Advanced modeling tools for laser-plasma accelerators (LPAs) 3/3

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Overview of lecture 3

- Modeling of LPAs using tools beyond standard PIC (computational gains and limitations):
  - Lorentz boosted frame;
  - Laser-envelope description (i.e., ponderomotive guiding center);
  - Quasi-static approximation;
  - Quasi-cylindrical modality;

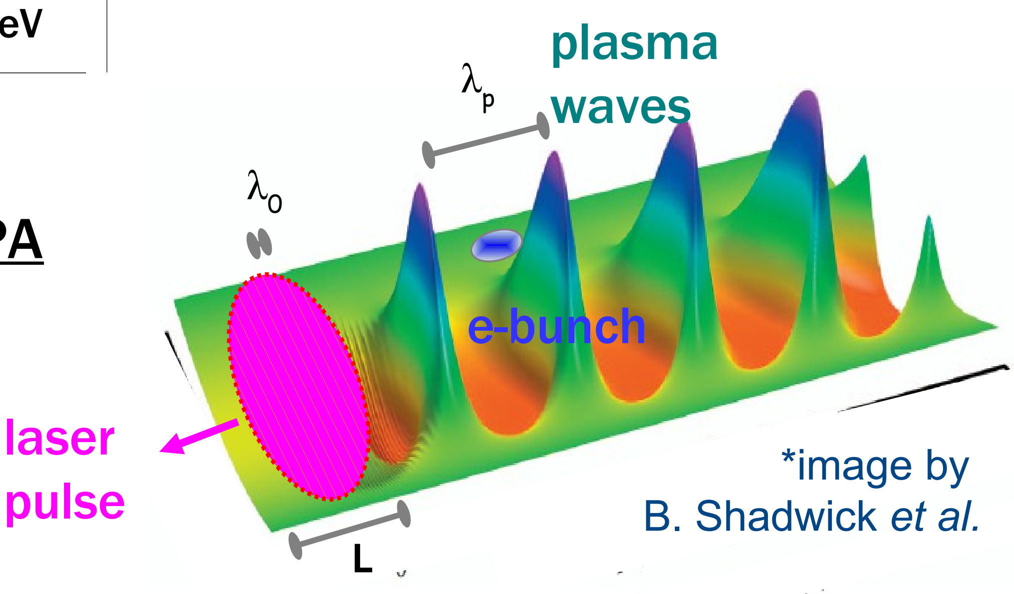
3D full-scale modeling of an LPAs over cm to m scales is challenging task

laser wavelength (λ_0)	~ µm
laser length (L)	~ few tens of µm
plasma wavelength (λ_p)	~10 µm @ 10^{19} cm^{-3} ~30 µm @ 10^{18} cm^{-3} ~100 µm @ 10^{17} cm^{-3}
interaction length (D)	~ mm @ 10^{19} cm^{-3} → 100 MeV ~ cm @ 10^{18} cm^{-3} → 1 GeV ~ m @ 10^{17} cm^{-3} → 10 GeV

- Simulation complexity ~$(D/\lambda_0)^{4/3}$
- Cost of 3D explicit PIC simulations:

- 10^4-10^5 CPUh for 100 MeV stage
- ~10^6 CPUh for 1 GeV stage
- ~10^7 -10^8 CPUh for 10 GeV stage

Ex: <u>Full 3D PIC modeling of 10 GeV LPA</u>
grid: 5000x500^2 ~10^9 points
particles: ~4x10^9 particles (4 ppc)
time steps: ~10^7 iterations



Understanding the physics of LPAs requires <u>detailed</u> numerical modeling

What we need (from the computational point of view):

- run 3D simulations (dimensionality matters!) of cm/m-scale laser-plasma interaction in a reasonable time (a few hours/days)

- perform, for a given problem, **several simulations** (exploration of the parameter space, optimization, convergence check, comparison with experiments, feedback with experiments for optimization, etc.)

<u>Reduced Models</u>
→ Neglecting some aspects of the physics depending on the particular problem that needs to be addressed, (reducing computational complexity)

<u>Lorentz Boosted Frame</u>
→ Different spatial/temporal scales in an LPA simulation do not scale the same way changing the reference frame. Simulation length can be greatly reduced going to an optimal (wake) reference frame.

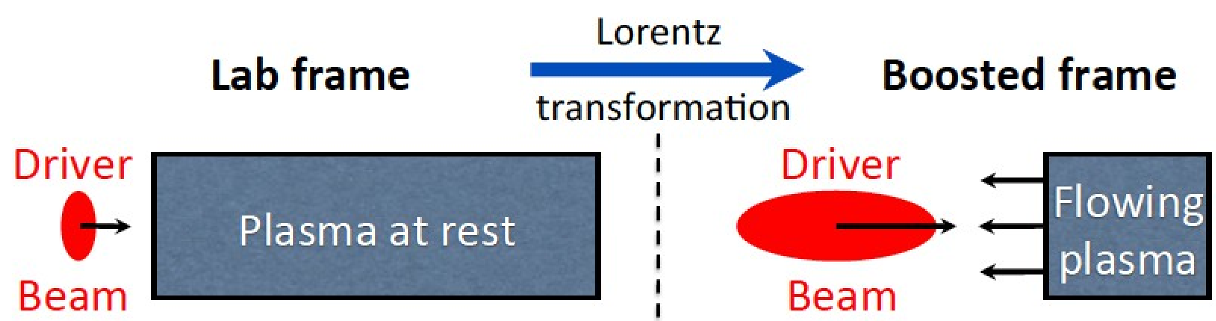
Modeling in a Lorentz boosted frame

Modeling an LPA in a Lorentz boosted frame

The space/time scales spanned by a system are not invariant under Lorentz transform
$\rightarrow$ the computational complexity of the problem can be reduced changing the reference frame

Laboratory Frame	Boosted Lorentz Frame (β_*)
$\lambda_0 \rightarrow$ laser wavelength $\ell \rightarrow$ laser length $L_p \rightarrow$ plasma length $c\Delta t < \Delta z \ll \lambda_0,\ \lambda_0 < \ell \ll L_p$	$\lambda_0' = \gamma_*(1+\beta_*)\,\lambda_0 > \lambda_0$ $\ell' = \gamma_*(1+\beta_*)\,\ell > \ell$ $L_p' = L_p/\gamma_* < L_p$
$\Rightarrow t_{simul} \sim (L_p + \ell)/c$ $\#\,\text{steps} = \frac{t_{simul}}{\Delta t} \propto \frac{L_p}{\lambda_0} \gg 1$ **large # of steps**	$\Rightarrow t'_{simul} \sim (L_p' + \ell')/(c(1+\beta_*))$ $\#\text{steps}' = \frac{t'_{simul}}{\Delta t'} \propto \frac{L_p}{\lambda_0 \gamma_*^2 (1+\beta_*)^2}$ **# of steps reduced** $(1/\gamma_*^2)$

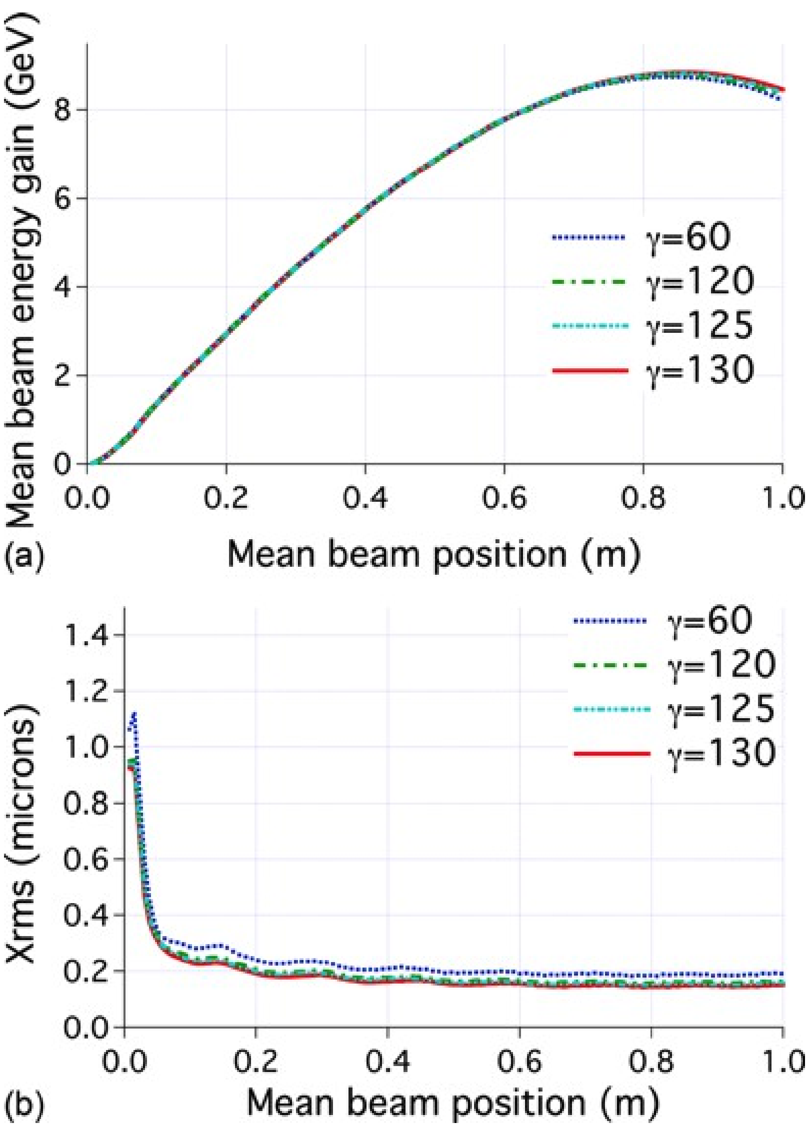
- Neglects backward propagating waves (blueshifted and so under-resolved in the BF);
- Diagnostic and initialization are more complicated;
- For any LPA there is an "optimal" frame, the frame of the wake: $\gamma_{opt} \sim k_0/k_p$
  $\rightarrow S \sim (\lambda_p/\lambda_0)^2$

