Speeding up simulations of relativistic systems using an optimal boosted frame

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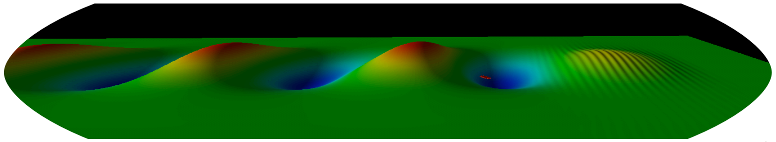

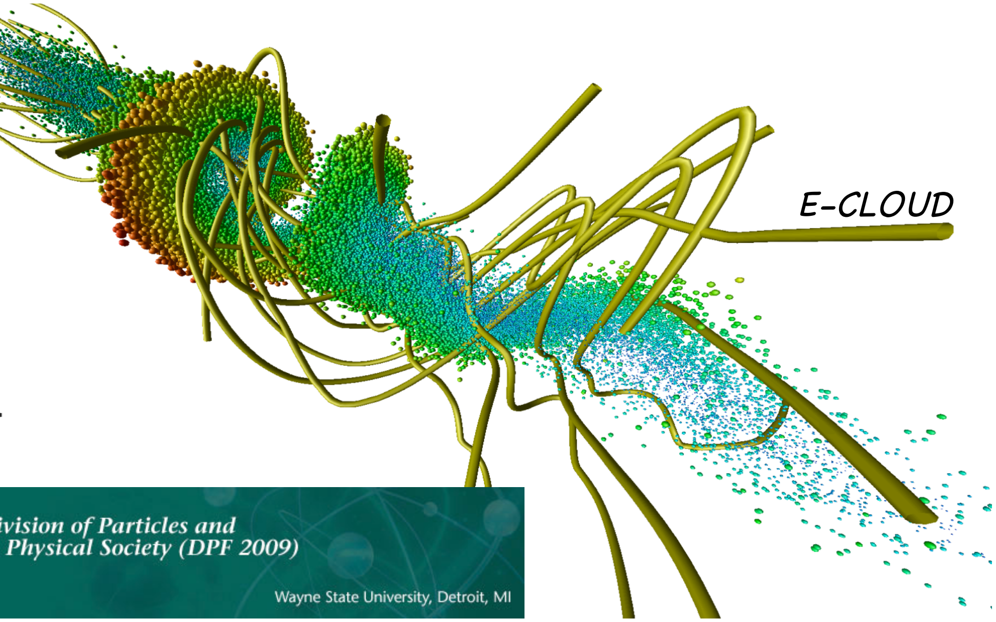

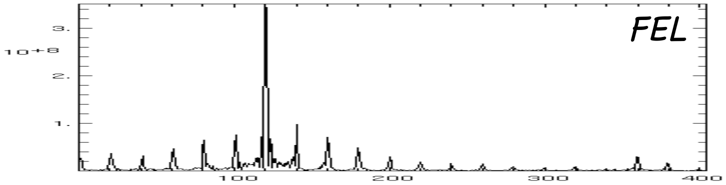

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Outline

- Concept
- Difficulties
- Examples of application
    - laser wakefield acceleration
    - electron cloud effects
    - free electron laser
- Conclusion

Special relativity

Lorentz transformation (LT) for v along x

$$t' = \gamma\,(t - vx/c^2) \qquad \gamma = (1-v^2/c^2)^{-1/2}$$
$$x' = \gamma\,(x - vt)$$
$$y' = y$$
$$z' = z$$

Time dilation/space contraction

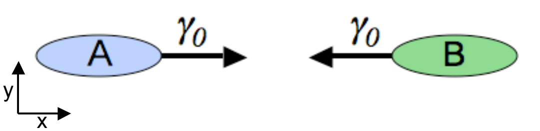
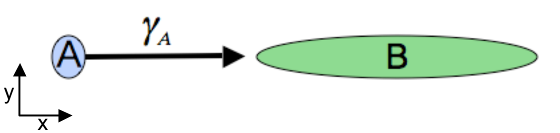
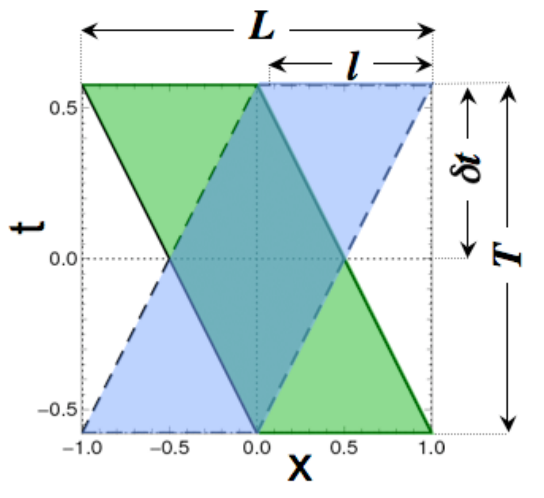
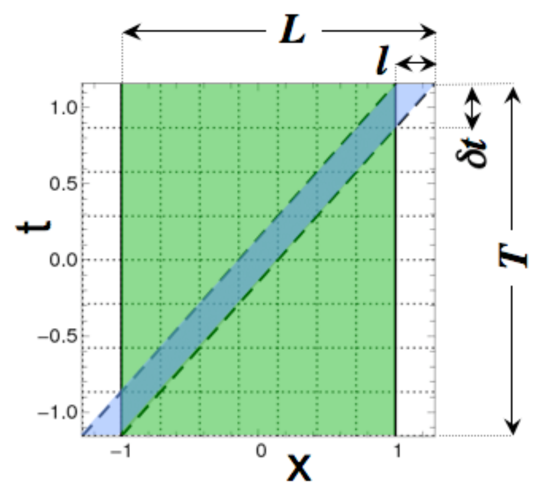
at rest: $\Delta t,\ \Delta x=0$ → in motion: $\Delta t'=\gamma\Delta t$

