Advanced modeling tools for laser-plasma accelerators (LPAs) 2/3

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Overview of lecture 2

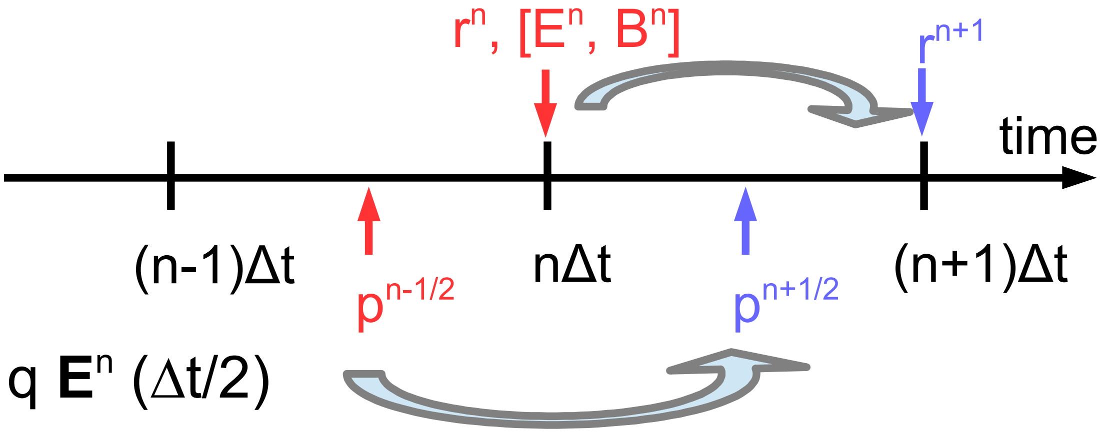
- Limitations of conventional PIC codes → numerical artifacts associated to finite resolution and/or poor sampling result in incorrect description of the physics:
  - error from particle pusher;
  - incorrect dispersion of EM waves on a grid;
  - unphysical kinetic effects.
- Solutions to some of the issues presented.

Errors from particle pusher

The Boris pusher (review)

- Conventional PIC codes use the Boris pusher (2nd order accurate) to integrate the equations of motion for the numerical particles

$$\begin{cases} \frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i \equiv \frac{\mathbf{p}_i}{m_i \gamma_i}, \\ \frac{d\mathbf{p}_i}{dt} = q_i \left(\mathbf{E}(\mathbf{r}_i, t) + \frac{\mathbf{v}_i}{c} \times \mathbf{B}(\mathbf{r}_i, t) \right) \end{cases}$$



momentum

$\mathbf{p}^{n-1/2} \rightarrow \mathbf{p}^- = \mathbf{p}^{n-1/2} + q\, \mathbf{E}^n\, (\Delta t/2)$

$\gamma^n = [1+(\mathbf{p}^-/mc)^2\,]^{1/2}$

$\mathbf{p}' = \mathbf{p}^- + \mathbf{p}^- \times \mathbf{t}$ $\quad\quad$ $\mathbf{t} = q\Delta t\mathbf{B}^n/2mc\gamma^n$

$\mathbf{p}^+ = \mathbf{p}^- + \mathbf{p}' \times \mathbf{s}$ $\quad\quad$ $\mathbf{s} = 2t/(1+|t|^2)$

$\mathbf{p}^- \rightarrow \mathbf{p}^+$: rotation around $\mathbf{B}^n$ by an angle $\arctan[q\Delta t\mathbf{B}^n/2mc\gamma^n]$

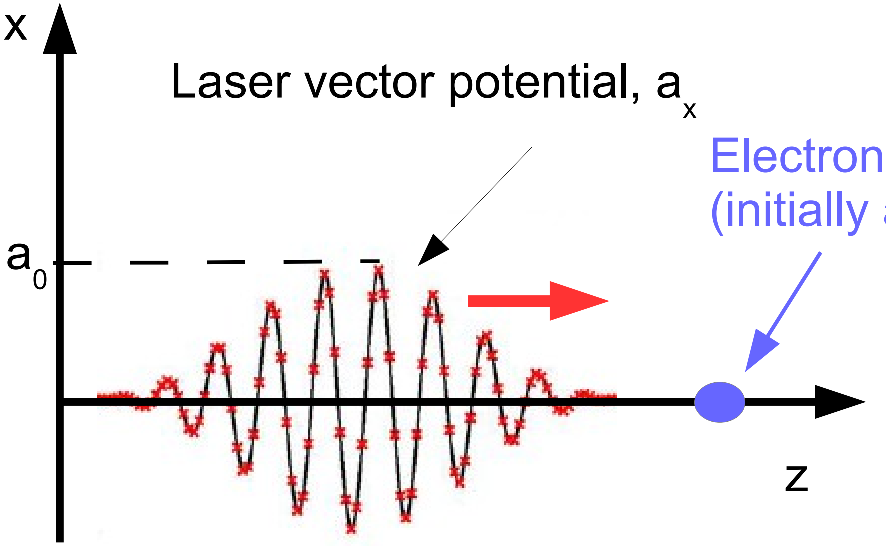
$\mathbf{p}^+ \rightarrow \mathbf{p}^{n+1/2} = \mathbf{p}^+ + q\, \mathbf{E}^n\, (\Delta t/2)$

position

$\mathbf{r}^{n+1} = \mathbf{r}^n + \mathbf{v}^{n+1/2}\Delta t$

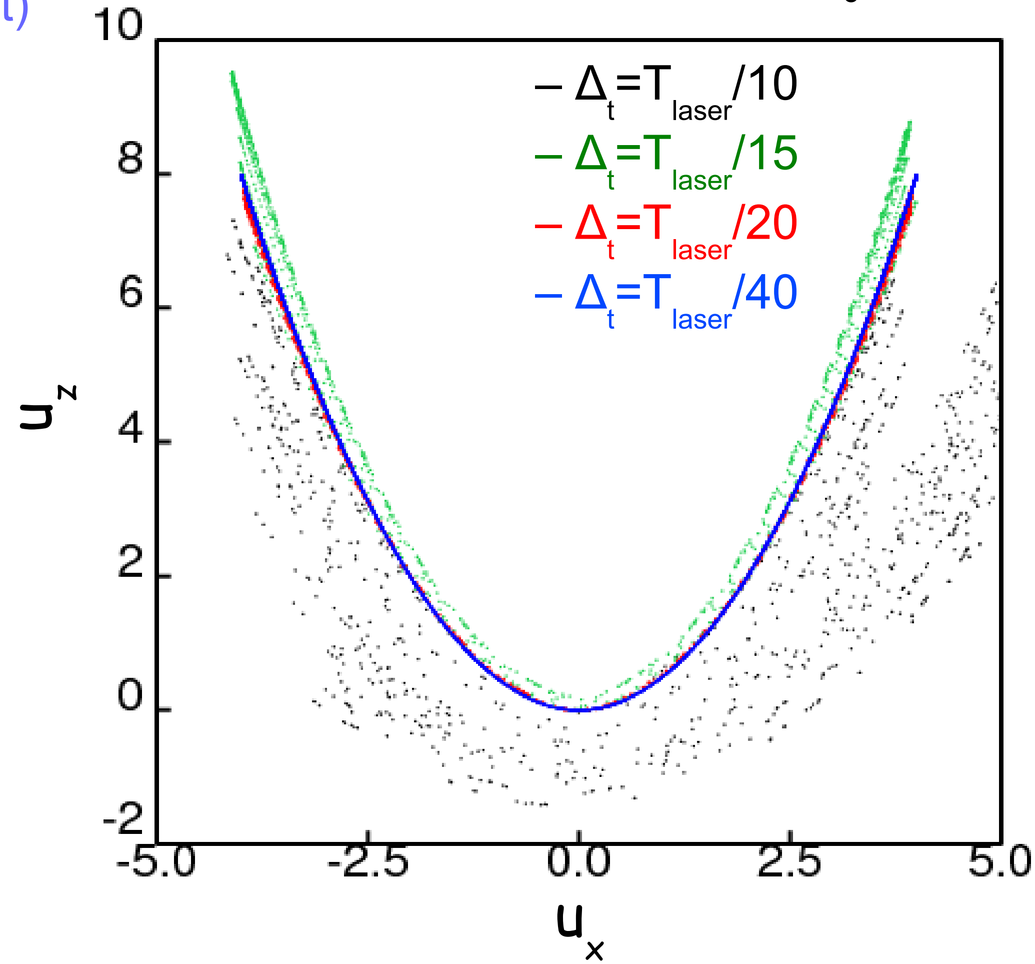
Test: particle in a 1D plane wave/1

- The motion of a particle (electron) in a 1D plane wave is integrable



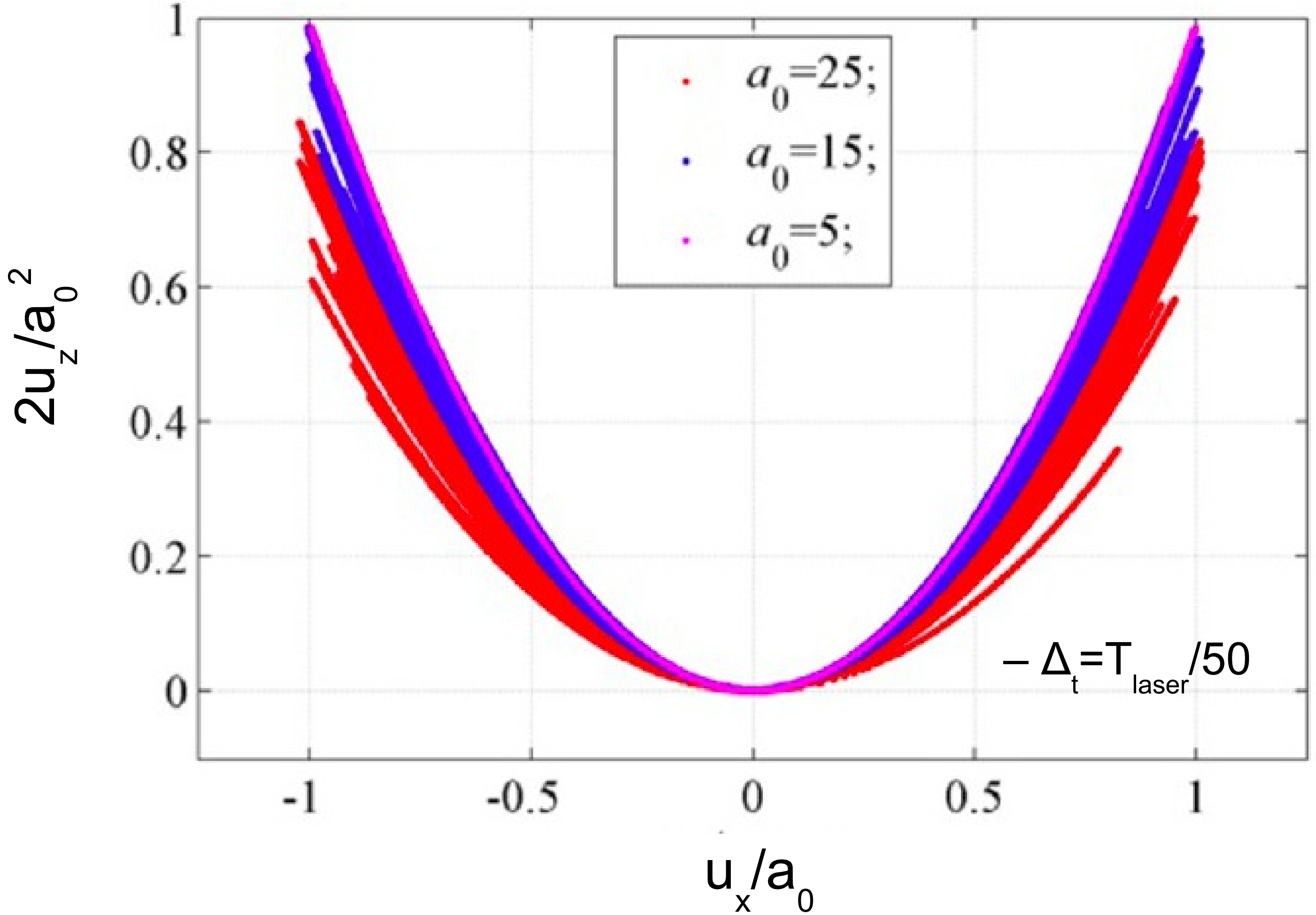
$$\begin{cases} u_z = p_z/mc = a_x^2/2 \\ u_x = p_x/mc = a_x \end{cases}$$