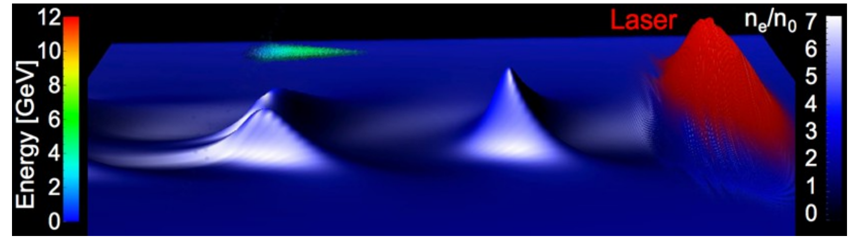


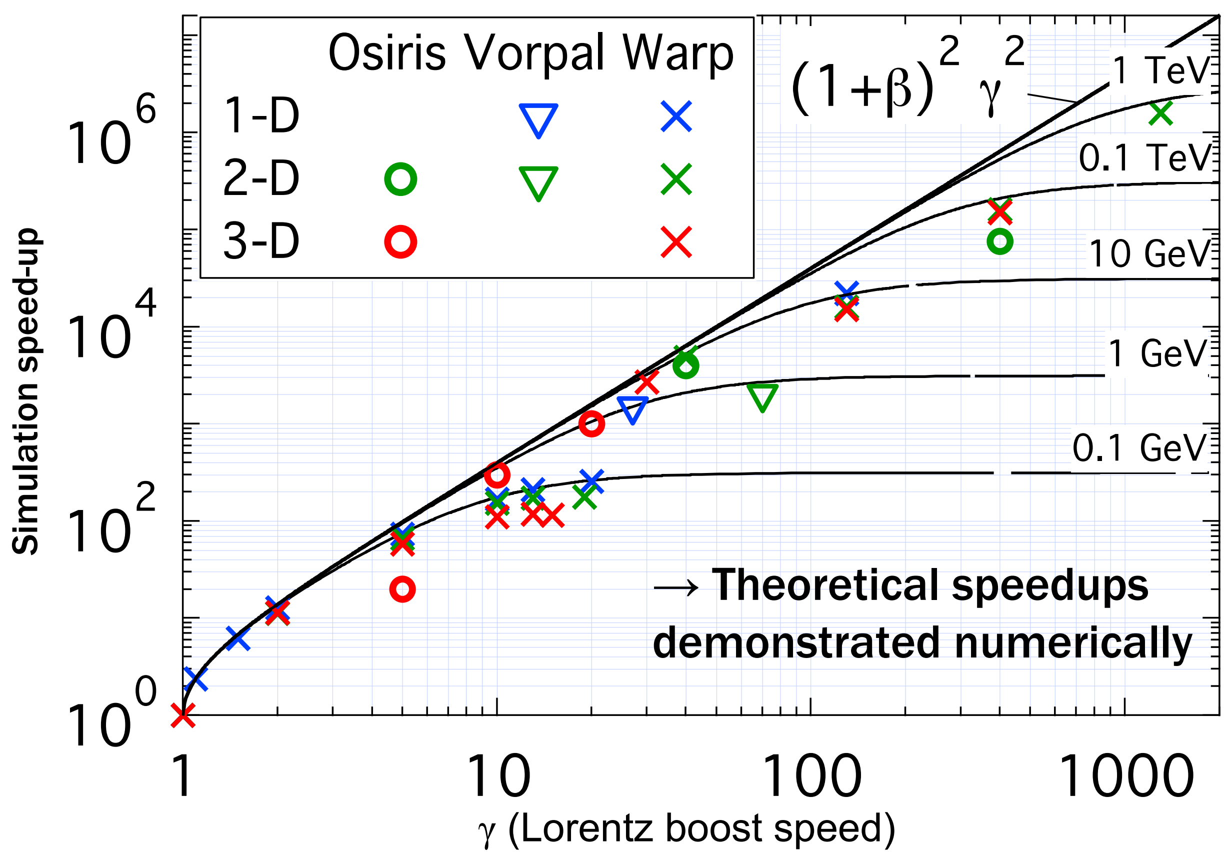
Vay, PRL 98, 130405 (2007)

Modeling an LPA in the BF provides large computational gains

Modeling of a ~10 GeV LPA stage

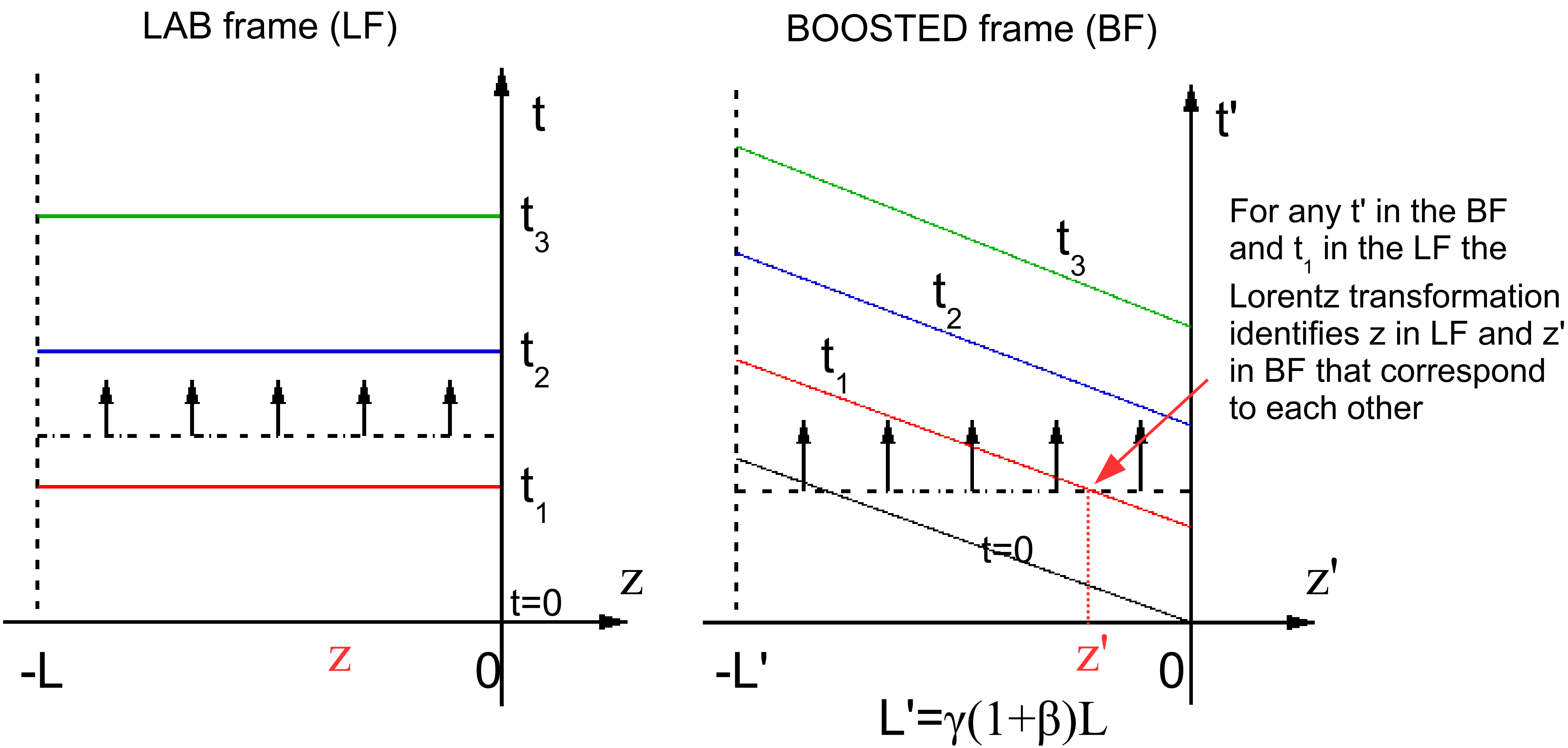






Simulation cost for 10 GeV LPA (3D) w/ WARP: 5,000 CPUh using LBF (reduction ~20,000)

Simulation initialization and diagnostics in the Lorentz boosted Frame

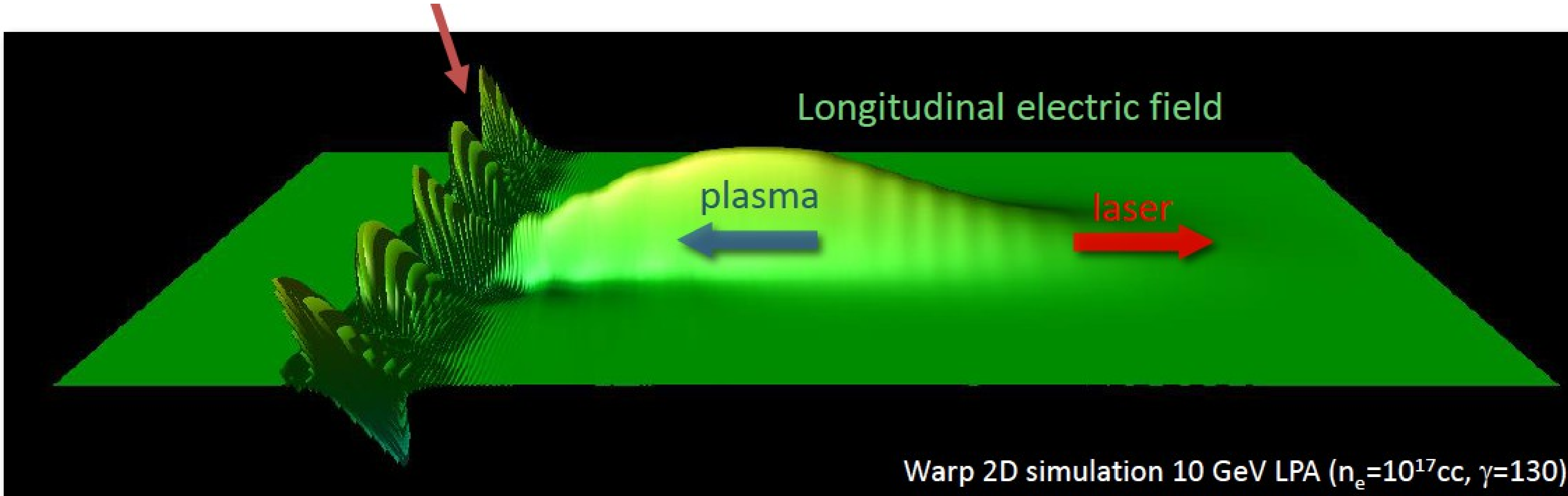


Initializing the simulation in the BF and obtaining output (diagnostics) in the LF while performing the simulation in the BF is challenging due to the mixing between space and time among BF and LF → use a moving planar antenna

Vay et al., Phys. Plasmas **18**, 123103 (2011)

Numerical Cherenkov Instability (NCI) prevents realization of the full potential of BF simulations

Snapshot of the electron density in a BF simulation



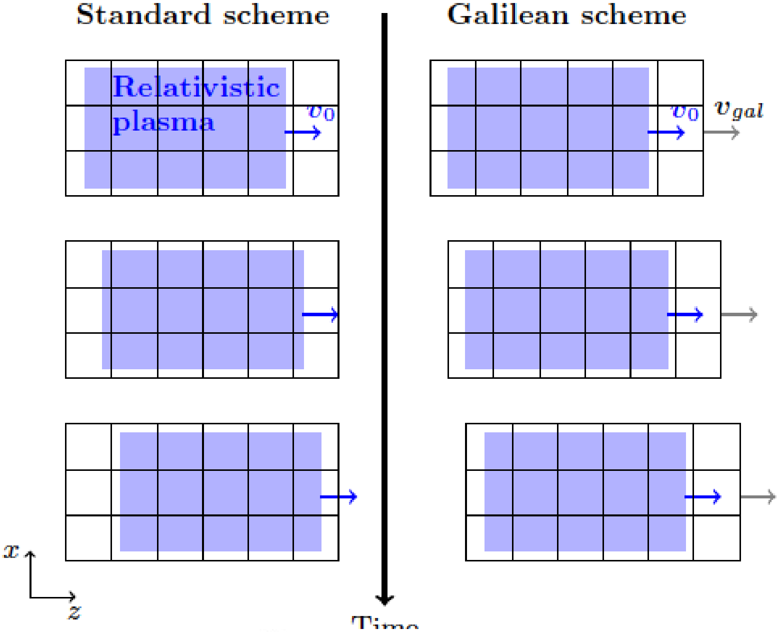
- NCI in PIC codes arises from coupling between distorted EM modes (e.g., EM with slow phase velocity) and spurious beam modes (drifting plasma);

- NCI prevents use of high boost velocities;

- Several solutions proposed over the years to mitigate the instability (see References) involving strong digital smoothing (filtering EM fields/currents) or arbitrary numerical corrections which are tuned specifically against the NCI and go beyond the natural discretization of the equations;

- Elegant solution found by M. Kirchen (DESY) and R. Lehe (LBNL) that completely eliminates NCI without an *ad hoc* assumption or treatment of the physics →

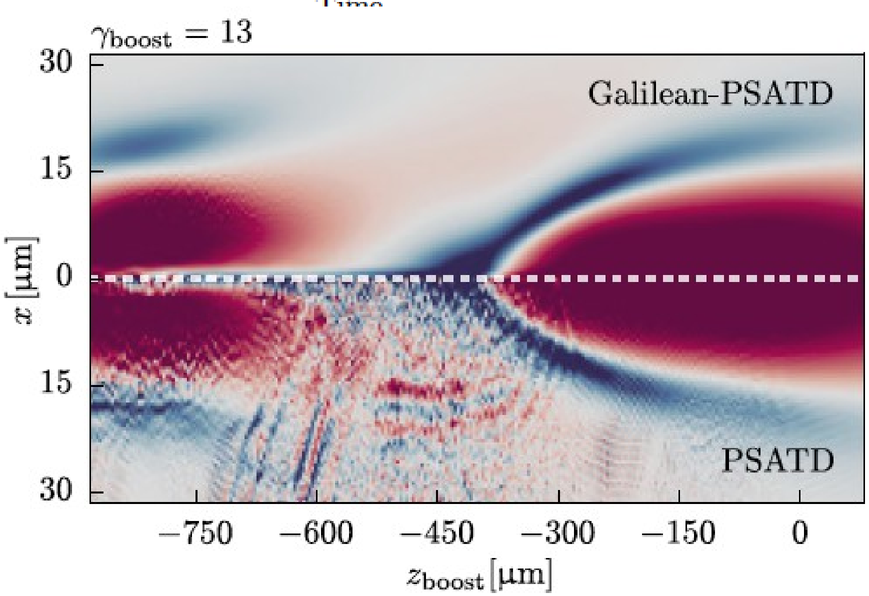
NCI can be eliminated by rewriting PIC equations using a coordinates system (Galilean transform) co-moving with the drifting plasma

