \Delta t + \zeta_x k_z^2 \sin(k\Delta t)\right)\cos\left(k_z' v \frac{\Delta t}{2}\right).$$

Then simplify and solve with Mathematica, Python or other…

*B. B. Godfrey, J. L. Vay, I. Haber, J. Comp. Phys. 248 (2013)

Growth rates from theory match Warp simulations





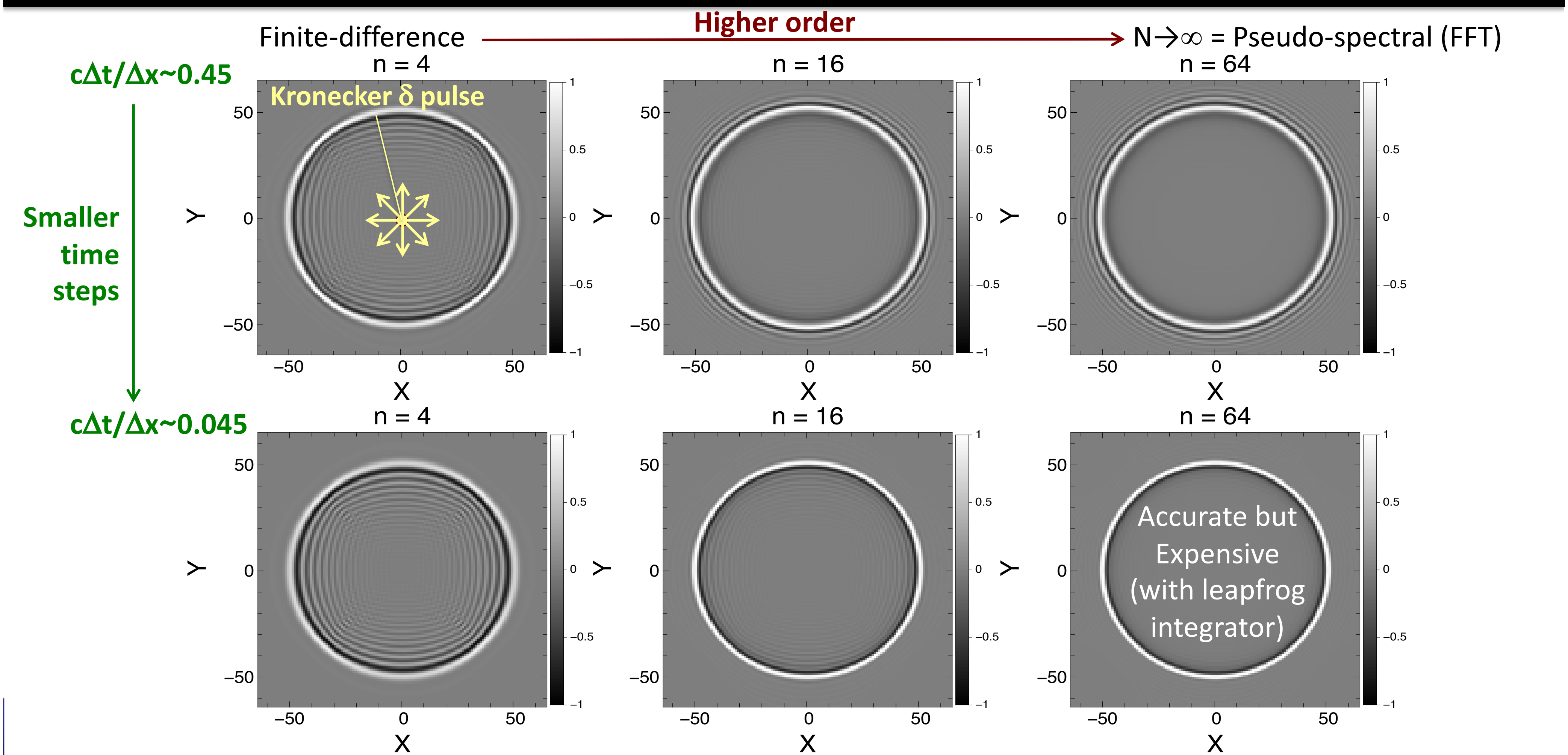
Warp run uses uniform drifting plasma with periodic BC.
Yee finite difference, energy conserving gather ($c\Delta t/\Delta x=0.7$)

Latest theory has led to ne insight and the development of very effective methods to mitigate the instability.

Best mitigation solution involves FFT-based Maxell solvers.