$\rightarrow u_z(t) = [u_x(t)]^2/2$



Test: particle in a 1D plane wave/2

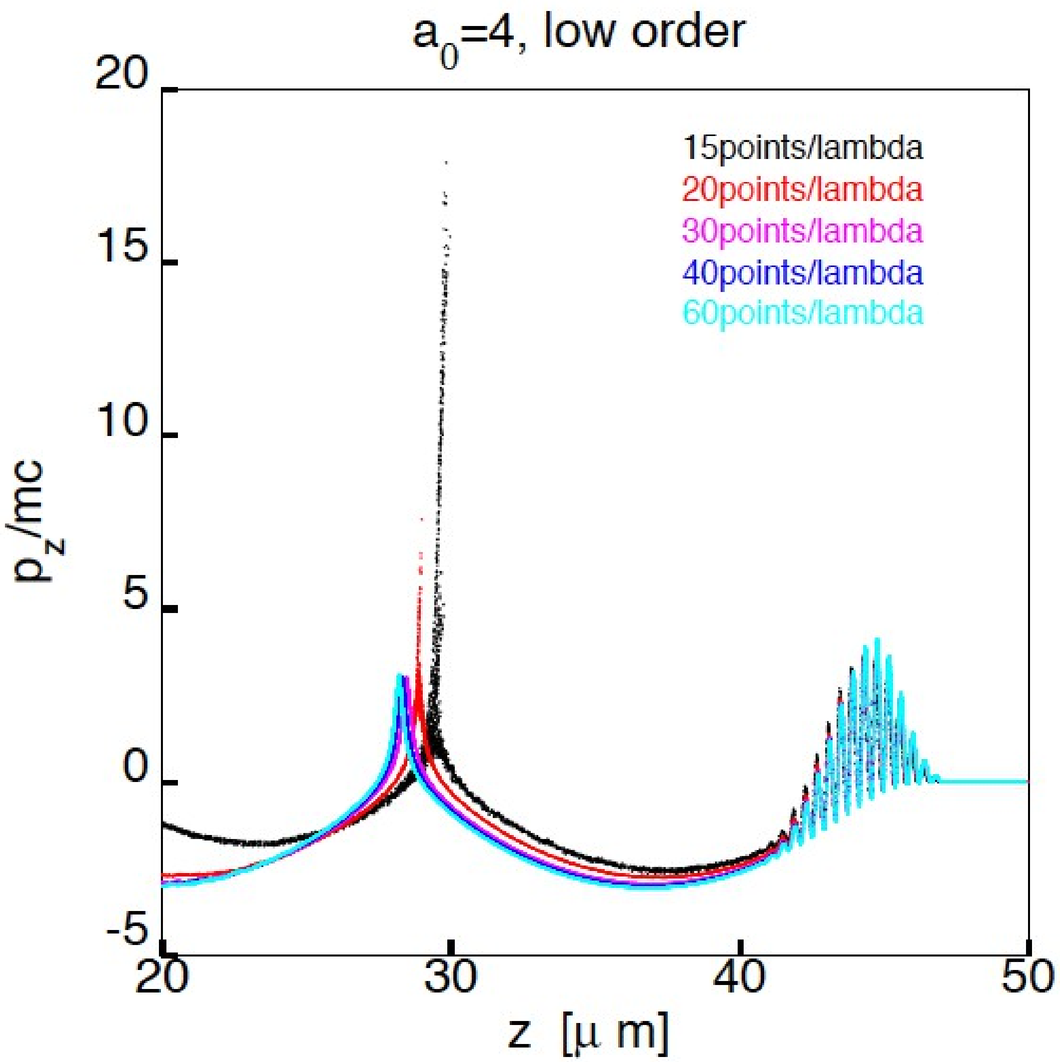
- Accuracy deteriorates with increasing wave amplitude



Arefiev et al, Phys. Plasma, 22, 013103 (2015)

N.B. a_0 can become very large in an LPA operating in a regime with $P/P_c >> 1$

Incorrect electron motion in the laser field affects wake excitation



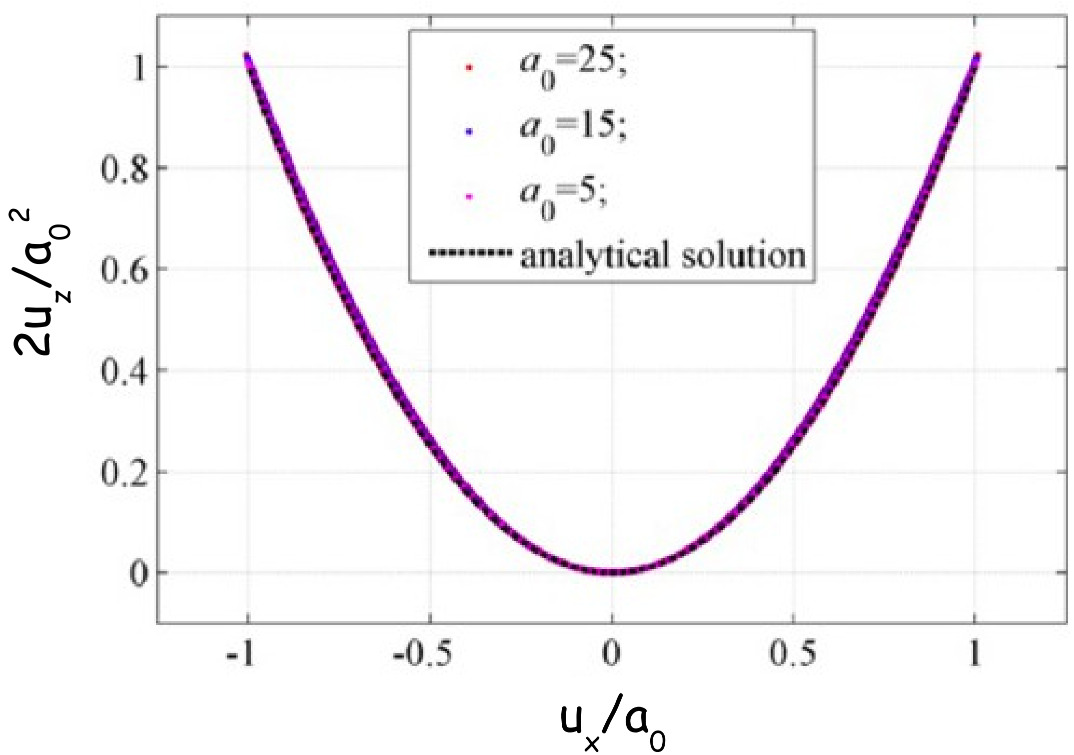
Convergence of the longitudinal phase space (z, p_z) in a self consistent simulation (laser $a_0 = 4$, $\tau = 10$ fs, density 10^{19} e/cm3, 30 particles/cell) changing the resolution

Sub-cycling is an efficient solution to the problem

- Good accuracy requires the time step to satisfy: $\Delta t/T_{laser} << 1/a_0$

  → criterion ensures that the rotation in B-field during Δt is small at locations where B is max

- Besides decreasing uniformly the time-step (expensive), a more efficient solution is to use adaptive sub-cycling



1. check the estimated rotation angle ψ in Δt

2. if $\psi > \psi_*$ (threshold) redefine Δt → Δt'=Δt/4 (repeat until suitable time step is found)

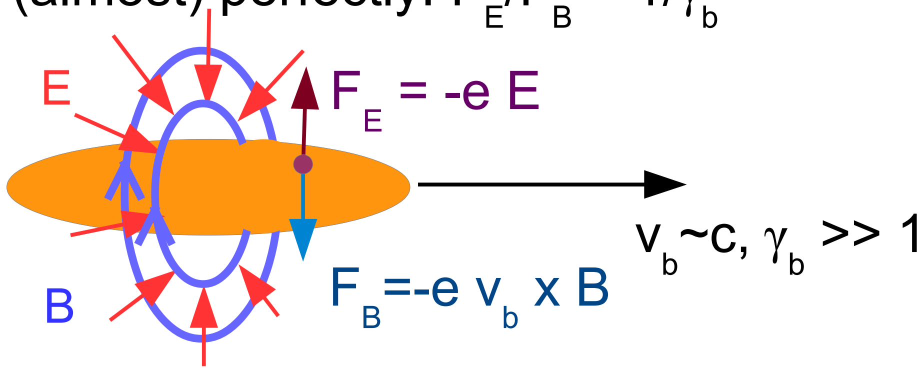
3. Revert to original time step when possible

a_0	ψ_*	Δt (%)	$\Delta t/4$ (%)	$\Delta t/16$ (%)	$\Delta t/64$ (%)
5	0.05	58	30	12	0
15	0.05	78	13	8	1
25	0.05	87	7	4	2

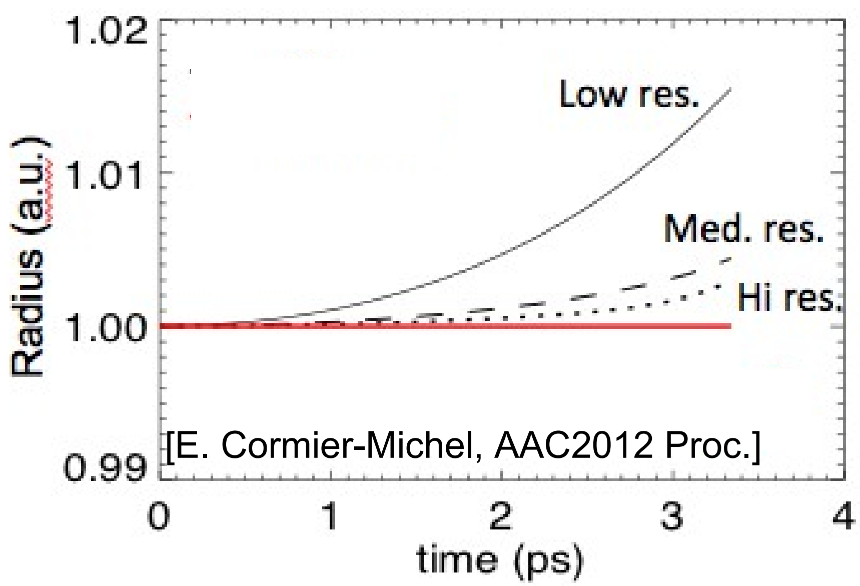
Arefiev et al, Phys. Plasma 22, 013103 (2015)

Spurious emittance growth for ultra-relativistic bunches due to spatial staggering of E and B

- For a highly relativistic bunch (γ_b >> 1), the electric (defocusing) and magnetic (focusing) forces experienced by a generic electron in the bunch due to the bunch self-fields should cancel (almost) perfectly: $F_E/F_B \sim 1/\gamma_b^2$



- E and B are spatially/temporally staggering → interpolation error → non-perfect cancellation between F_E and F_B causes emittance growth for bunches with ultra low emittance (problem for "collider" applications)



→ Problem can be mitigated by using nodal fields (no spatial staggering, but requires going beyond Yee)

→ Problem can be mitigated using "beam frame Poisson solve" technique [bunch self field computed in the rest frame of the bunch and then added to the wakefield] (E. Cormier-Michel, AAC2012 Proc.)

