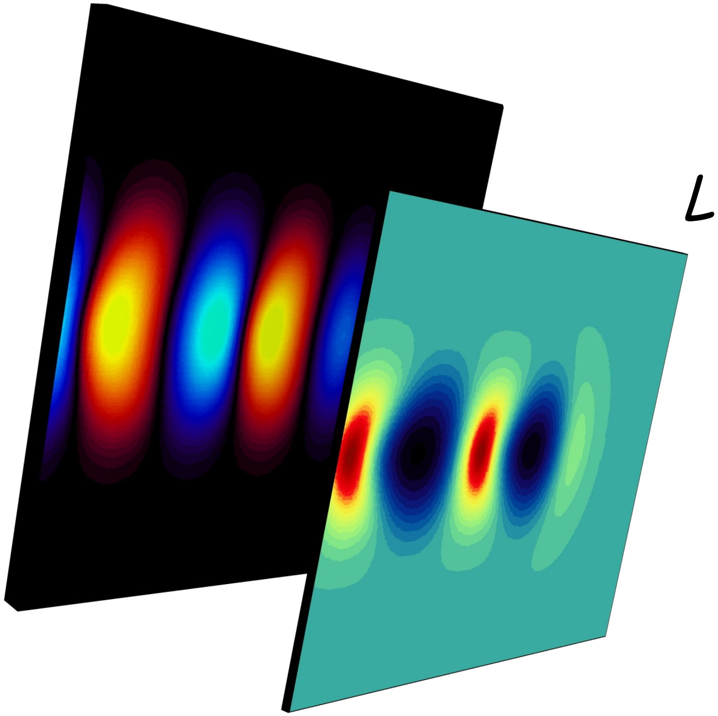
Efficient Modeling of Laser-Plasma Accelerators Using the Ponderomotive-Based Code INF&RNO



Carlo Benedetti
Lawrence Berkeley National Laboratory

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Coworkers

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F. Rossi, P. Londrillo, G. Servizi & G. Turchetti

Department of Physics, University of Bologna, Italy

Overview

- challenges in modeling laser-plasma accelerators (LPAs) over distances ranging from cm to m scales

- the code INF&RNO (INtegrated Fluid & paRticle simulatioN cOde)
  - ✓ basic equations, numerics and features of the code
  - ✓ validation tests and performance

- applications
  - ✓ modeling of current LOASIS experiments (tunable LPA)
  - ✓ modeling of 10 GeV LPA stage for BELLA (BErkeley Lab Laser Accelerator)

- conclusions

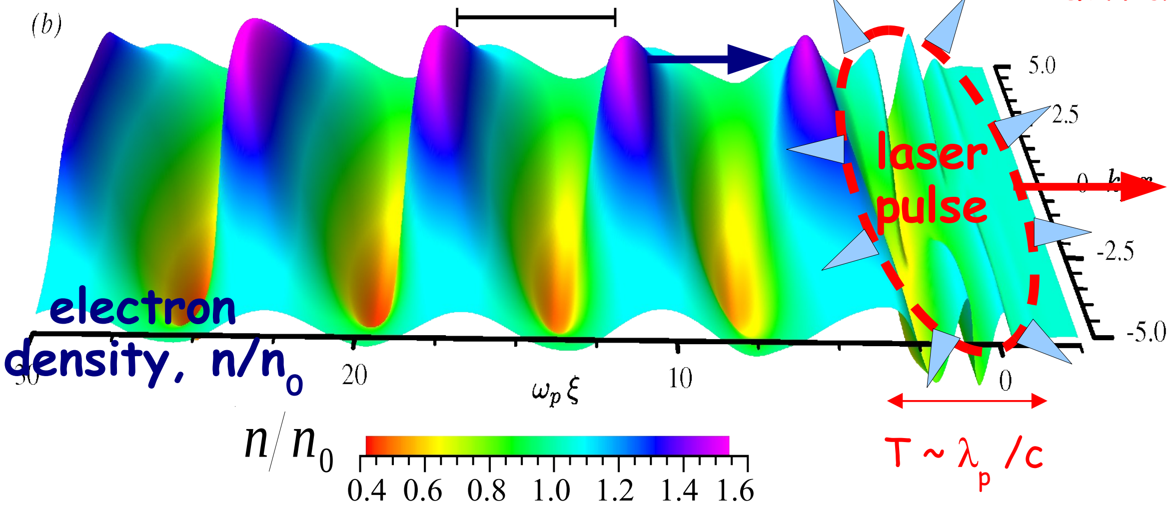
Laser-plasma accelerators*: 1-100 GV/m accelerating gradients

- **Plasma waves**

$\lambda_p \sim n_0^{-1/2}$
$\approx$ 10-100 µm

$v_{phase} \sim v_{laser} \sim c$

laser:
ultra-short (T ~ tens of fs)
ultra-intense ($I_0 > 10^{18}$ W/cm^2)



T ~ λ_p /c

$$a_0 = eA_0^{laser}/mc^2 \propto (I_0 \lambda_0^2)^{1/2}$$

ponderomotive force:

$$F_p \sim -(1/2\gamma)\ \mathrm{grad}\ (a^2/2)$$

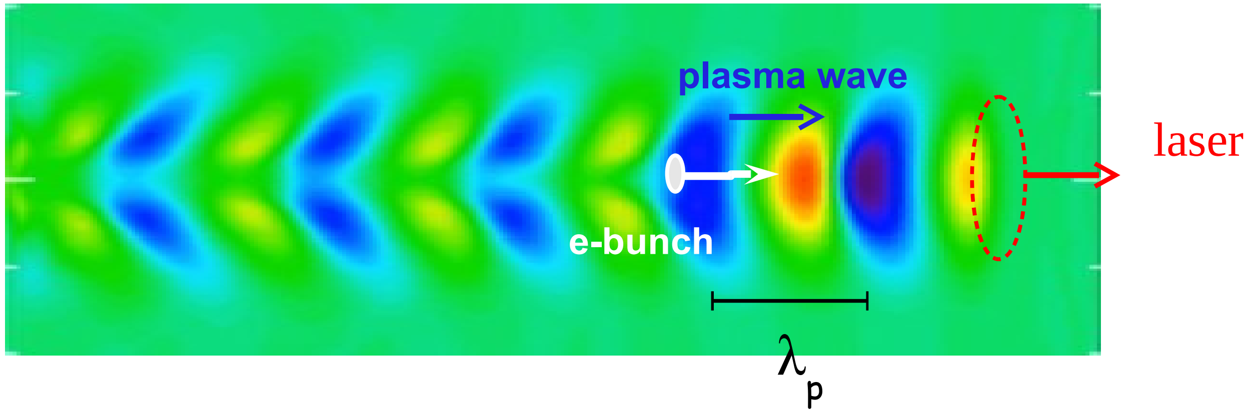
- **Wakefields** (due to charge separation: ion at rest VS displaced electrons)

$$E_z \sim mc\omega_p/e \sim 100\ [\mathrm{V/m}] \times (n_0[\mathrm{cm}^{-3}])^{1/2}$$

e.g.: for $n_0 \sim 10^{18}$ cm^{-3}, $I_0 \sim 10^{18}$ W/cm^2 ===> **E_z ~ 100 GV/m**,
~ 10^3 larger than conventional RF accelerators

*Tajima and Dawson, PRL (1979)

Energy gain in a (single stage) LPA



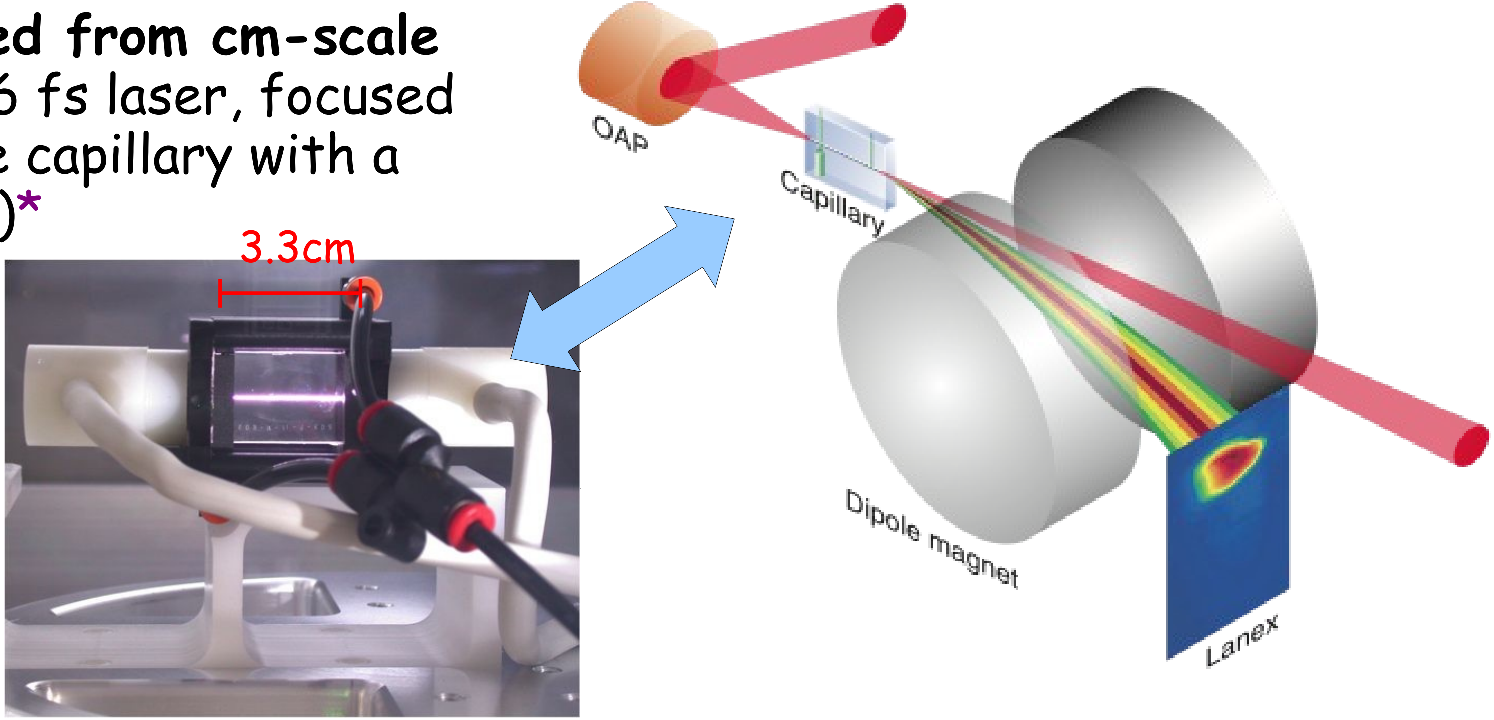
Limits to single stage energy gain:

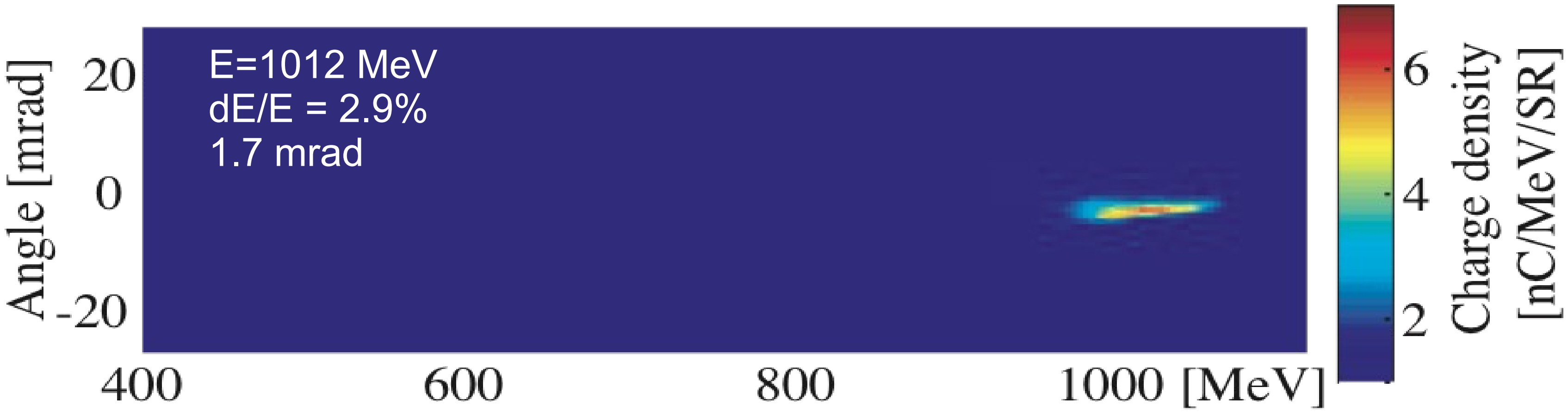
- laser diffraction (~ Rayleigh range)
  → mitigated by transverse plasma density tailoring (plasma channel) and/or self-focusing
- beam-wave dephasing
  $\beta_{bunch} \sim 1$, $\beta_{wave} \sim 1-\lambda_0^2/(2\lambda_p^2) \rightarrow$ slippage $L_d \propto \lambda_p / (\beta_{bunch}-\beta_{wave}) \sim n_0^{-3/2}$
  → mitigated by longitudinal density tailoring
- laser energy depletion → energy loss into plasma wave excitation

Energy gain (single stage) ~ n_0^{-1}

Experimental demonstration: 1 GeV high-quality beam from LPA

GeV e-bunch produced from cm-scale plasma (using 1.5 J, 46 fs laser, focused on a **3.3 cm** discharge capillary with a density of 4x10^{18} cm^{-3})*





*Leemans *et al.*, Nature Phys. (2006); Nakamura *et al.*, Phys. Plasmas (2007)

3D full-scale modeling of an LPA over cm to m scales is a 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

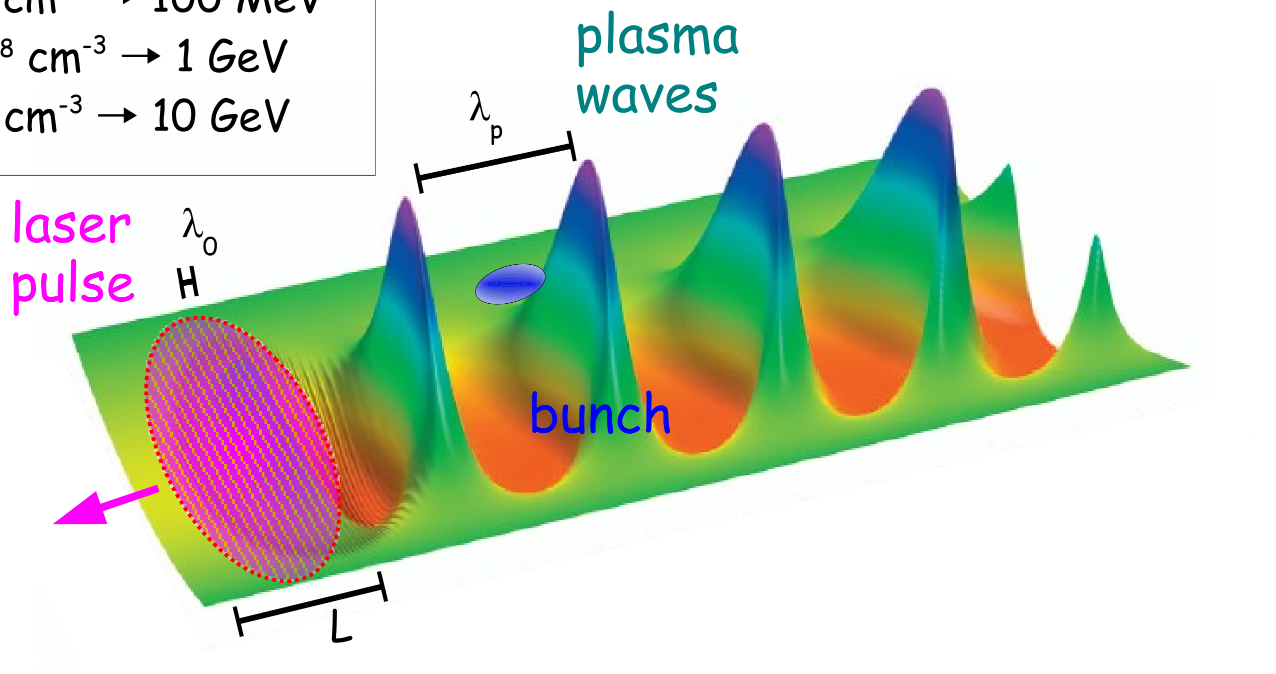
Simulation complexity:

$\propto (D/\lambda_0) \times (\lambda_p/\lambda_0)$

$\propto (D/\lambda_0)^{4/3}$ [if D is deph. length]

3D explicit PIC simulation:

- ✓ 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~~



The INF&RNO framework: motivations

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, different simulations (exploration of the parameter space, optimization, convergence check, etc..)

Reduced Models[#,%,^,&,@]

[drawbacks/issues: neglecting some aspects of the physics depending on the particular approximation made]

[#] Mora & Antonsen, Phys. Plas. (1997) [WAKE]
[%] Huang, et al., JCP (2006) [QuickPIC]
[^] Lifshitz, et al., JCP (2009) [CALDER-circ]
[&] Cowan, et al., JCP (2011) [VORPAL/envelope]
[@] Benedetti, et al., AAC2010 + submitted (2012) [INF&RNO]

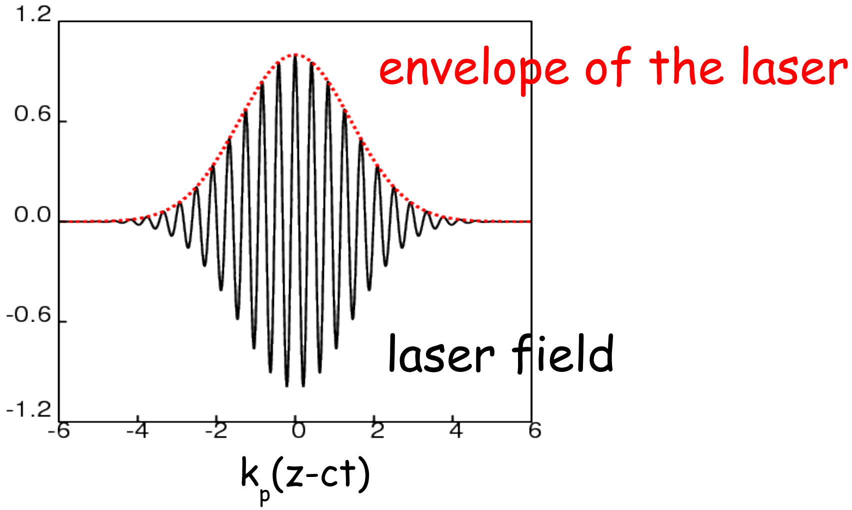
Boosted Lorentz Frame[*]

[drawbacks/issues: control of numerical instabilities, self-injection to be investigated, under-resolved physics (e.g. RBS)]

[*] Vay, PRL (2007)

INF&RNO* is orders of magnitude faster than full PIC codes still retaining physical fidelity

INF&RNO ingredients:



- envelope model for the laser
  - ✓ no λ_{laser}
  - ✓ axisymmetric
- 2D cylindrical (r-z)
  - ✓ self-focusing & diffraction for the laser as in 3D
  - ✓ significant reduction of the computational complexity
    ... but only axisymmetric physics
- ponderomotive approximation to describe laser → plasma interaction
  - ✓ (analytical) averaging over fast oscillations in the laser field
  - ✓ => scales @ λ_{laser} are removed from the plasma model
- PIC & (cold) fluid
  - ✓ fluid → noiseless and accurate for linear/mildly nonlinear regimes
  - ✓ integrated modalities (e.g., PIC for injection, fluid acceleration)
  - ✓ hybrid simulations (e.g., fluid background + externally injected bunch)