$\Delta x,\ \Delta t=0$ $\qquad$ $\Delta x'=\Delta x/\gamma$

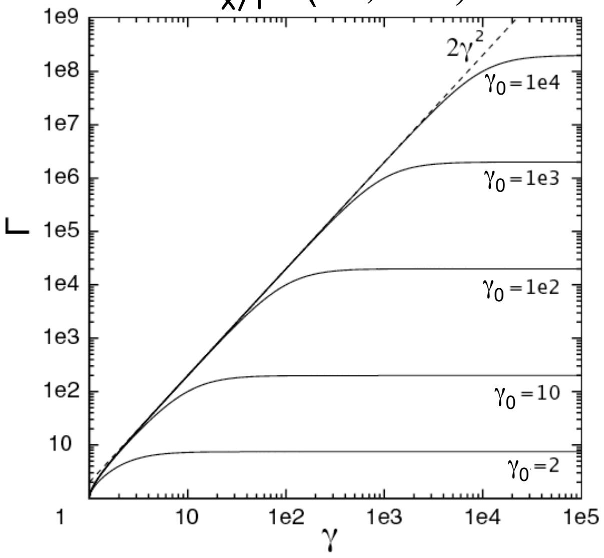
Lorentz invariant (invariant to change of reference frame)

$$\Delta s^2 = \Delta x^2+\Delta y^2+\Delta z^2-c^2\Delta t^2 = \Delta x'^2+\Delta y'^2+\Delta z'^2-c^2\Delta t'^2$$

Range of space and time scales spawned by two identical beams crossing each other

	F_0-center of mass frame	F_B-rest frame of "B"
space		
space+time		

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



- Γ is not invariant under the Lorentz transformation: $\Gamma_{x/t} \propto \gamma^2$.
- There exists an "optimum" frame which minimizes it.
- Result is general and applies to light beams too.

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

Consequence for computer simulations

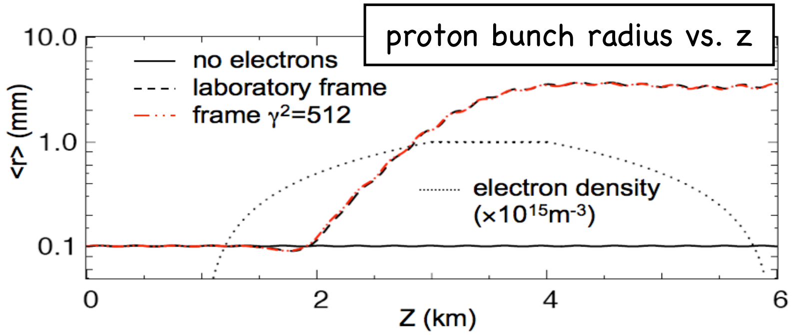
of computational steps grows with the full range of space and time scales involved

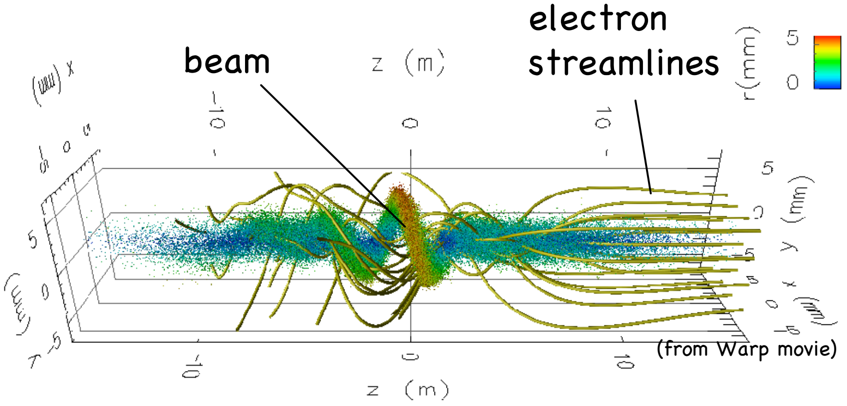
Choosing optimum frame of reference to minimize range can lead to dramatic speed-up for relativistic matter-matter or light-matter interactions.

Calculation of e-cloud induced instability of a proton bunch*

- Proton energy: γ=500 in Lab
- L=5 km, continuous focusing

Code: Warp (Particle-In-Cell)


proton bunch radius vs. z



(from Warp movie)

CPU time (2 quad-core procs):

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

Speedup x1000

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

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Seems simple but ⚠. Algorithms which work in one frame may break in another. Example: the Boris particle pusher.

- Boris pusher ubiquitous
  - In first attempt of e-cloud calculation using the Boris pusher, the beam was lost in a few betatron periods!
  - Position push: $\mathbf{X}^{n+1/2} = \mathbf{X}^{n-1/2} + \mathbf{V}^{n}\,\Delta t$ -- no issue
  - Velocity push: $\gamma^{n+1}\mathbf{V}^{n+1} = \gamma^{n}\mathbf{V}^{n} + \frac{q\,\Delta t}{m}\left(\mathbf{E}^{n+1/2} + \frac{\gamma^{n+1}\mathbf{V}^{n+1} + \gamma^{n}\mathbf{V}^{n}}{2\,\gamma^{n+1/2}} \times \mathbf{B}^{n+1/2}\right)$

    issue: $\mathbf{E}+v\times\mathbf{B}=0$ implies $\mathbf{E}=\mathbf{B}=0$ => large errors when $\mathbf{E}+v\times\mathbf{B}\approx 0$ (e.g. relativistic beams).

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

- Not used before because of implicitness. We solved it analytically*

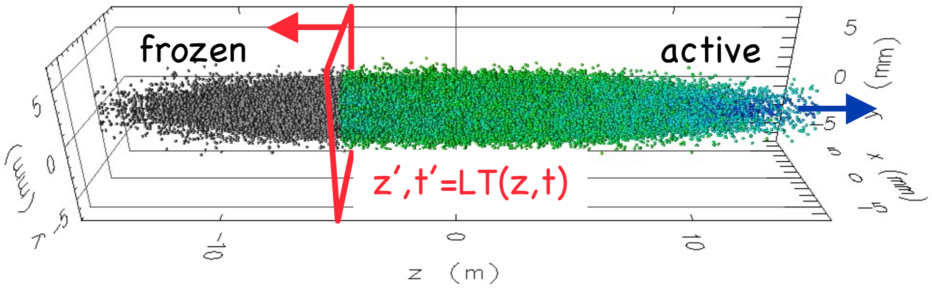
$$\begin{cases} \gamma^{i+1} = \sqrt{\dfrac{\sigma + \sqrt{\sigma^2 + 4(\tau^2 + u^{*2})}}{2}} \\ \mathbf{u}^{i+1} = [\mathbf{u}' + (\mathbf{u}' \cdot \mathbf{t})\mathbf{t} + \mathbf{u}' \times \mathbf{t}]/(1+t^2) \end{cases}$$