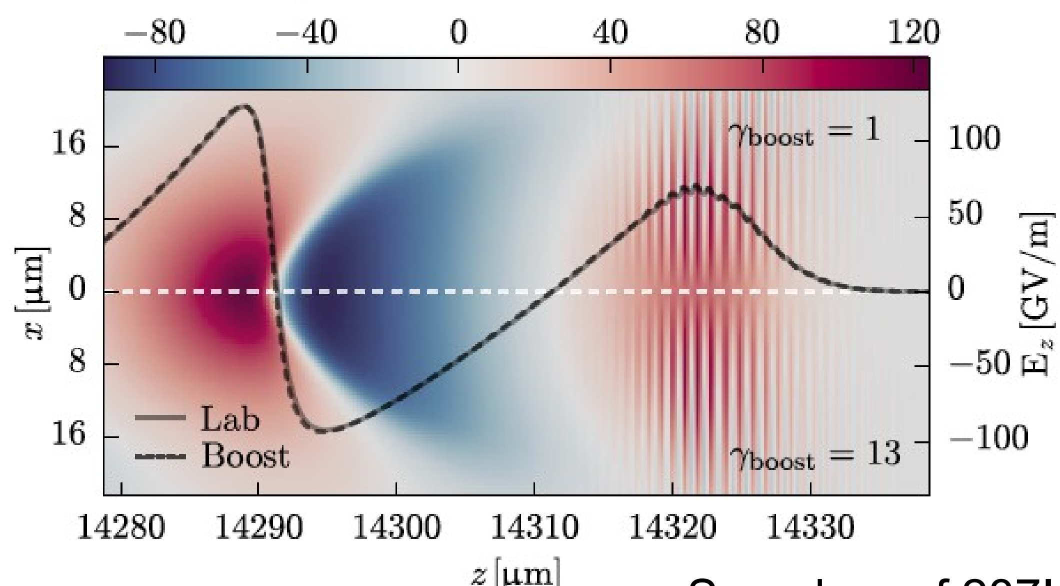


- PIC equations rewritten using a coordinates system co-moving with the plasma (Galilean transform): $z'=z-v_0t$ (v_0 velocity of drifting plasma in BF)

- Use PSATD scheme (i.e., solve Maxwell's equation in Fourier space + analytical integration over Δt)

→ Intrinsically free of NCI for drifting plasma





Speed-up of 287!

M. Kirchen et al., Phys. Plasmas 23, 100704 (2016) R. Lehe et al., Phys Rev. E 2016, 053305 (2016)

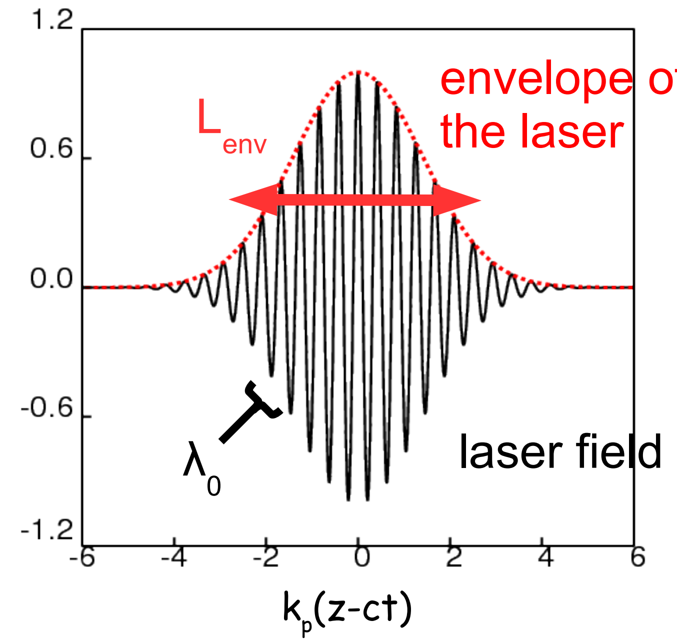
Laser-envelope description

Laser-envelope description (pond. guiding center)

- In an LPA, the laser envelope usually satisfies L_{env} (~10s of um) >> λ_0 (~ 1 um)
- Plasma electrons quiver in the fast laser field
- There is a time scale separation between the fast laser fields (ω_0) and the slow wakefield (ω_p), typically $\omega_p \ll \omega_0$

→ **ponderomotive approximation**: electron motion averaged (analytically) over fast laser oscillations

→ laser **decomposed** into fast phase and slow envelope, only the latter is evolved



Laser vector potential → $$a_\perp(\zeta,\tau) = \overbrace{\frac{\hat{a}(\zeta,\tau)}{2}}^{\text{slow}}\overbrace{e^{ik_0\zeta}}^{\text{fast}} + \text{c.c.}$$

Electron equation of motion → $$\frac{d\mathbf{p}}{dt} = \underbrace{-\frac{mc^2}{4\bar{\gamma}}\nabla|\hat{a}|^2}_{\text{averaged ponderomotive force}} \underbrace{- e\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right)}_{\text{wake contribution}} \qquad \bar{\gamma} = \left(1 + \frac{|\mathbf{p}|^2}{m^2c^2} + \frac{|\hat{a}|^2}{2}\right)^{1/2}$$

=> Envelope description removes scale @ λ_0 from the simulation [$\sim(\lambda_p/\lambda_0)^2$ speed-up]

=> Envelope generally axisymmetric → modeling in 2D cylindrical geometry possible

Complete set of equations to be solved in an envelope code

Laser envelope equation

$$\left(\nabla_\perp^2 + 2i\frac{k_0}{c}\frac{\partial}{\partial\tau} + \frac{2}{c}\frac{\partial^2}{\partial\zeta\partial\tau} - \frac{1}{c^2}\frac{\partial^2}{\partial\tau^2}\right)\hat{a} = k_{p0}^2\frac{\overline{n}}{n_0\overline{\gamma}}\hat{a}$$

Laser driver and wake are decoupled (good for diagnostics)

Wakefield description (Maxwell equations) [slow fields ~ ω_p]

$$\frac{\partial \mathbf{E}}{\partial t} = c\nabla\times\mathbf{B} - 4\pi\mathbf{J} \qquad \frac{\partial \mathbf{B}}{\partial t} = -c\nabla\times\mathbf{E}$$

Plasma description (equations of motion for numerical particles sampling the plasma)

$$\frac{d\mathbf{p}}{dt} = -\frac{mc^2}{4\overline{\gamma}}\nabla|\hat{a}|^2 - e\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right)$$

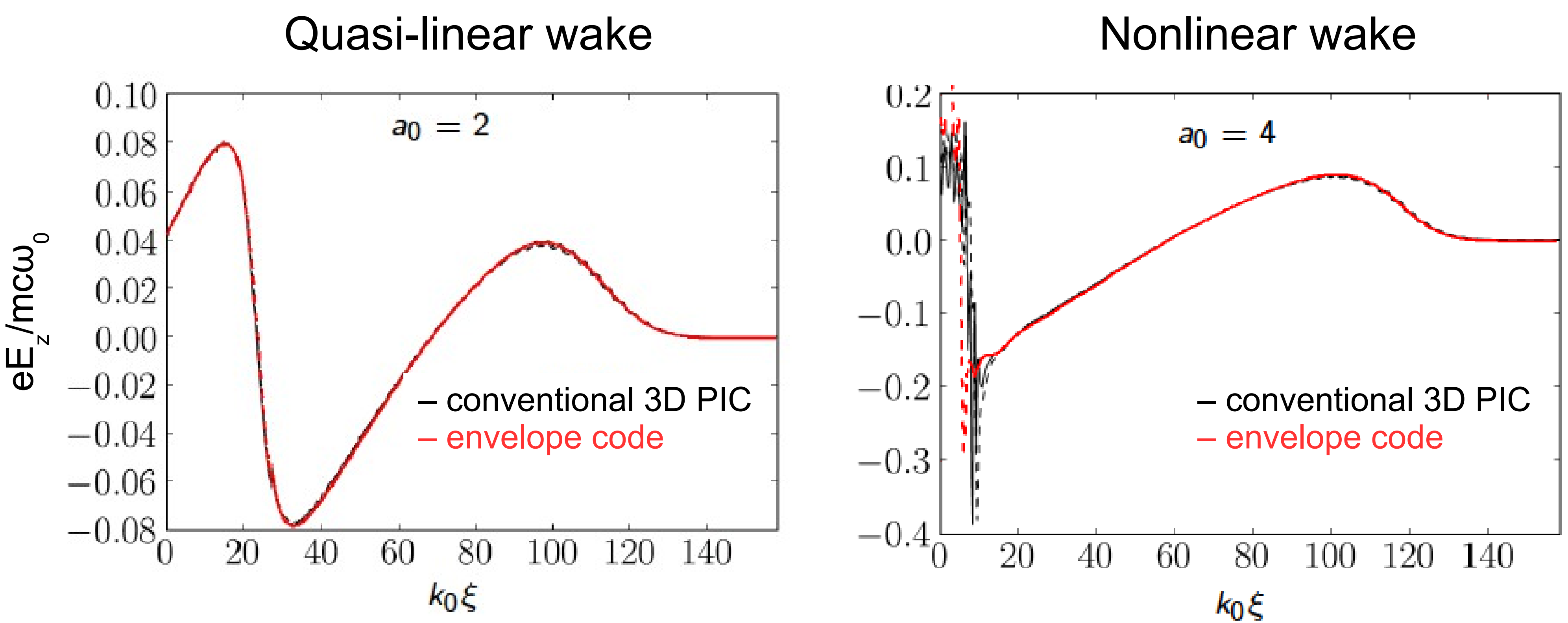
$$\frac{d\mathbf{r}}{dt} = \mathbf{v} = \frac{\mathbf{p}}{\overline{\gamma}}$$

$$\overline{\gamma} = \left(1 + \frac{|\mathbf{p}|^2}{m^2c^2} + \frac{|\hat{a}|^2}{2}\right)^{1/2}$$

→ coupling between the equations provided by **J** and $\overline{n}$

Wakefield structure and amplitude in excellent agreement with results obtained with conventional 3D PIC

→ Lineout of the longitudinal wakefield, E_z



==> averaged ponderomotive approximation works **very well** for laser and plasma parameters of interest for current and future LPA experiments