* Benedetti *et al.*, Proc. of AAC10 (2010); Benedetti *et al.*, Proc. of PAC11 (2011); Benedetti *et al.*, JCP, submitted

The *INF&RNO* framework: physical model

The code adopts the "comoving" normalized variables $\xi = k_p(z - ct)$, $\tau = \omega_p t$

- laser pulse (envelope)

* deep into depletion
* rel. invariance
* backwards propag waves

$$a_\perp = \frac{\hat{a}(\xi, r)}{2} e^{i(k_0/k_p)\xi} + c.c. \quad \rightarrow \quad \left(\nabla_\perp^2 + 2i\frac{k_0}{k_p}\frac{\partial}{\partial\tau} + 2\frac{\partial^2}{\partial\xi\partial\tau} \boxed{-\frac{\partial^2}{\partial\tau^2}}\right)\hat{a} = \frac{\delta}{\gamma_{\text{fluid}}}\hat{a}$$

- wakefield (fully electromagnetic)

$$\frac{\partial E_r}{\partial\tau} = \frac{\partial(E_r - B_\phi)}{\partial\xi} - J_r \qquad \frac{\partial E_z}{\partial\tau} = \frac{\partial E_z}{\partial\xi} + \frac{1}{r}\frac{\partial(rB_\phi)}{\partial r} - J_z \qquad \frac{\partial B_\phi}{\partial\tau} = -\frac{\partial(E_r - B_\phi)}{\partial\xi} + \frac{\partial E_z}{\partial r}$$

- plasma

$$\text{PIC} \rightarrow \begin{cases} \forall j = 1, \ldots, N_p \\ \frac{d\xi_j}{d\tau} = \beta_{z,j} - 1 \qquad \frac{du_{z,j}}{d\tau} = -\frac{\partial\gamma_j}{\partial\xi} - E_z - \beta_r B_\phi \\ \frac{dr_j}{d\tau} = \beta_{r,j} \qquad \frac{du_{r,j}}{d\tau} = -\frac{\partial\gamma_j}{\partial r} - E_r + \beta_z B_\phi \\ \gamma_j = \sqrt{1 + |\hat{a}|^2/2 + u_{z,j}^2 + u_{r,j}^2} \end{cases} \qquad \text{fluid} \rightarrow \begin{cases} \frac{\partial\delta}{\partial\tau} = \frac{\partial\delta}{\partial\xi} - \nabla\cdot(\vec{\beta}\delta) \\ \frac{\partial(\delta u_j)}{\partial\tau} = \frac{\partial(\delta u_j)}{\partial\xi} - \nabla\cdot(\vec{\beta}\delta u_j) + \\ \quad + \delta\left(-(\mathbf{E} + \vec{\beta}\times\mathbf{B}) - \frac{1}{2\gamma_{\text{fluid}}}\nabla\frac{|\hat{a}|^2}{2}\right)_j \\ \gamma_{\text{fluid}} = \sqrt{1 + |\hat{a}|^2/2 + u_z^2 + u_r^2} \end{cases}$$

where δ is the density and $\mathbf{J}$ the current density

The *INF&RNO* framework: numerical aspects

- longitudinal derivatives:
  - 2nd order **upwind** FD scheme → $(\partial_\xi f)_{i,j}=(-3f_{i,j} + 4f_{i+1,j} - f_{i+2,j}) /2\Delta_\xi$
  - BC easy to implement (unidirectionl "information" flux using ξ)

- transverse (radial) derivatives:
  - 2nd order **centered** FD scheme → $(\partial_r f)_{i,j}=(f_{i,j+1} - f_{i,j-1}) /2\Delta_r$
  - fields are not singular in r=0, from symmetry we have

$$\partial_r E_z = 0, \quad E_r = B_\phi = 0, \quad \lim_{r\to 0} E_r/r = \partial E_r/\partial r|_0, \quad \lim_{r\to 0} B_\phi/r = \partial B_\phi/\partial r|_0$$

- time integration for plasma / EM wakefield: **RK2** [fluid] / **RK4** [PIC]

- **quadratic shape** function for force interpolation/current deposition [PIC]

- **digital filtering** for current and/or fields smoothing [PIC]
  - N*binomial filter (1, 2, 1) + compensator
  - compact low-pass filter*: $\beta F_{i-1}+F_i+ \beta F_{i+1} = \sum_{k=0,2} a_k(\beta) (f_{i+k}+ f_{i-k})/2$

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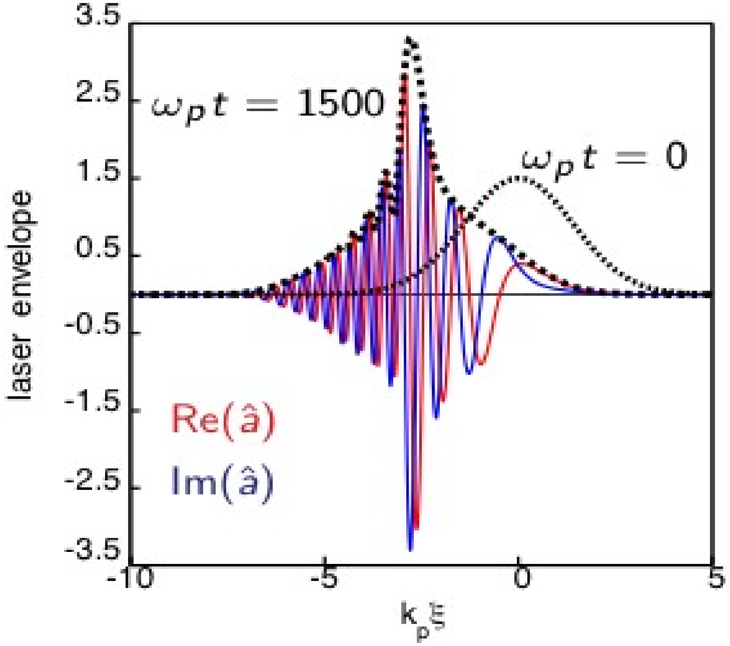
* Shang, JCP (1999)

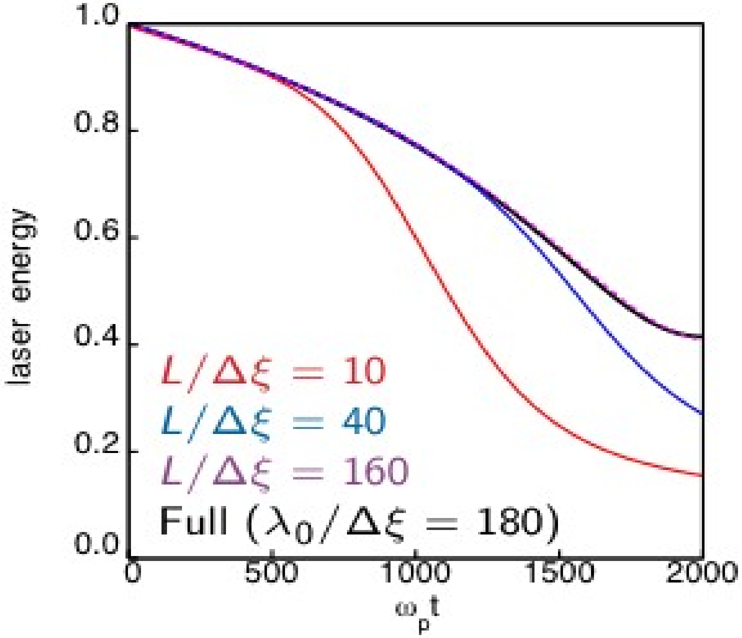
The *INF&RNO* framework: improved laser envelope solver/1

- envelope description: $a_{laser} = \underset{\text{“slow”}}{\underset{\uparrow}{\hat{a}}}\ \underset{\text{“fast”}}{\underset{\uparrow}{\exp[ik_0}}(z-ct)]/2 + \text{c.c.}$

  - early times: NO need to resolve λ_0 (~ 1 μm), only $L_{env} \sim \lambda_p$ (~ 10-100 μm)
  - later times: laser-pulse redshifting → structures **smaller** than L_{env} **arise** in $\hat{a}$ (mainly in Re[$\hat{a}$] and Im[$\hat{a}$]) 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?