Arbitrary-order Maxwell solver offers flexibility in accuracy

(on centered or staggered grids)

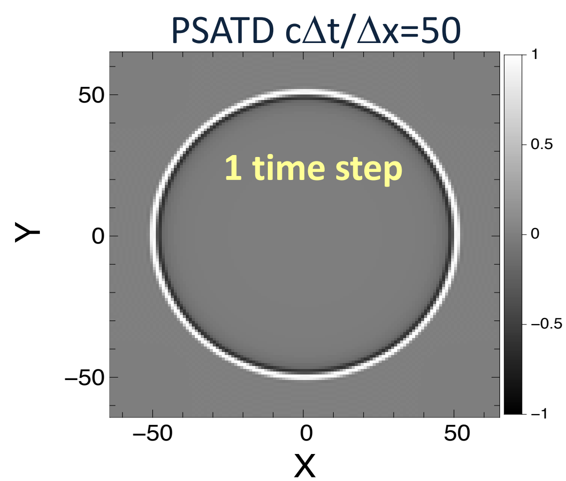


Analytical integration in Fourier space offers infinite order

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

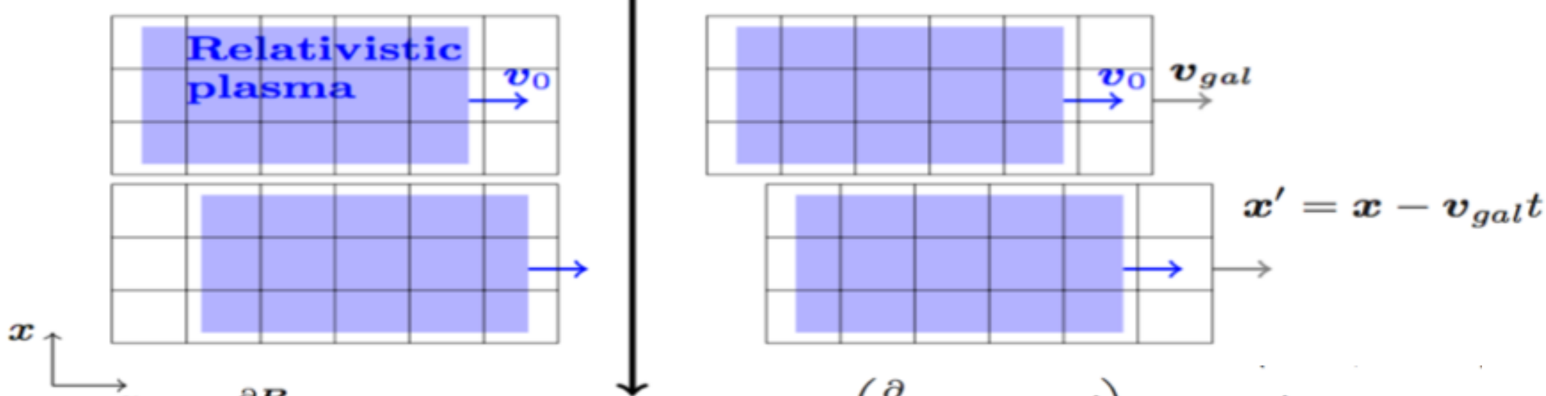
Both arbitrary order FDTD and PSATD to be implemented in WarpX.

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

PSATD also enables integration in Galilean frame

Use Galilean coordinates that follow the relativistic plasma.