(with $\mathbf{u} = \gamma\mathbf{v}$, $\mathbf{u}' = \mathbf{u}^{\mathbf{i}} + \frac{q\Delta t}{m}\left(\mathbf{E}^{i+1/2} + \frac{\mathbf{v}^{i}}{2} \times \mathbf{B}^{i+1/2}\right)$, $\boldsymbol{\tau} = (q\Delta t/2m)\mathbf{B}^{i+1/2}$; $u^{*} = \mathbf{u}' \cdot \boldsymbol{\tau}/c$, $\sigma = \gamma'^2 - \tau^2$, $\gamma' = \sqrt{1 + u'^2/c^2}$, $\mathbf{t} = \boldsymbol{\tau}/\gamma^{i+1}$).

*J.-L. Vay, *Phys. Plasmas* **15**, 056701 (2008)

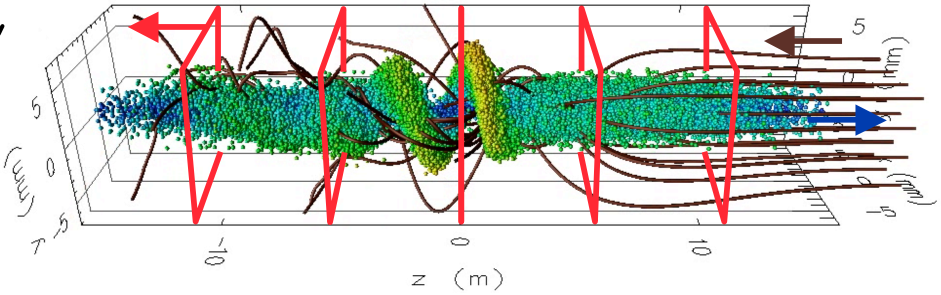
Other possible complication: inputs/outputs

- Often, initial conditions known and output desired in laboratory frame
  - relativity of simultaneity => inject/collect at plane(s) ⊥ to direction of boost.
- Injection through a moving plane in boosted frame (fix in lab frame)
  - fields include frozen particles,
  - same for laser in EM calculations.



- Diagnostics: collect data at a collection of planes
  - fixed in lab fr., moving in boosted fr.,
  - interpolation in space and/or time,
  - already done routinely with Warp

  for comparison with experimental data, often known at given stations in lab.



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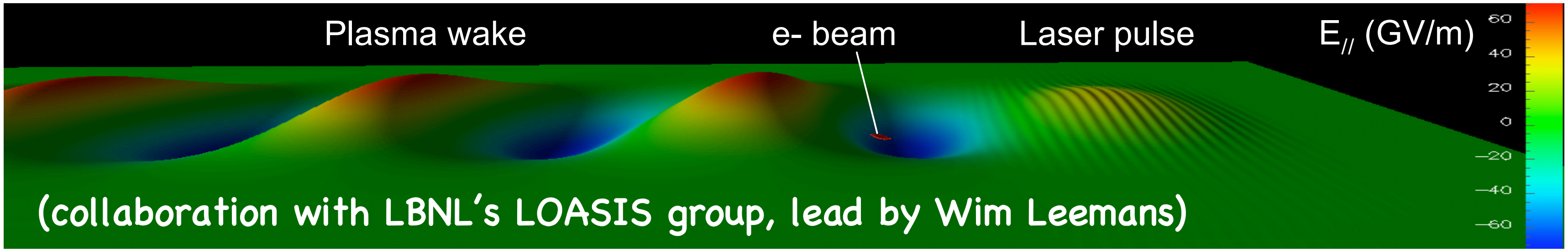
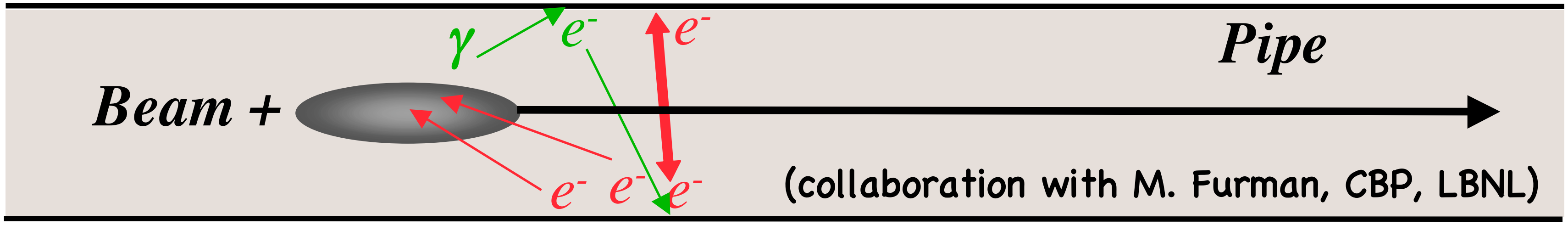
Several areas in which simulations in a boosted may be beneficial were identified

Laser-plasma wakefield accelerators



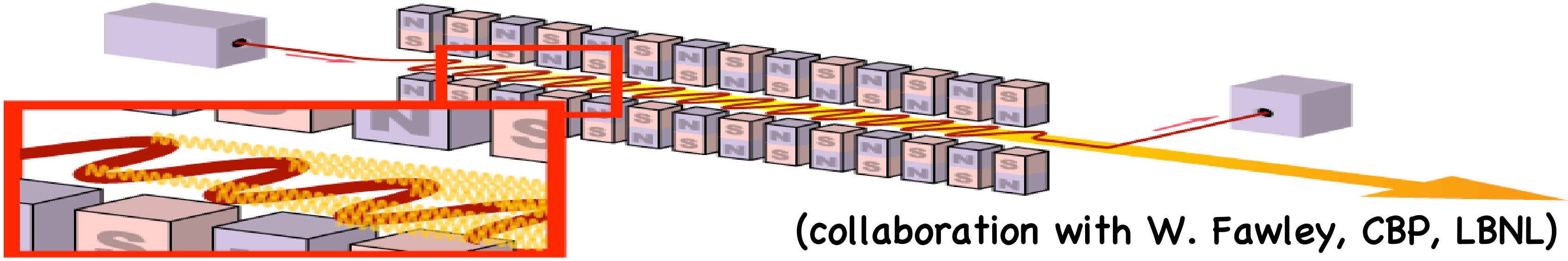
(collaboration with LBNL's LOASIS group, lead by Wim Leemans)