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

The *INF&RNO* framework: improved laser envelope solver/2

- envelope evolution equation is discretized in time using using a 2nd order Crank-Nicholson scheme

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

- FD form for ∂/∂ξ → **unable to deal** with unresolved structures in â

- INF&RNO uses a polar representation for â when computing ∂/∂ξ

(cartesian) (polar)

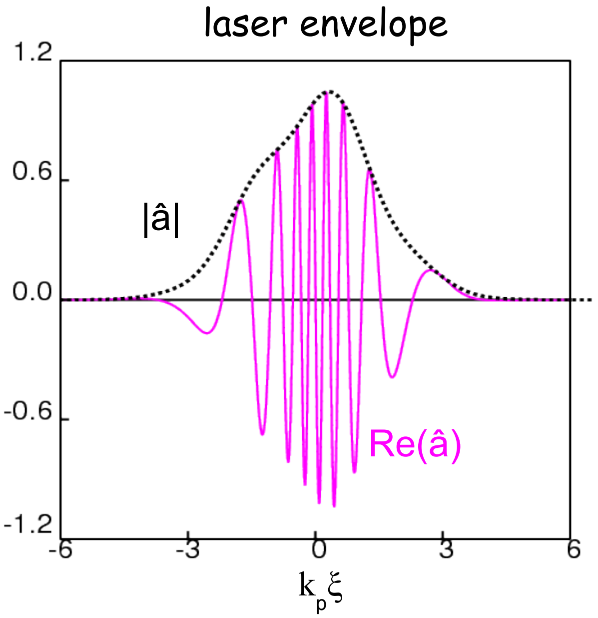
$$\hat{a}=\Re[\hat{a}]+i\Im[\hat{a}]=|\hat{a}|e^{i\theta}$$

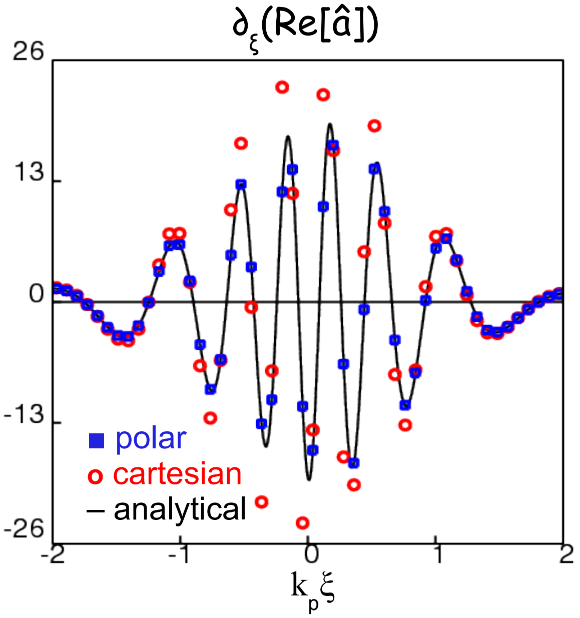
(cartesian)

(polar)

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

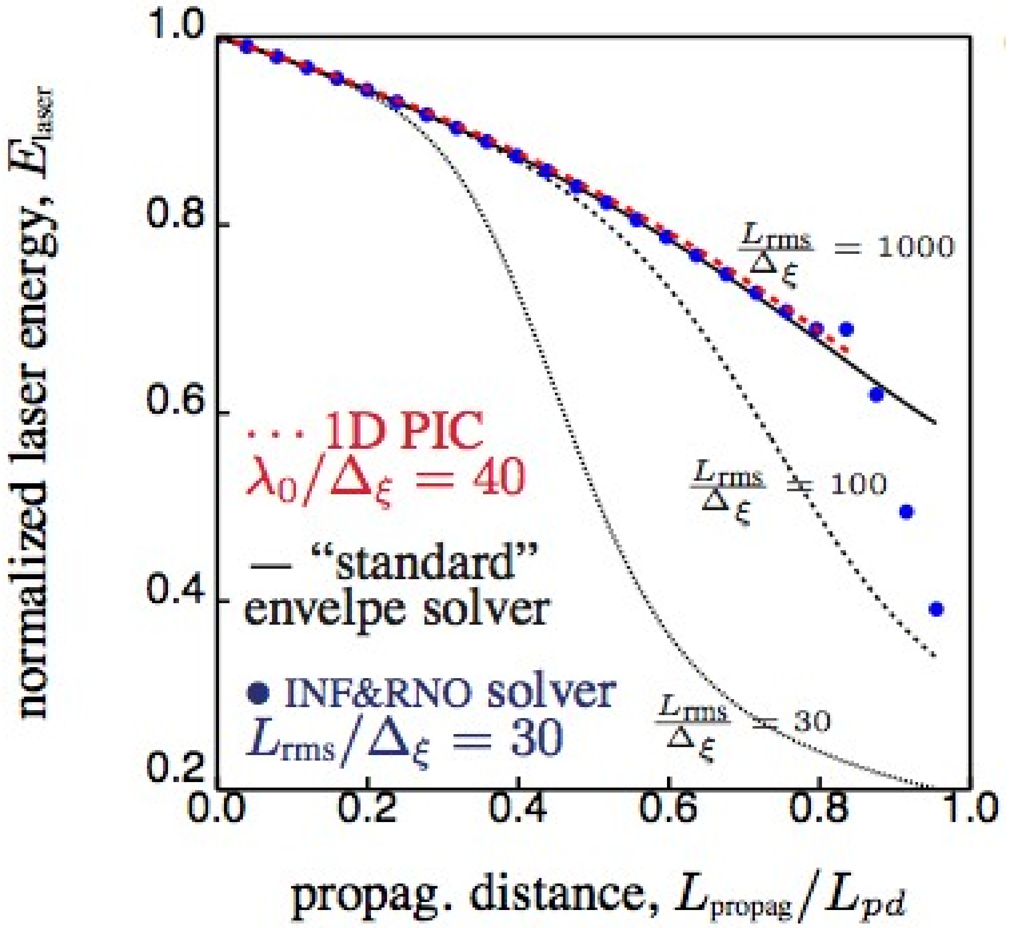
smoother behavior compared to **Re[â]** and **Im[â]**

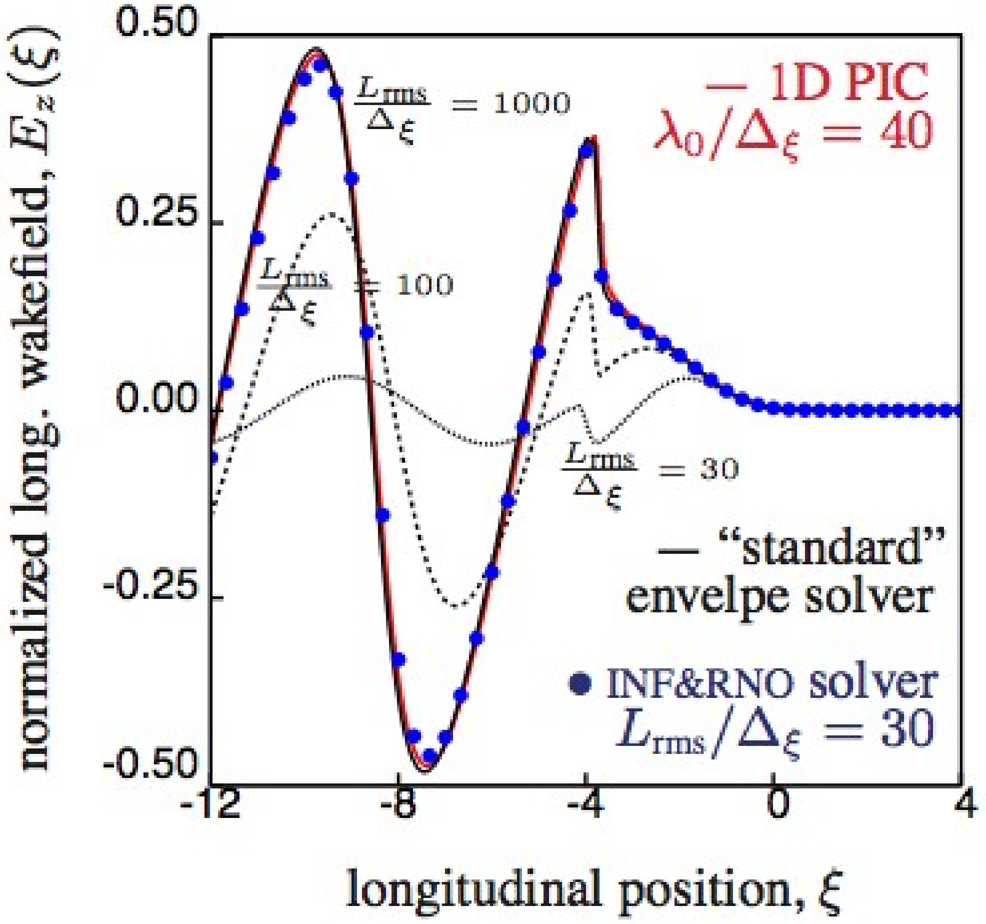




The *INF&RNO* framework: improved laser envelope solver/3

1D sim.: a_0=1, k_0/k_p=100, L_{rms} = 1 (parameters of interest for a 10 GeV LPA stage)





pump depletion length (resonant pulse): $L_{pd} \approx \lambda_p^3/\lambda_0^2 \approx 80$ cm

The *INF&RNO* framework: Lorentz Boosted Frame* (LBF) modeling/1

- The spatial/temporal scales involved in a LPA simulation DO NOT scale in the same way changing the reference frame

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

==> the LF ***is not*** the optimal frame to run a LPA simulation

==> simulation in the LBF is shorter (optimal frame is the one of the wake)

==> OK ***iff*** backwards propagating waves are negligible!

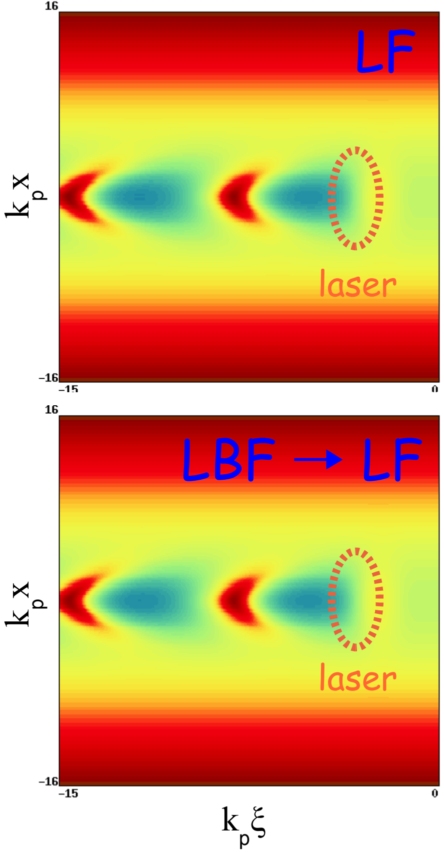
==> diagnostic more complicated (LBF ↔ LF loss of simultaneity)