Envelope codes reproduce correct laser group velocity in vacuum and plasmas

Plasma profile:

$$n(r) = n_0 + (\pi r_e r_m)^{-1}\left(\frac{r}{r_m}\right)^2$$

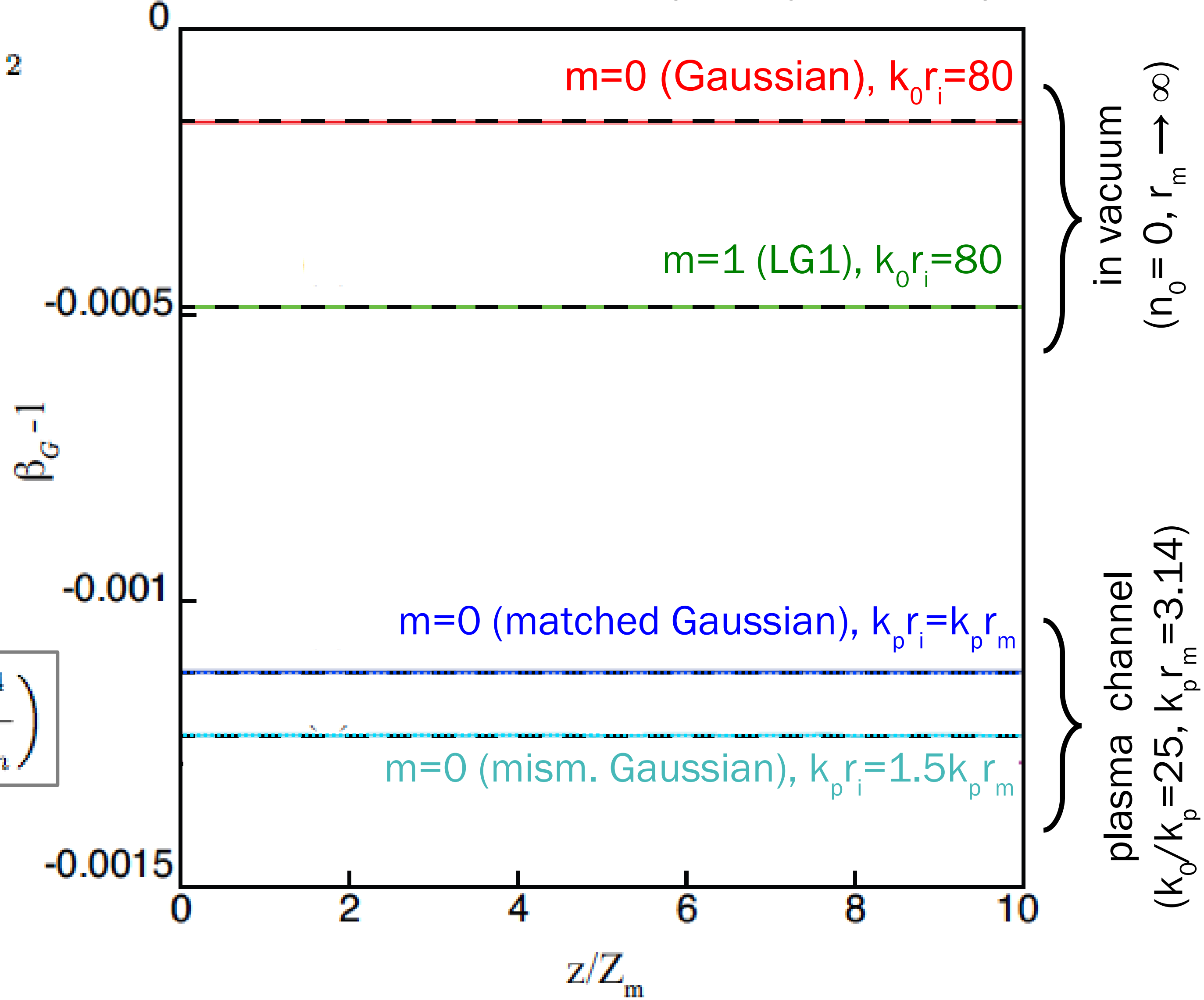
Laser profile:

$$\hat{a}_\perp \sim L_m^0\left(\frac{2r^2}{w_0^2}\right)e^{-r^2/w_0^2}$$

Laser velocity:

$$\boxed{\beta_g = 1 - \frac{k_p^2}{2k_0^2} - \frac{1+2m}{k_0^2 r_i^2}\left(1+\frac{r_i^4}{r_m^4}\right)}$$

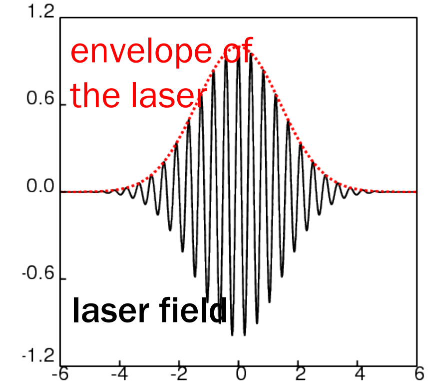
(theory in black)



*Schroeder, *et al.*, POP (2011); Benedetti, *et al.*, PRE (2015)

Correct numerical modeling of a strongly depleted laser pulse is challenging

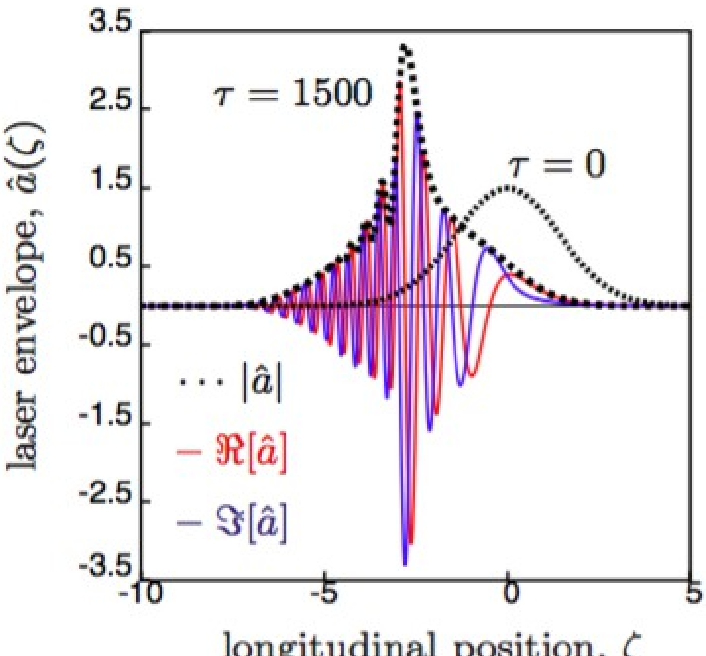
Envelope description: $a_{laser} = \hat{a} \exp[ik_0(z-ct)]/2 + c.c.$



$$\left(\nabla_\perp^2 + 2i\frac{k_0}{c}\frac{\partial}{\partial\tau} + \frac{2}{c}\frac{\partial^2}{\partial\zeta\partial\tau} - \frac{1}{c^2}\frac{\partial^2}{\partial\tau^2}\right)\hat{a} = k_{p0}^2\frac{\overline{n}}{n_0\overline{\gamma}}\hat{a}$$

- early times: NO need to resolve λ_0 (~1 μm), only $L_{env} \sim \lambda_p$(~ 10-100 μm)
- later times: spectral modification (i.e., laser-pulse redshifting) → structures **smaller** than L_{env} **arise** in â (mainly in Re[â] and Im[â]) and **need to be captured***

a_0=1.5
k_0/k_p=20
L_{env} = 1



Is it possible to have a good description of a depleted laser at a "reasonably low" resolution (in space and time)?

*Benedetti *at al.*, AAC2010
Cowan *et al.*, JCP (2011)
Zhu *et al.*, POP (2012)

Ingredients for an efficient laser envelope solver

- Envelope evolution equation discretized in time using a 2nd order Crank-Nicholson implicit scheme → **enable large time steps**

$$-\frac{\hat{a}^{n+1}-2\hat{a}^{n}+\hat{a}^{n-1}}{\Delta_\tau^2}+2\left(i\frac{k_0}{k_p}+\boxed{\frac{\partial}{\partial\xi}}\right)\frac{\hat{a}^{n+1}-\hat{a}^{n-1}}{2\Delta_\tau}=-\nabla_\perp^2\frac{\hat{a}^{n+1}+\hat{a}^{n-1}}{2}+\frac{\delta^n}{\gamma^n_{\text{fluid}}(\hat{a}^n)}\frac{\hat{a}^{n+1}+\hat{a}^{n-1}}{2}$$

- Use a **polar** representation for â when computing $\partial/\partial\xi$

(cartesian) (polar)

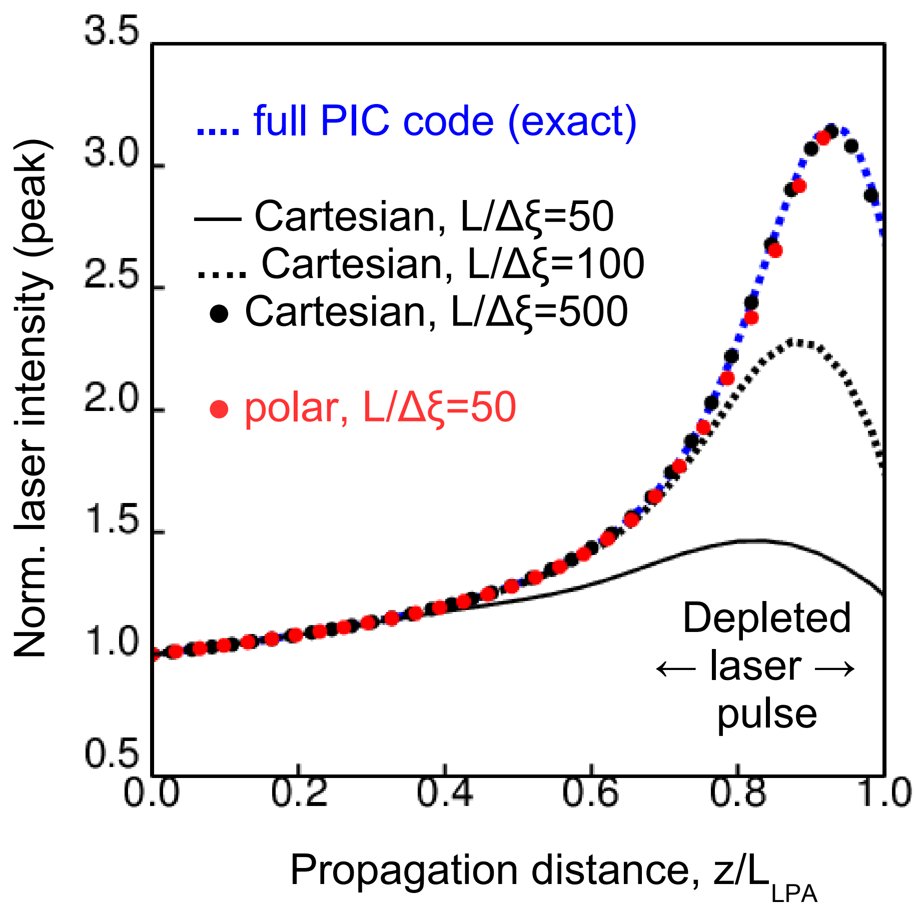
$$\hat{a}=\Re[\hat{a}]+i\Im[\hat{a}]=|\hat{a}|e^{i\theta}$$

(cartesian)

$$\partial_\xi\hat{a}=\begin{cases}\partial_\xi\left(\Re[\hat{a}]\right)+i\partial_\xi\left(\Im[\hat{a}]\right)\\ \\ \underbrace{\partial_\xi\left(|\hat{a}|\right)}e^{i\theta}+i\underbrace{(\partial_\xi\theta)}\hat{a}\end{cases}$$

(polar)

"smoother" behavior compared to **Re[â]** and **Im[â]**→ **easier to differentiate numerically!**