Standard PSATD PIC | **Galilean PSATD PIC**



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

Time

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

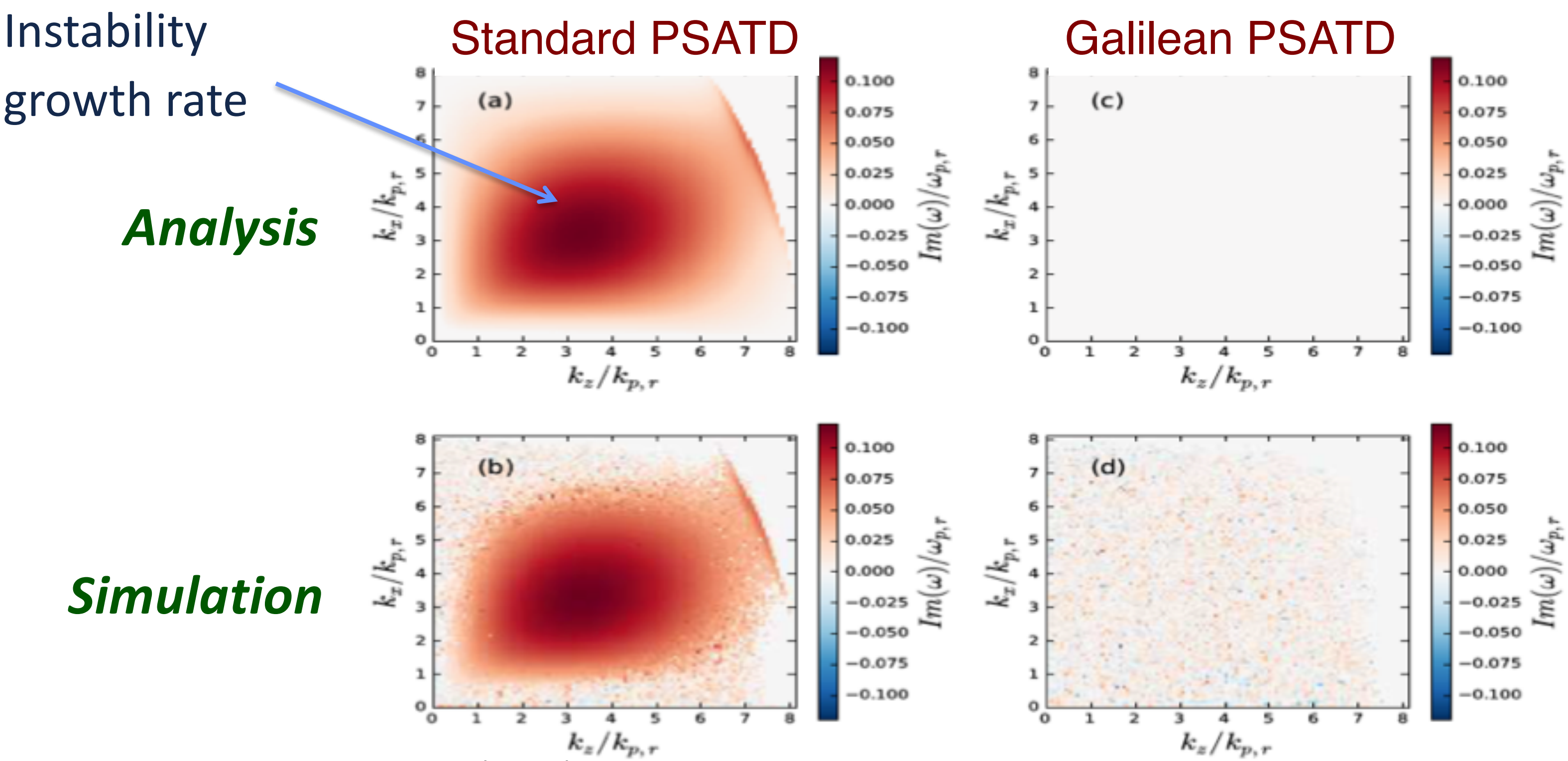
+ integrate analytically, assuming $j(x,t)$ $j(x',t)$ is constant over one timestep.

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

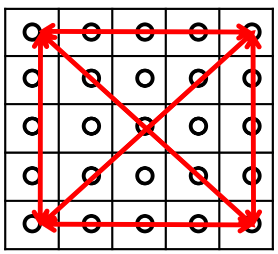
Uniform plasma streaming in 2D periodic box



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

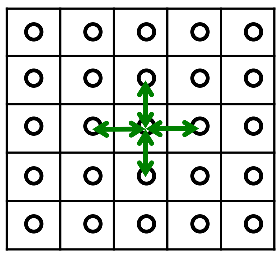
Spectral solvers involve global operations → harder to scale to large # of cores

