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

Self-Consistent Simulations of Beam and Plasma Systems
Steven M. Lund, Jean-Luc Vay, Rémi Lehe and Daniel Winklehner
Colorado State U., Ft. Collins, CO, 13-17 June, 2016

A3. Special Topics

Jean-Luc Vay
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

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:

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

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

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

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.

Lorentz invariant particle pusher

Replace Boris velocity pusher

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

with

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

Looks implicit but solvable analytically

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

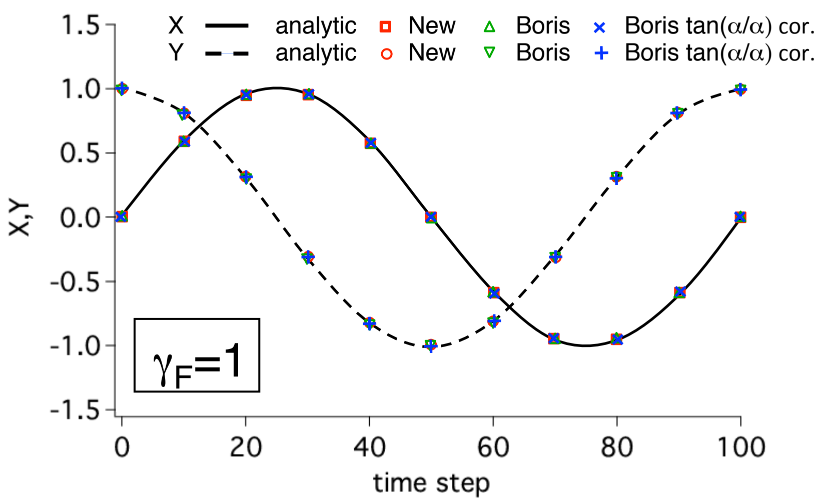
with

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

Lorentz invariant particle pusher: test w/ 1 particle

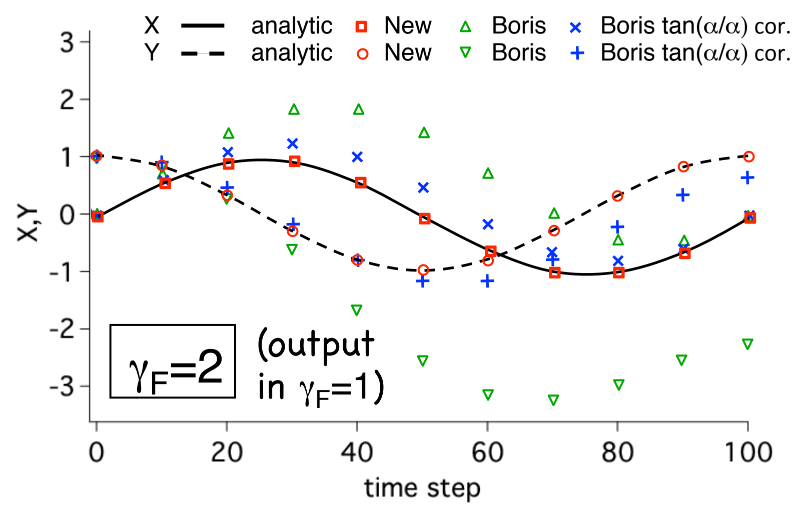
Lab frame

particle cycling in constant B field



Boosted frame γ=2

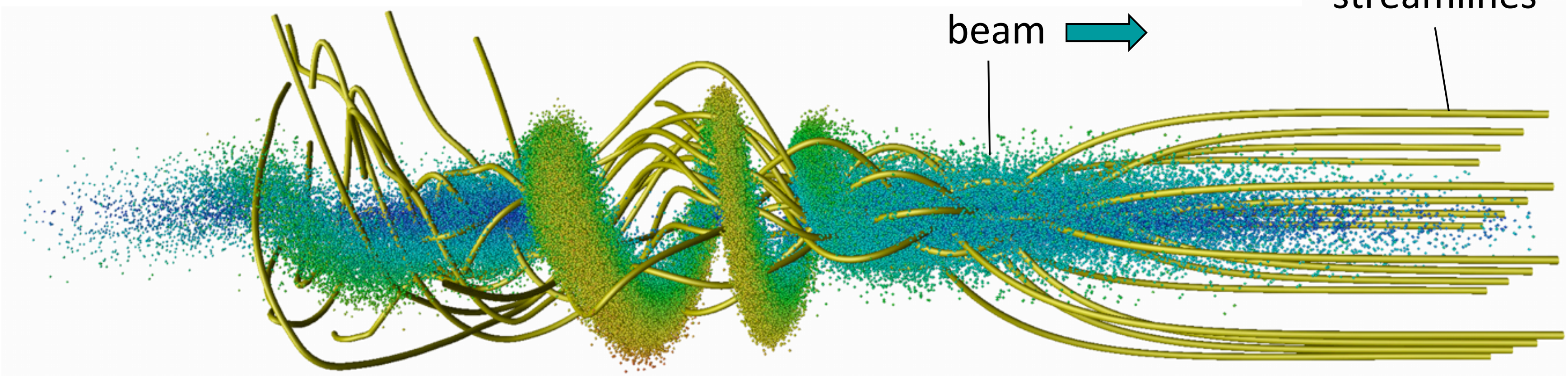
ExB drift adds to gyration



Application to modeling of two-stream instability

Calculation of e-cloud induced instability of a proton bunch

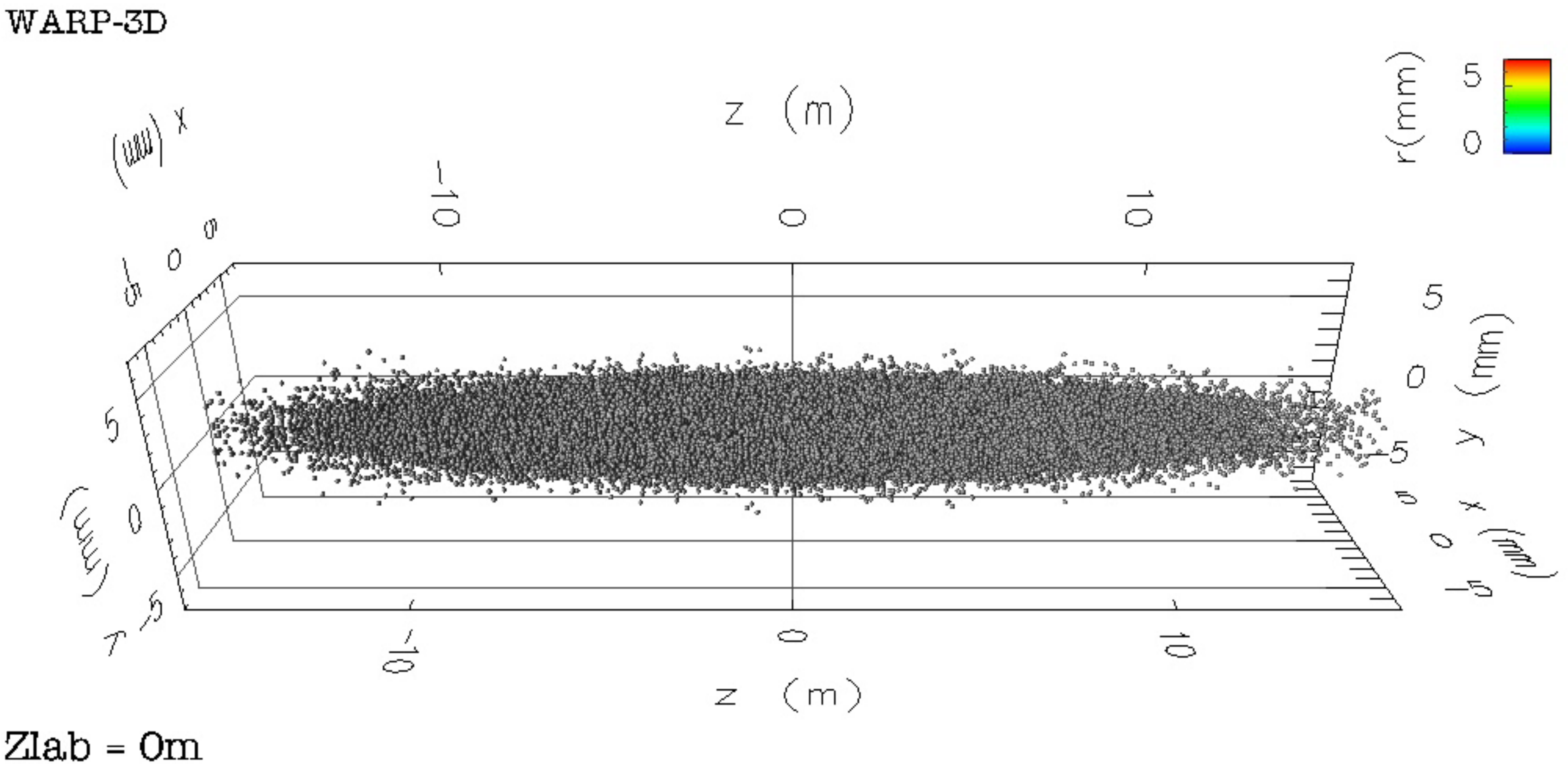
- Proton beam: γ=500, σ_z=13 cm
- L=5 km, continuous focusing



Beam was lost after a few betatron oscillations with Boris pusher.

Accurate result was obtained with new pusher.