Electron cloud driven beam instabilities



(collaboration with M. Furman, CBP, LBNL)

Free electron lasers/coherent synchrotron radiation

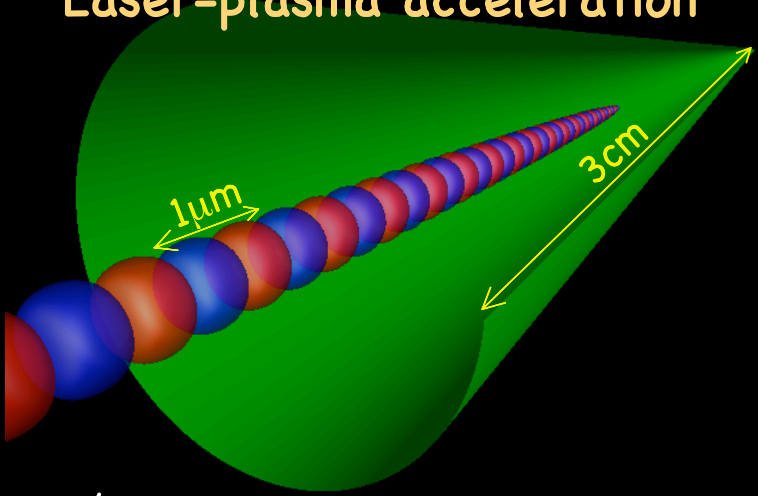


(collaboration with W. Fawley, CBP, LBNL)

Large scale range renders simulation difficult, if not impractical, in lab frame

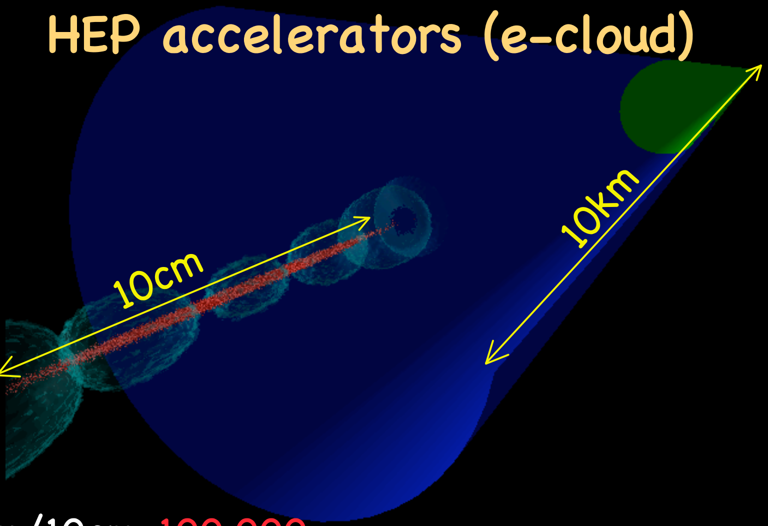
laboratory frame

Laser-plasma acceleration



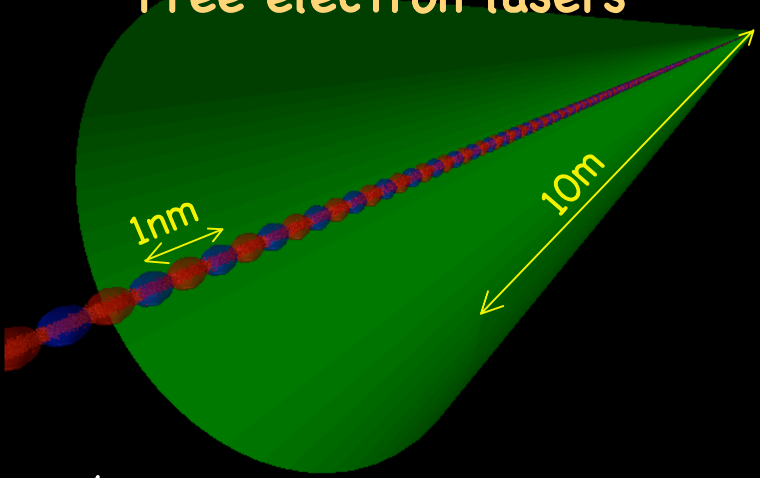
3cm/1μm=30,000.

HEP accelerators (e-cloud)



10km/10cm=100,000.

Free electron lasers

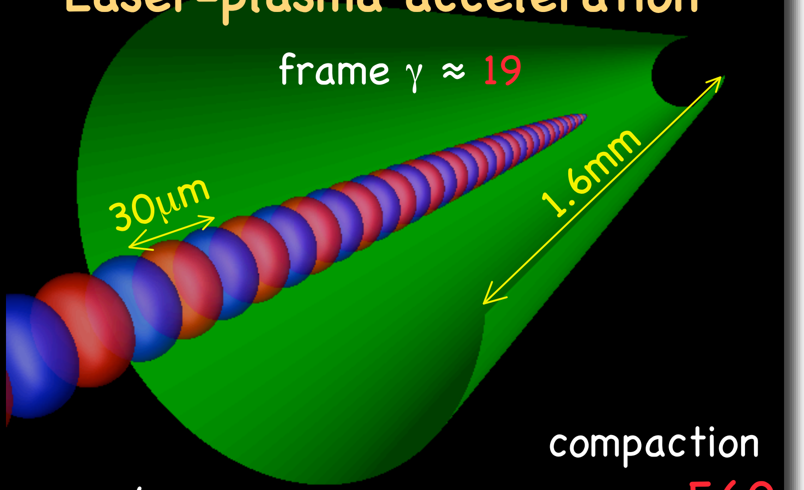


10m/1nm=10,000,000,000.