Spectral — **global "costly" communications**



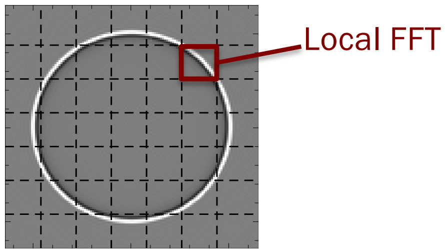
vs

Finite Difference (FDTD) — **local "cheap" communications**



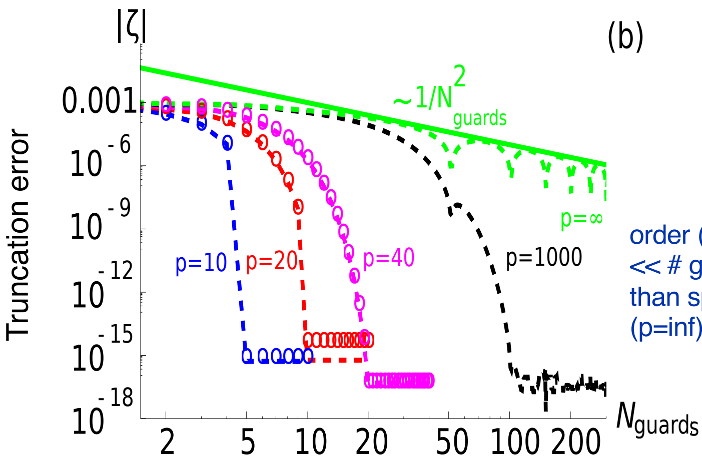
Harder to scale | **Easier to scale**

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



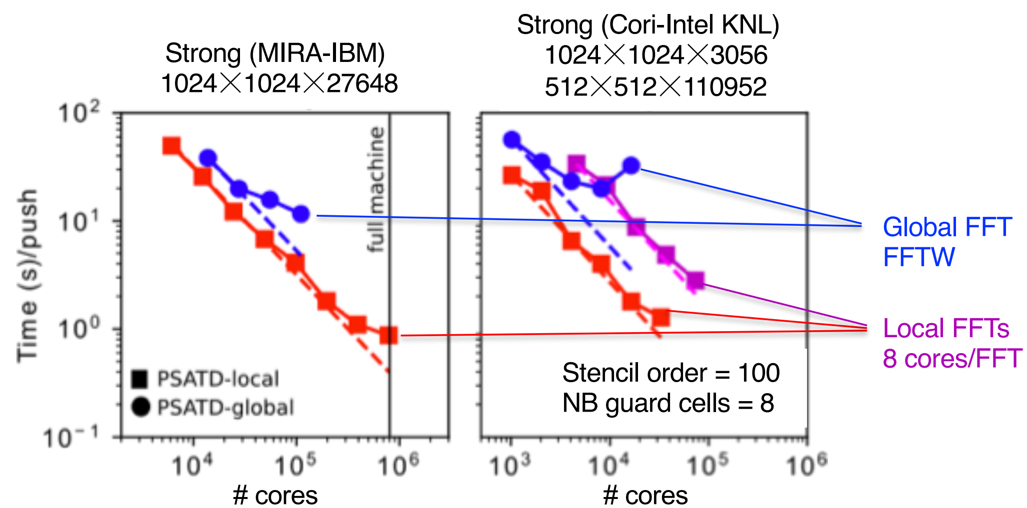
Finite-order stencil offers scalable ultra-high order solver

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



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

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



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. **119**, 155001 (2017)

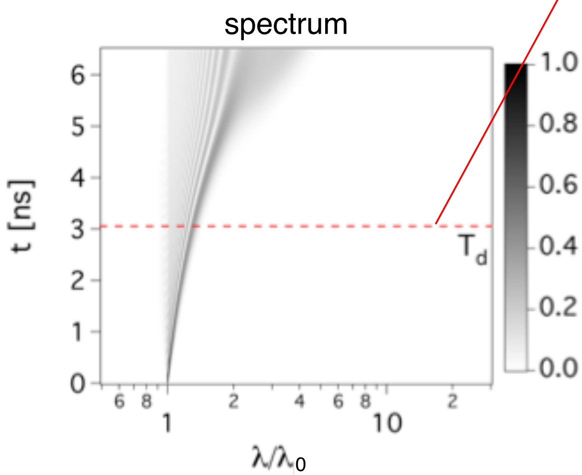
Complication: physics looks different in boosted frame

Time history of laser spectrum on axis (relative to laser λ_0 in vacuum)

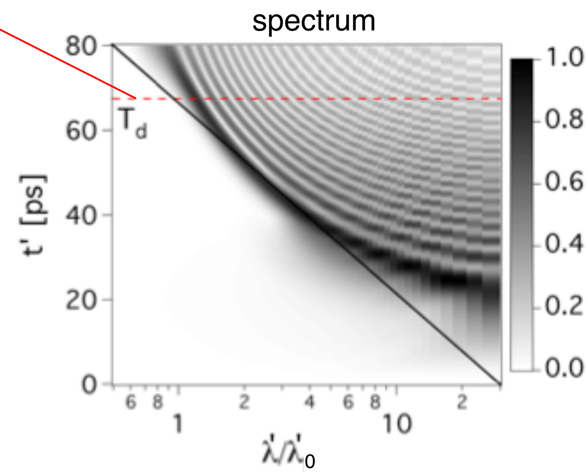
Spectrum very different in lab and boosted frames