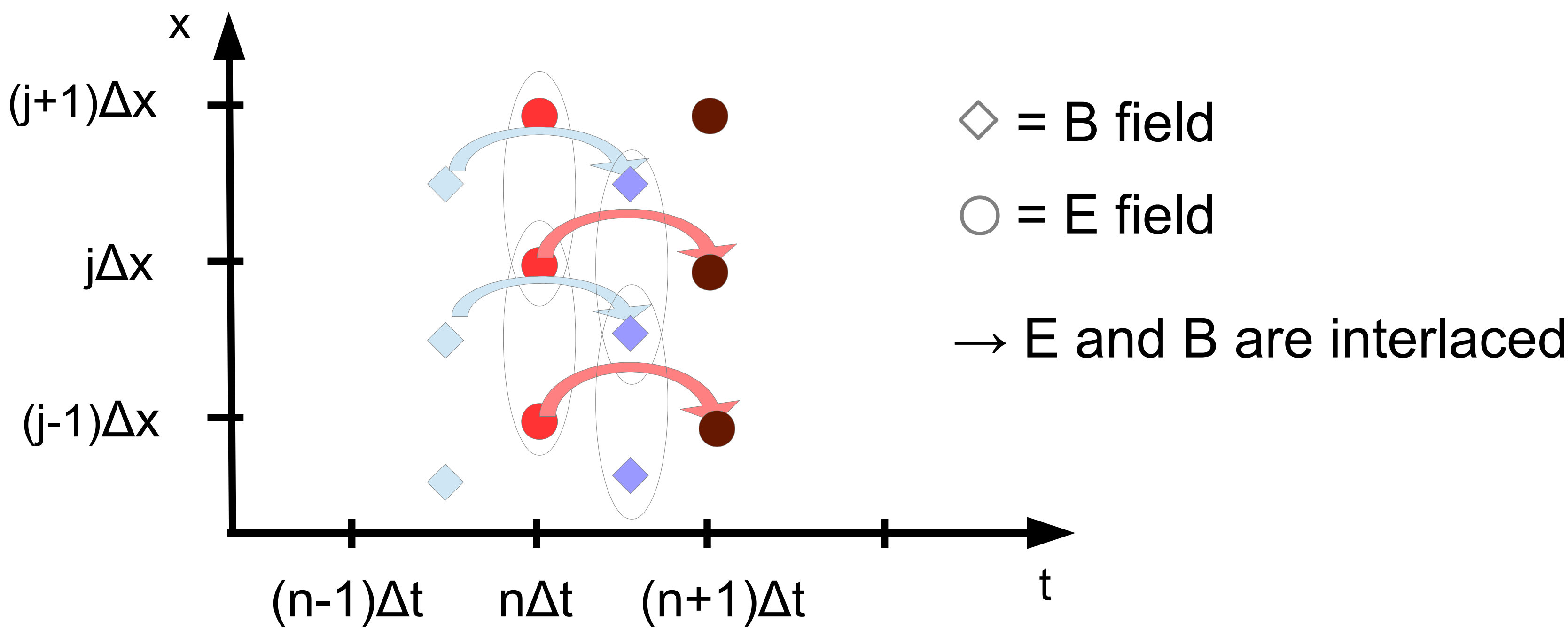
Incorrect dispersion of EM waves on a grid

Discretized Maxwell equations (review)

- In conventional PIC codes Maxwell equations are discretized in space and time according to the Yee scheme (2nd order accuracy via staggering in space and time)

(1D in vacuum) $[E_x = E,\ B_y = B]$

$$\begin{cases} \dfrac{\partial \mathbf{E}}{\partial t} = c\nabla \times \mathbf{B} \\ \dfrac{\partial \mathbf{B}}{\partial t} = -c\nabla \times \mathbf{E} \end{cases} \longrightarrow \begin{cases} (E^{n+1}_{j} - E^{n}_{j})/\Delta t = -c\,(B^{n+1/2}_{j+1/2} - B^{n+1/2}_{j-1/2})/\Delta z \\ (B^{n+1/2}_{j+1/2} - B^{n-1/2}_{j+1/2})/\Delta t = -c\,(E^{n}_{j+1} - E^{n}_{j})/\Delta z \end{cases}$$



Von Neumann analysis of 1D discretized wave equation

$$(E^{n+1}_j - 2E^n_j + E^{n+1}_j)/\Delta t^2 = c^2(E^n_{j+1} - 2E^n_j + E^n_{j-1})/\Delta z^2 \quad (1)$$

$$[\partial^2 E/\partial t^2 = c^2\, \partial^2 E/\partial z^2 \text{ for } \Delta z \rightarrow 0 \text{ and } \Delta t \rightarrow 0]$$

$$E = E_0 \exp(ikz - i\omega t) \rightarrow E^n_j = E_0 \exp(ikj\Delta z - i\omega n\Delta t) \text{ in Eq. (1)}$$

Wave number (k) Frequency (ω)

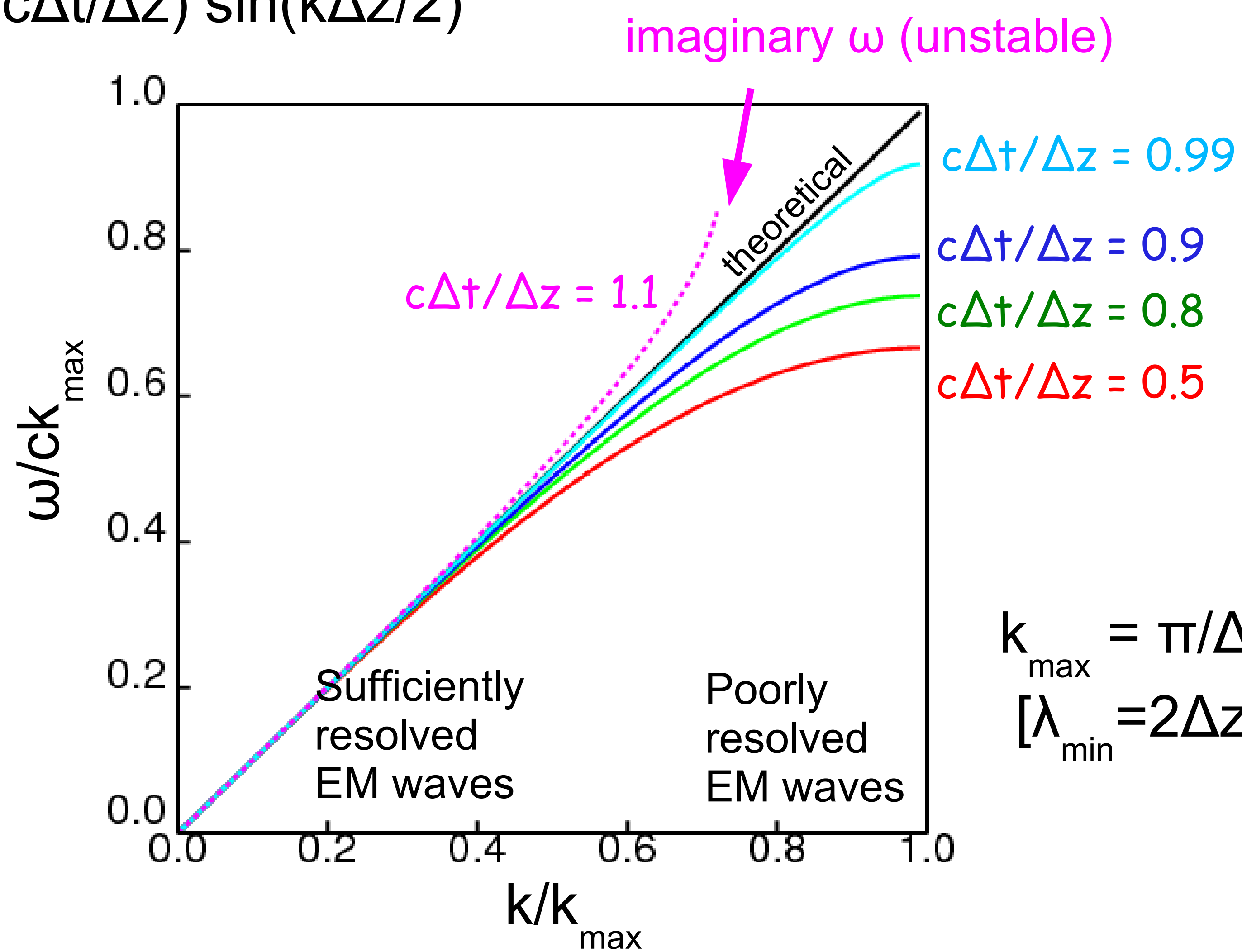
1D dispersion relation

$$\frac{1}{c^2\Delta t^2}\sin^2\left(\frac{\omega\Delta t}{2}\right) = \frac{1}{\Delta z^2}\sin^2\left(\frac{k\Delta z}{2}\right)$$

$$[\omega^2 = c^2k^2 \text{ for } \Delta z \rightarrow 0 \text{ and } \Delta t \rightarrow 0]$$

Numerical dispersion of EM waves on a grid [1D]/1

$\sin(\omega\Delta t/2) = (c\Delta t/\Delta z)\sin(k\Delta z/2)$



$k_{max} = \pi/\Delta z$
$[\lambda_{min} = 2\Delta z]$

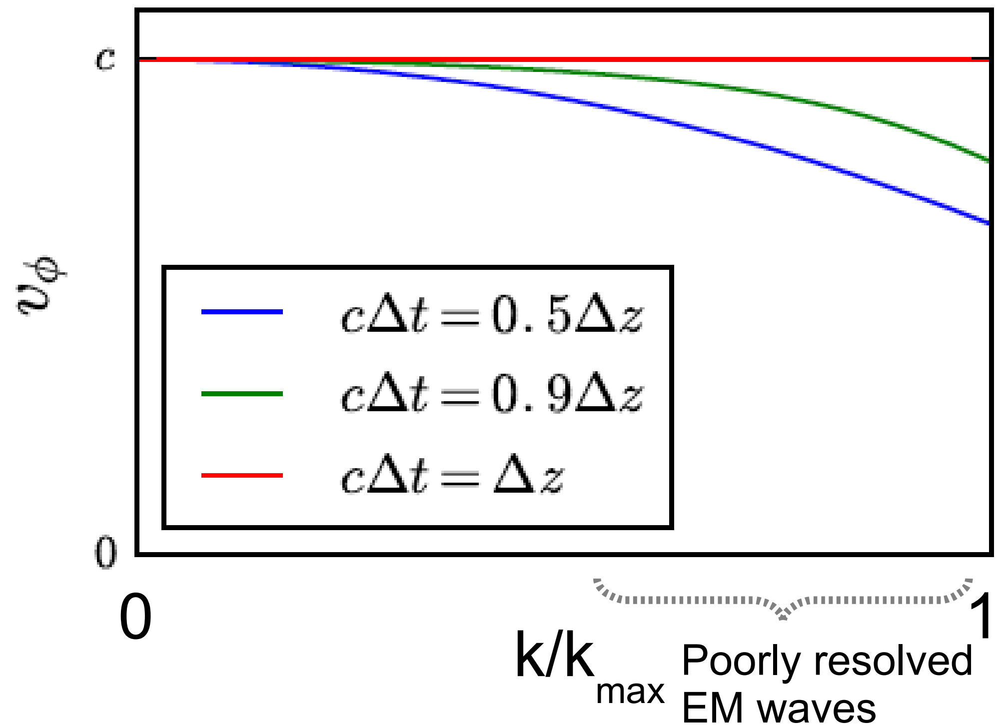
- Standard PIC codes are **unstable** if $c\Delta t > \Delta z$ [Courant/CFL limit] (in an EM code signals cannot travel faster than the speed of light)

- EM waves in PIC have a k-dependent (and $\Delta t/\Delta z$-dependent) velocity ($\neq c$)

Numerical dispersion of EM waves on a grid [1D]/2

- Phase velocity of EM waves on a grid $v_\Phi = \omega/k$

$$v_\phi = \pm \frac{2}{k\Delta t} \arcsin\left(\frac{c\Delta t}{\Delta z} \sin\left(\frac{k\Delta z}{2}\right)\right)$$



- The shorter is the wavelength, the slower is the phase velocity;
- A k-dependent phase velocity implies a k-dependent group velocity (e.g., the laser group velocity is lower than the right one, this remains true for propagation in plasma);
- Best results for $c\Delta t = \Delta z$;

Numerical dispersion of EM waves on a grid [3D]/1

- Von Neumann analysis in 3D gives

3D Discrete dispersion relation

$$\frac{\sin^2\left(\frac{\omega\Delta t}{2}\right)}{c^2\Delta t^2} = \frac{\sin^2\left(\frac{k_x\Delta x}{2}\right)}{\Delta x^2} + \frac{\sin^2\left(\frac{k_y\Delta y}{2}\right)}{\Delta y^2} + \frac{\sin^2\left(\frac{k_z\Delta z}{2}\right)}{\Delta z^2}$$

[$\omega^2 = c^2(k_x^2 + k_y^2 + k_z^2)$ for $\Delta x, \Delta y, \Delta z, \Delta t \rightarrow 0$]