Application to modeling of two-stream instability



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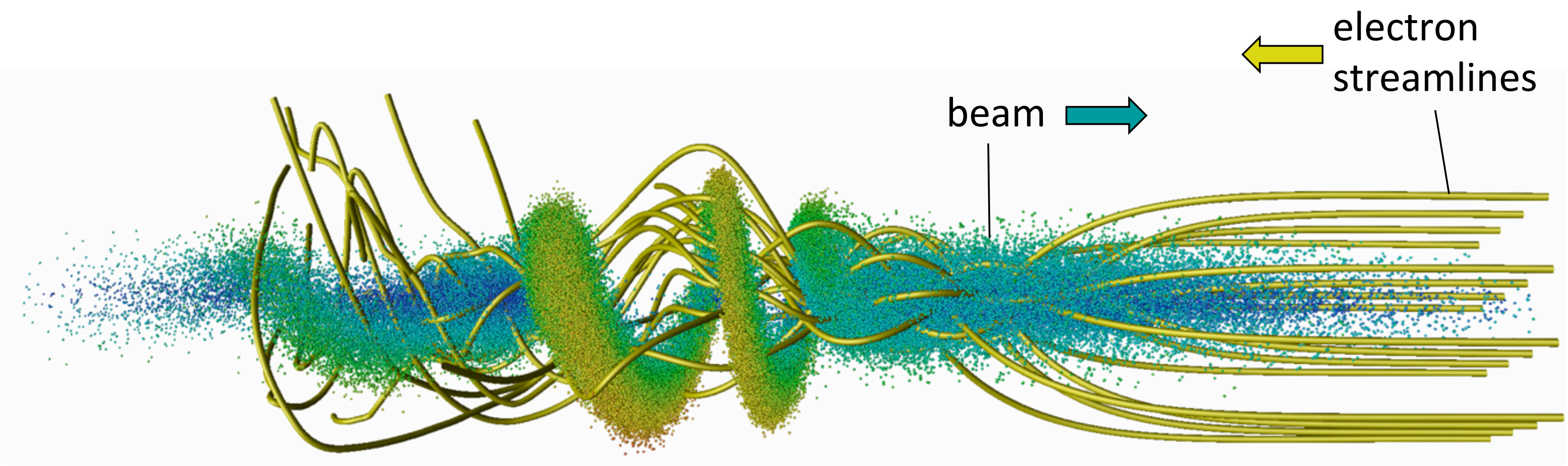
Modeling of two-stream instability is expensive

Need to follow short (σ_z=13 cm) and stiff (γ=500) proton beam for 5 km:

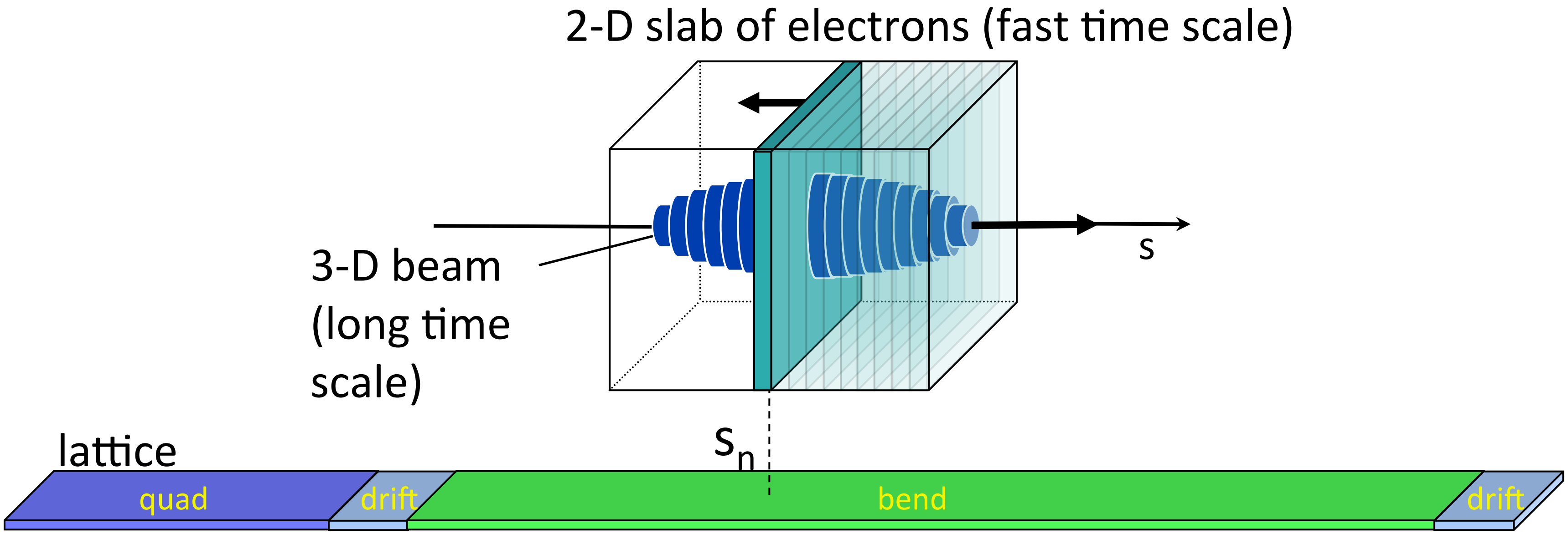
- mobile background electrons react in fraction of beam ➔ small time steps



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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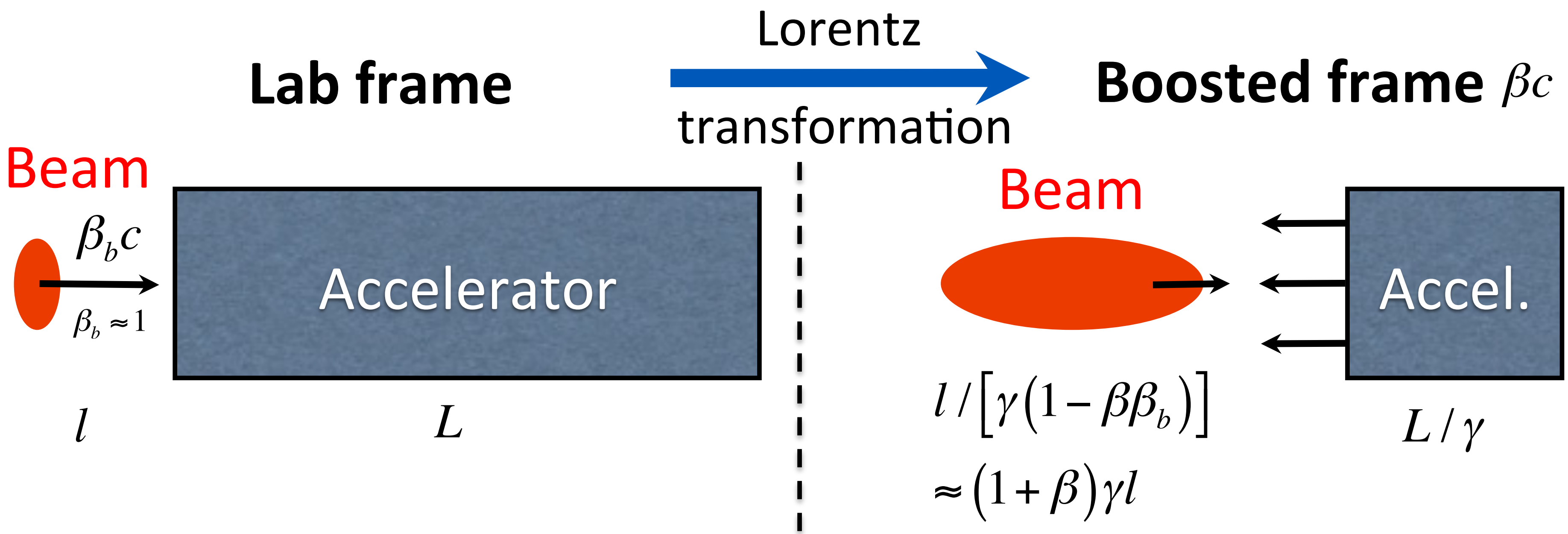
Optimal Lorentz boosted frame



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.

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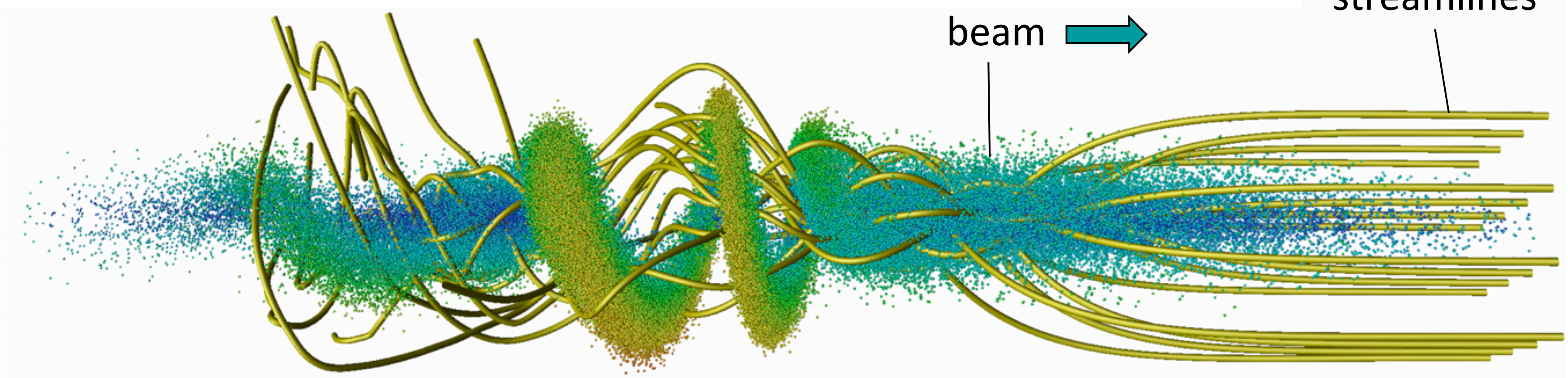
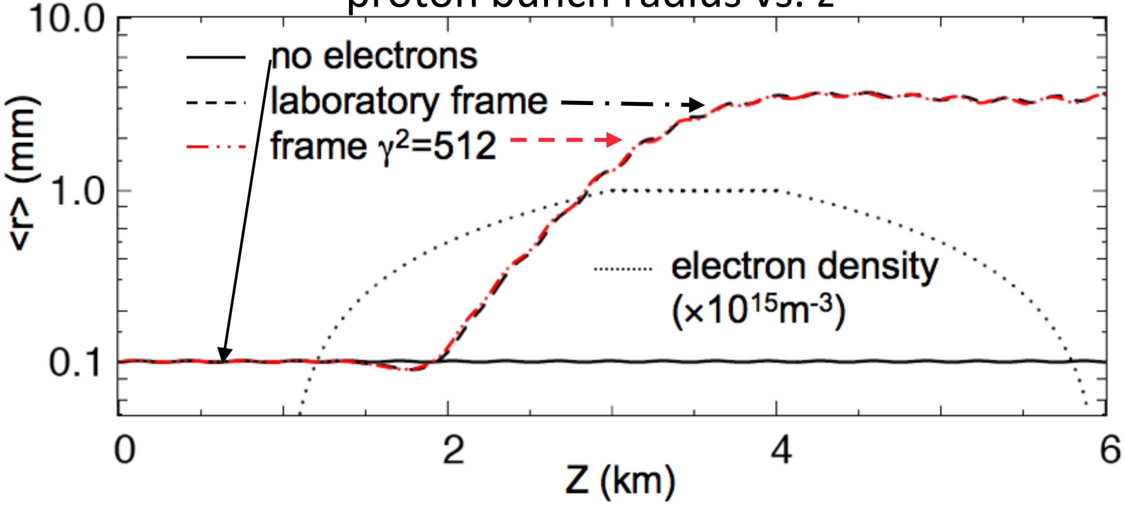


proton bunch radius vs. z



CPU time (on 8 cores in 2006):