Lorentz transformation => large level of compaction of scales range

Hendrik Lorentz

Laser-plasma acceleration

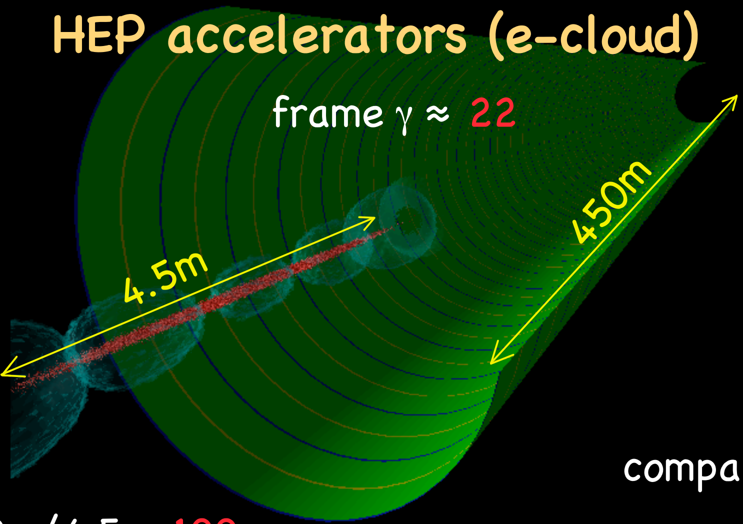


1.6mm/30μm=53.

compaction

x560

HEP accelerators (e-cloud)

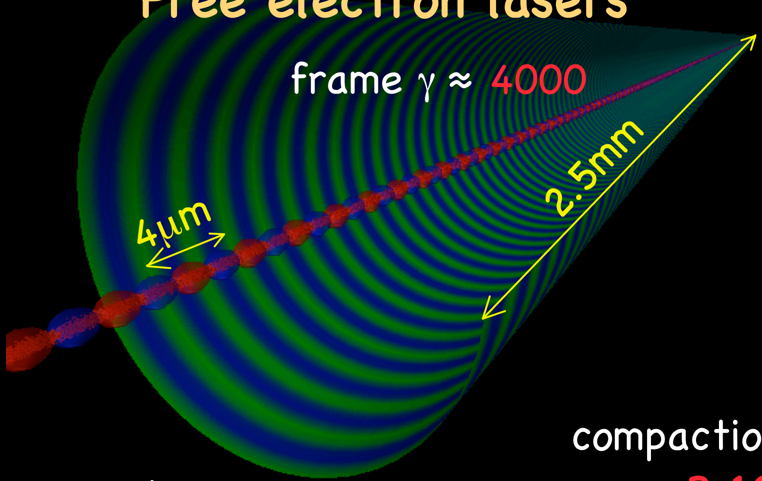


450m/4.5m=100.

compaction

$\times 10^3$

Free electron lasers



2.5mm/4μm=625.

compaction

$\times 3.10^7$

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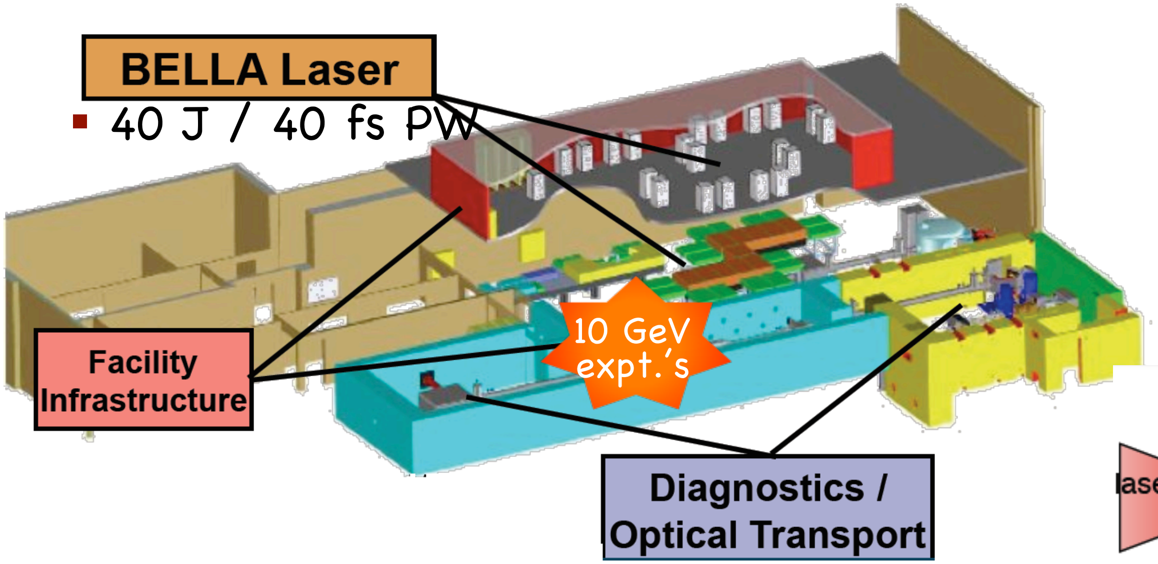
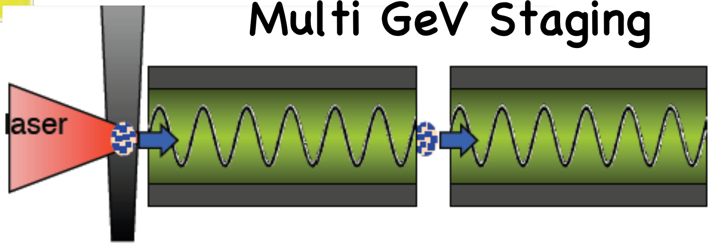
BELLA 40 J PW Laser – Components for a Laser Plasma Collider



Injection + 10 GeV stages

Emittance preservation

Multi GeV Staging



Simulating 10 GeV stages explicitly (PIC) in lab frame needs ~1G CPU•hours ⇒ impractical*

Predictions have relied on theory, reduced models (fluid, envelope, quasistatic), scaling:

– Energy gain	$\propto n^{-1}$	: 10 GeV at 10^{17}/cc	⇒ 100 MeV at 10^{19}/cc
– Length	$\propto n^{-3/2}$	: 1m at 10^{17}/cc	⇒ 1mm at 10^{19}/cc
– Gradient	$\propto n^{1/2}$	: 10 GV/m at 10^{17}/cc	⇒ 100 GV/m at 10^{19}/cc

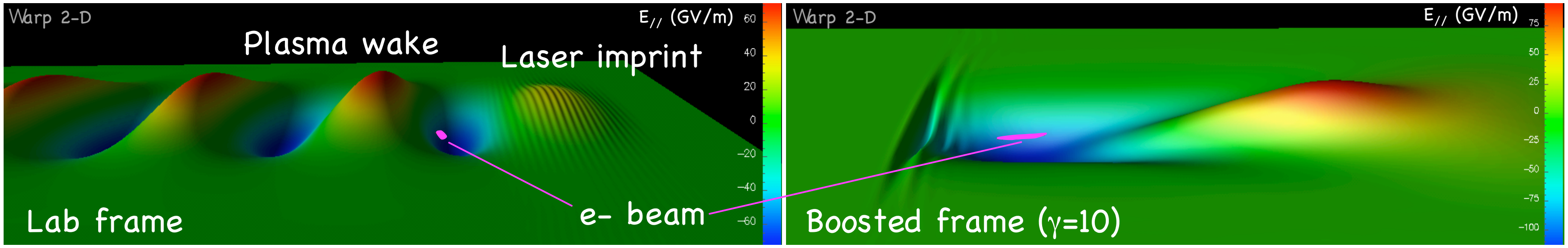
Can simulations of full scale 10 GeV stages be practical using a Lorentz boosted ref. frame?

- difficulty: backward emitted radiation frequency upshifted in boosted frame.

*Geddes et al, Proc. PAC'09

Scaled simulations of a 10 GeV LWFA stage
(λ=0.8μm, a_0=1, k_pL=2, L_p=1.5mm in lab)

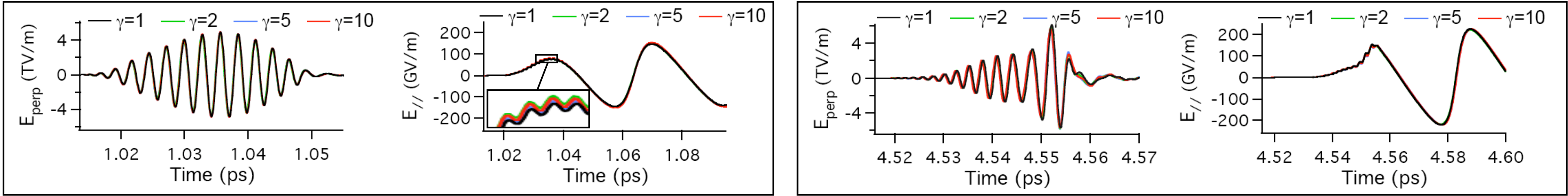
Snapshots of surface plot of // electric field in lab frame and boosted frame at γ=10



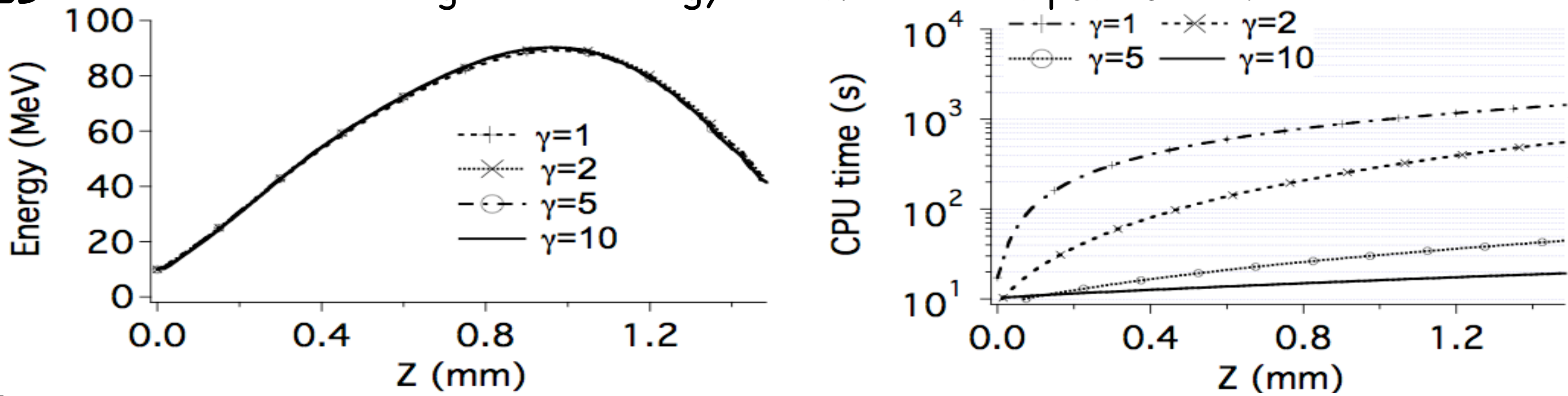
2D ⊥ and // electric field history in lab frame

Station z=0.154mm

Station z=1.354mm



2D Average beam energy and CPU time vs position in lab frame



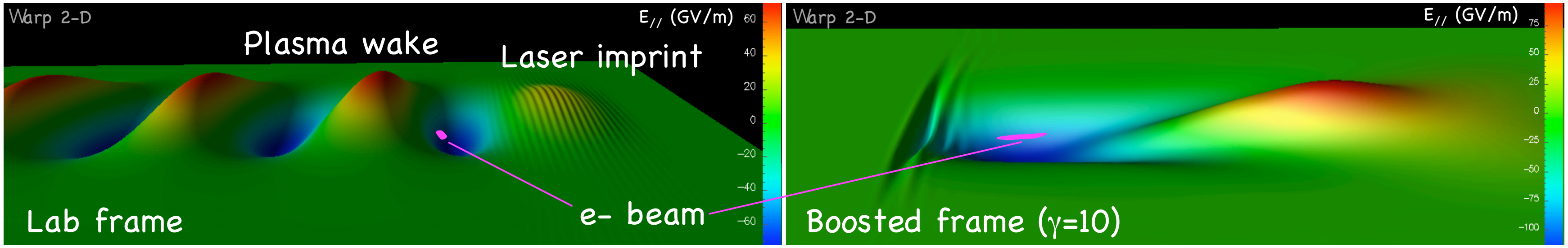
1,500s

speedup x75

20s

Scaled simulations of a 10 GeV LWFA stage
(λ=0.8μm, a_0=1, k_pL=2, L_p=1.5mm in lab)