Lab frame

Dephasing time

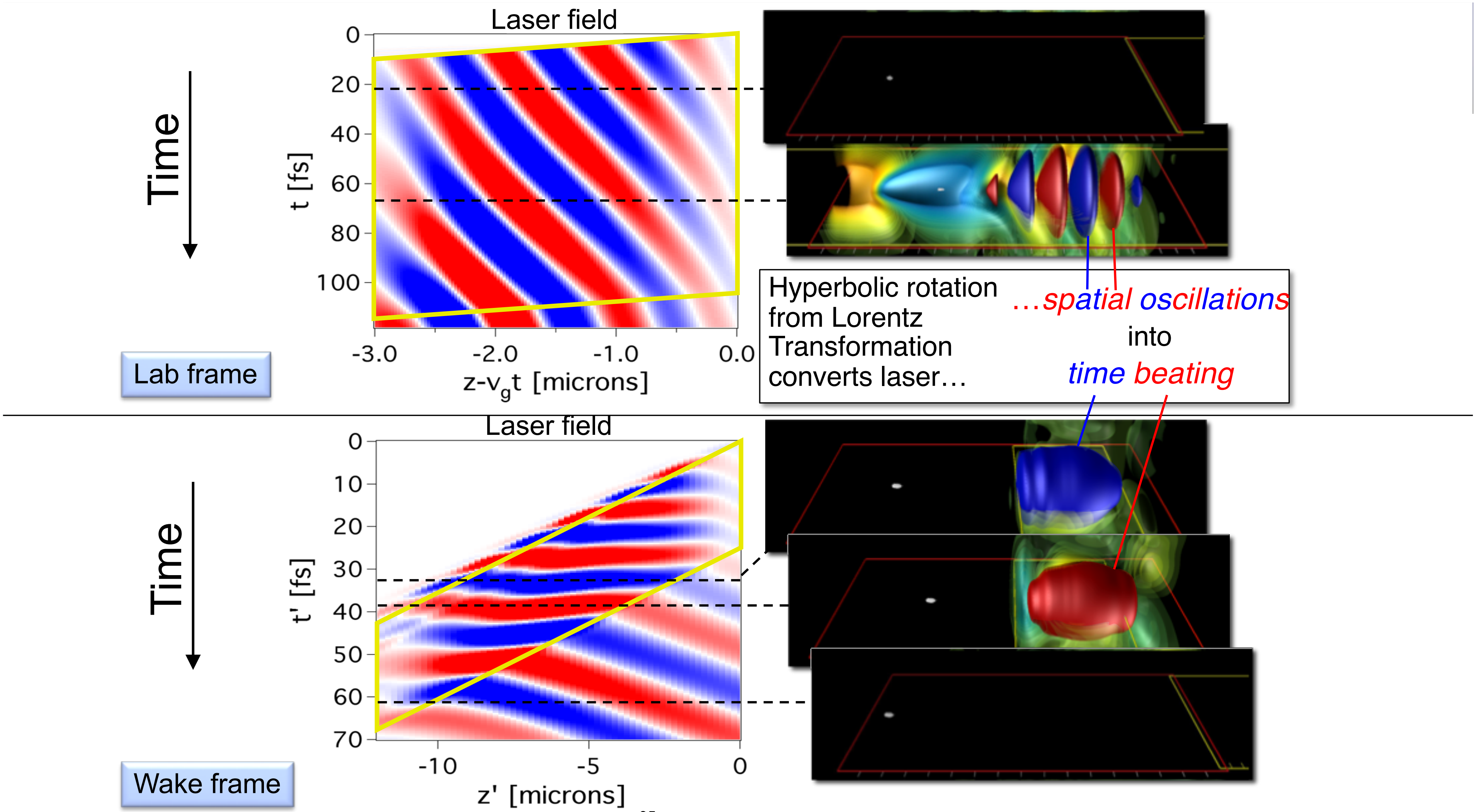


Frame of wake (γ=130)