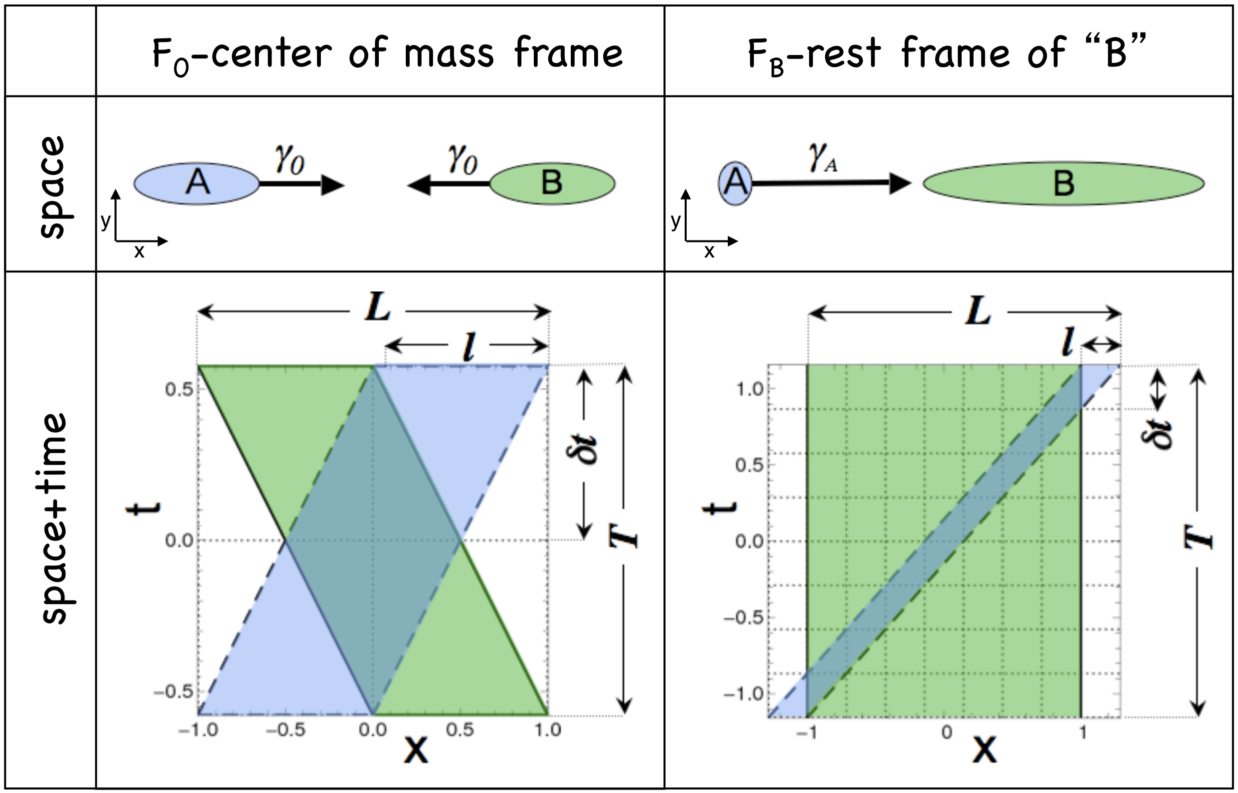
- **lab frame: >2 weeks**
- **frame with γ^2=512: <30 min**

Speedup x1000

Generalization of optimal boosted frame approach

General formulation:

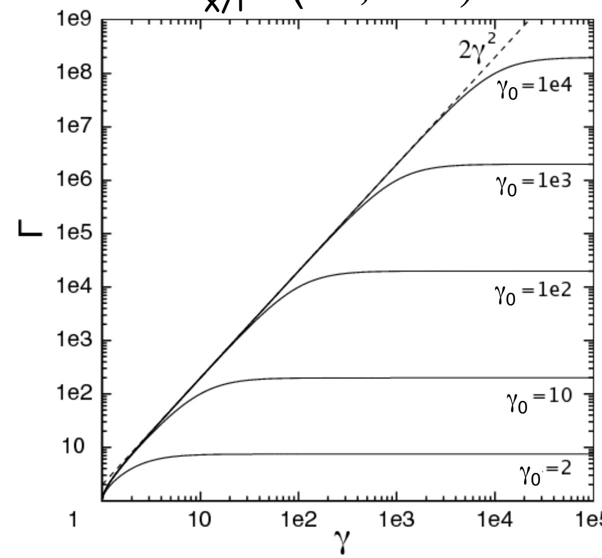
crossing of 2 relativistic objects



Range of space/time scales

$\Gamma_{x/t} \propto \gamma^2$

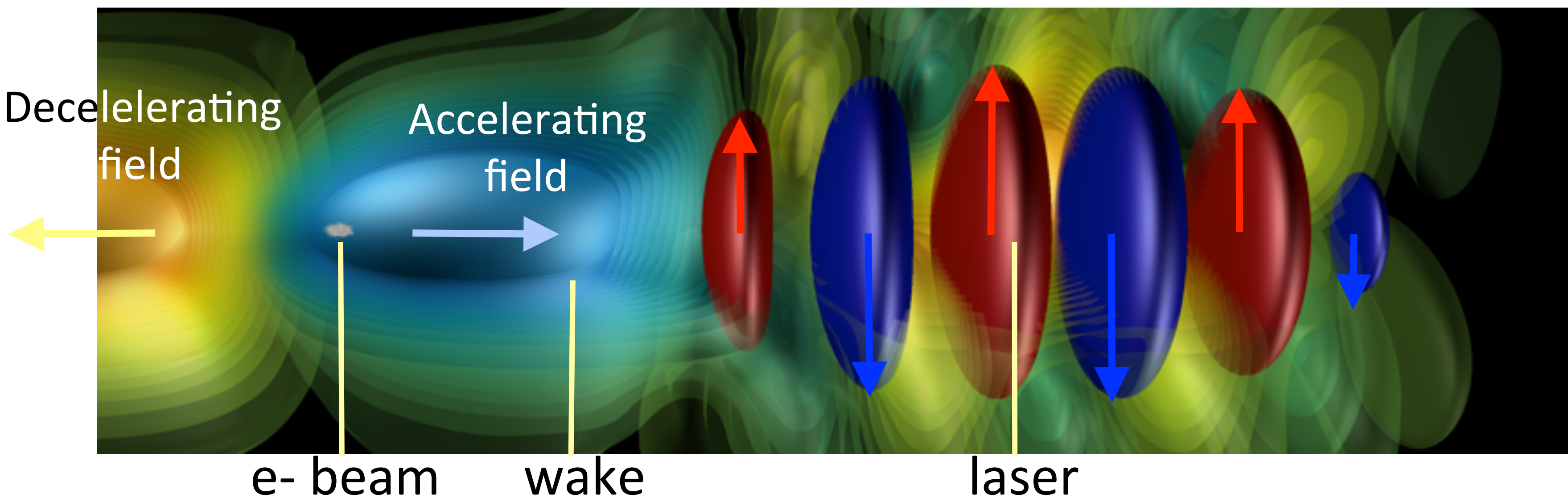
$\Gamma_{x/t} = (L/l, T/\delta t)^*$



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

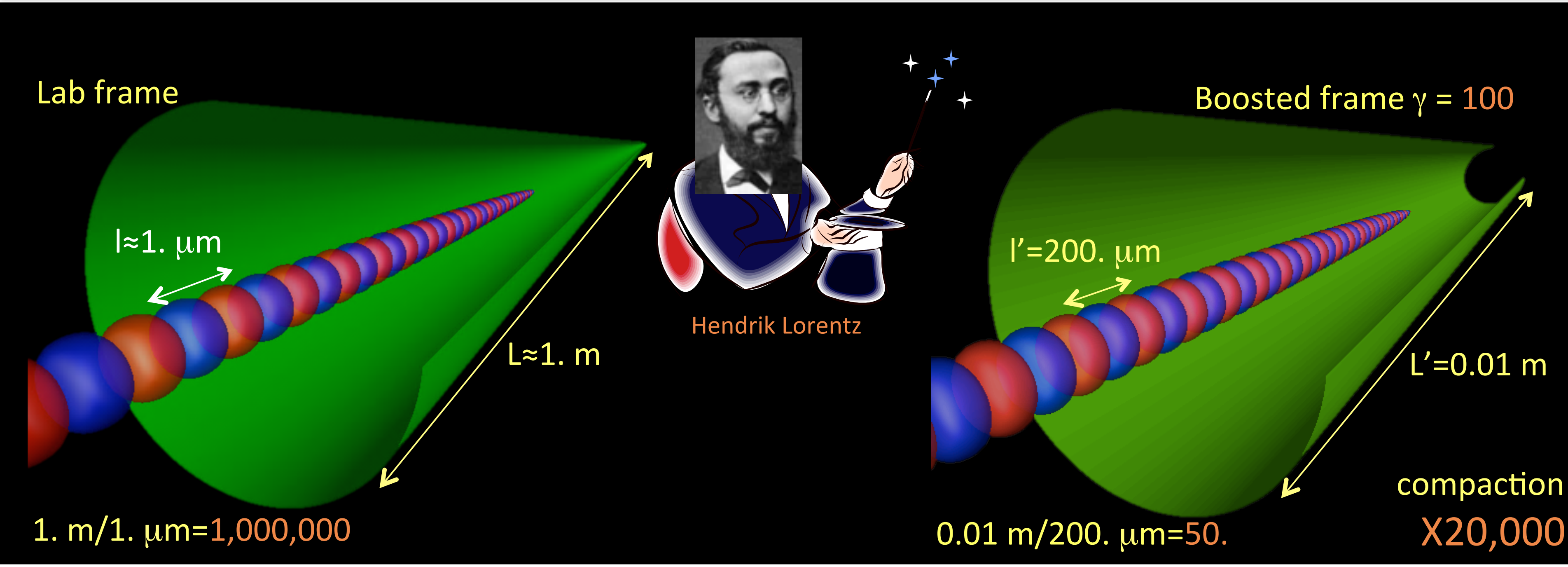
For a 10 GeV scale stage:

~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

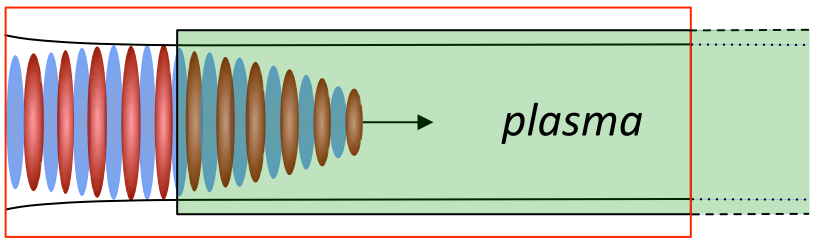


Alternate or <u>complementary</u> solutions: quasistatic, laser envelope, azimuthal Fourier decomposition ("Circ"), …

Laser injection through moving plane solves initialization issue in LBF

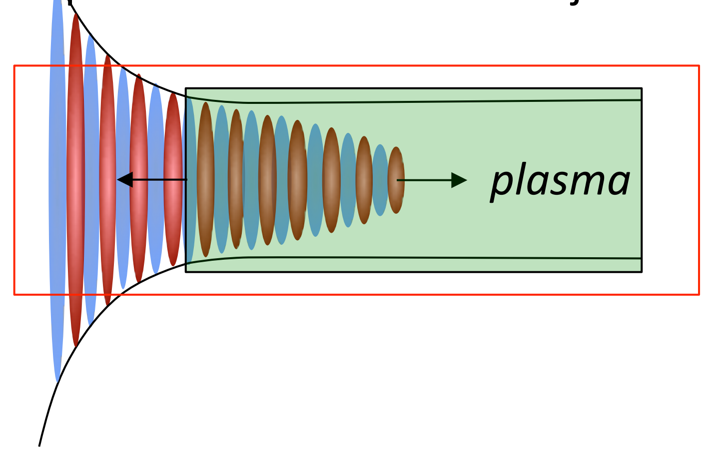
Lab frame

Standard laser injection
from left boundary or all at once

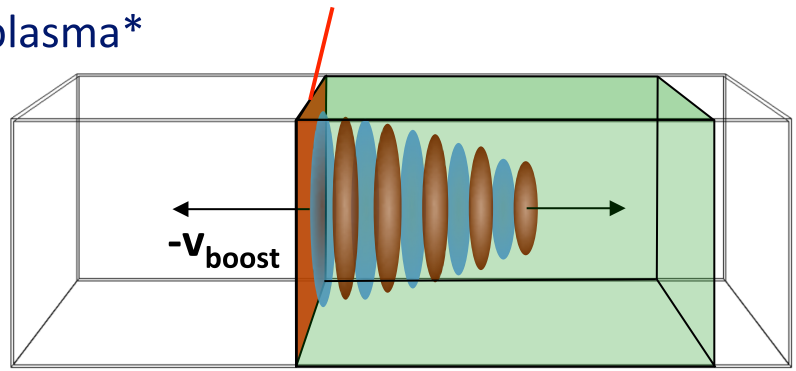


Boosted frame

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

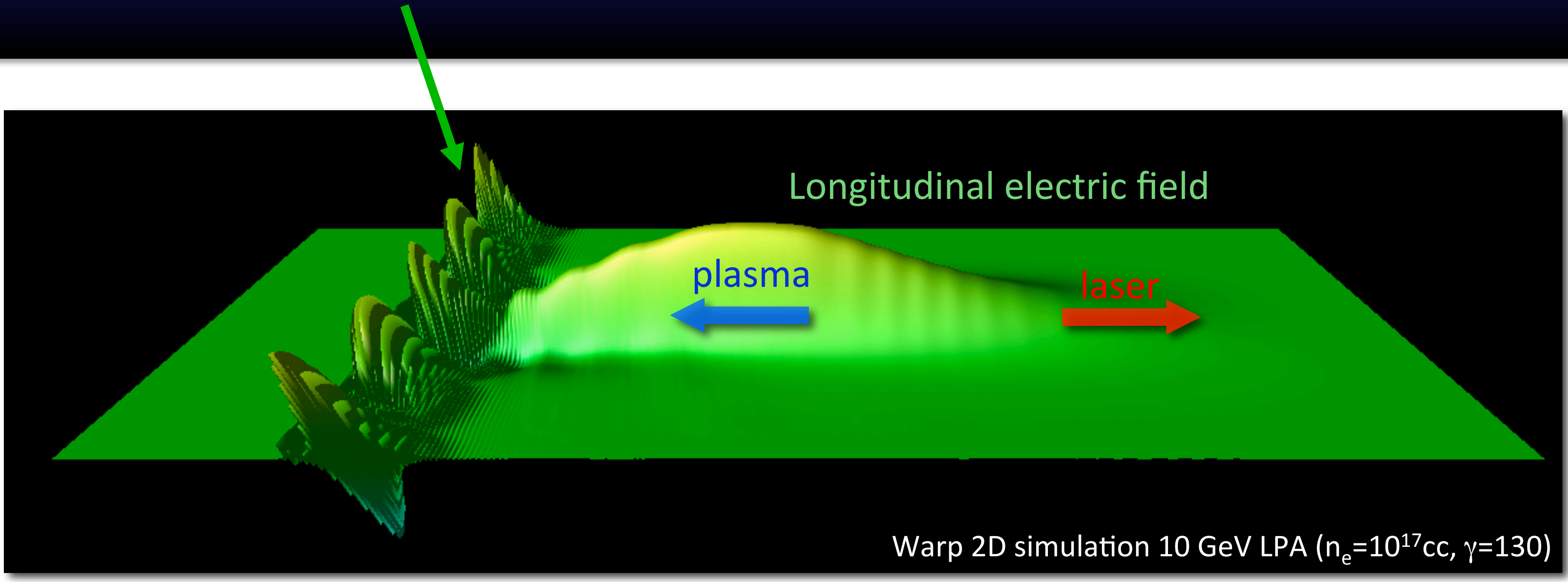


Solution: injection through a **moving planar antenna** in front of plasma*



- 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 ($\geq$100)



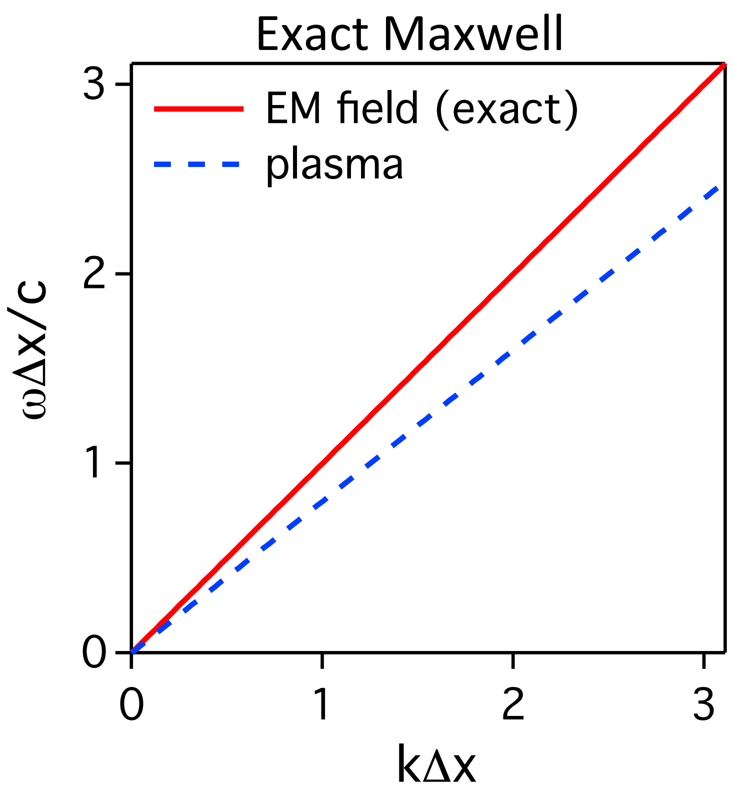
Is it numerical Cherenkov instability?

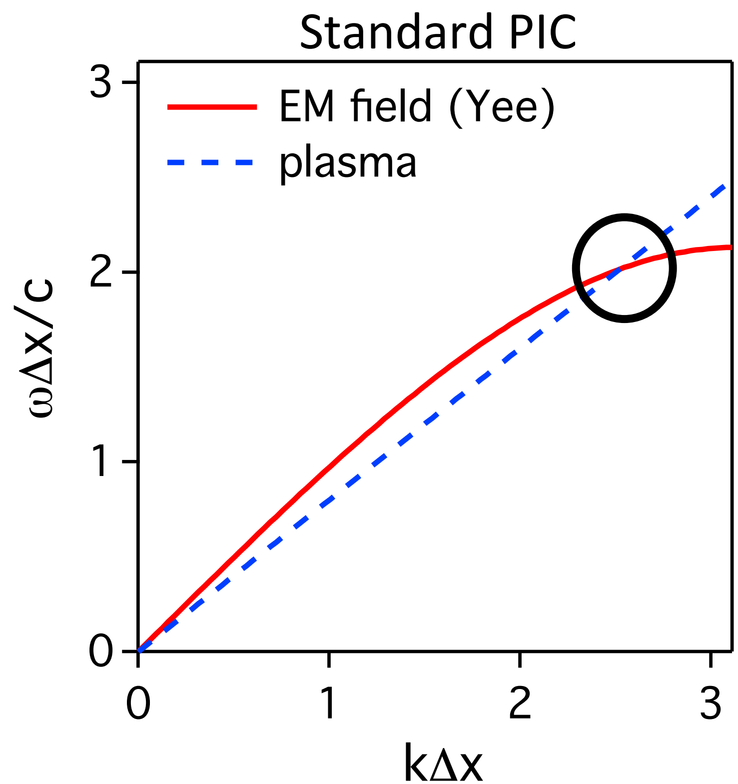
BTW, what is “numerical Cherenkov instability”?