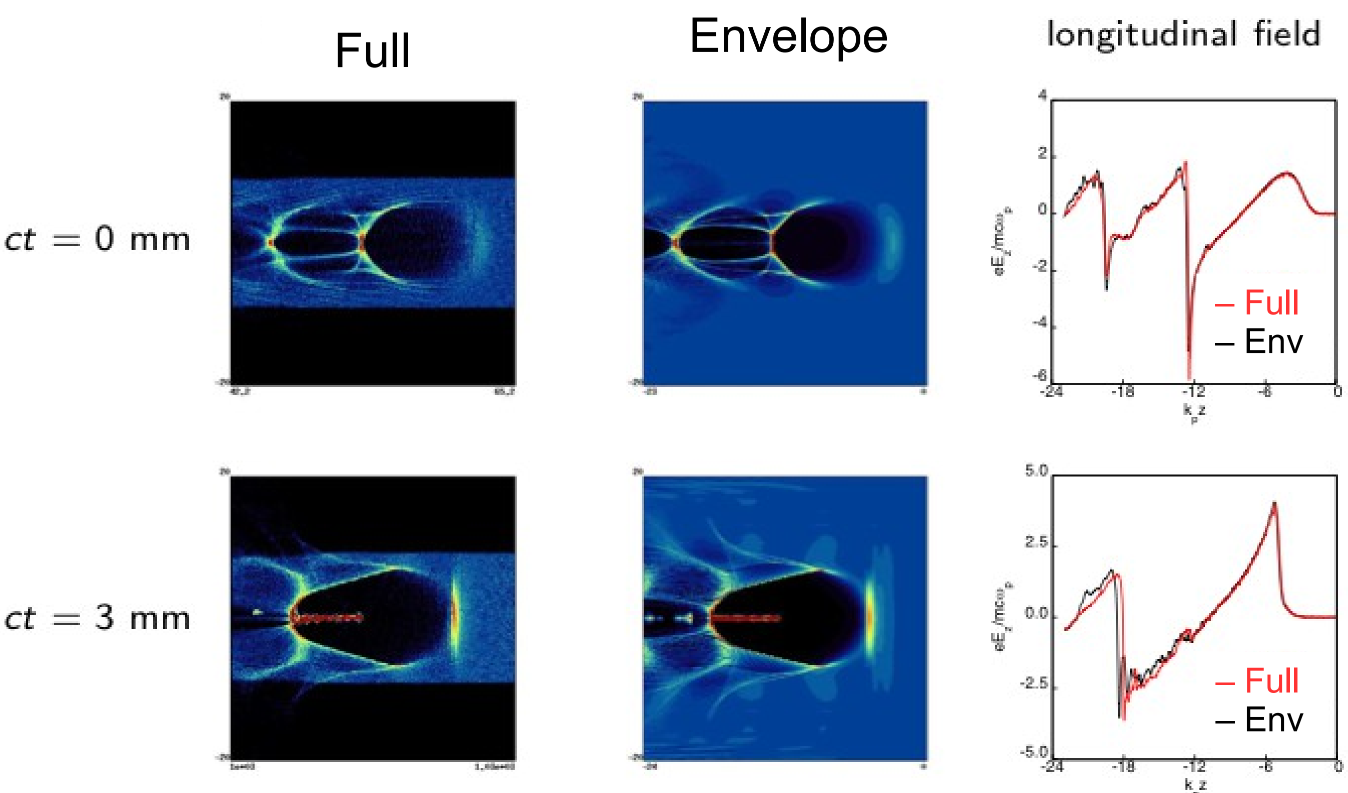


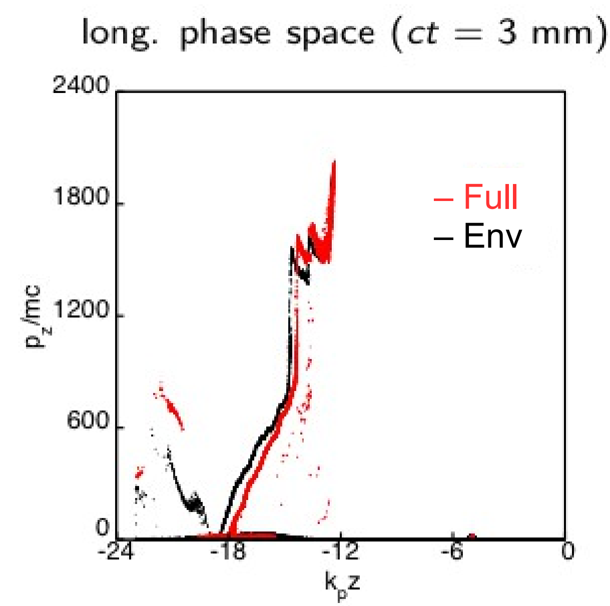
Modeling performed with 2D-cylindrical envelope scheme provides significant speedup compared to full 3D PIC still retaining physical fidelity

n_0 [e/cm^3]	k_0/k_p	a_0	τ [fs]	w_0 [μm]	L_{sym} [mm]
$3 \cdot 10^{18}$	24	5	30	16	3.2

box: 23×20 - res: $1/30 \times 1/20$ - $\Delta t = 0.25 \Delta z$ -

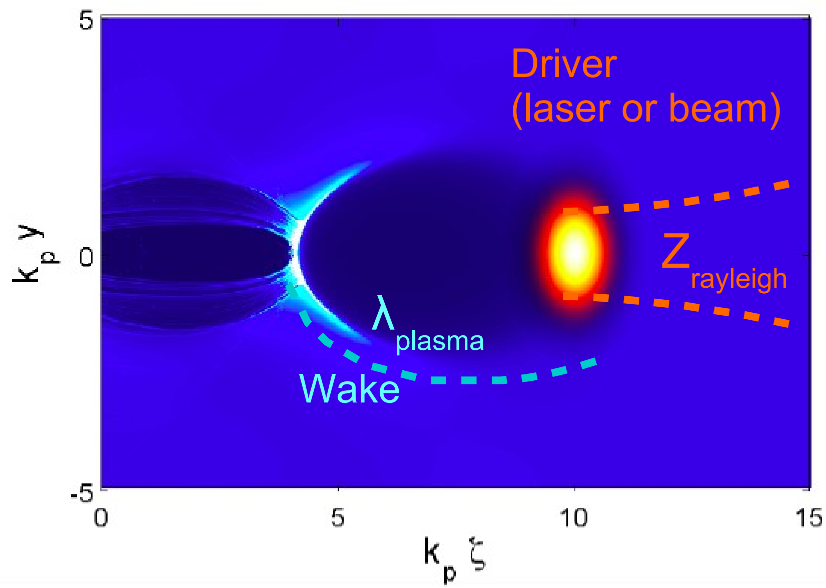
Envelope code > 300 times faster than 3D explicit PIC code





Quasi-static approximation

Quasi-static approximation takes advantage of the time scale separation between driver and plasma evolution



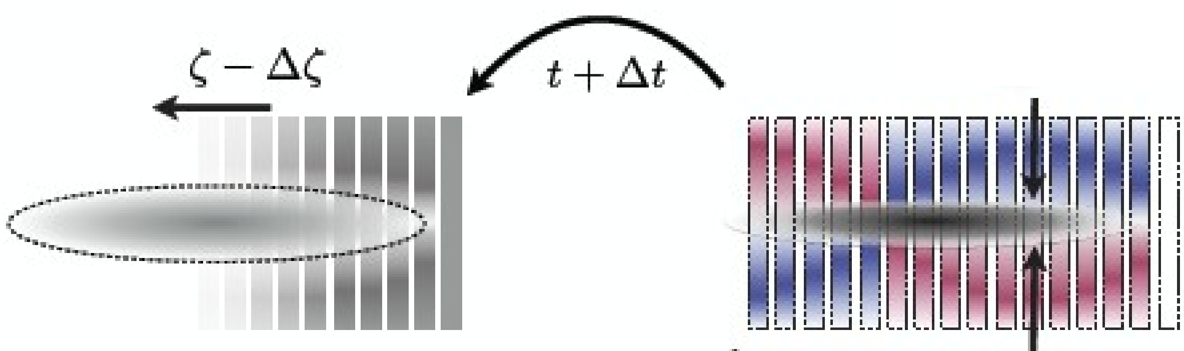
The laser (or beam) driver is evolving on a time scale much longer compare to the plasma response

$$T_{laser} \sim Z_{rayleigh}/c$$

$$T_{plasma} \sim \omega_p^{-1}$$

$$T_{laser}/T_{plasma} \sim (k_0/k_p)(k_p w_0)^2 \gg 1$$

→ **neglect** time-dependence in all the quantities related to the wake
→ **retain** time-dependence only in the evolution of the driver



Driver is frozen while a plasma slice is passed through the driver and the wakefield is computed

wakefield is frozen while driver is advanced in time

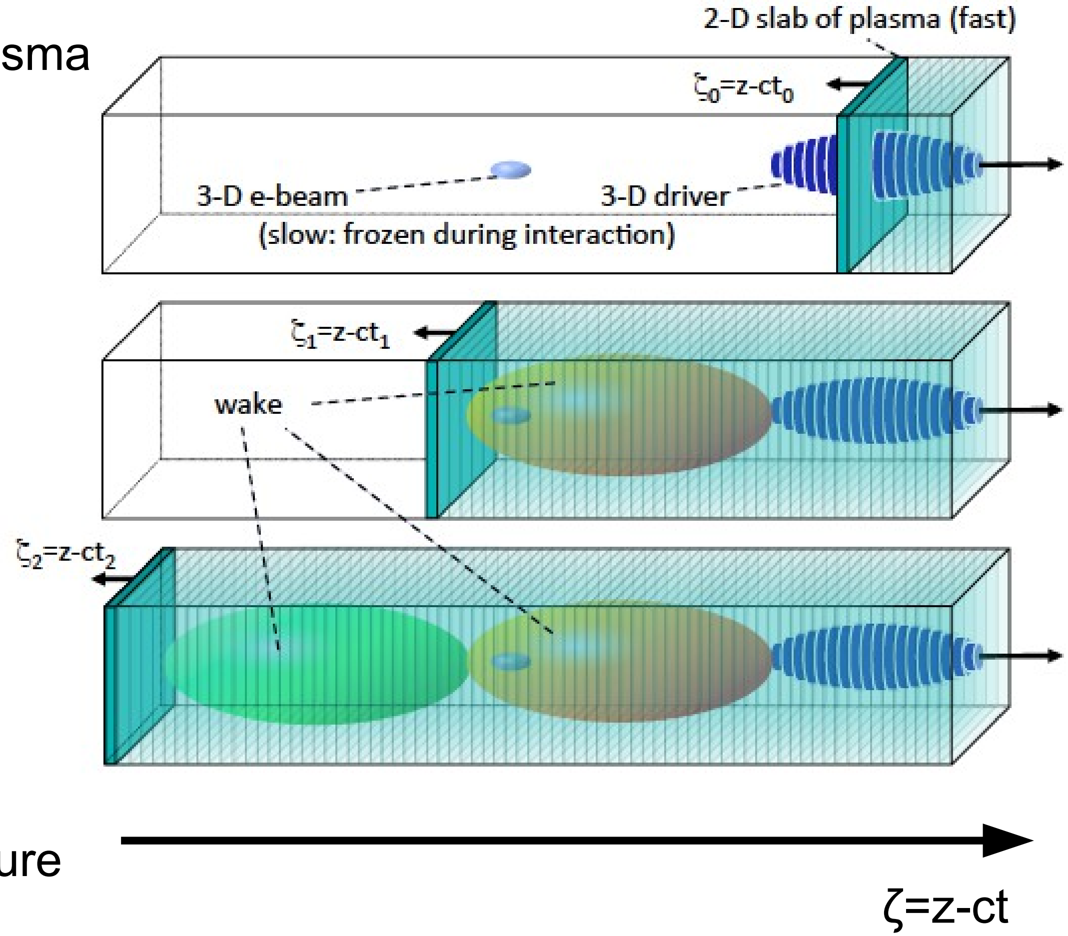
Δt set according to driver evolution (much bigger than in conv. PIC): # of time steps reduced by ~$(\lambda_p/\lambda_0)^2$

*Sprangle , *et al.*, PRL (1990)
Mora, Antonsen, Phys. Plas. (1997)

Outline of the wake calculation in the quasi-static approximation (different in different codes)

1. Determine position and momentum of plasma particles on slice ζ (computed from ζ+dζ)

$$\begin{cases} \frac{dr}{d\xi} = -\frac{u_r}{1+\psi} \\ \frac{du_r}{d\xi} = \frac{F_{laser} + \gamma(E_r - B_\phi)}{1+\psi} + B_\phi \\ \frac{d\psi}{d\xi} = \frac{u_r}{1+\psi}(E_r - B_\phi) - E_z \\ \gamma - u_z - \psi = 1 \end{cases}$$



2. Deposit charge/current in the slice ζ

3. Solve PDEs for the fields in the slice ζ (requires implementation of iterative procedure to obtain a solution)

$$\nabla_\perp^2 E_z = \frac{1}{r}\frac{d}{dr}(rJ_r) \qquad \frac{\partial(E_r - B_\phi)}{d\xi} = J_r \qquad \frac{1}{r}\frac{d}{dr}(rB_\phi) = J_z - \frac{\partial E_z}{\partial \xi}$$