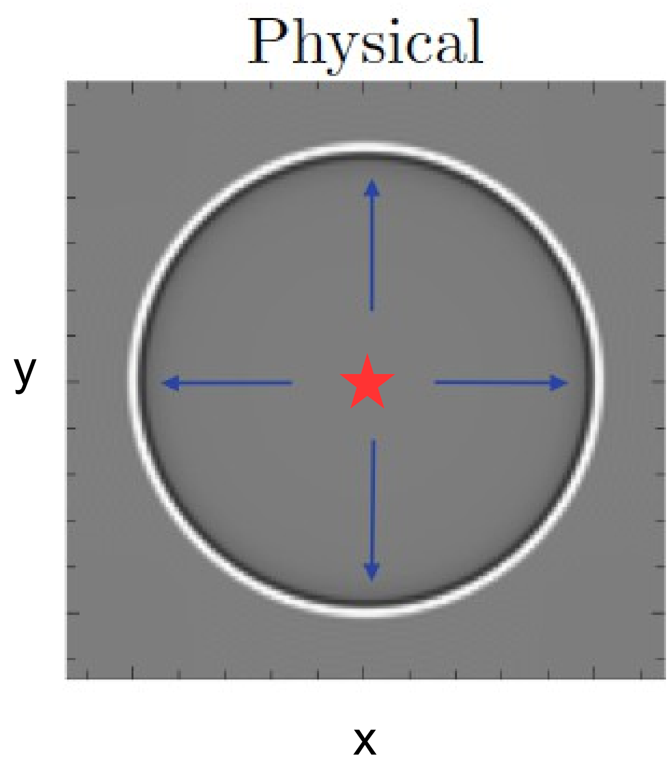
Courant limit (a.k.a CFL limit) in 3D

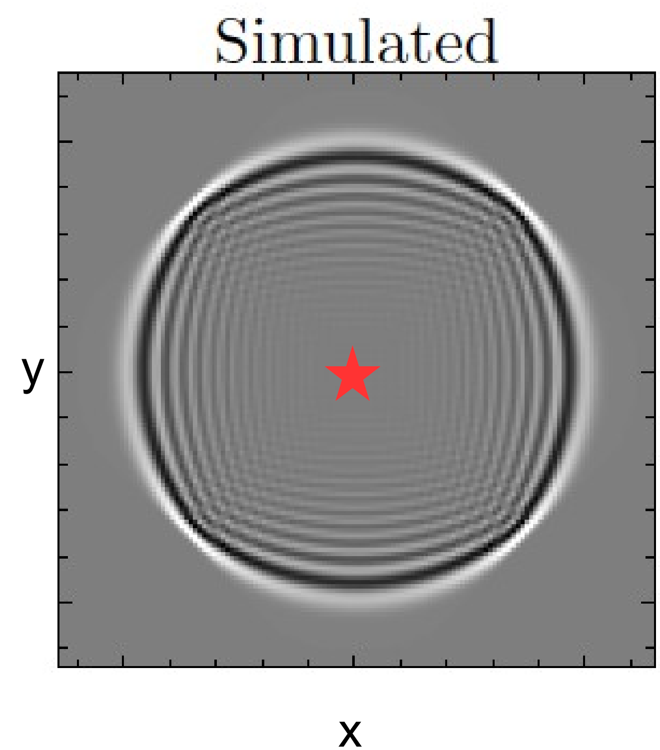
$$c\Delta t \leq \frac{1}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$ $<\Delta z$ (long.)

- Velocity depends on the wavelength and propagation direction;
- Waves are **always** slower than c along the main axes (x, y, or z);
- Correct phase velocity can be obtained along the 3D diagonal ($k_x=k_y=k_z$) if $\Delta x=\Delta y=\Delta z$ and $c\Delta t=\Delta z/\sqrt{3}$ (CFL condition);

Numerical dispersion of EM waves on a grid [3D]/2

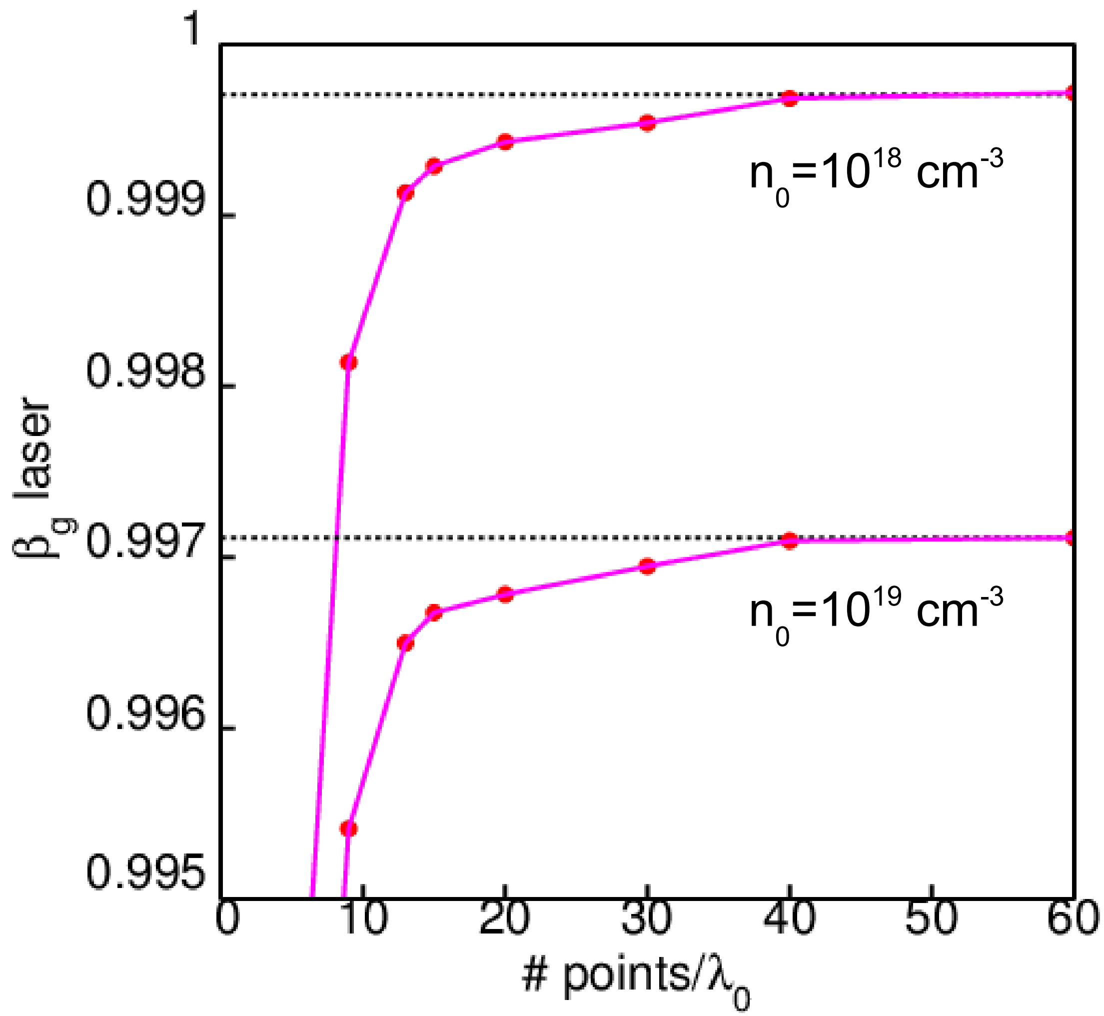
Example: expanding electromagnetic wave (anisotropic propagation)





Numerical dispersion results in incorrect laser propagation in plasma

$\beta_g \approx 1 - \lambda_0^2/(2\lambda_p^2)$ [1D limit], $a_0 \ll 1$

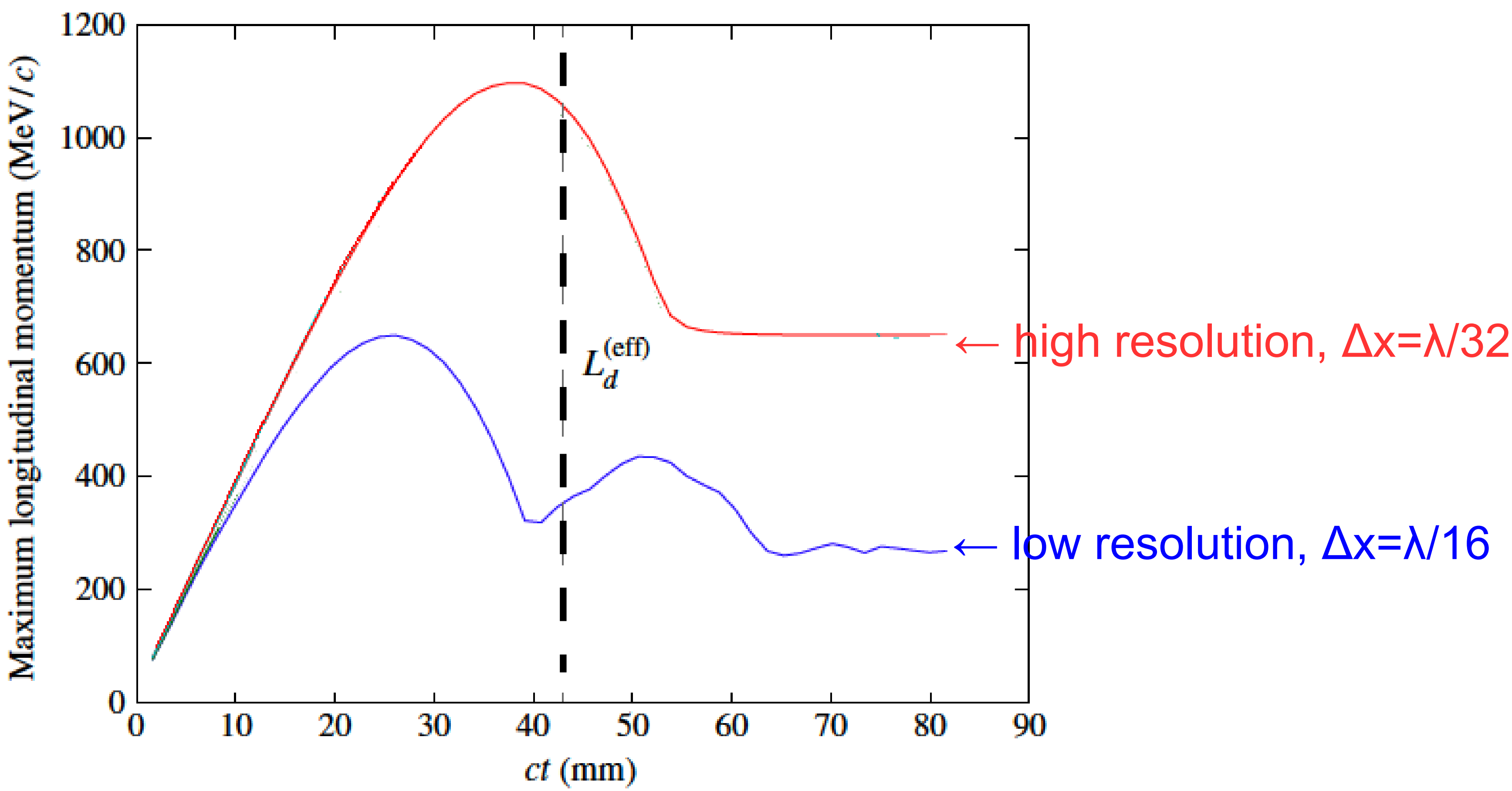


Incorrect laser propagation results in numerical dephasing (incorrect LPA description)

Slower laser results in smaller energy gain for e-bunch in an LPA (the e-bunch catches up with the laser → shorter dephasing length).