Relativistic plasmas PIC subject to "numerical Cherenkov"

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

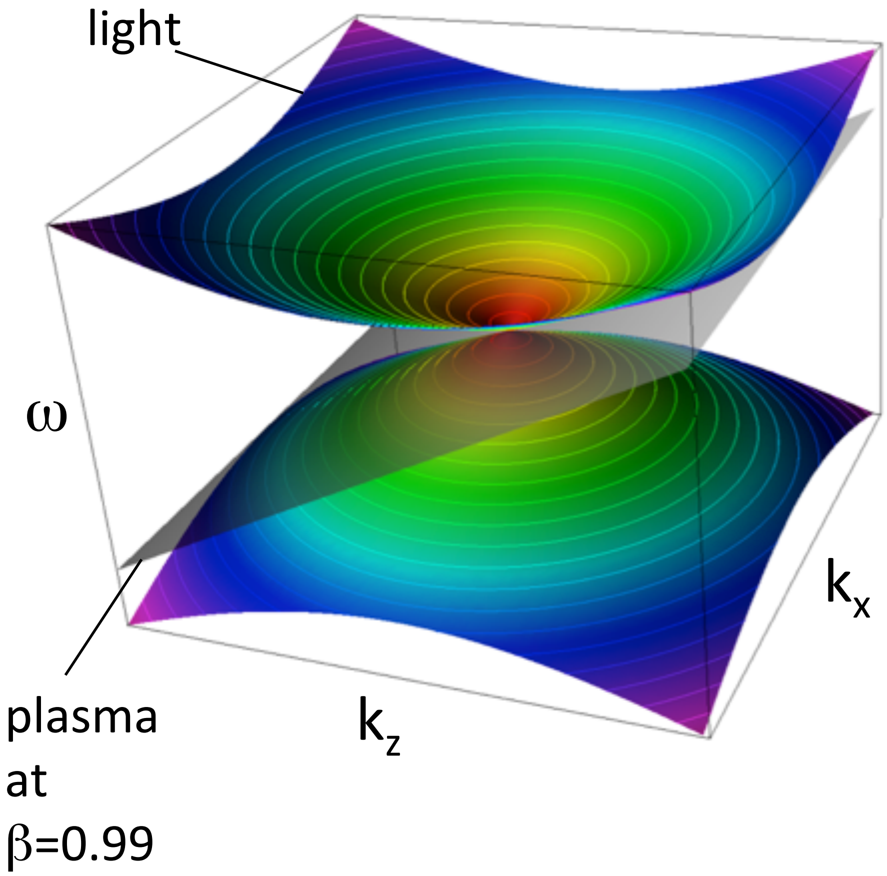
Numerical dispersion leads to crossing of EM field and plasma modes -> instability.