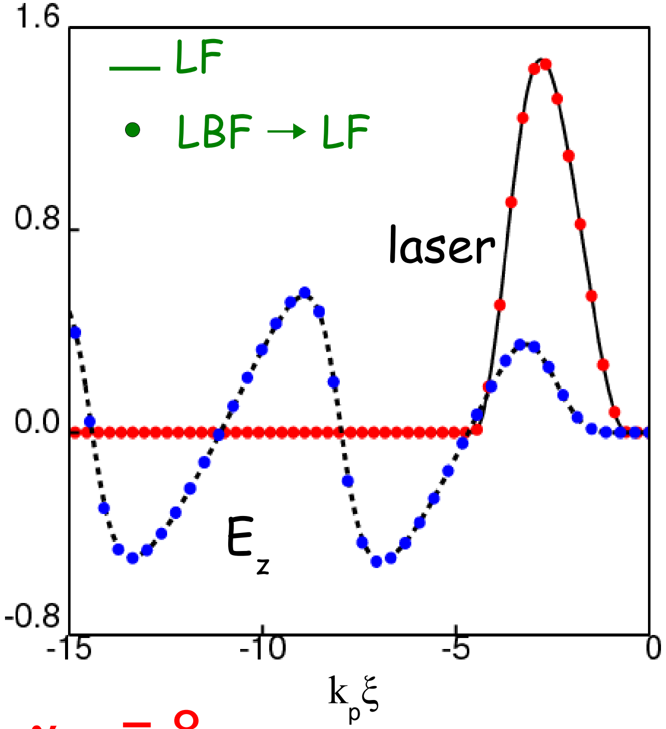
* Vay, PRL (2007); Vay, *et al.*, JCP (2011)

The *INF&RNO* framework: Lorentz Boosted Frame modeling/2

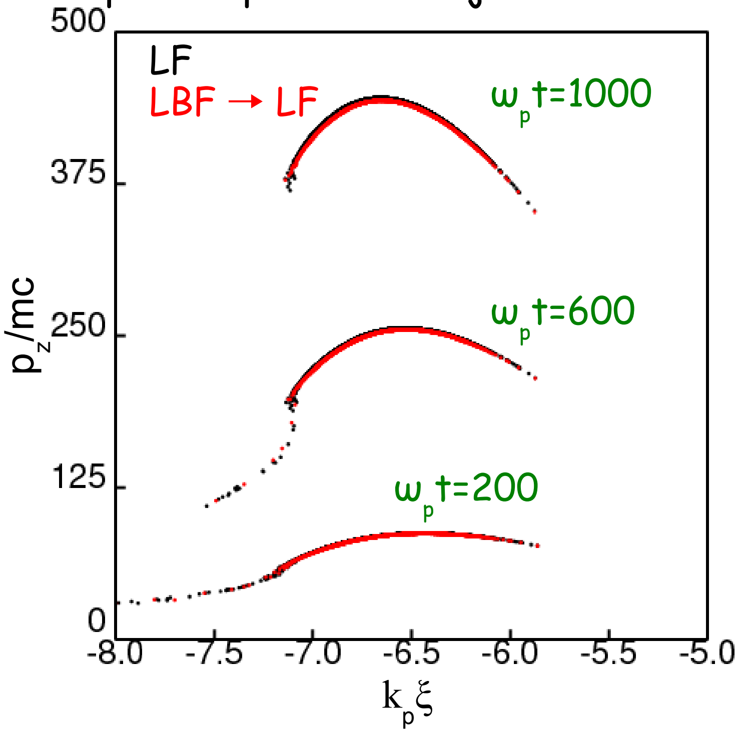
- LBF modeling implemented in INF&RNO/fluid (INF&RNO/PIC underway):
  - ✓ input/output in the Lab frame (swiping plane*, ***transparent*** for the user)
  - ✓ no instability observed at high γ_{LBF} (reported in 2D/3D PIC runs)
  - ✓ some of the approx. in the envelope model are not Lorentz invariant (limit max γ_{LBF})

electron density





phase space: ext. injected bunch



γ_{LBF}= 8

LF= 16h 47' VS LBF=15'

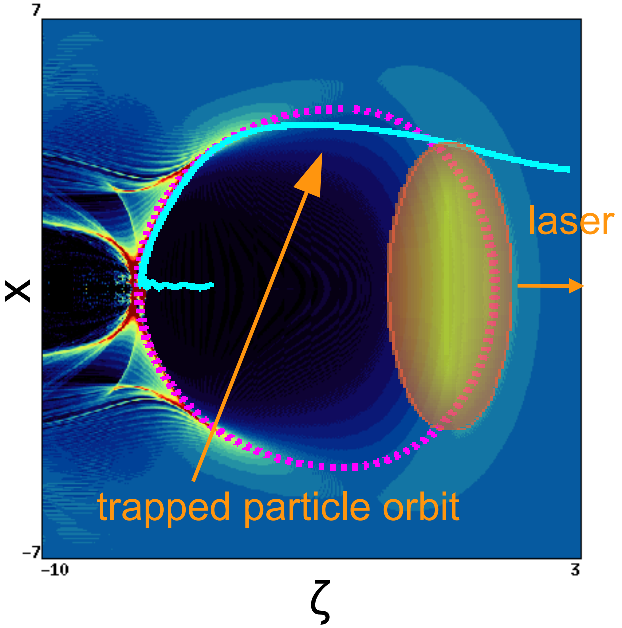
* Vay, JCP (2011)

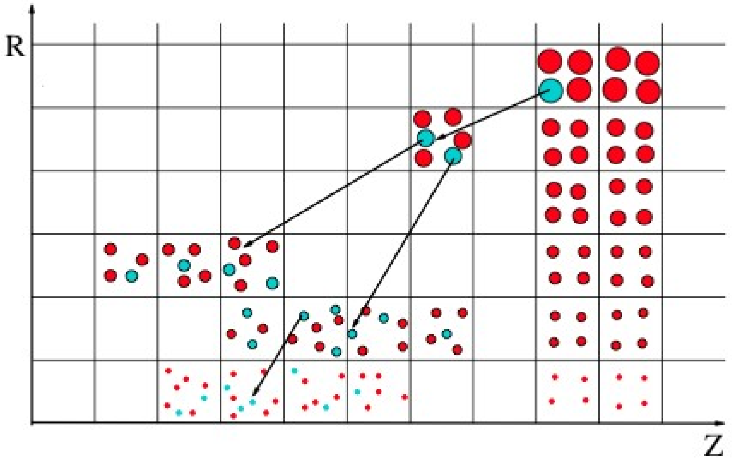
The *INF&RNO* framework: particle resampling to reduce noise

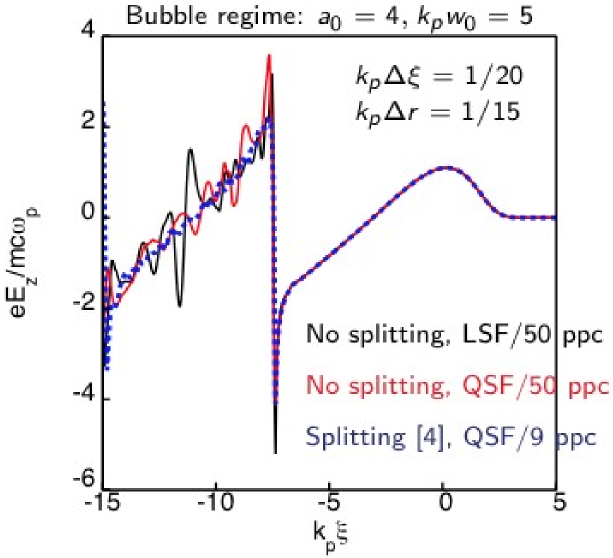
- "adaptive" **particle resampling** (useful for "quick" runs)
  - numerical particles loaded ~ uniformly in the computational domain
  - charge of a particle $q_i \propto r_{0,i}$ (particles born at large radii are "heavier")
  - "heavy" particles generate "spikes" in density/current when $r_i \sim 0$

→ *particles are* ***split into fragments*** *as* $r_i \to 0$

  - drawbacks: small violation of the local charge/energy conservation (total charge and momentum are conserved), heating of the plasma



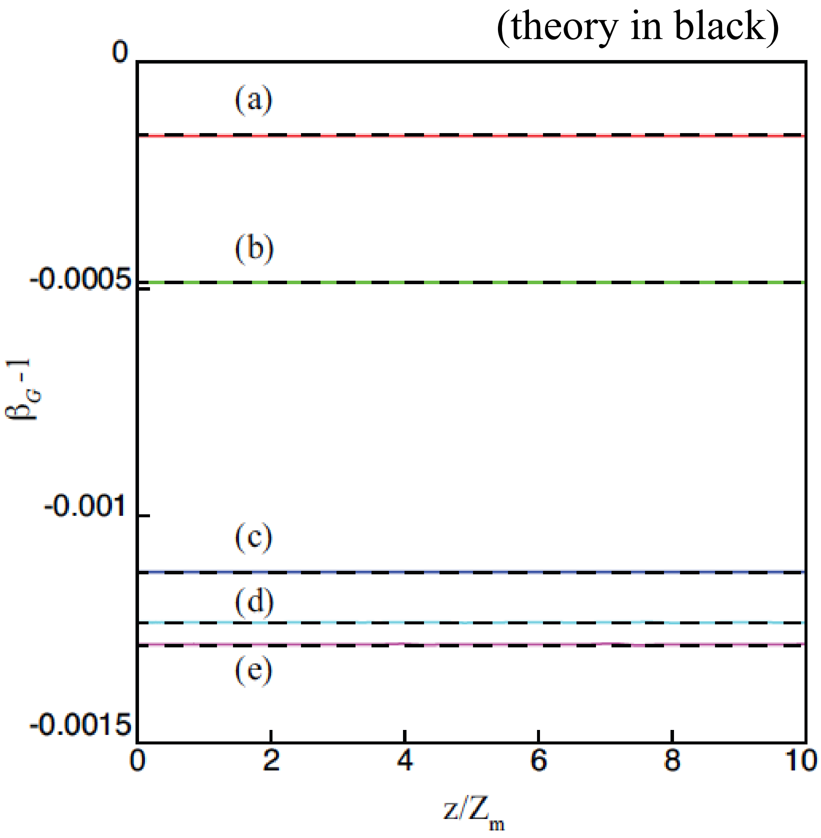




Benchmark 1/3: laser pulse velocity

Propagation velocity of a low intensity (a_0=0.01) laser pulse* in vacuum or plasma

$$\begin{cases} n(r) = n_0 + (\pi r_e r_m^2)^{-1} \left(\frac{r}{r_m}\right)^2 \\ \hat{a}_\perp \sim L_m^0 \left(\frac{2r^2}{w_0^2}\right) e^{-r^2/w_0^2} \end{cases} \qquad \beta_g = 1 - \frac{k_p^2}{2k_0^2} - \frac{1+2m}{k_0^2 r_i^2}\left[1 + \frac{r_i^4}{r_m^4} + \frac{r_i^2}{r_m^2}\left(\frac{\partial(r_i/r_m)}{\partial(z/Z_m)}\right)^2\right]$$



m=0 (Gaussian), $k_0 r_i$=80

m=1 (LG1), $k_0 r_i$=80

vacuum propagation (n_0= 0, $r_m \to \infty$)

m=0 (matched Gaussian), $k_p r_i = k_p r_m$

m=0 (mismatched Gaussian), $k_p r_i = 1.5 k_p r_m$

m=0 (Gaussian, converging at the entrance of the channel), $k_p r_i = \sqrt{2} k_p r_m$, $dr_i/dz \neq 0$