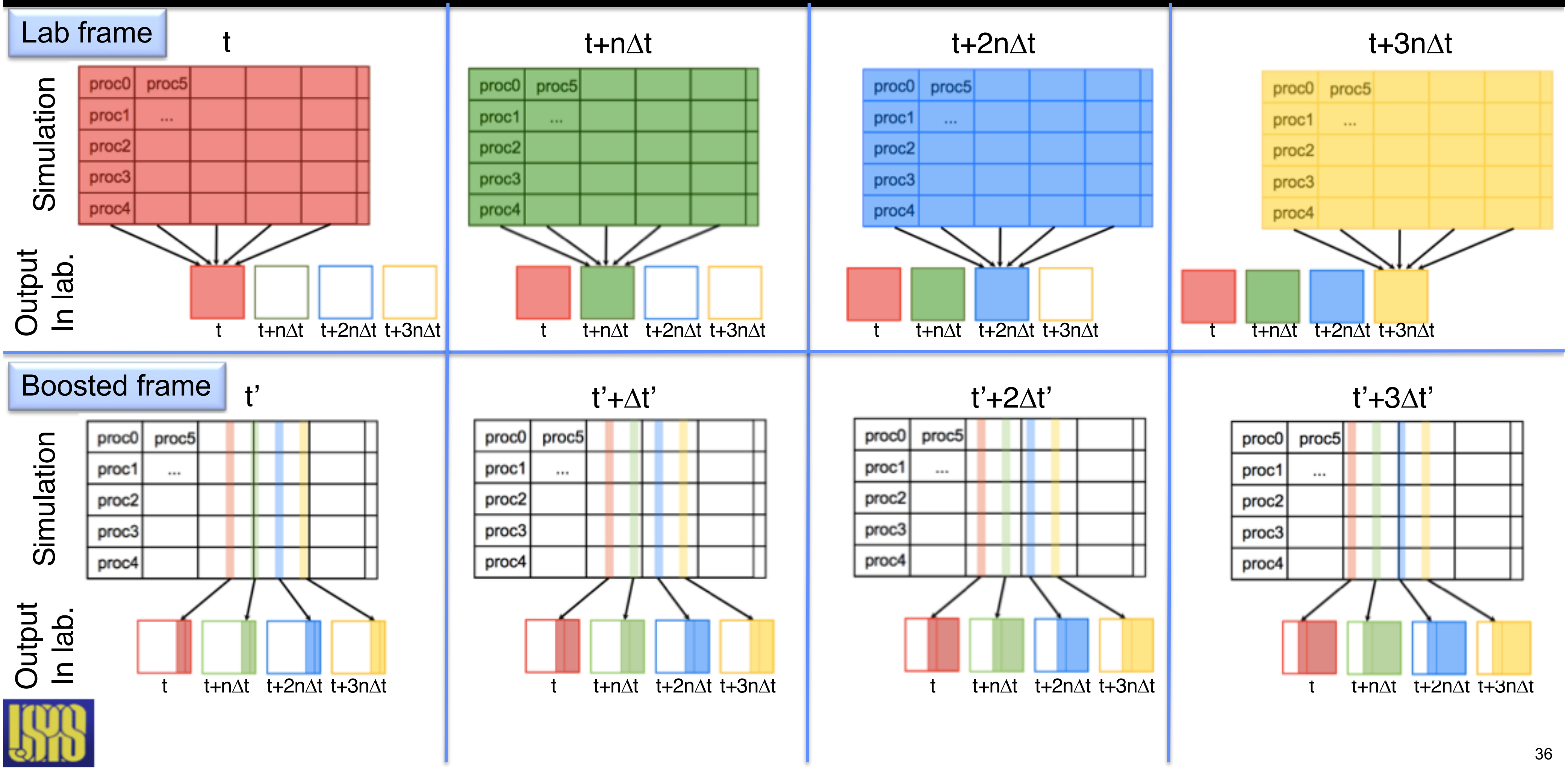


Content concentrated around λ_0

Content concentrated at much larger λ'