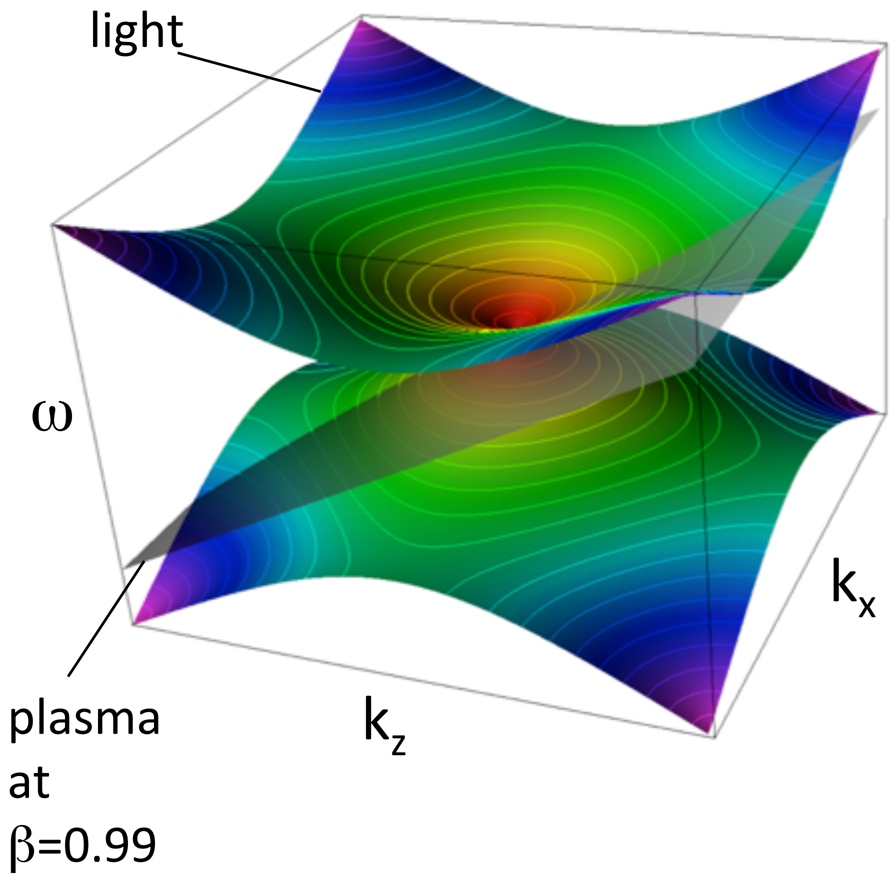


Space/time discretization aliases → more crossings in 2/3-D

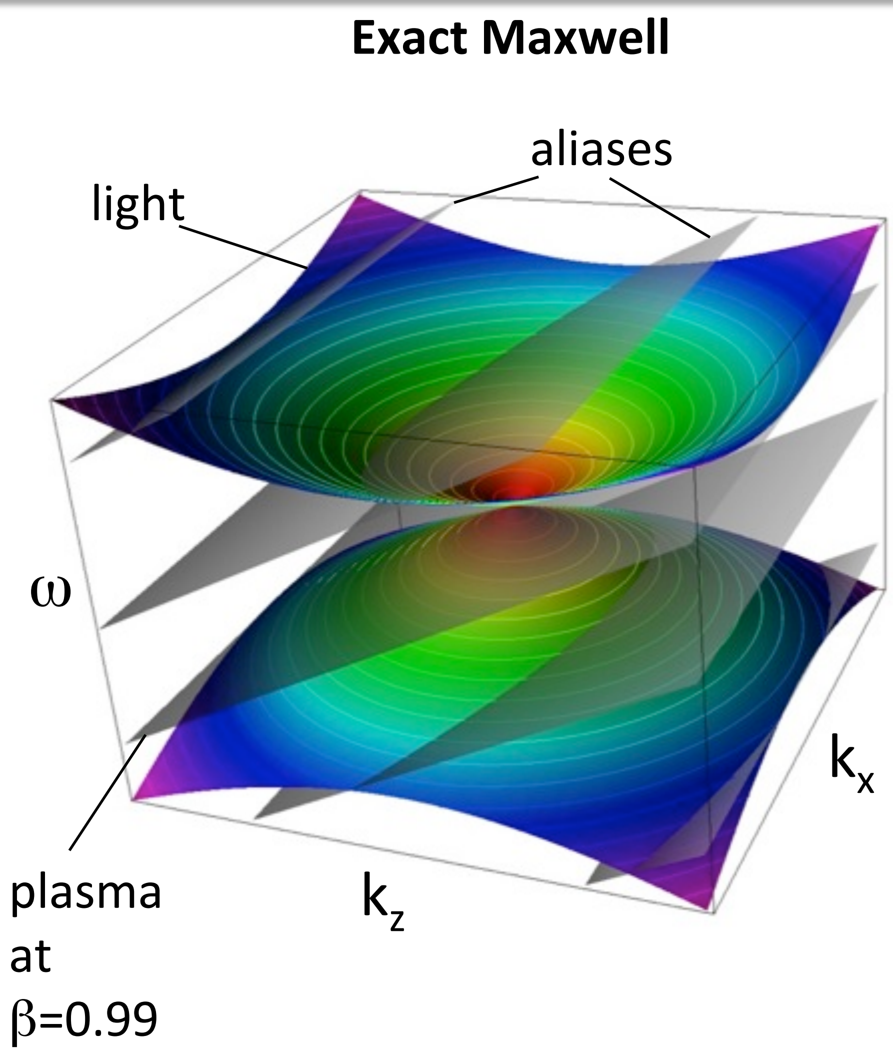
Exact Maxwell

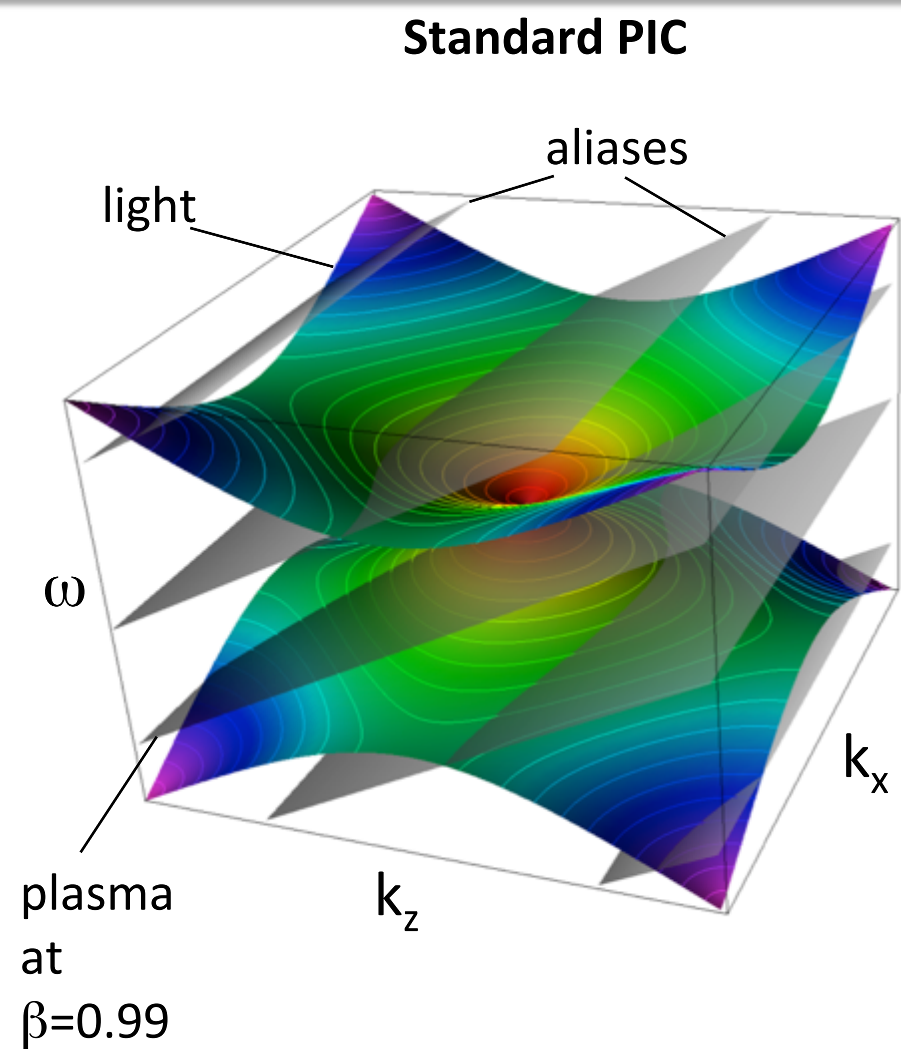


Standard PIC



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

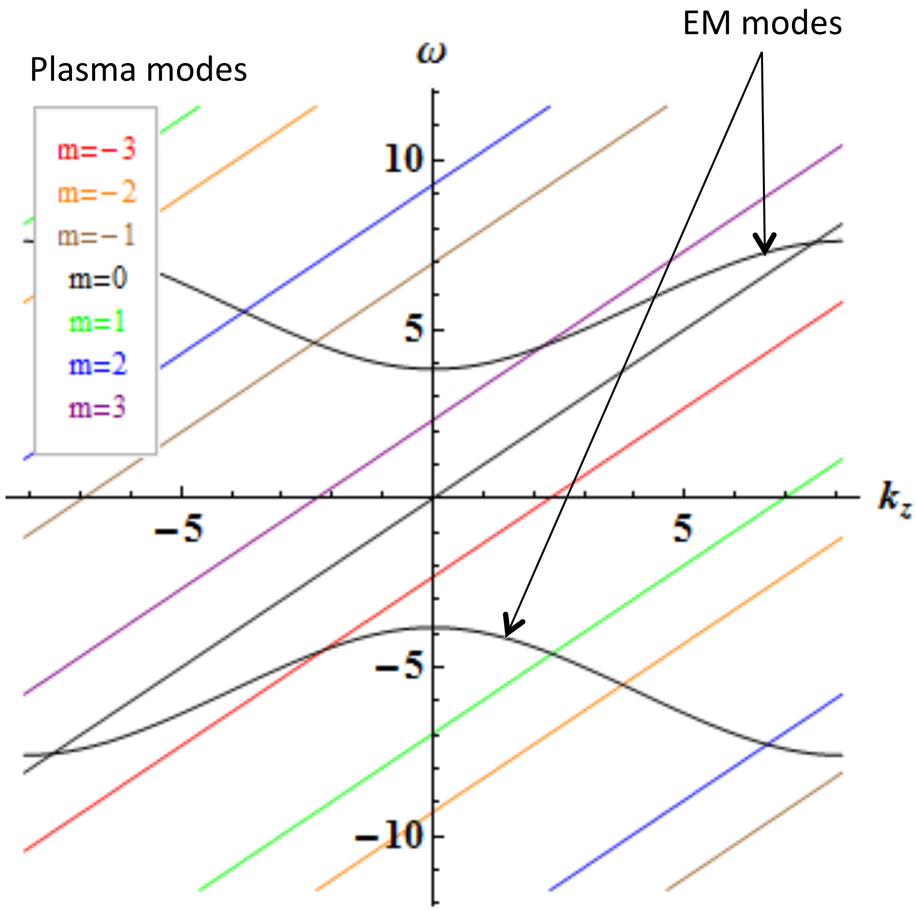




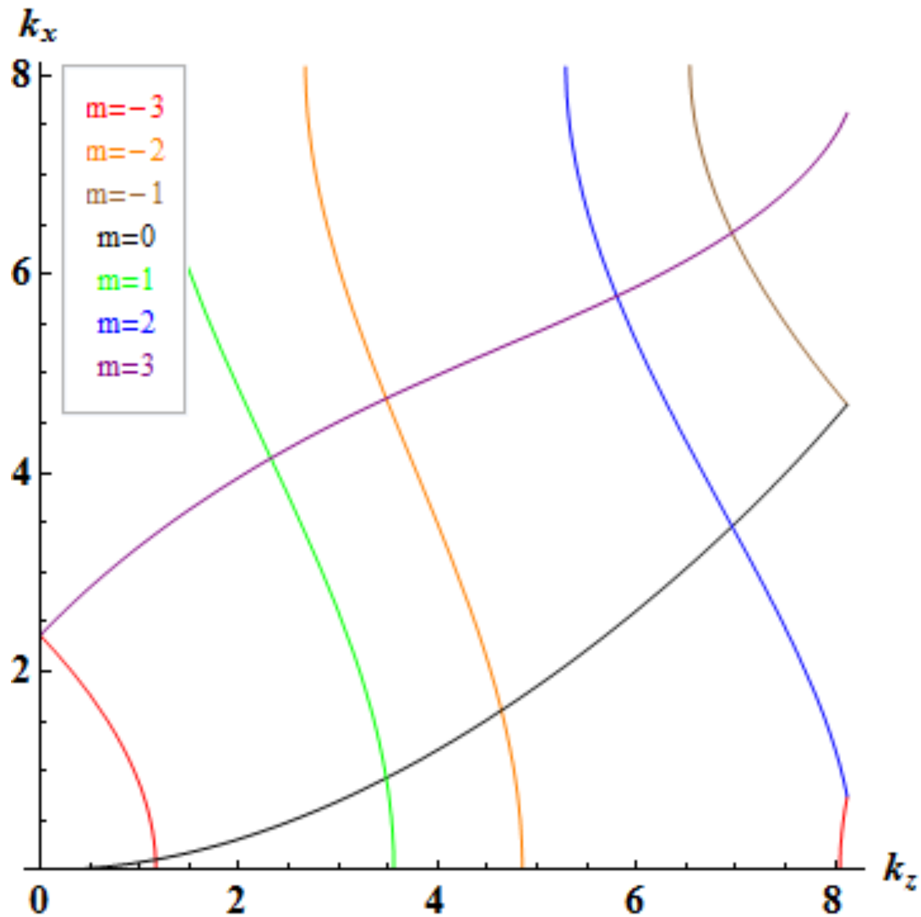
Analysis calls for full PIC numerical dispersion relation

Maps of unstable modes

Normal modes
at k_x=0.5π/Δx for cΔt=0.7Δz



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)

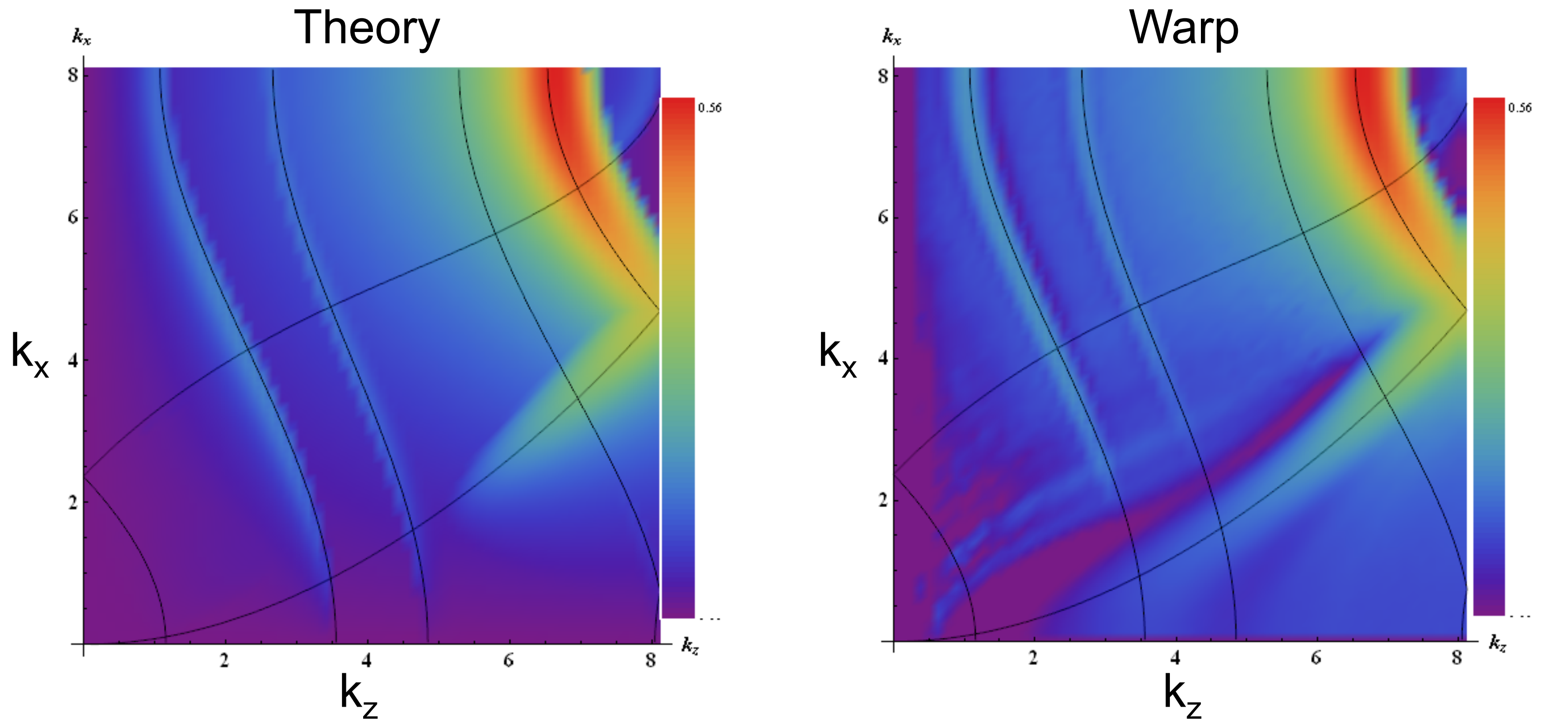
$$\eta_z = \cot\left[(\omega - k_z' v)\frac{\Delta t}{2}\right]\left(k k_z^2 \Delta t + \zeta_z k_x^2 \sin(k\Delta t)\right)\sin\left(k_z' v \frac{\Delta t}{2}\right) + \left(k\Delta t - \zeta_x \sin(k\Delta t)\right) k_z^2 \cos\left(k_z' v\frac{\Delta t}{2}\right),$$