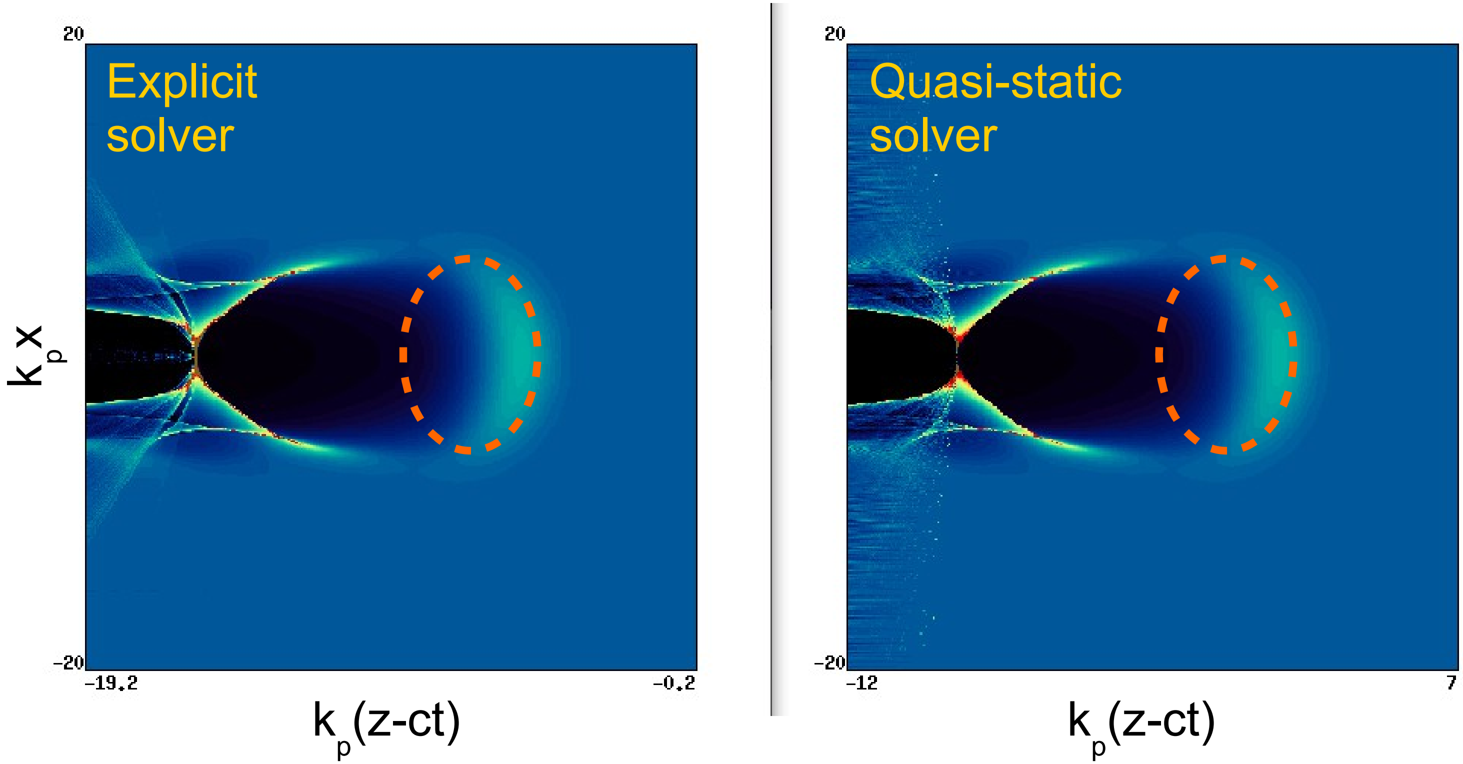
(Poisson-like equations)

4. shift plasma slice (go to 1) and repeat until the end of the computational box is reached.

C. Huang al., JCP 217, 658 (2006); T. Mehrling et al., PPCF 56, 084012 (2014)

Quasi-static approximation provides accurate description of the wakefield structure

Ex: bubble wake generated by an intense laser driver, a_0=5



→ QSA particularly useful in describing dark-current-free LPA stages (bunch has to be provided): fast laser evolution and correct wake description

N.B. QSA solver **cannot** model some aspects of kinetic physics like particle self-injection (for trapped particles, plasma → bunch, the time scale separation does not hold)

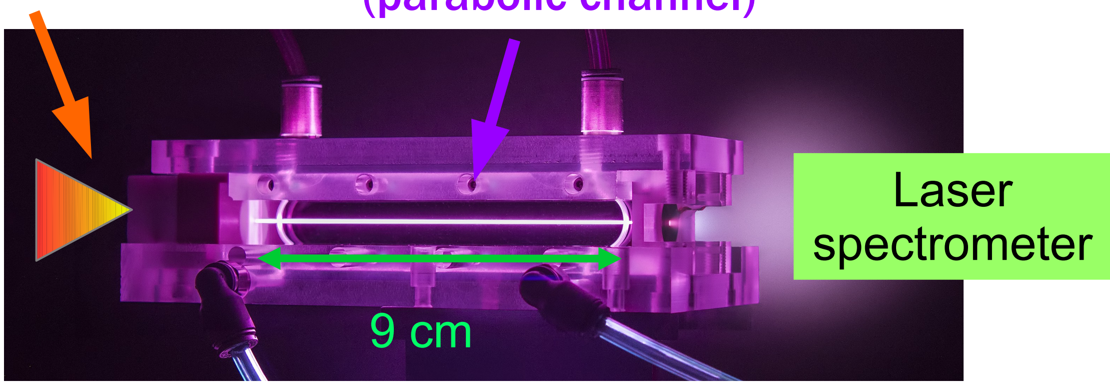
Laser envelope description (LED) + Quasi-static approximation (QSA): examples of the computational gains

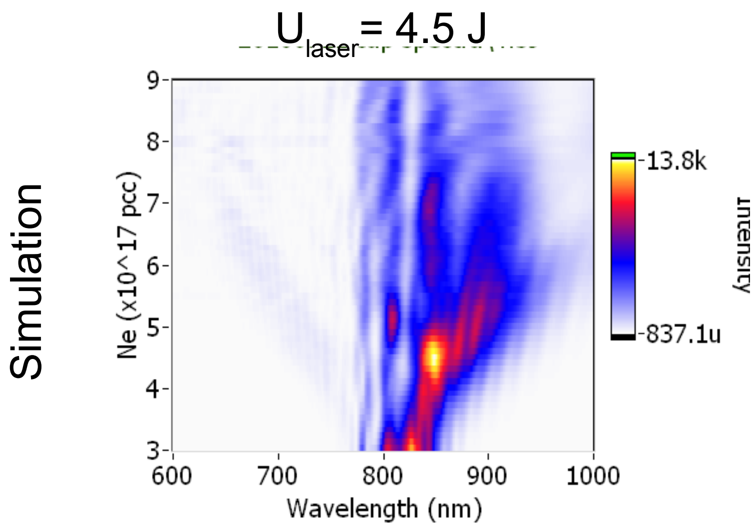
LED + QSA allow for detailed modeling of LPAs and close comparison with experiments/1

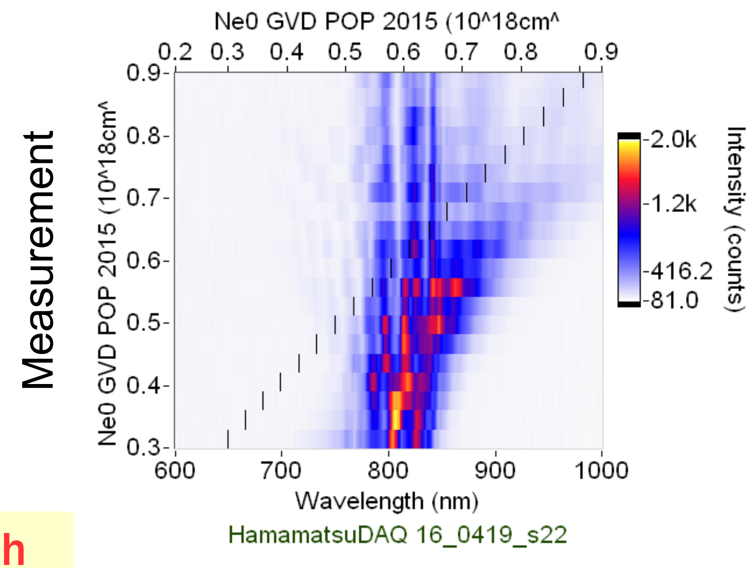
Comparison between measured and simulated post-interaction laser optical spectra used as independent density diagnostic*.

Laser:
U= 4.5 J
T= 30 fs
w_0= 53 um

Plasma (capillary):
L=9 cm
n_0=(3-9) x 10^{17} cm^{-3}
(parabolic channel)







- 80 simulations (density scan) of a 9 cm LPA;
- modeling reproduces key features in laser spectra

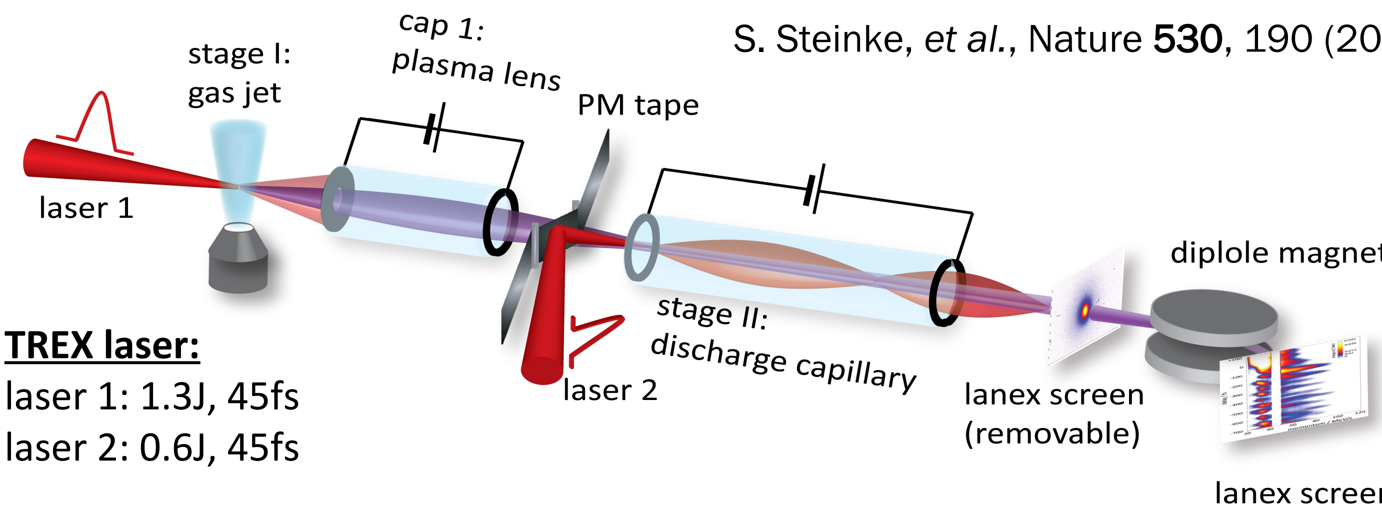
9 cm LPA (nonlinear regime) simulation cost: ~10 CPUh (reduction ~10^6 compared to conventional 3D PIC)

*Leemans, *et al.*, PRL (2014)

LED + QSA allow for detailed modeling of LPAs and close comparison with experiments/2

Staging of independent LPAs.