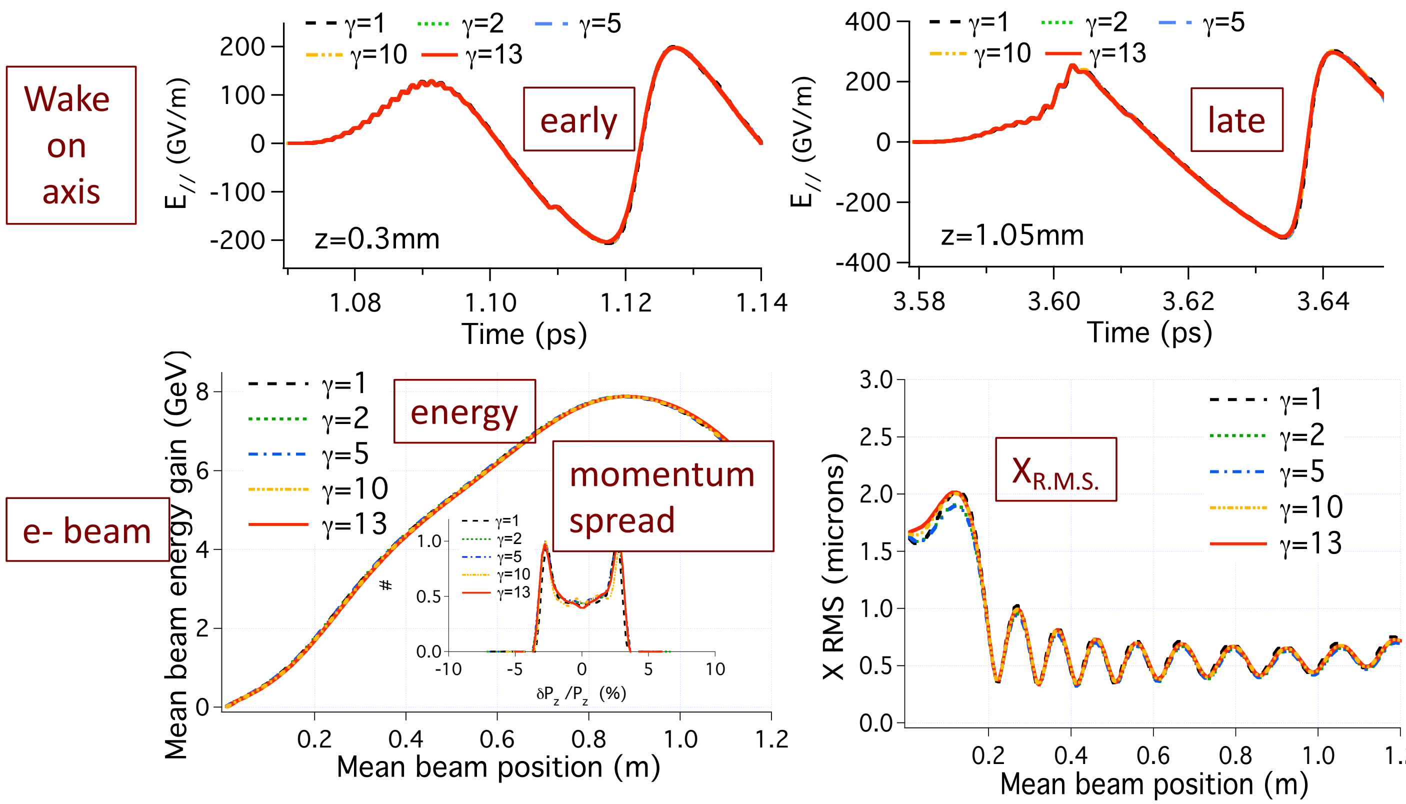

Laser field
Time
t [fs]
0
20
40
60
80
100
-3.0
-2.0
-1.0
0.0
z-v_gt [microns]
Lab frame
Hyperbolic rotation from Lorentz Transformation converts laser…
…spatial oscillations
into
time beating
Laser field
Time
t' [fs]
0
10
20
30
40
50
60
70
-10
-5
0
z' [microns]
Wake frame

BF modeling requires transforming data back to laboratory frame



Very high precision validation of BF method with Warp

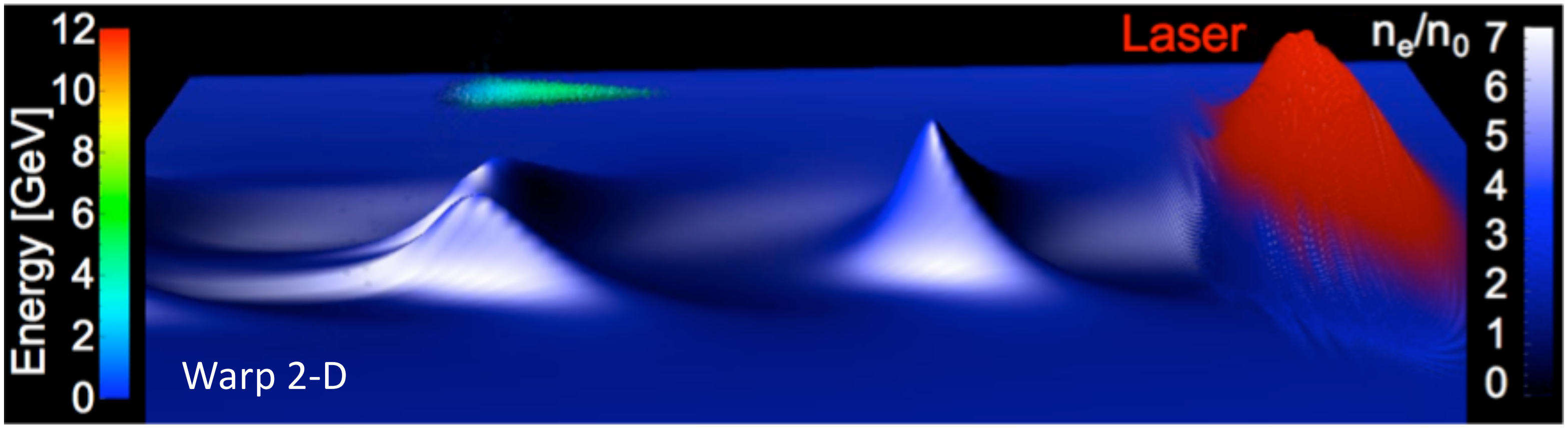
Simulations in various frames (γ=1,2,5,10,13) are almost undistinguishable.