n_0=10^{18} cm^{-3} (channel)
a_0=1
k_pL=1
k_pw=5

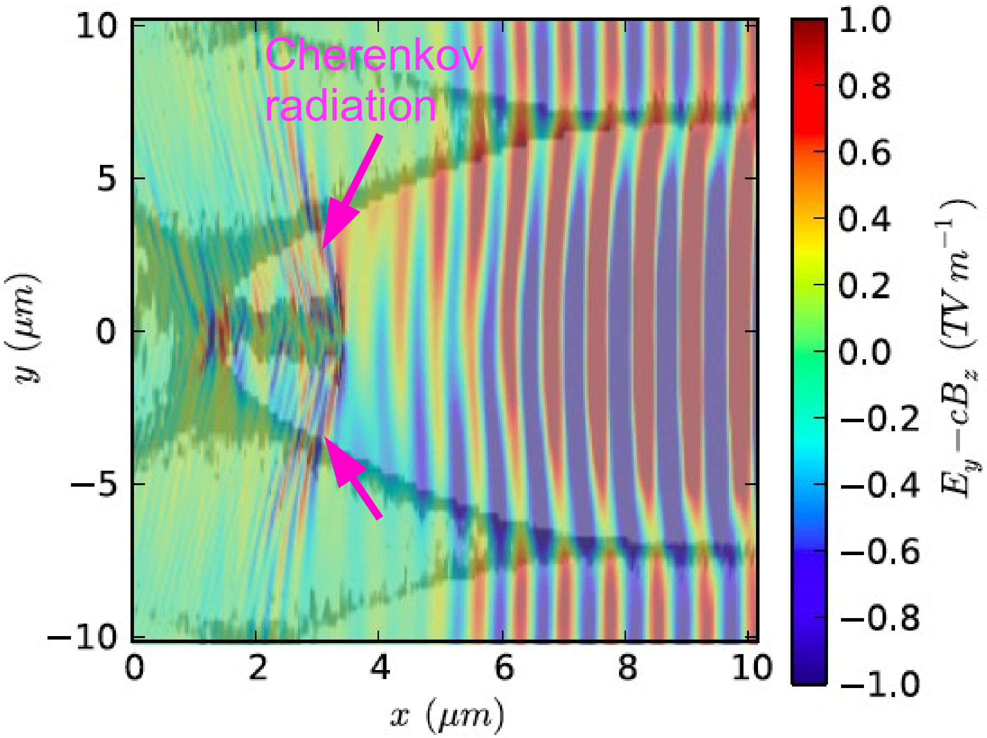
L_{deph}=4.3 cm



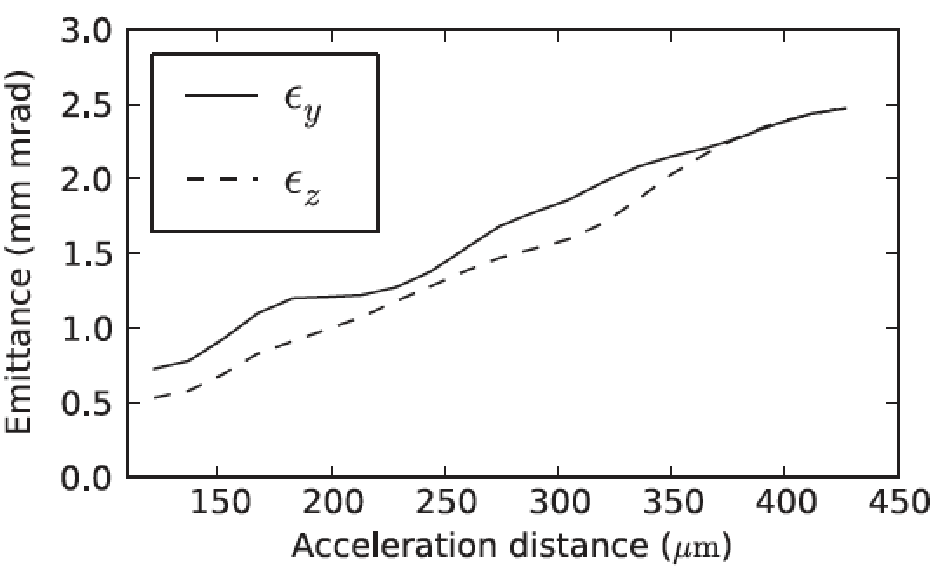
Cowan et al, PRSTAB 16, 041303 (2013)

Incorrect phase velocity for EM waves results in spurious numerical Cherenkov radiation

- Cherenkov radiation – whether physical or numerical – occurs when phase velocity of EM waves is < c. Relativistic particles traveling at ~c can excite these waves.
- In a PIC code where Maxwell equations are solved with Yee scheme EM waves have a phase velocity < c (numerical artifact) → **spurious Cherenkov radiation**



→ Cherenkov radiation induces spurious bunch emittance growth (degradation of bunch quality)



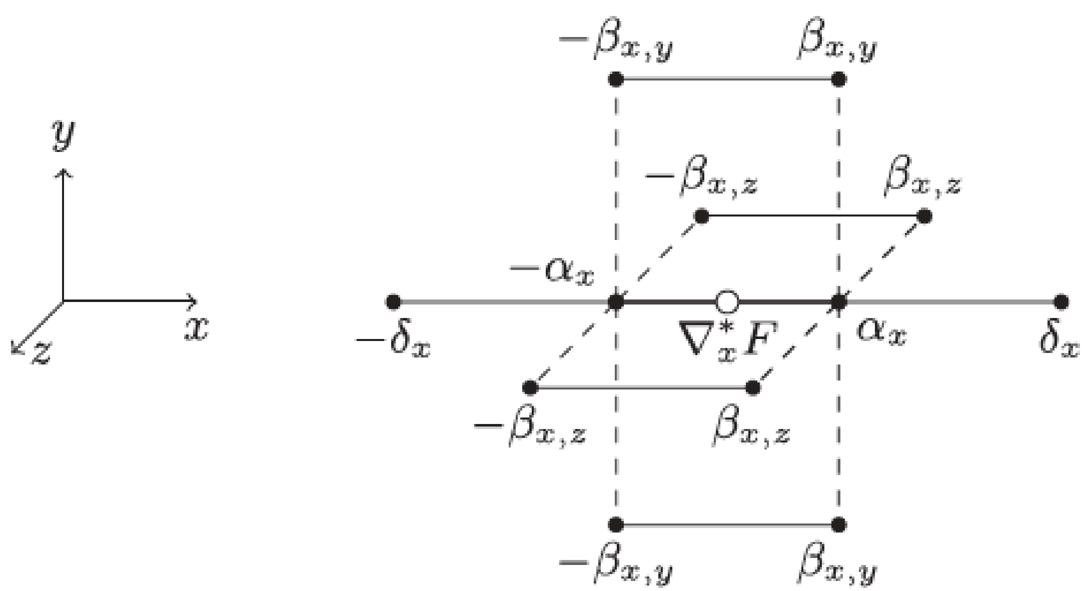
Lehe et al, PRSTAB 16, 021301 (2013)

Numerical dispersion improved via non-standard FDTD schemes

Standard		Non-standard
$D_t\mathbf{B} = -\nabla\times\mathbf{E}$ $D_t\mathbf{E} = \nabla\times\mathbf{B} - \mathbf{J}$	→	$D_t\mathbf{B} = -\nabla^*\times\mathbf{E}$ $D_t\mathbf{E} = \nabla\times\mathbf{B} - \mathbf{J}$

Ex.: Modified curl* operator (longitudinal component)

$$\nabla^*_x F|^n_{i+1/2,j,k} = \alpha_x(F^n_{i+1,j,k} - F^n_{i,j,k})/\Delta x + \beta_{x,y}(F^n_{i+1,j+1,k} - F^n_{i,j+1,k})/\Delta x + \beta_{x,y}(F^n_{i+1,j-1,k} - F^n_{i,j-1,k})/\Delta x$$
$$+ \beta_{x,z}(F^n_{i+1,j,k+1} - F^n_{i,j,k+1})/\Delta x + \beta_{x,z}(F^n_{i+1,j,k-1} - F^n_{i,j,k-1})/\Delta x + \delta_x(F^n_{i+2,j,k} - F^n_{i-1,j,k})/\Delta x$$



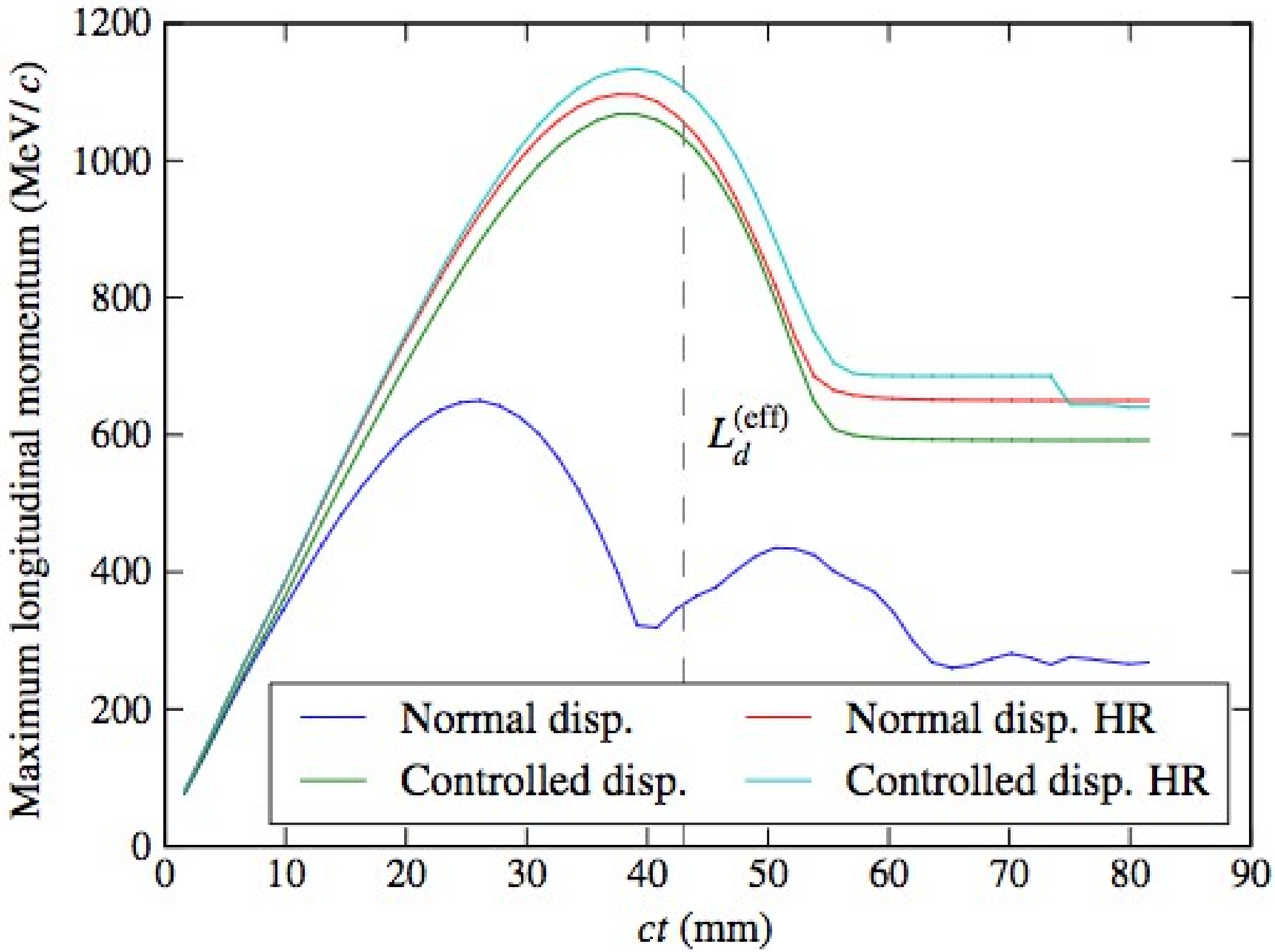
- Standard FDTD (Yee)
  α_x=1,
  $\beta_{x,y}$=$\beta_{x,z}$=0, δ_x=0
- The choice of the coefficients allows to "tune" the dispersion properties of the solver (several options available, e.g. no dispersion along longitudinal axis)

*Lehe et al, PRSTAB 16, 021301 (2013)