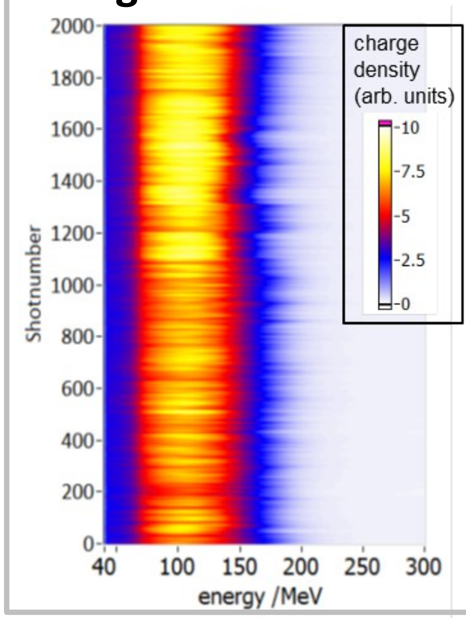
S. Steinke, *et al.*, Nature **530**, 190 (2016)



TREX laser:

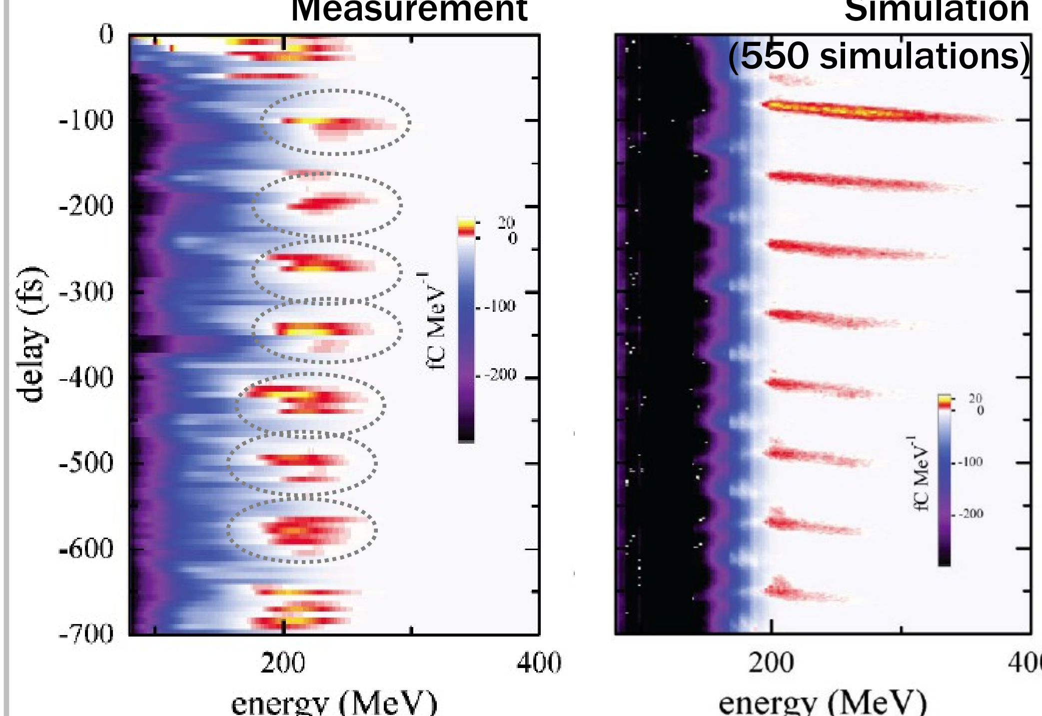
laser 1: 1.3J, 45fs
laser 2: 0.6J, 45fs

Stage I



Staging simulation cost: ~15 CPUh (reduction ~60,000 compared to conventional 3D PIC)

Stage II



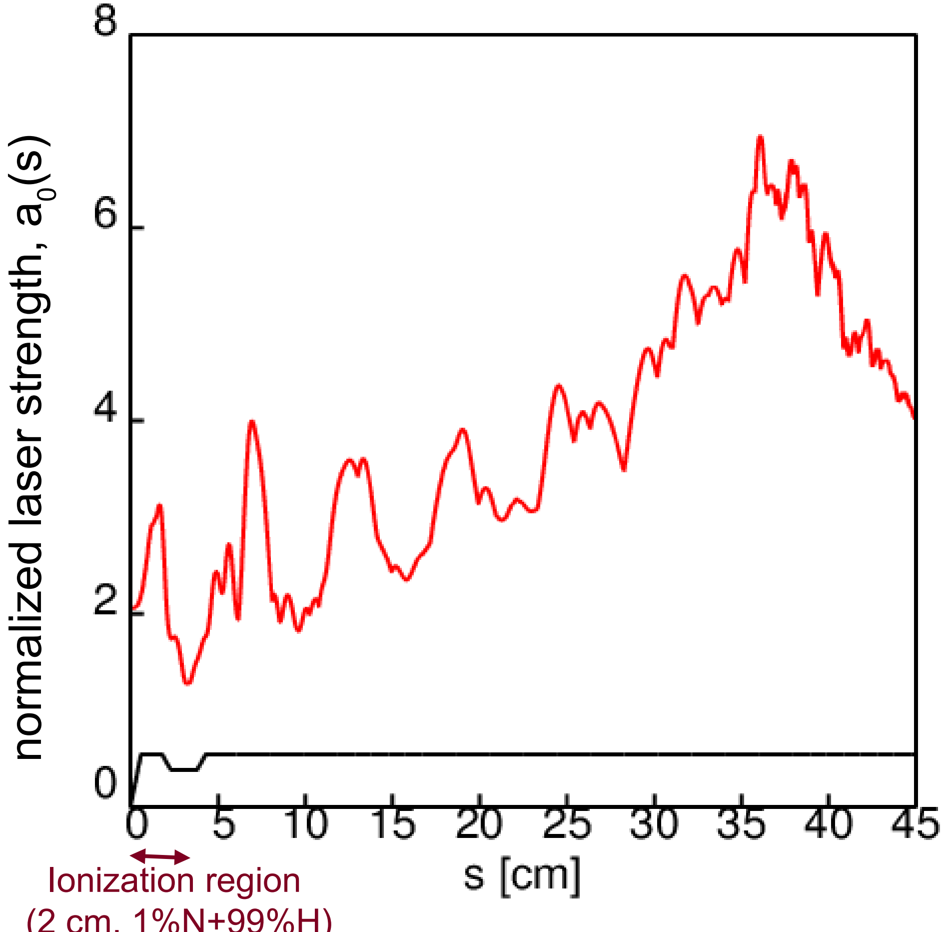
← Electron spectra measured after STAGE-II as a function of the delay between STAGE-II laser and bunch (waterfall plot)

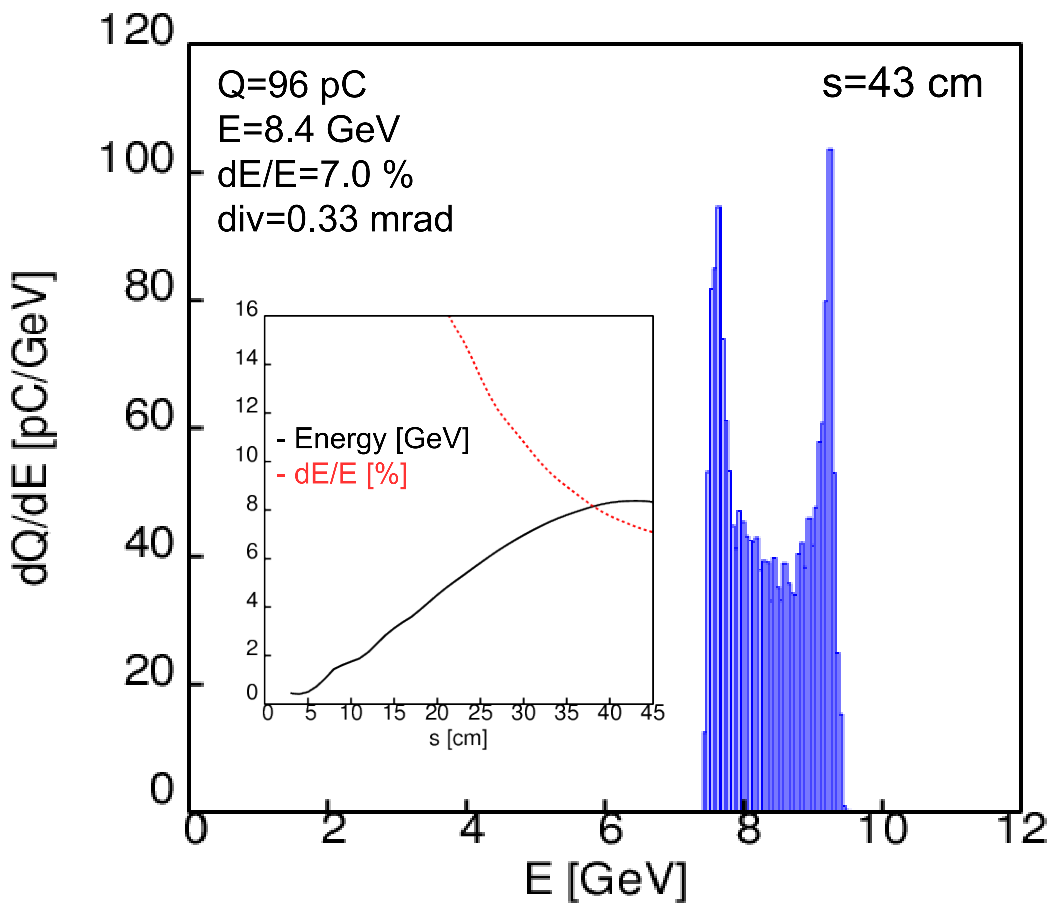
+100 MeV energy gain, 3% capturing efficiency

LED + QSA allow for (very) efficient modeling of 10 GeV-class LPA stages in the quasi-linear regime

Laser (BELLA): U=36 J, w_0=60 μm (spot size expanded w/ near field clipping), T=66 fs

Plasma target: capillary discharge+laser heater (MHD) → n_0=1.6x10^{17} cm^{-3}, $R_{matched}$=70 μm





10 GeV simulation cost: ~50 CPUh (reduction ~10^6 compared to conventional 3D PIC code)

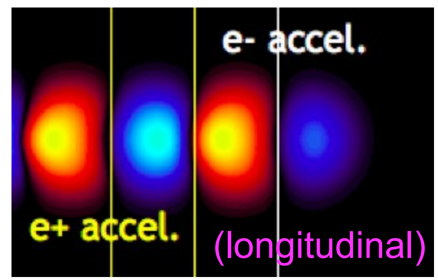
N.B. No optimization for the injector (work in progress)

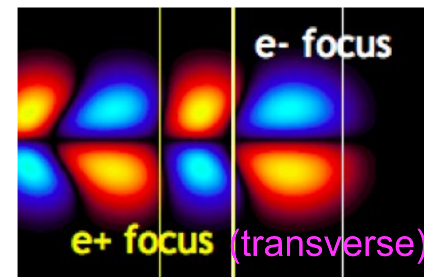
Quasi-cylindrical modality

Motivation for a quasi-cylindrical modality

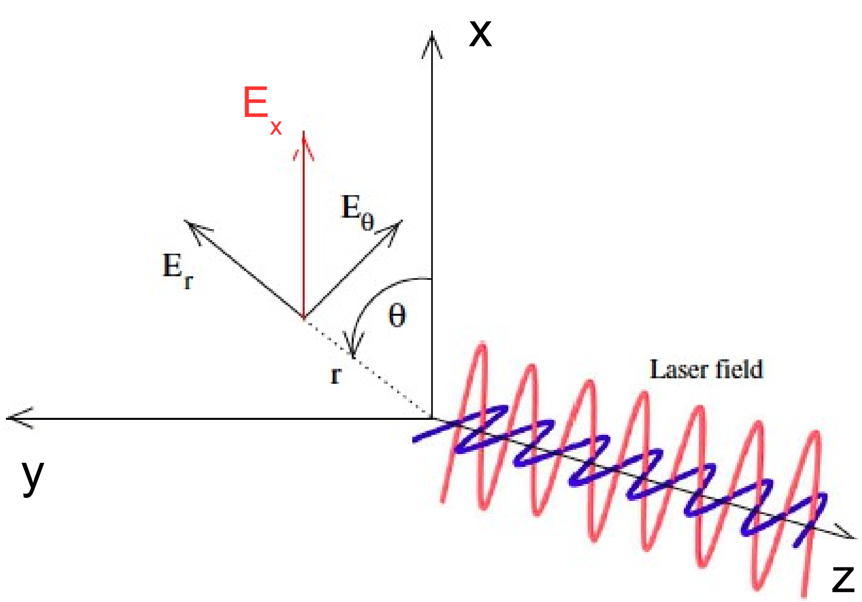
- Modeling of LPAs require a 3D description of the physics [laser evolution, wakefield structure, (self-)injection dynamics, etc.];
- For a driver with a **symmetric envelope**, the wake and laser field structure is “quasi-cylindrical”, i.e., when described in cylindrical geometry (z, r, θ) it contains a **few** azimuthal modes (simple functional dependence from θ)