Warp-3D – a_0=1, n_0=10^{19}cm^{-3} (~100 MeV) scaled to 10^{17}cm^{-3} (~10 GeV).
Detailed validation for a0>1 (non-linear regime) is underway.

Enabling simulations that were previously untractable

Simulation of 10 GeV stage for BELLA project (LBNL)

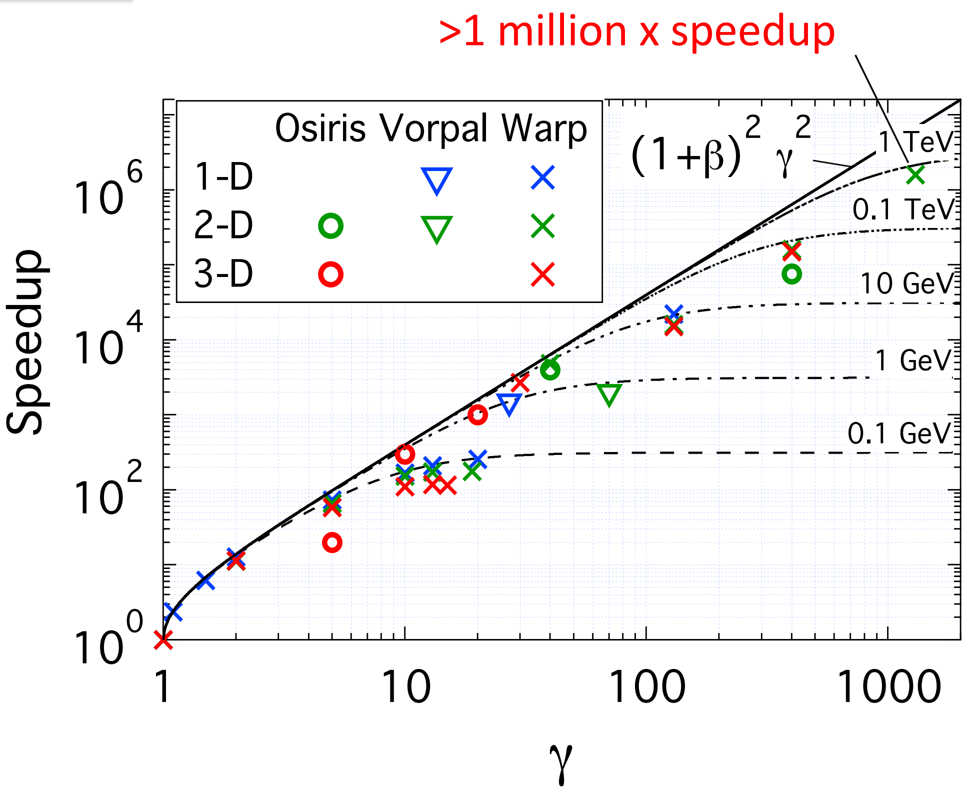


State-of-the-art PIC simulations of 10 GeV stages:

2006 (lab) in 1D: ~ 5k CPU-hours ➔ 2011 (boost) in 3D: ~ 1k CPU-hours

Current state-of-the-art in lab: 2-D RZ simulations in ~2 weeks on thousands of cores.
Other approach: quasistatic solver with advanced laser envelope model (e.g. INF&RNO).

Speedup verified to over a million



Warp:

1. J.-L. Vay, et al., *Phys. Plasmas* **18** 123103 (2011)
2. J.-L. Vay, et al., *Phys. Plasmas (letter)* **18** 030701 (2011)
3. J.-L. Vay, et al., *J. Comput. Phys.* **230** 5908 (2011)
4. J.-L. Vay et al, PAC Proc. (2009)

Osiris:

1. S. Martins, et al., *Nat. Phys.* **6** 311 (2010)
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3. S. Martins, et al., *Phys. Plasmas* **17** 056705 (2010)
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Vorpal:

1. D. Bruhwiler, et al., *AIP Conf. Proc* **1086** 29 (2009)

Special topics summary

- Modeling of relativistic beams/plasmas with full PIC may benefit from “non-standard” algorithms
  - Lorentz invariant particle pusher
  - Quasistatic approximation
  - Optimal Lorentz boosted frame
- Quasistatic is well established method, but requires writing dedicated code or module
- Boosted frame approach is newer and uses standard PIC at core, needing only extensions

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