Correct laser propagation with non-standard FDTD

n_0=10^{18} cm^{-3}
(channel)
a_0=1
k_pL=1
k_pw=5

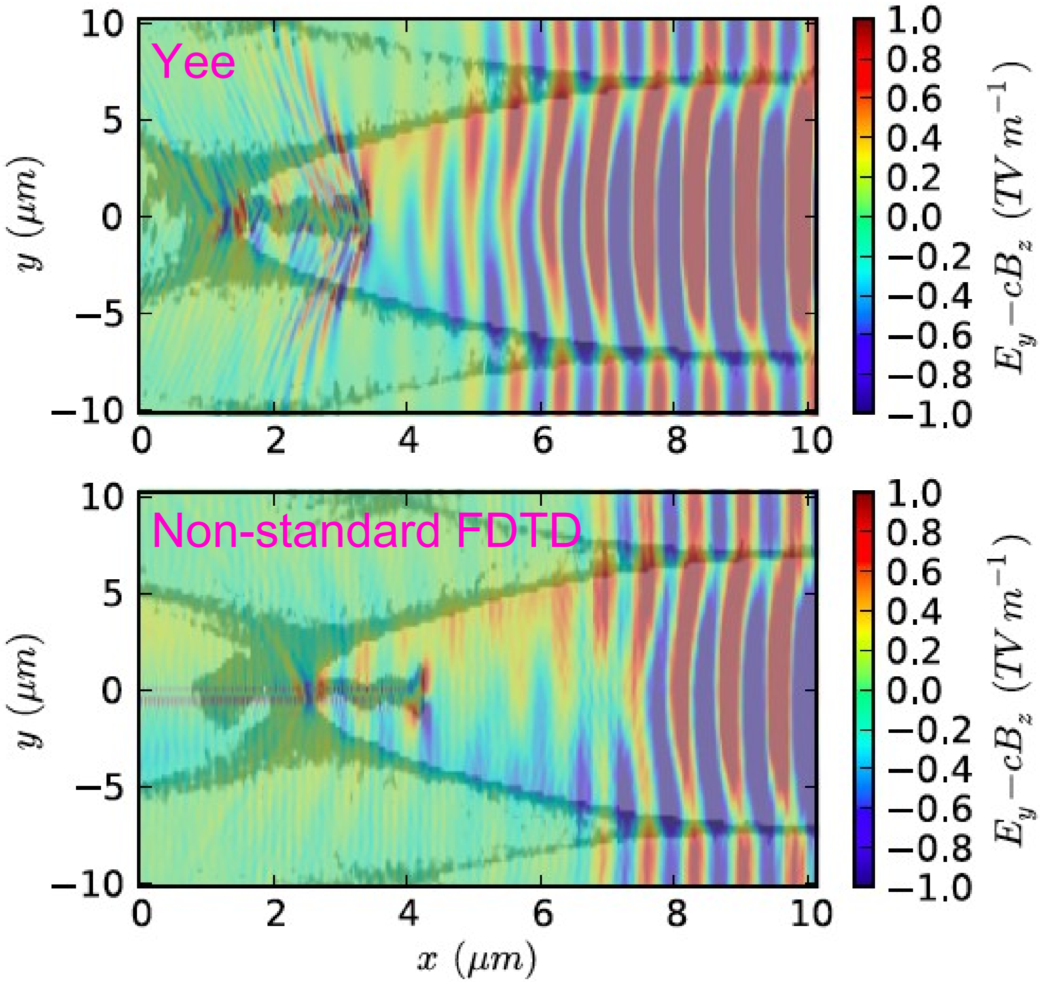
L_{deph}=4.3 cm



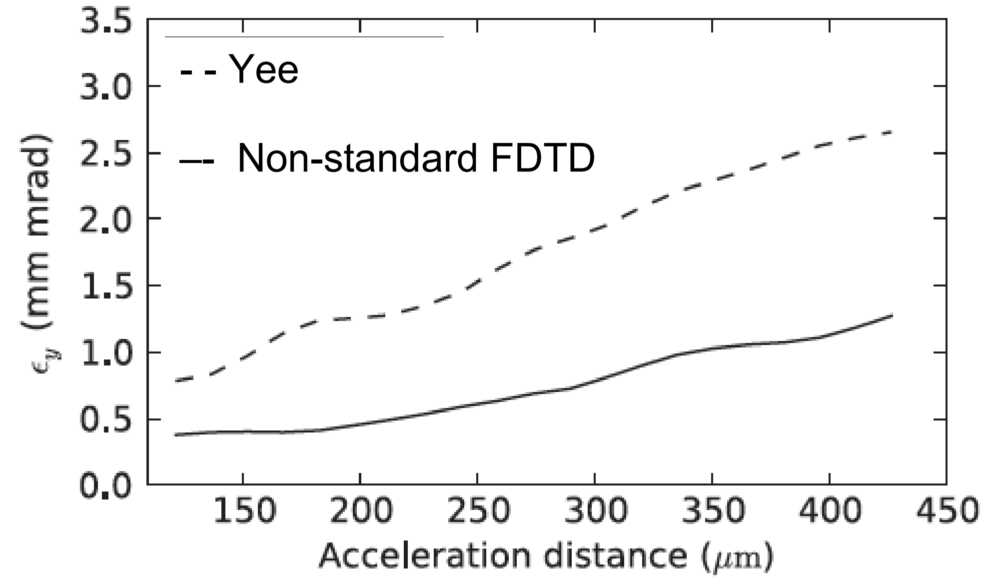
LR: Δz=λ/16
HR: Δz=λ/32

Cowan et al, PRSTAB 16, 041303 (2013)

Suppression of numerical Cherenkov radiation with non-standard FDTD



→ No spurious Cherenkov radiation around the bunch



→ Less emittance growth

Lehe et al, PRSTAB 16, 021301 (2013)

Improved dispersion with high-order finite difference schemes in space and time/1

Temporal evolution => Runge-Kutta 4 (for particles and fields)

Spatial derivatives $\Rightarrow$ **(compact) high order schemes** [S.K. Lele, JCP **103**, 16 (1992)]
Denoting by f_i/f'_i the function/derivative on the $i-th$ grid point

$$\alpha f'_{i-1} + f'_i + \alpha f'_{i+1} = a\,\frac{f_{i+1}-f_{i-1}}{2h} + b\,\frac{f_{i+2}-f_{i-2}}{4h} + c\,\frac{f_{i+3}-f_{i-3}}{6h} \qquad (*)$$

$\Rightarrow$ relation between a, b, c and α by matching the Taylor expansion of (*)
$\Rightarrow$ if $\alpha \neq 0$, f'_i obtained by solving a **tri-diagonal** linear system
$\Rightarrow$ "classical" 2^{nd} order: $\alpha = b = c = 0,\ a = 1$

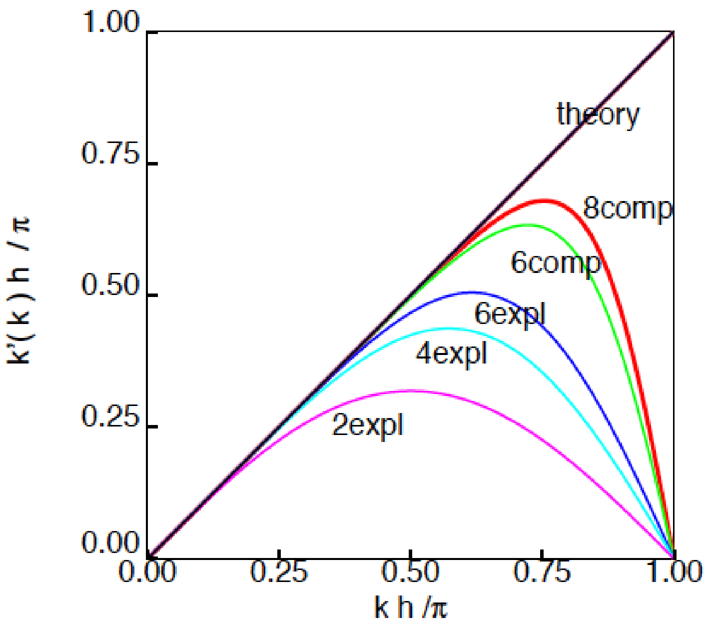
*** Improvement of the spectral accuracy ***
considering (on the grid) the "test" function

$$f \sim \exp(i\,k\,x)$$

its numerical derivative $\partial/\partial x$ is

$$f' \sim ik'(k)\exp(i\,k\,x)$$

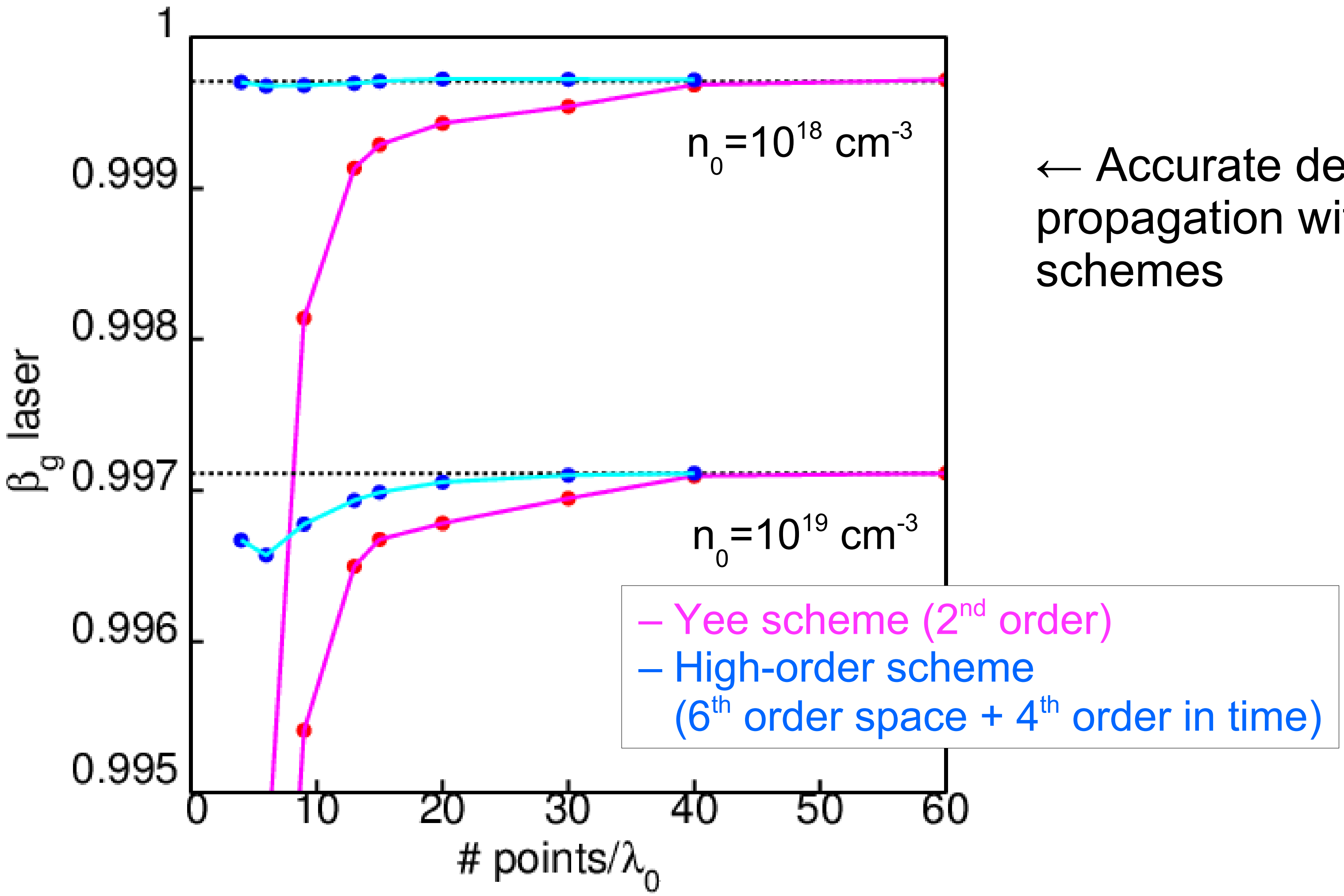
where, in general, $k'(k) \neq k$ $\quad\Rightarrow\Rightarrow\Rightarrow\Rightarrow$



Benedetti et al, IEEE Transactions on Plasma Science 36, 1790 (2008)

Improved dispersion with high-order finite difference schemes in space and time/2

$\beta_g \approx 1 - \lambda_0^2/(2\lambda_p^2)$ [1D limit], $a_0 << 1$



← Accurate description of laser propagation with high-order schemes

Pseudo Spectral Analytical Time Domain (PSATD) scheme

- PSATD scheme [1] features a Fourier representation for Maxwell equations
  - derivatives → multiplications in k-space
  - analytical time integration over Δt (if source assumed constant)

$$\frac{\partial \tilde{\mathbf{E}}}{\partial t} = i\mathbf{k} \times \tilde{\mathbf{B}} - \tilde{\mathbf{J}}$$
$$\frac{\partial \tilde{\mathbf{B}}}{\partial t} = -i\mathbf{k} \times \tilde{\mathbf{E}}$$

→

$$\begin{aligned}
\tilde{\mathbf{E}}^{n+1} &= C\tilde{\mathbf{E}}^{n} + iS\hat{\mathbf{k}} \times \tilde{\mathbf{B}}^{n} - \frac{S}{k}\tilde{\mathbf{J}}^{n+1/2} \\
&+ (1-C)\hat{\mathbf{k}}(\hat{\mathbf{k}} \cdot \tilde{\mathbf{E}}^{n}) \\
&+ \hat{\mathbf{k}}(\hat{\mathbf{k}} \cdot \tilde{\mathbf{J}}^{n+1/2})(\frac{S}{k} - \Delta t), \\
\tilde{\mathbf{B}}^{n+1} &= C\tilde{\mathbf{B}}^{n} - iS\hat{\mathbf{k}} \times \tilde{\mathbf{E}}^{n} \\
&+ i\frac{1-C}{k}\hat{\mathbf{k}} \times \tilde{\mathbf{J}}^{n+1/2}.
\end{aligned}$$

where C=cos(kΔt) S=sin(kΔt)

==> no CFL condition
==> **strongly** mitigates numerical dispersion problems (better at low density, no dispersion in vacuum)