Wake → (almost) symmetric





Laser polarized along x →



Symmetric pulse [$r=(x^2+y^2)^{1/2}$]

$$\mathbf{E} = E_0(r,\zeta)\hat{x}$$

$$= \underbrace{\underbrace{\cos\theta E_0(r,\zeta)\hat{r}}_{E_r} - \underbrace{\sin\theta E_0(r,\zeta)\hat{n}}_{E_\theta}}_{\text{Simple } \theta\text{-dependence}}$$

The Quasi-cylindrical (quasi-3D) modality: overview

- Represent the fields in cylindrical coordinates using a Fourier decomposition in θ

$$E_r(z,r,\theta) = \hat{E}_{r,0}(z,r) + \hat{E}_{r,1}(z,r)e^{i\theta} + \hat{E}_{r,2}(z,r)e^{2i\theta} + \cdots$$

→ similar expressions for all the components of **E**, **B** and **J**
→ truncate the series at a **low** order (usually 1 or 2) [**quasi-cylindrical assumption!**]
→ use 2D (z,r) grids to represent the "coefficients" $\hat{E}_{r,m}$(z,r) for all the fields [gridless in θ]

- Solve Maxwell's equations*
→ equations for different azimuthal modes decouple (i.e., equations for m=0 are solved independently from m=1, etc..)
→ "standard" 2ndorder* or PSATD schemes are available

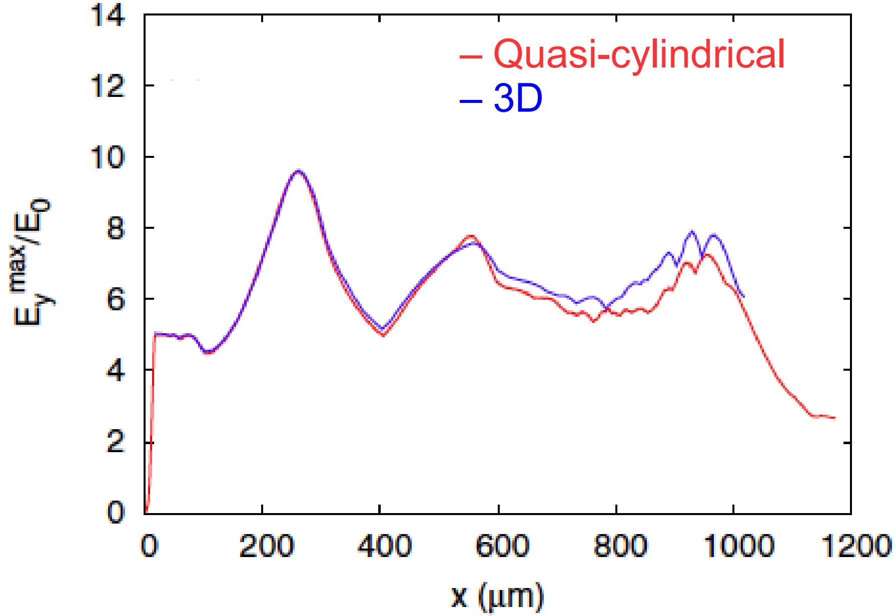
- Push particles
→ equations for the numerical particles are solved in 3D Cartesian coordinates (requires reconstructing the fields in Cartesian geometry but avoids problems related to "singularity" in r=0)
→ particle quiver in the laser field modeled (no averaged ponderomotive approx.)

*Lifschitz et al., Journal of Computational Physics 228, 1803 (2009)

Quasi-cylindrical codes reproduce 3D physics at a ~2D computational cost → large savings

a_0=5
T_0=30 fs
w_0=9 um
$n_0=1.2\times10^{19}$ cm^{-3}
(uniform density)

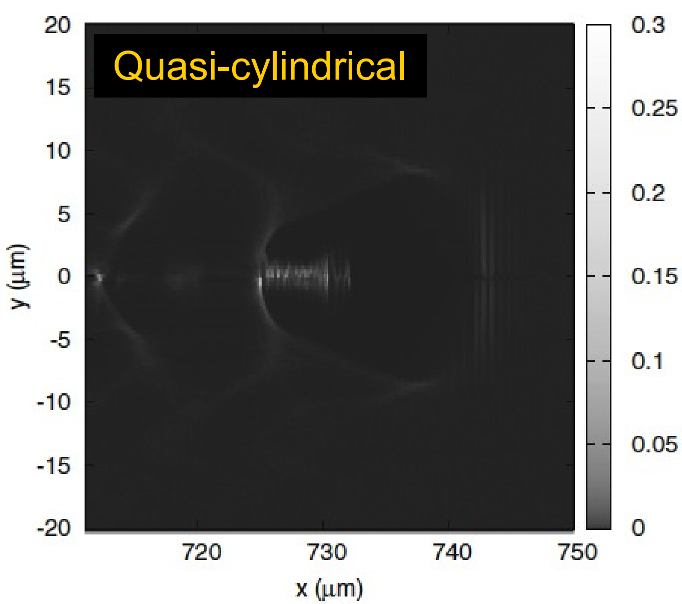
Laser field evolution

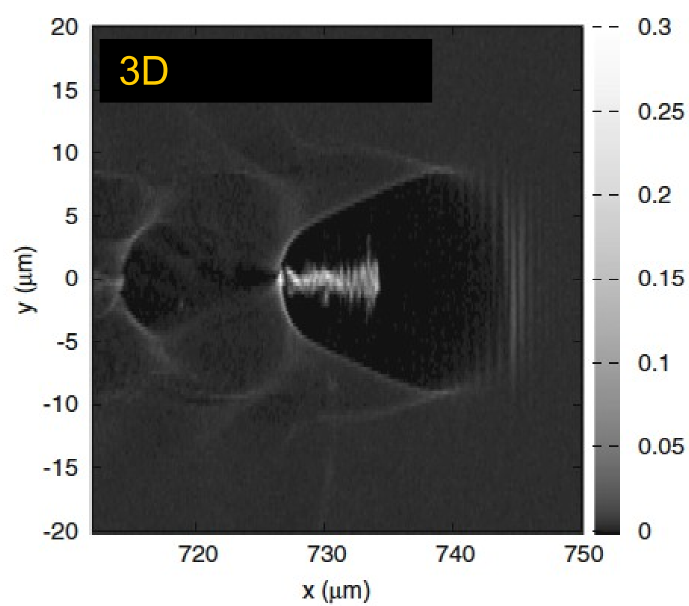


Simulation with CALDER (CALDER-circ):

3D → 7000 CPUh
Quasi-cylindrical → 70 CPUh

Electron density →

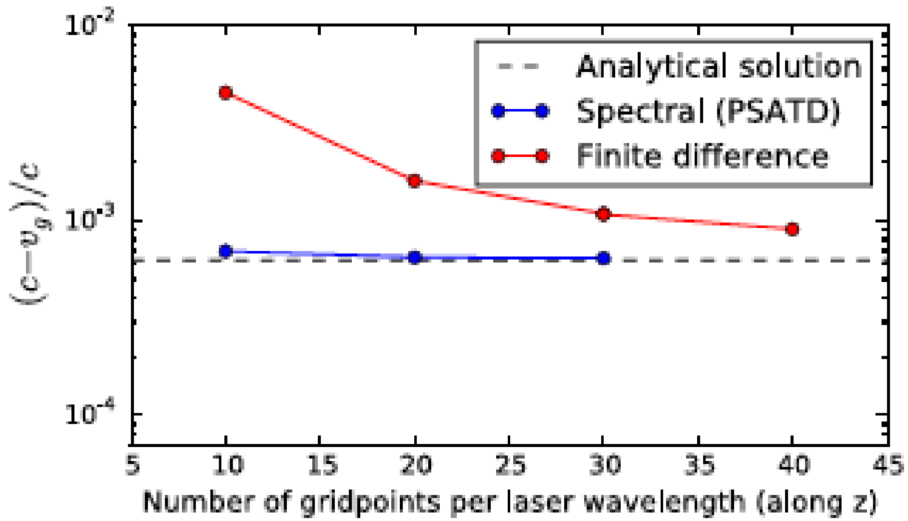




Combining quasi-cylindrical + spectral (FBPIC)

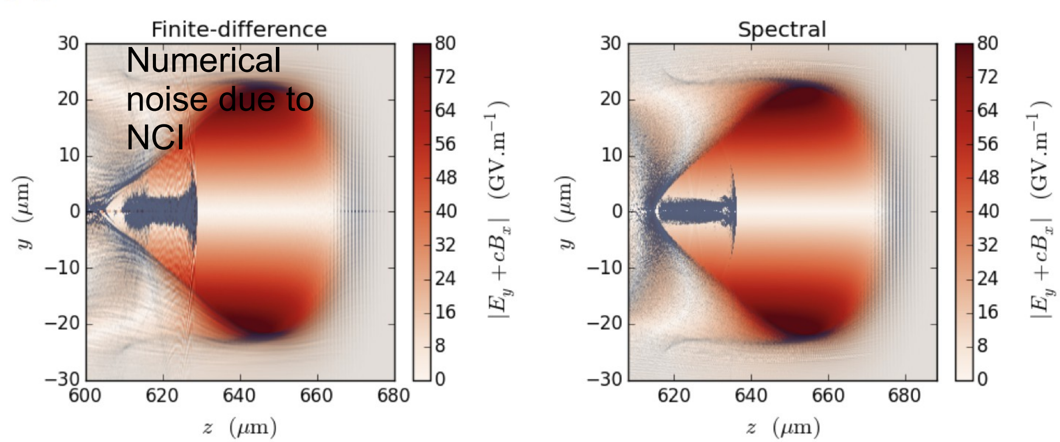
Advantages of a quasi-cylindrical modality (computational savings) combined with the advantages of a spectral field solver (superior description of EM waves propagation)

Correct laser group velocity →



Typical laser-wakefield simulation:

Suppression of NCI →



R. Lehe et al., Computer Physics Communications 203, 66 (2016)

References

Lorentz boosted frame:
- J.-L. Vay, PRL 98, 130405 (2007)
- J.-L. Vay et al., Phys. Plasmas 18, 123103 (2011)

Mitigation of NCI in Lorentz boosted frame:
- B. B. Godfrey and J. L. Vay, Computer Physics Communications 196, 221 (2015)
- P. Yu et al., Computer Physics Communications 192, 32 (2015)
- P. Yu et al., Computer Physics Communications 197, 144 (2015)
- R. Lehe et al., Phys Rev. E 2016, 053305 (2016)
- M. Kirchen et al., Phys. Plasmas 23, 100704 (2016)

Laser-envelope description:

C. Benedetti, et al., AIP Conference Proceedings 1299, 250 (2010)
C. Benedetti, et al., AIP Conference Proceedings 1812, 050005 (2017)
D. Gordon, IEEE Transactions on Plasma Science 35, 1486 (2007)
B. M. Cowan, et al., J. Comp. Phys. 230, 61 (2011)

Quasi-static approximation:
- P. Mora and T. Antonsen, Phys. Plasmas 4, 217 (1997)
- C. Huang al., Journal of Computational Physics 217, 658 (2006)
- W. An et al., Journal of Computational Physics 250, 165 (2013)
- T. Mehrling et al., Plasma Physics and Controlled Fusion 56, 084012 (2014)

Quasi-cylindrical:
- A. F. Lifschitz et al., Journal of Computational Physics 228, 1803 (2009)
- A. Davidson et al., Journal of Computational Physics 281, 1063 (2015)
- R. Lehe et al., Computer Physics Communications 203, 66 (2016)