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

Then simplify and solve with Mathematica…

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

Growth rates from theory match Warp simulations



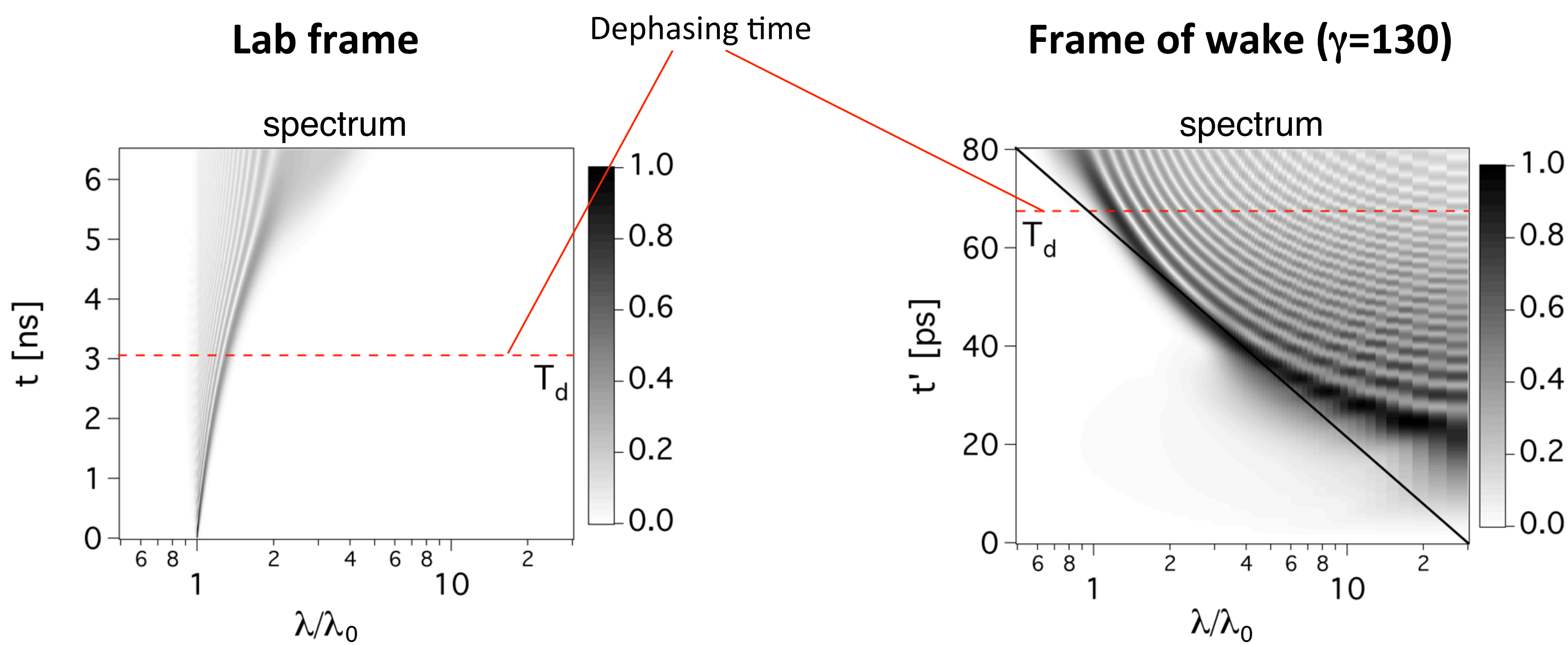
Warp run uses uniform drifting plasma with periodic BC.
Yee finite difference, energy conserving gather ($c\Delta t/\Delta x=0.7$)

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

Physics in boosted frame also allows the use of wideband filtering

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

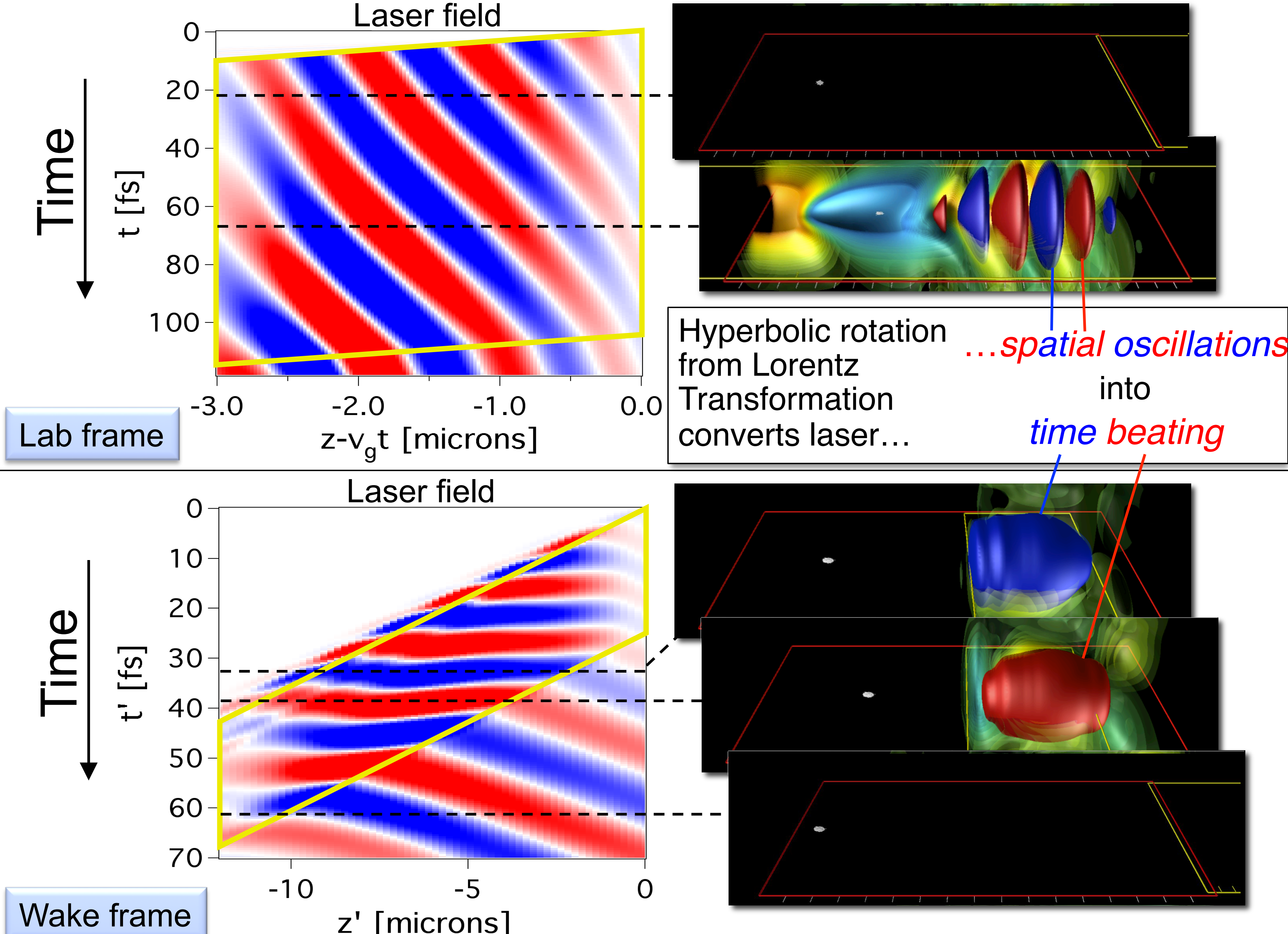
Spectrum very different in lab and boosted frames