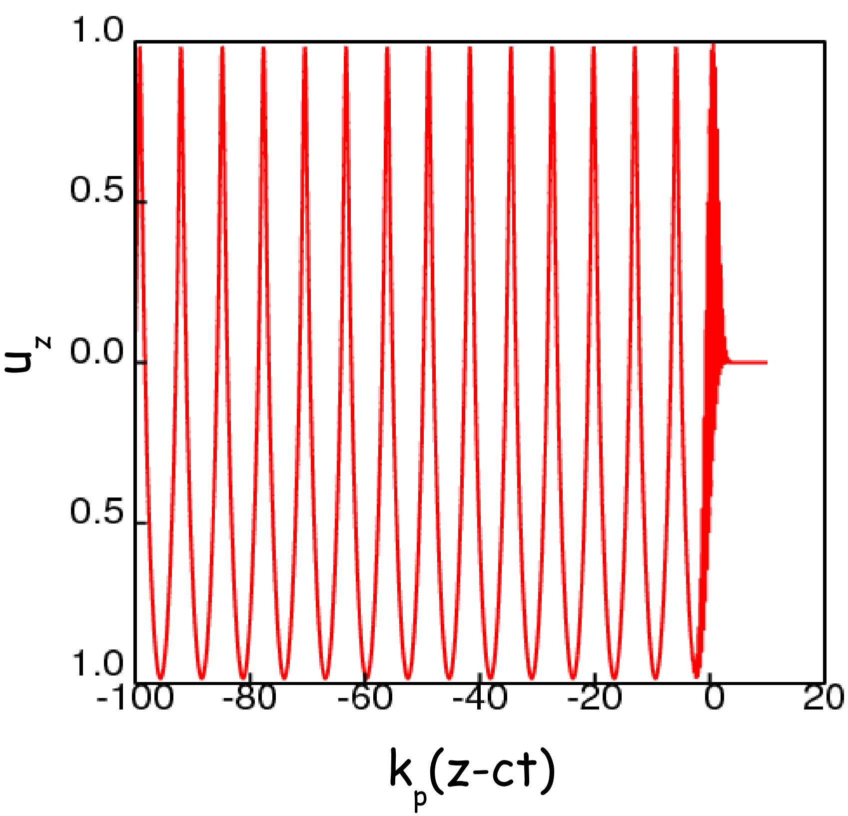
1. I. Haber et al., Advances In Electromagnetic Simulation Techniques, in Proc. Sixth Conf. Num. Sim. Plasmas, (Berkeley, Ca, 1251 1973)
2. J.-L. Vay et al., Journal of Computational Physics 243, 260 (2013)

Unphysical kinetic effects

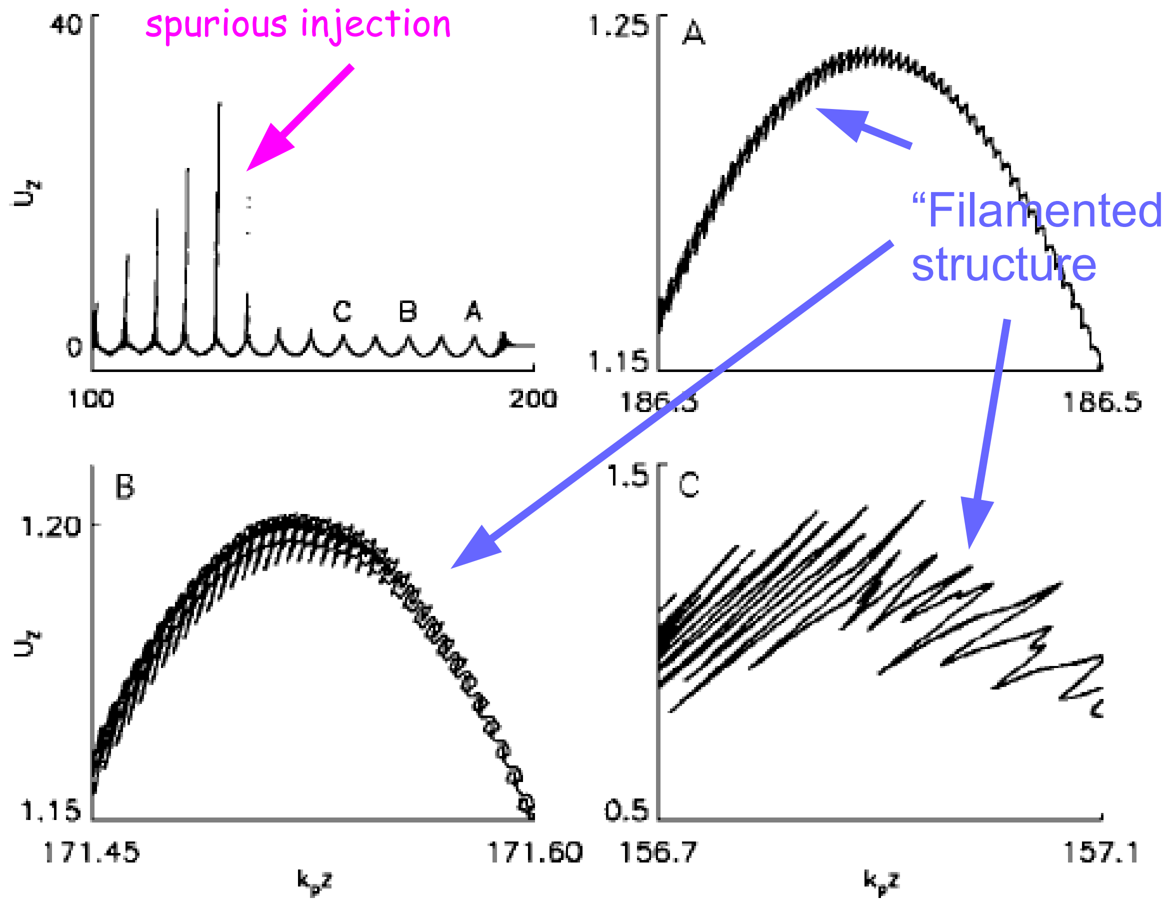
PIC simulations of LPAs show unphysical kinetic heating (≠ grid heating)/1

FLUID (exact Vlasov solution) VS PIC simulation of a dark current free LPA (a_0=2, k_0/k_p=10, k_pL=2)

Fluid simulation



PIC simulation

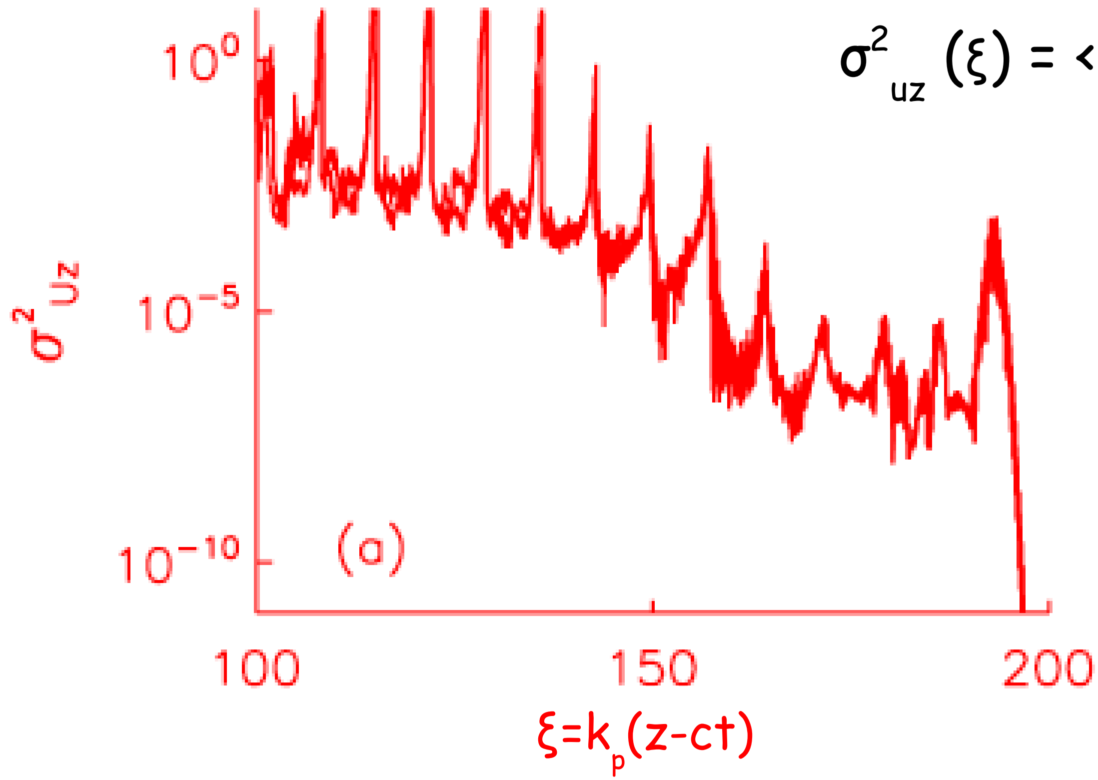


→ Spurious (unphysical) particle injection

Cormier-Michel et al., Phys. Rev. E 78, 016404 (2008)

PIC simulations of LPAs show unphysical kinetic heating (≠ grid heating)/2

Temperature of the plasma behind the laser (initially the plasma is cold)



$\sigma^2_{uz}(\xi) = \langle(u_z-\langle u_z\rangle)^2\rangle \approx k_B T/mc^2$

$\lambda_D = (k_b T/4\pi n_0 e^2)^{1/2}$

$k_g = 2\pi/\Delta z$

→ faster growth than "standard" grid heating* (unresolved λ_D);

→ temperatures greatly exceeds the value for which $k_g\lambda_D \sim 1$;

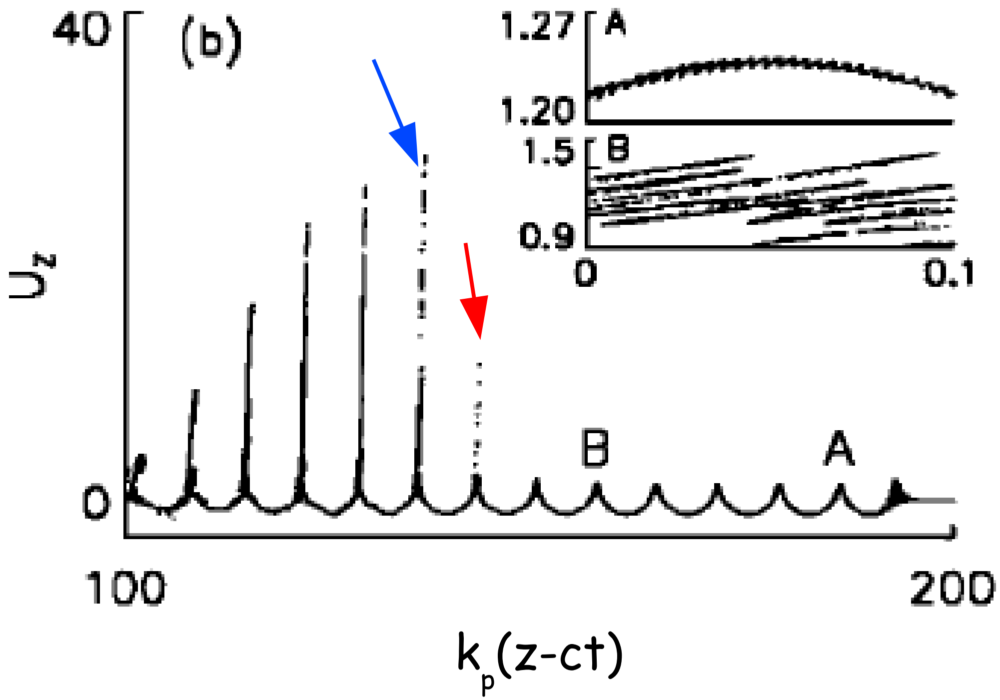
→ origin not well understood (but clearly related to interpolation, resolution, particle sampling, etc.);

*C. K. Birdsall and A. B. Langdon, Plasma Physics Via Computer Simulation (Adam-Hilger, 1991)

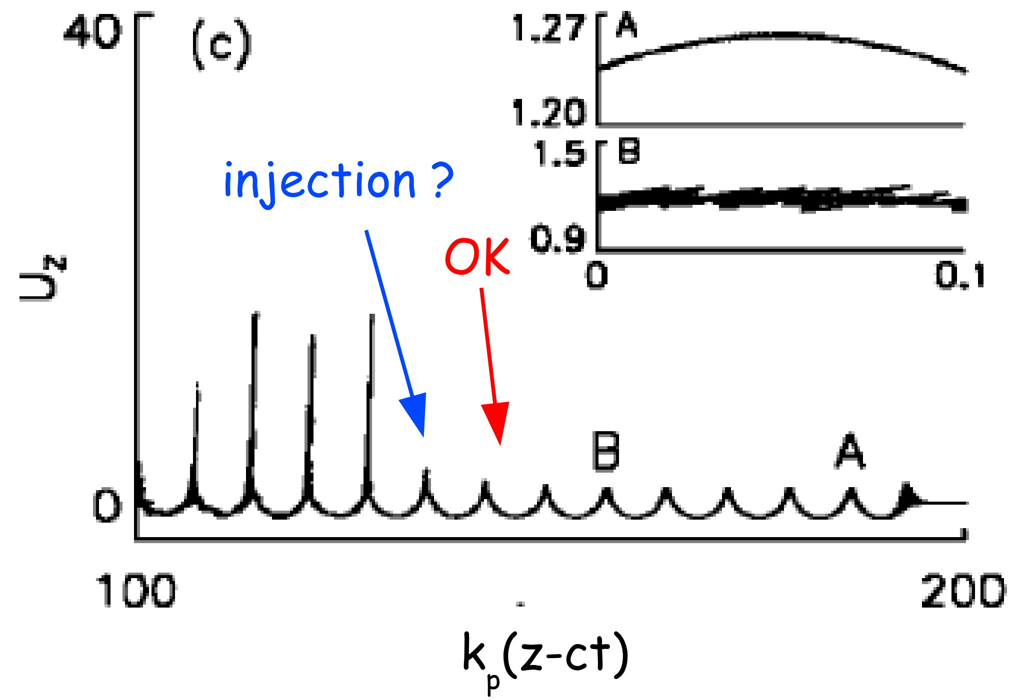
Reducing the spurious kinetic heating by increasing the resolution