Snapshots of surface plot of // electric field in lab frame and boosted frame at γ=10

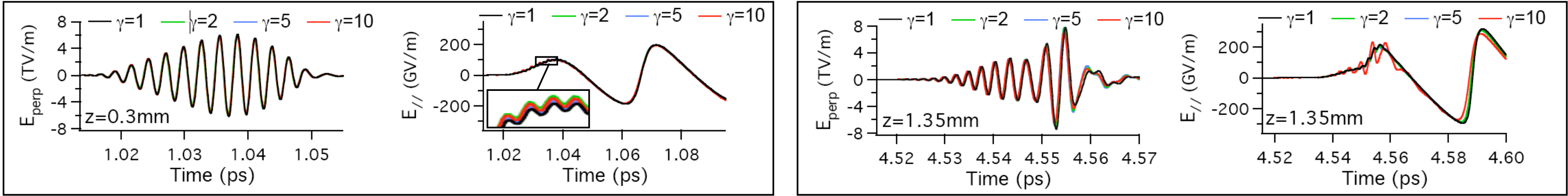


3D

⊥ and // electric field history in lab frame

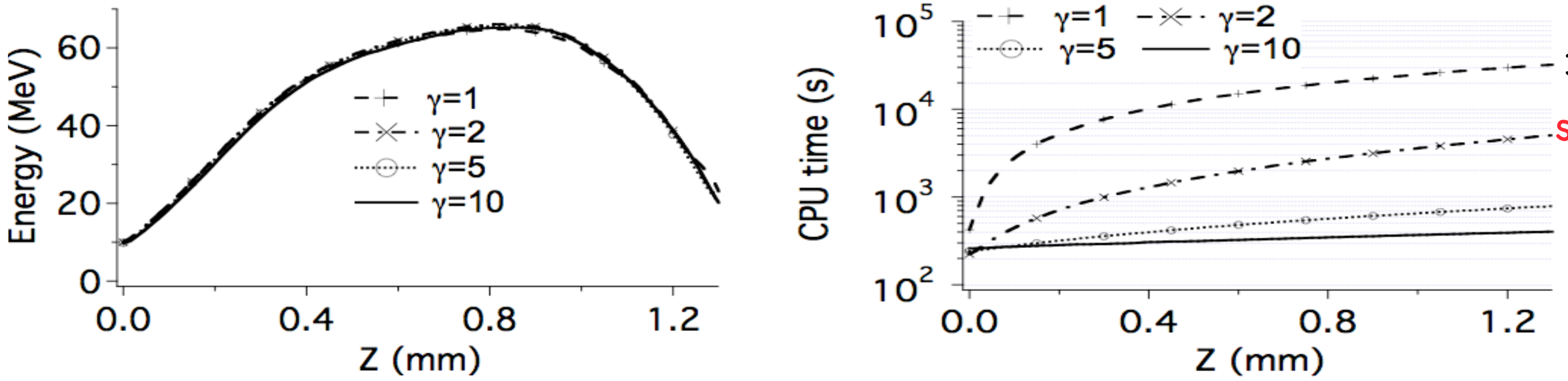
Station z=0.3mm

Station z=1.354mm



3D

Average beam energy and CPU time vs position in lab frame



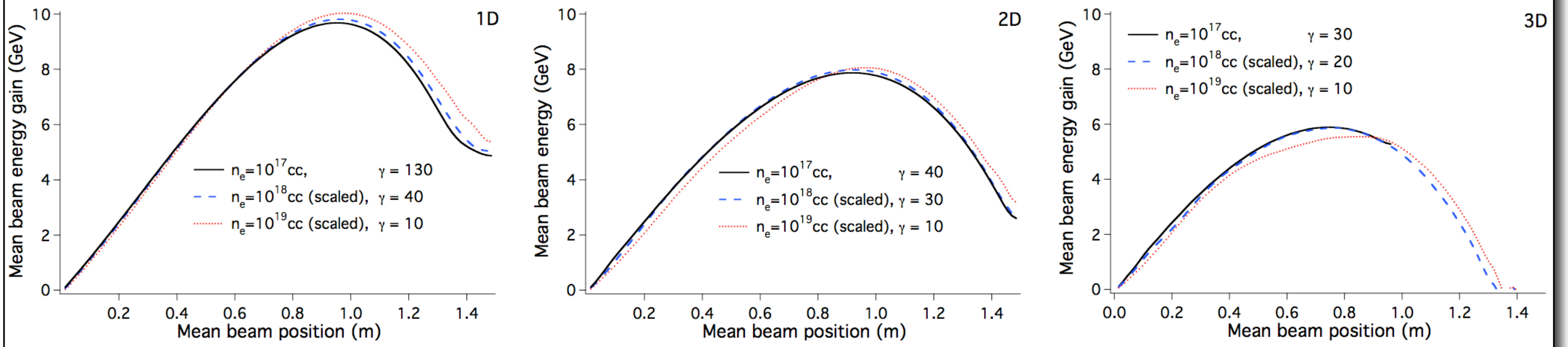
30,000s

speedup x75

400s

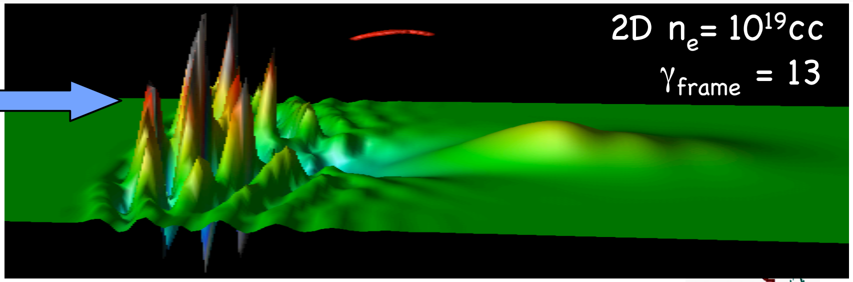
Full scale simulations of a 10 GeV LWFA stage

Simulations in 1D/2D/3D at plasma densities of 10^{19}cc, 10^{18}cc and 10^{17}cc show good agreement on (scaled) beam energy gain:



- 1D: max γ_{frame} = 130 ⇒ speedup > 10,000
- 2D: max γ_{frame} = 40 ⇒ speedup > 1,000
- 3D: max γ_{frame} = 30 ⇒ speedup > 500
  - 24h using 256 CPUs ⇒ more than one year x 256 CPUs in lab frame!