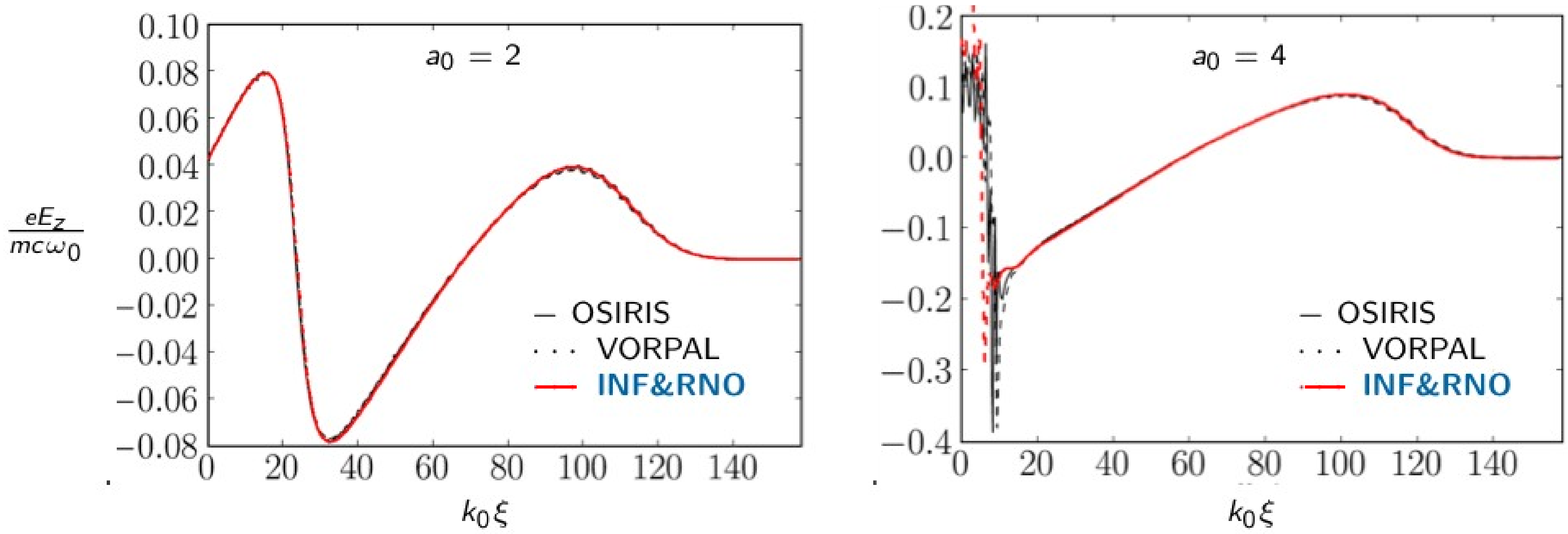
plasma channel (k_0/k_p=25, $k_p r_m$=3.14)

*Schroeder, *et al.*, Phys. Plasmas (2011)

Benchmark 2/3: comparison with “full” 3D PIC/1

Comparison with VORPAL and OSIRIS*

a_0	$k_p w_0$	k_0/k_p	numerics
2,4	5.7	11.2	$k_p\Delta\xi = 1/30$, $k_p\Delta r = 1/10$, 20ppc, QSF



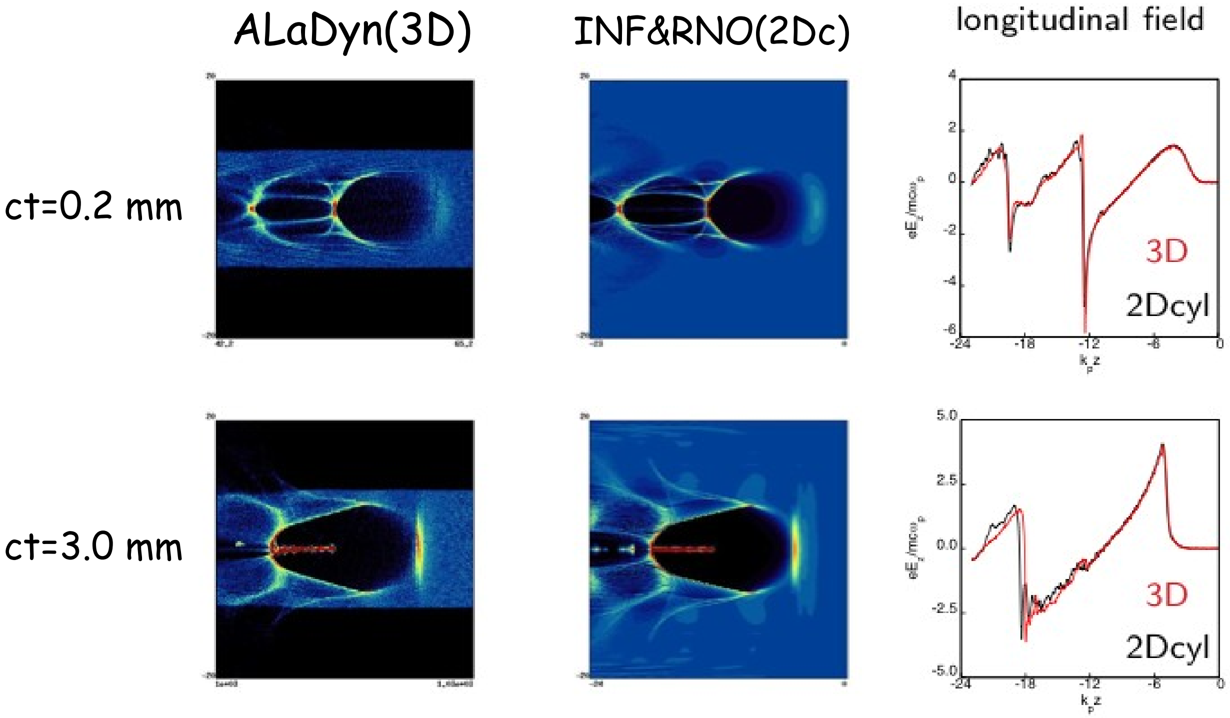
* Paul *et al.*, Proc. of AAC08 (2008)

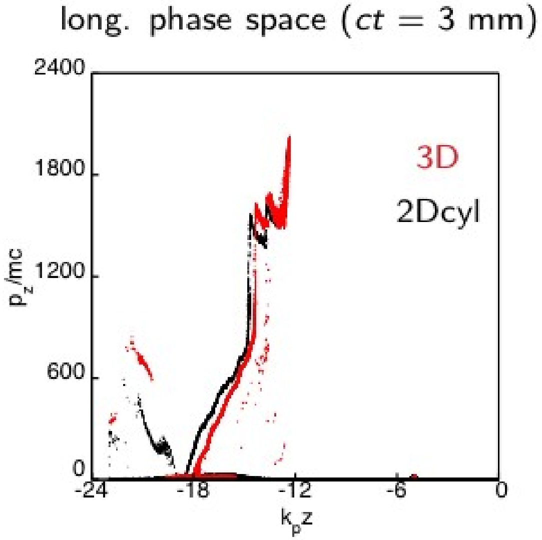
Benchmark 3/3: comparison with "full" 3D PIC/2

Comparison with 3D PIC code ALaDyn*

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: $1/30 \times 1/20$ - $\Delta t = 0.25\Delta z$ - QSF - split [2] - filter [250]





* Benedetti *et al.*, IEEE TPS (2008); Benedetti *et al.*, NIM A (2009)

Performance of INF&RNO

- code written in C/C++ & parallelized with MPI (1D longitudinal domain decomp.)