Content concentrated around λ_0

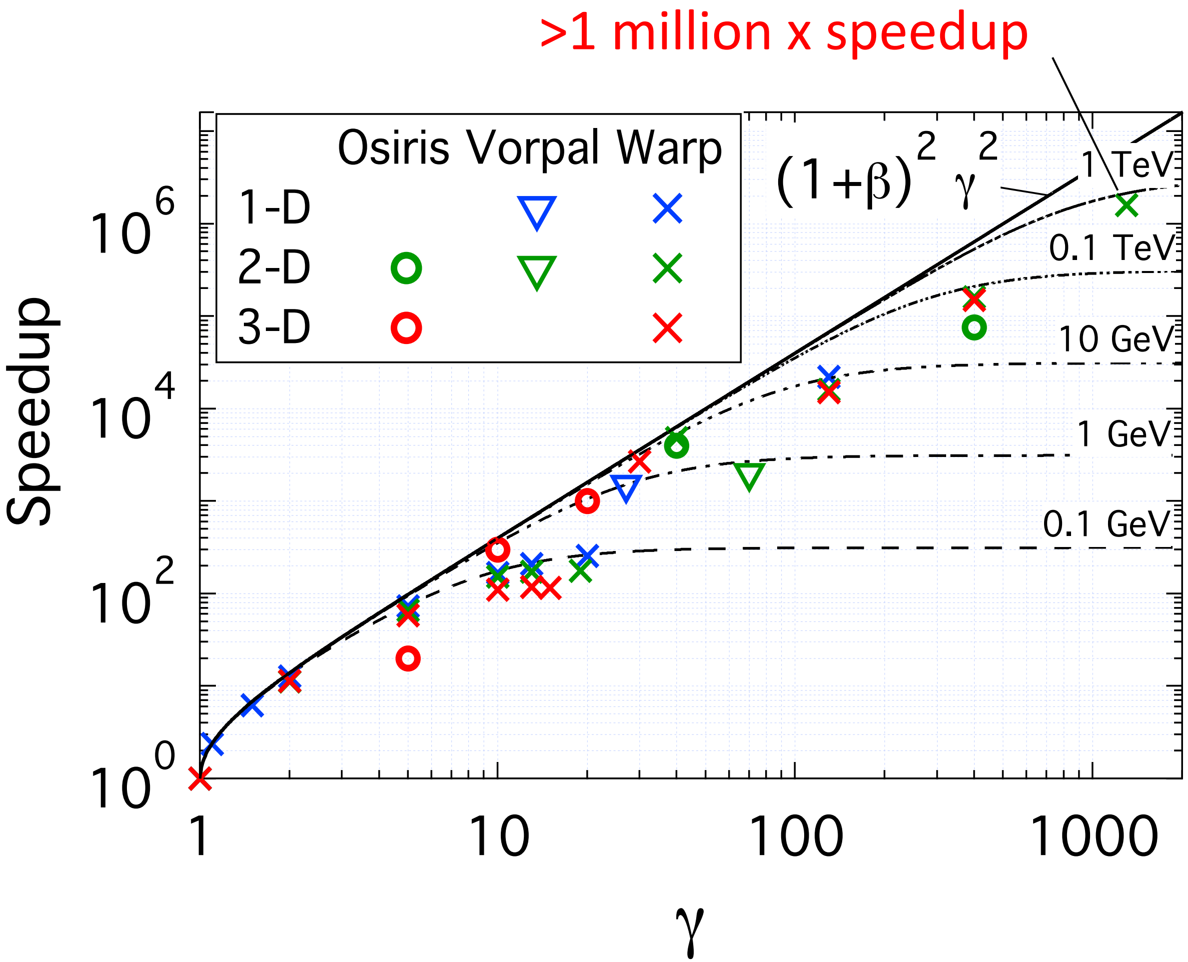
Content concentrated at much larger λ

More filtering possible without altering physics*.



Laser field
Time
t [fs]
0
20
40
60
80
100
-3.0
-2.0
-1.0
0.0
z-v_g t [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

Speedup verified by us and others 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)
2. S. Martins, et al., *Comput. Phys. Comm.* **181** 869 (2010)
3. S. Martins, et al., *Phys. Plasmas* **17** 056705 (2010)
4. S. Martins et al, PAC Proc. (2009)

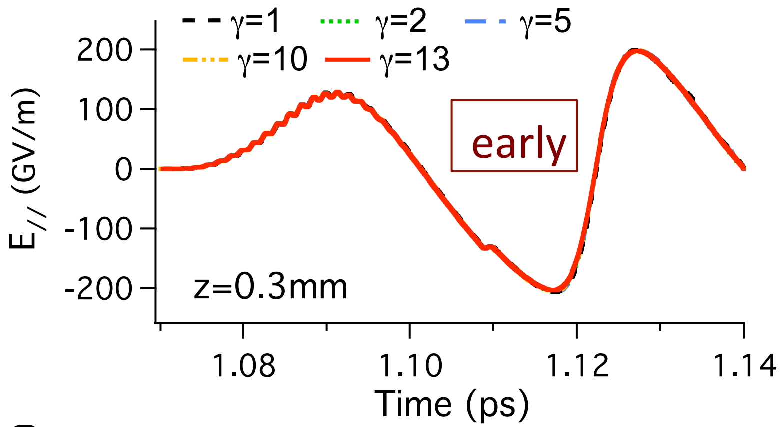
Vorpal:

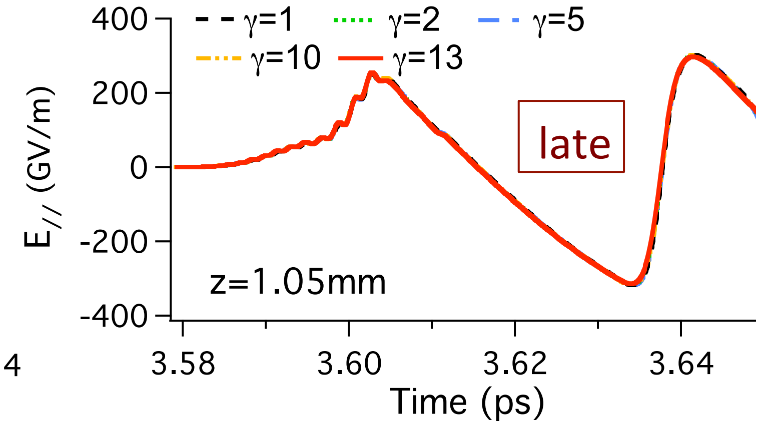
1. D. Bruhwiler, et al., *AIP Conf. Proc* **1086** 29 (2009)

Very high precision validation of BF method with Warp

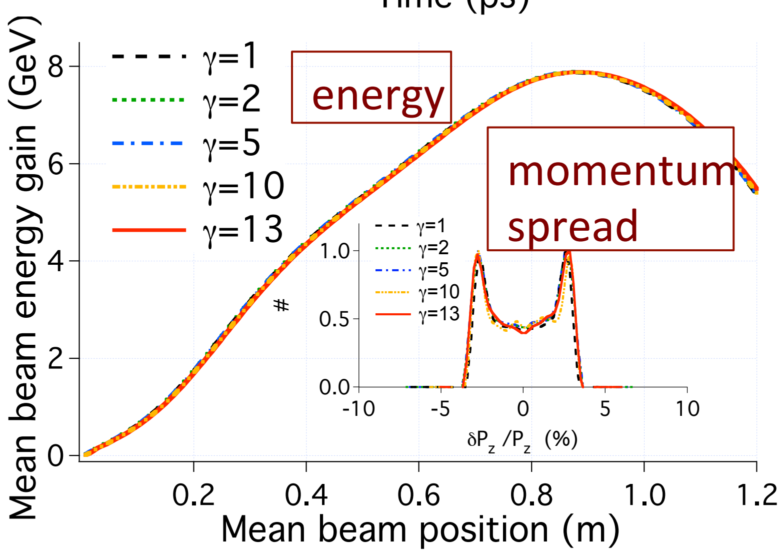
Simulations in various frames (γ=1,2,5,10,13) are almost undistinguishable.

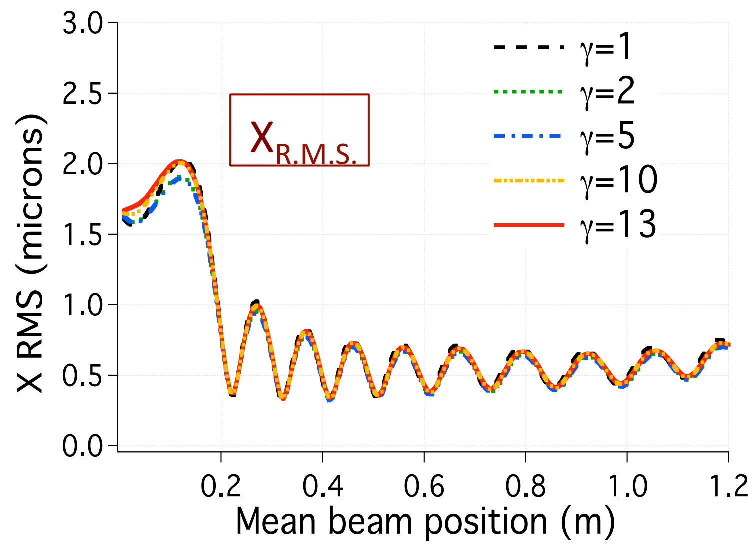
Wake on axis





e- beam

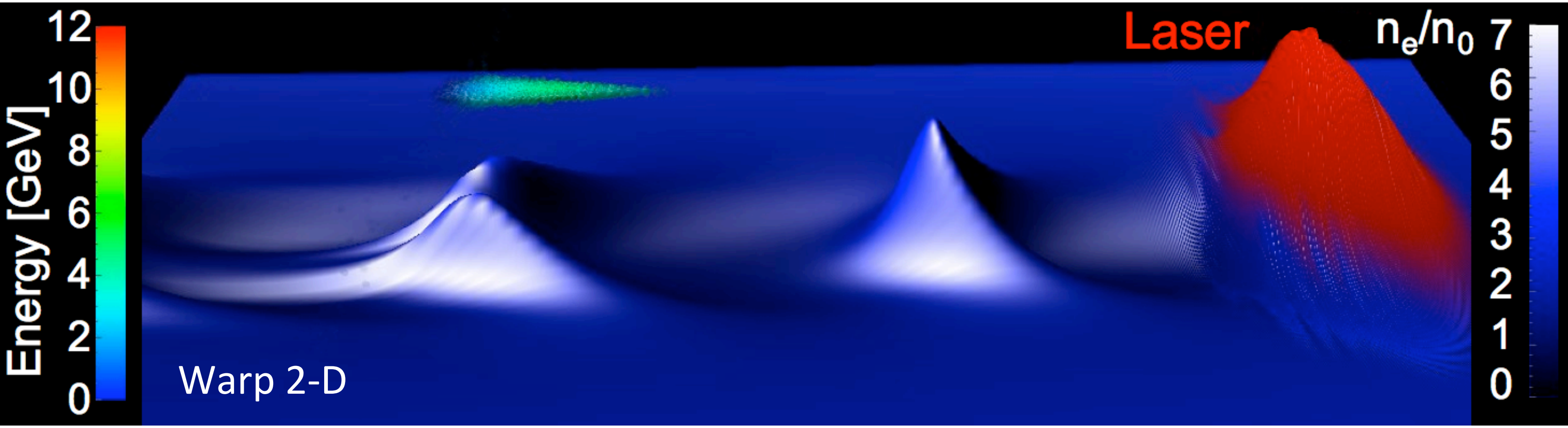




Warp-3D – a_0=1, n_0=10^{19}cm^{-3} (~100 MeV) scaled to 10^{17}cm^{-3} (~10 GeV).
Detailed validation for a0>1 (non-linear regime) is underway.

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.

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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