Max γ_{frame} achieved in 2D and 3D limited by instability developing at front of plasma



origin and cures are being studied…

*similar work by Bruhwiler et al (Tech X), Martins et al (UCLA/IST)

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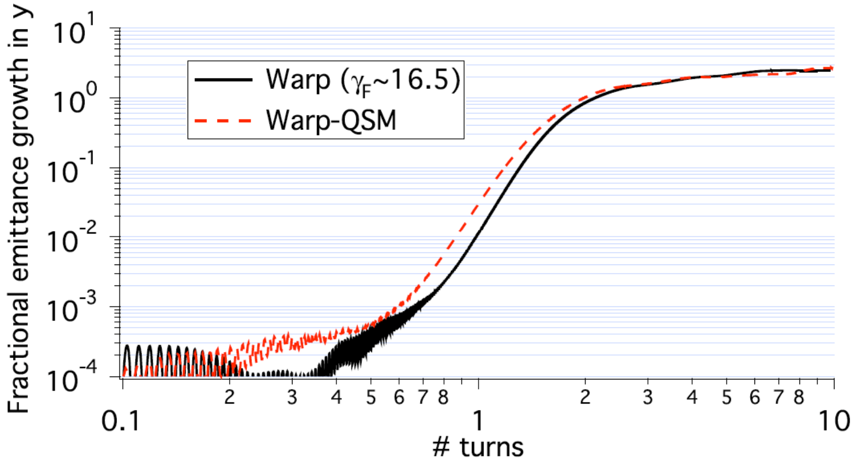
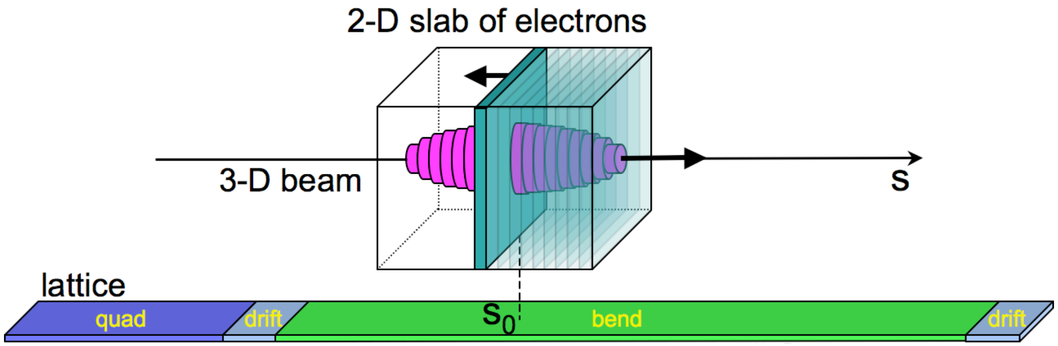
E-cloud: benchmarking against quasistatic model for LHC scenario

- Excellent agreement on emittance growth between boosted frame full PIC and “quasistatic” for e-cloud driven transverse instability in continuous focusing model of LHC

Electron cloud density	ρ_e	10^{14} m^{-3}
Bunch population	N_b	1.1×10^{11}
Beta functions	$\beta_{x,y}$	66.0, 71.54 m
rms bunch length	σ_z	0.13 m
rms beam size	$\sigma_{x,y}$	0.884 mm
rms momentum spread	δ_{rms}	0
Circumference	C	26.659 km
Nominal tunes	$Q_{x,y}$	64.28, 59.31
Relativistic factor	γ	479.6
Pipe radius	R_p	2.2 cm (with flat tops at ±1.8 cm)
Initial beam position offset	δy	0.1 σ_y
Dipole field (electrons only)	B_{y0}	8.39 T



- The “quasistatic” approximation uses the separation of time scales for pushing beam and e-cloud macro-particles with different “time steps”



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FEL in Boosted-Frame E&M Code

- Physics ignored by Eikonal codes but accessible to boosted frame approach:
  - Backward wave emission
  - Wide-angle emission (generally highly red-shifted)
  - CSE for all undulator, e-beam configurations
    - Emission from very short beams
    - Emission from beams with rapidly-varying envelope properties
    - Emission from beams bunched with “multiple colors”
  - Properties of *very* high gain systems ($L_G/\lambda_u < 5$)
  - FEL emission from beams in multiple harmonic undulators
    - Biharmonic (or triharmonic undulators)
    - Effects of adiabatic match sections
  - FEL emission in waveguides where v_{group} strongly varying with ω (normally relevant to microwave FEL’s operating near cutoff)
- Overall computational speed impressive compared to *full* E&M *but much slower than standard eikonal method*: Not likely to become dominant paradigm for short wavelength FEL’s but *might* be useful for very high gain microwave/far-IR devices or situations with wideband spectral output

Conclusion and outlook

- The range of scales of a system is not a Lorentz invariant $(\propto\gamma^2)$, and there exists an optimum frame minimizing it => orders of magnitude speedup predicted for some simulations.
- Calculating in a boosted frame more demanding, eventually:
  - developed new particle pusher for e-cloud problems,
  - added capabilities for injection/diagnostics in boosted frame.
- Orders of magnitude speedup demonstrated for a class of first-principle simulations of multiscale problems: laser-plasma acceleration, e-cloud in HEP accelerators, free electron lasers.
- Explore other applications: CSR, astrophysics,...
- Can we develop methods which costs do not depend on frame?