Changing resolution Δz (N_{ppc}=400, linear interpolation)

$\Delta_z=\lambda_0/30$



$\Delta_z=\lambda_0/60$

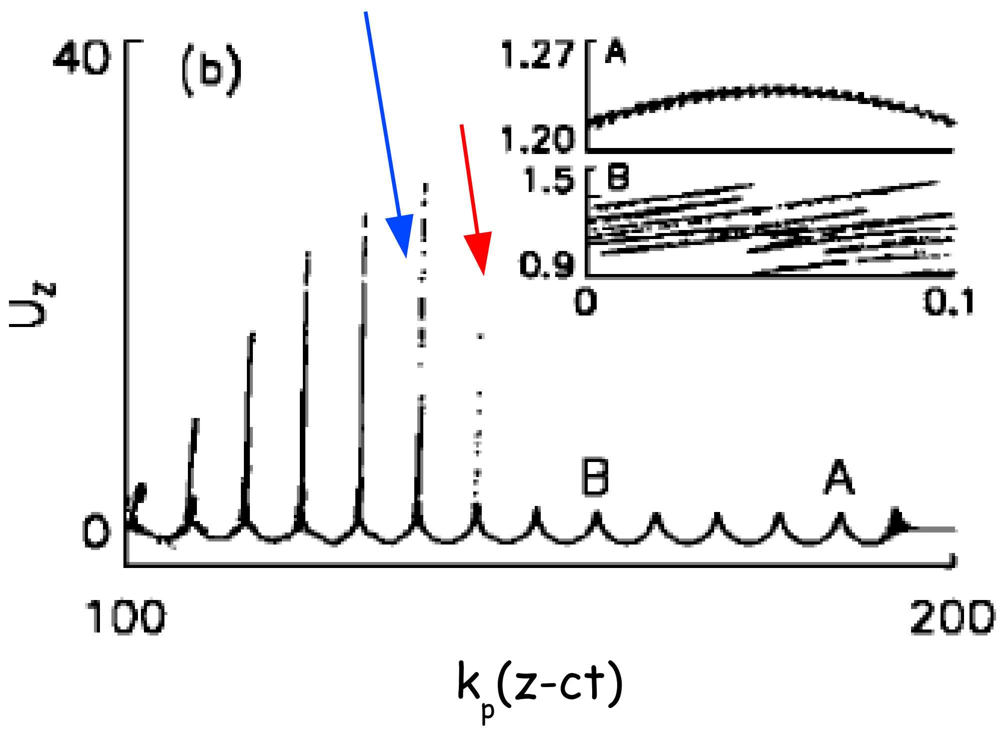


→ Computational cost ~ Δz^{-2}

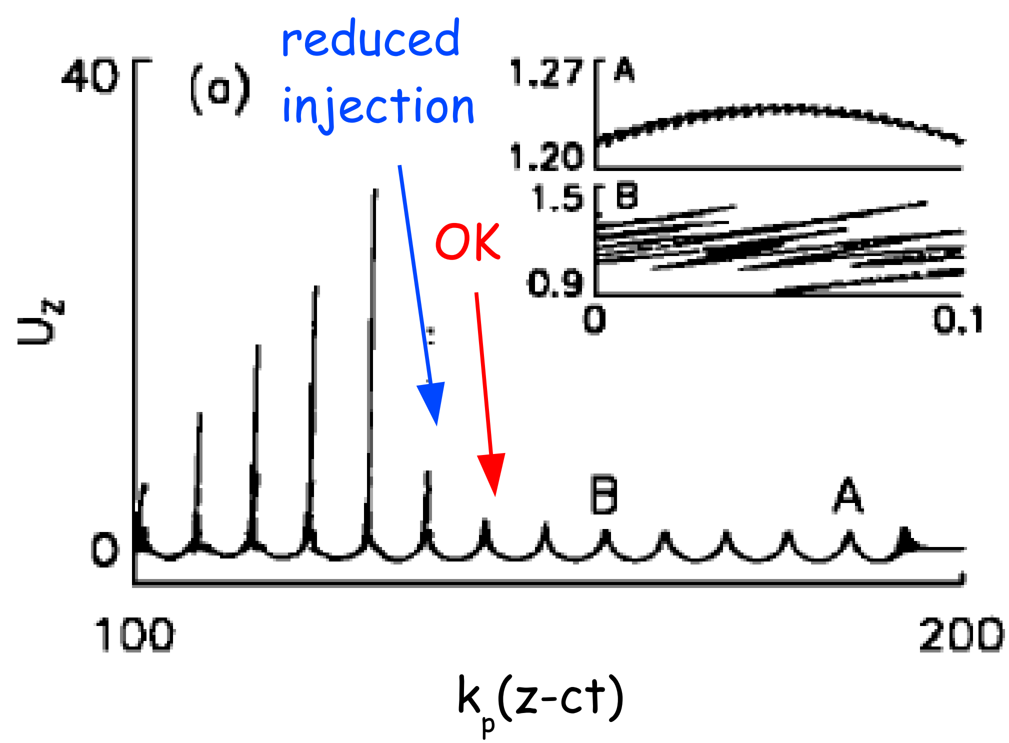
Reducing the spurious kinetic heating by increasing the number of particles per cell

Changing the number of PPC (Δz =1/30, linear interpolation)

Nppc = 100



Nppc = 400

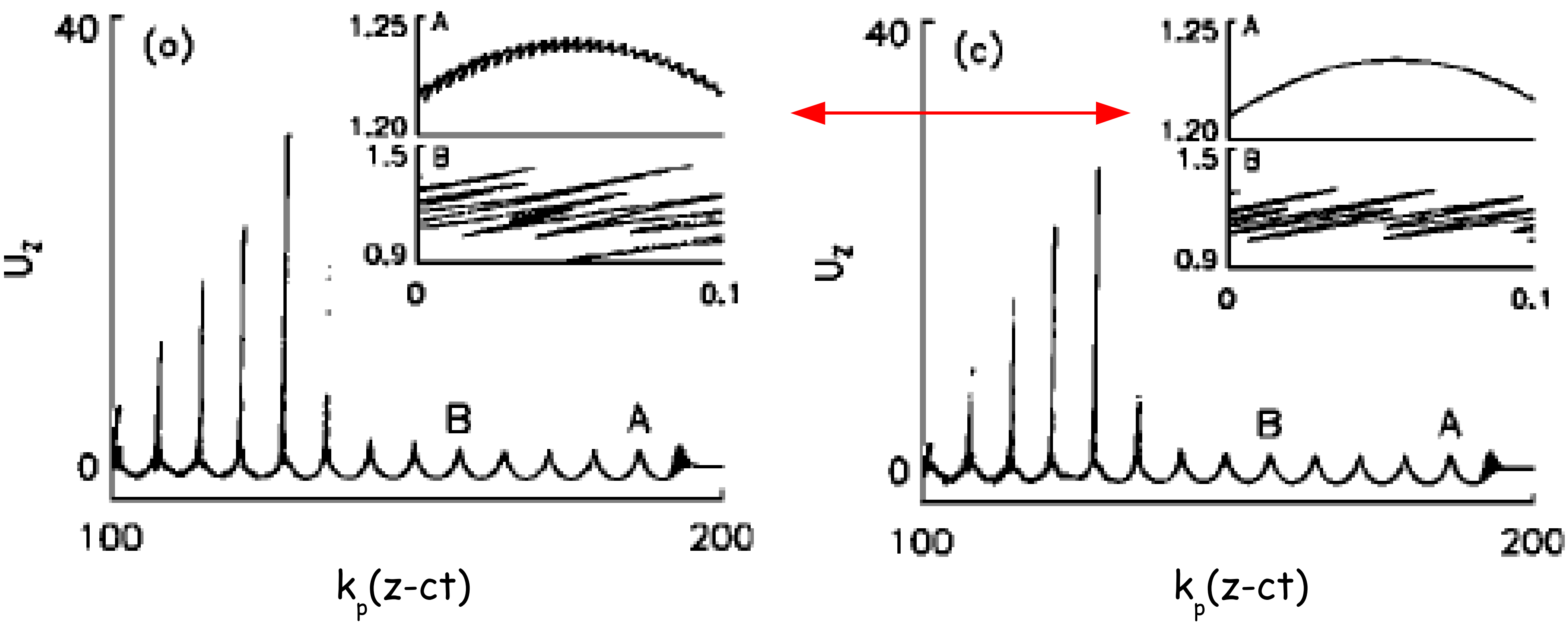


→ Computational cost ~ Nppc

Reducing the spurious kinetic heating by increasing the order of the shape function

Changing shape-function (Nppc=400, $\Delta z=\lambda_0/30$)

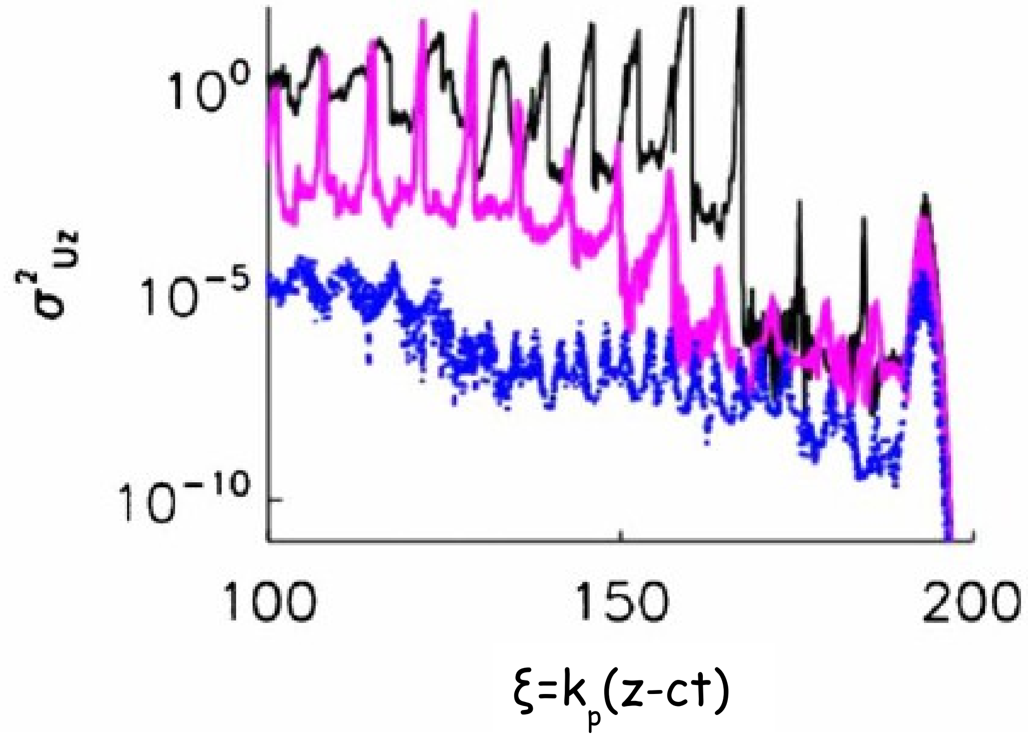
g_0 (linear interpolation) g_1 (quadratic interpolation)



→ Computational cost ~ $(n+2)^d$

Spurious kinetic heating stronger at higher laser intensity

Temperature in the plasma for different laser intensities (Nppc=400, $\Delta z=\lambda_0/36$)



- $a_0=3$
- $a_0=2$
- $a_0=1$

Summary on spurious kinetic heating

- Plasma momentum spread increases rapidly as a function of distance behind the drive laser pulse even when it shouldn't;

- Spurious heating much faster than conventional grid heating in thermal plasmas, final “temperature” much higher;

- Particle phase space develops a complex “filamented” structure;

- Numerical particle orbits develop errors in momentum/position compared to the fluid orbit;

- Affects self-injection dynamics;

- Spurious kinetic heating can be controlled by increasing resolution, increasing number particles per cell and increasing the order of the interpolation. However, **very slow convergence** for a large box (i.e., several plasma periods);

- Analysis performed in 1D but trends apply to 2D (and 3D). In 2D effect of laser polarization important.

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