- code performance on a MacBookPro laptop (2.5GHz, 4GBRAM, 1333MHz DDR3)

FLUID (RK2)	PIC (RK4)
0.8 μs / (grid point * time step)	1.1 μs / (particle push * time step)

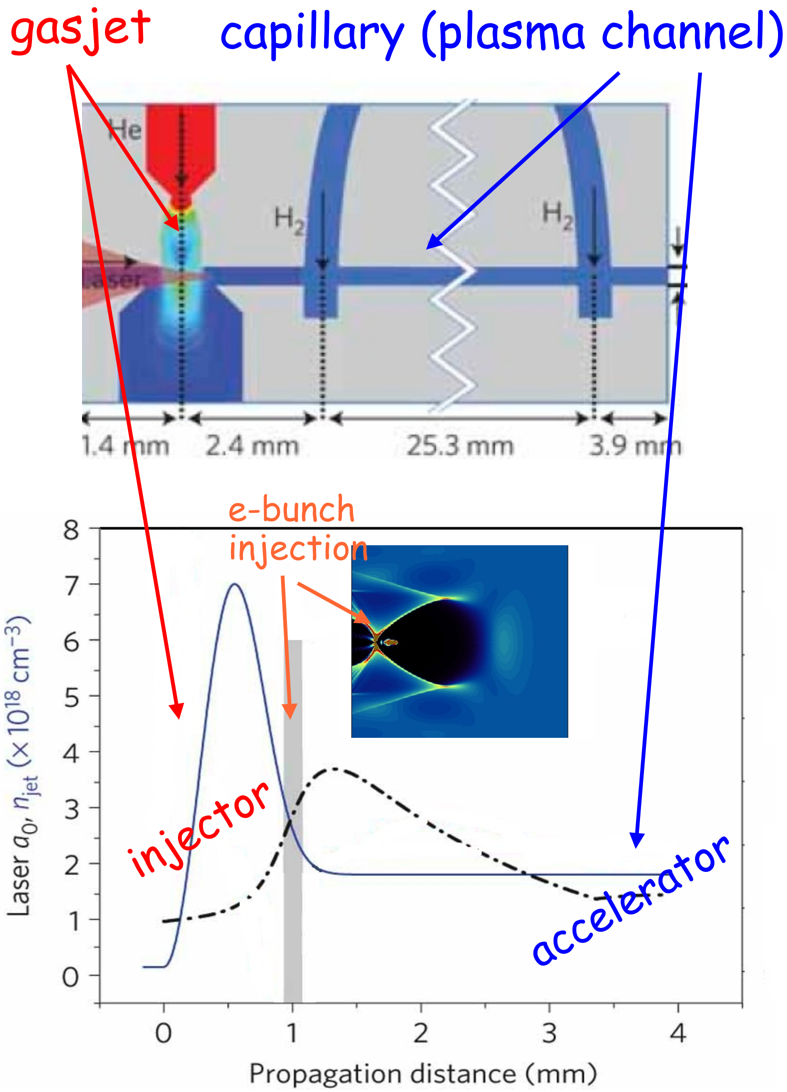
- Examples of simulation cost

  - ✓ 100 MeV stage (~10^{19} cm^{-3}, ~ mm) / PIC → **~10^2** CPUh
  - ✓ 1 GeV stage (~10^{18} cm^{-3}, ~ cm) / PIC → **~10^3–10^4** CPUh
  - ✓ 10 GeV stage quasi-lin. (~10^{17} cm^{-3}, ~m) / FLUID → **~10^3** CPUh
  - ✓ 10 GeV stage quasi-lin. (~10^{17} cm^{-3}, ~m) / FLUID + LBF[γ_{LBF}=10] → **~20** CPUh
  - ✓ 10 GeV stage bubble (~10^{17} cm^{-3}, ~ 10 cm) / PIC → **~10^4–10^5** CPUh

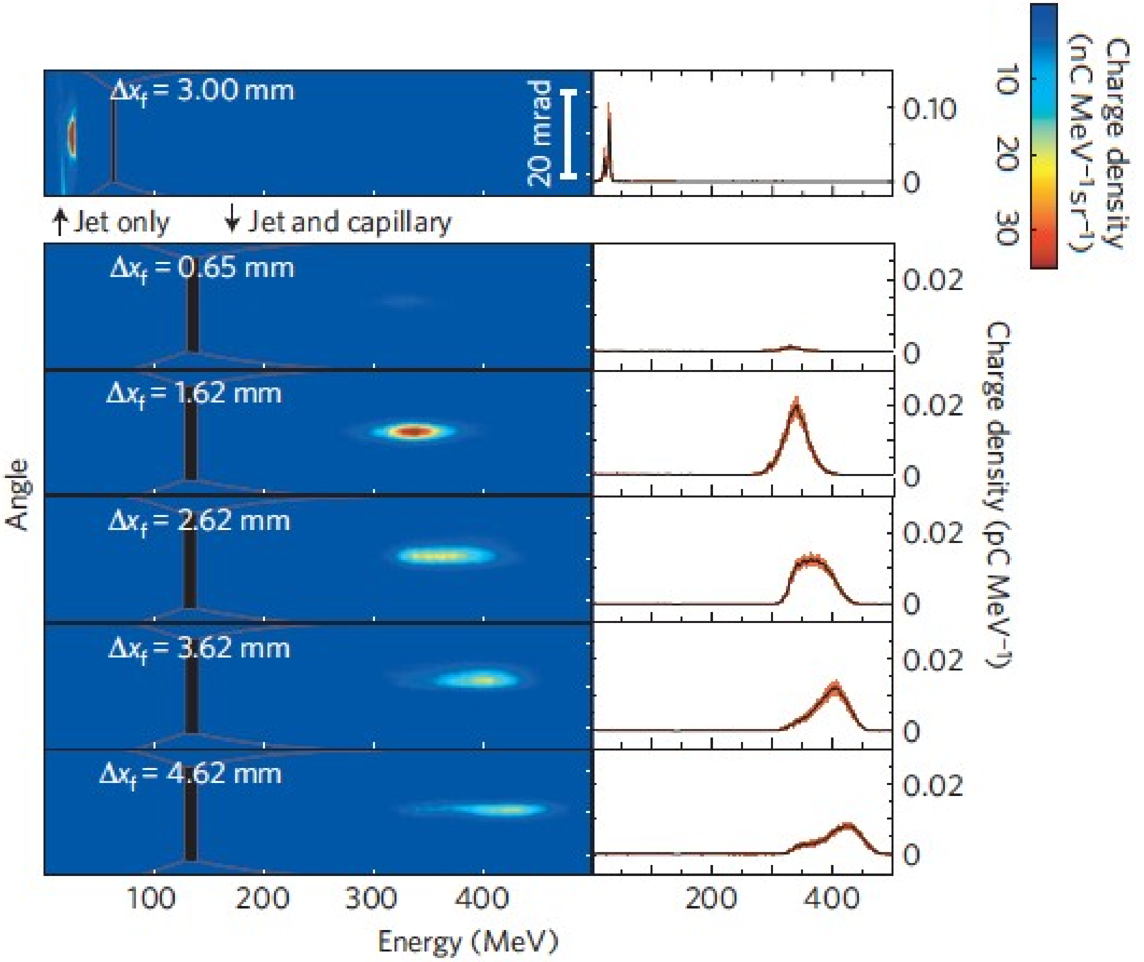
==> gain between 2 and 5 orders
of magnitude in the simulation time

INF&RNO is used to successfully model current experiments at LOASIS

Tunable laser plasma accelerator based on longitudinal density tailoring*



Electrons **injected** at density gradient + **coupling** of injected electrons to a lower density, separately tunable plasma for further **acceleration**.



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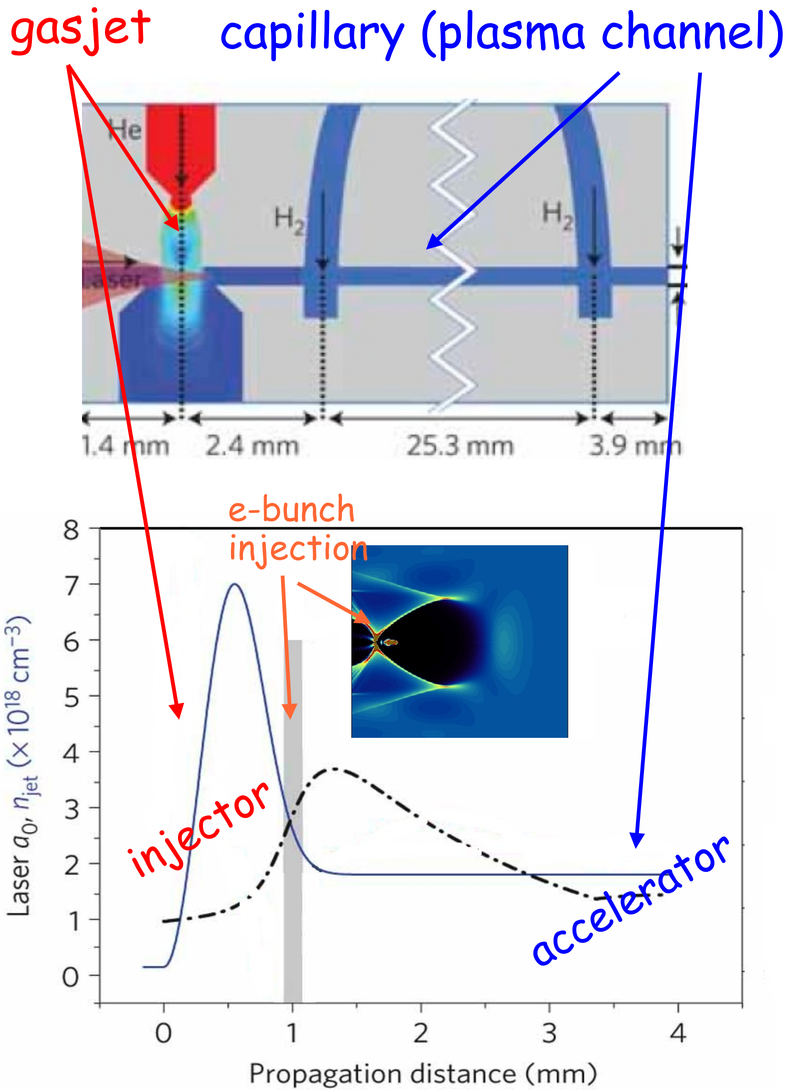
* Gonsalves *et al.*, Nature Phys. (2011)

INF&RNO is used to successfully model current experiments at LOASIS

Tunable laser plasma accelerator based on longitudinal density tailoring*


gasjet

capillary (plasma channel)

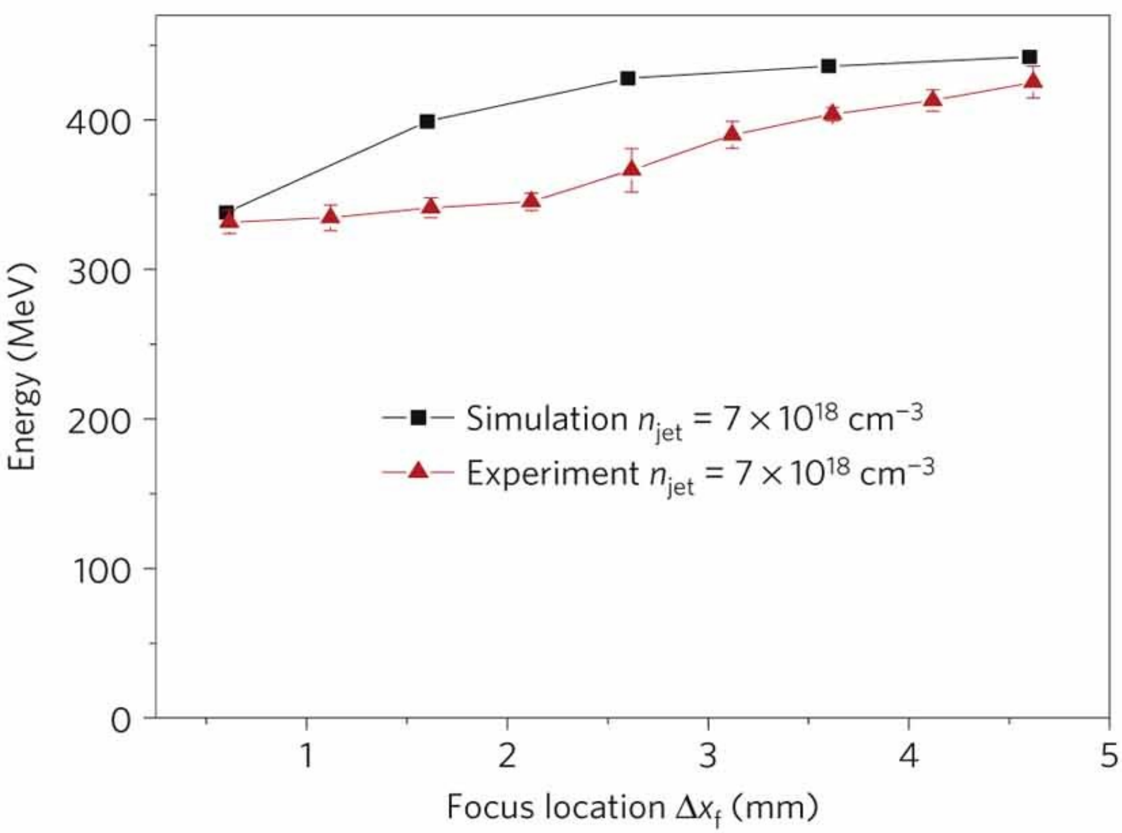
e-bunch injection

injector

accelerator

Electrons **injected** at density gradient + **coupling** of injected electrons to a lower density, separately tunable plasma for further **acceleration**.

Final energy



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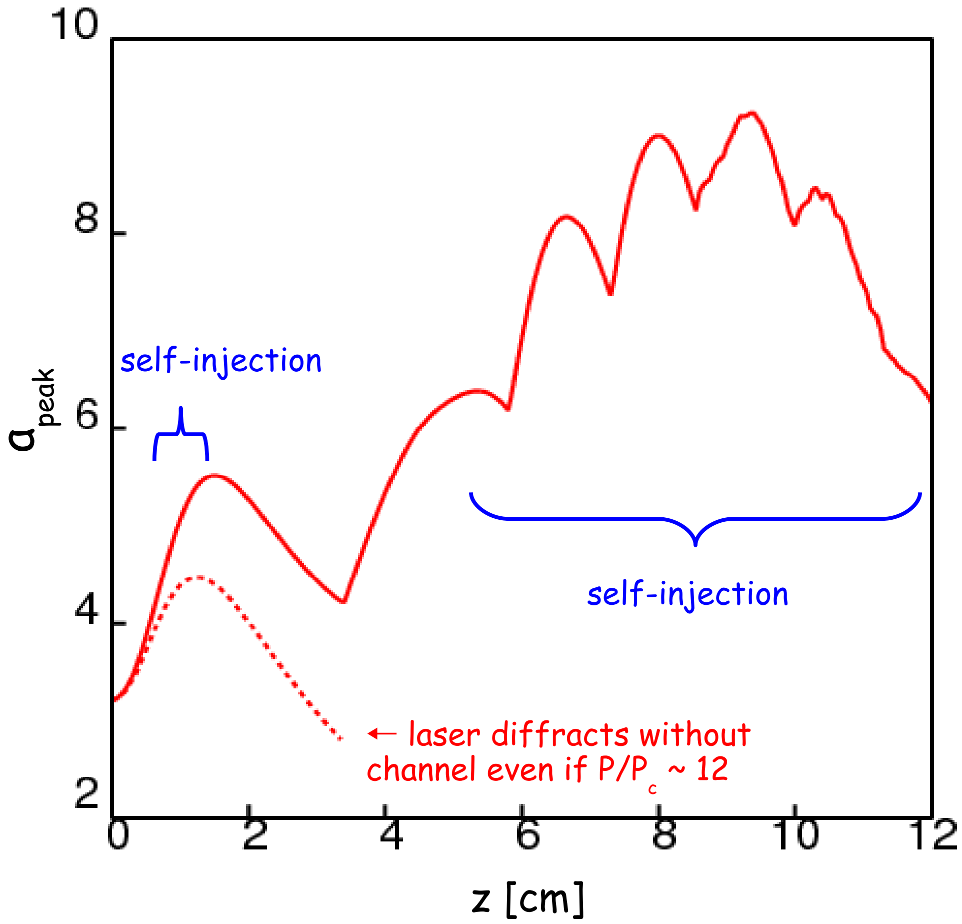
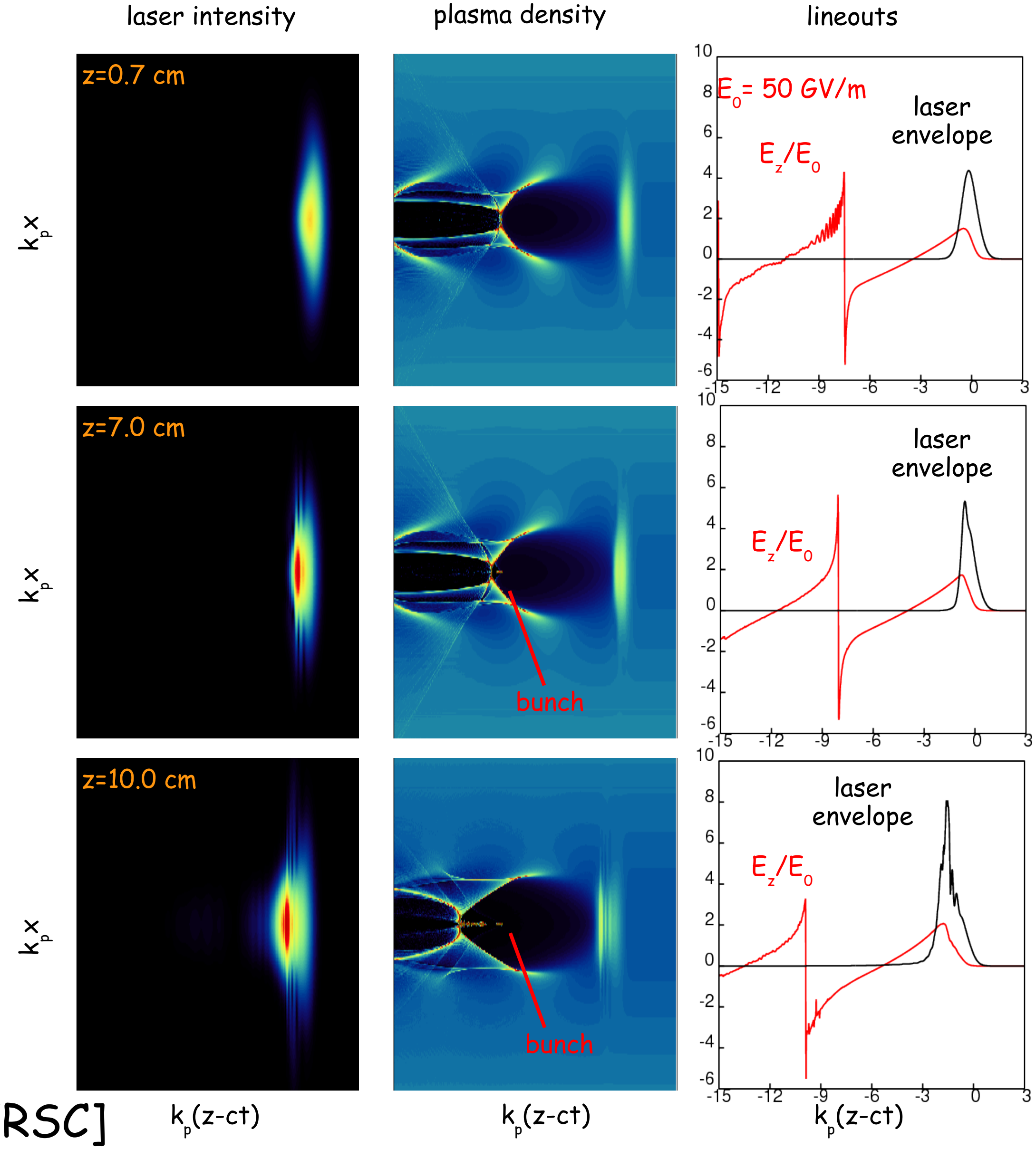
10 GeV-class LPA stage (BELLA) in the (nonlinear) bubble regime

BELLA laser: T_{laser} ~ 40 fs, E_{laser} ~ 40 J (~ 1 PW)
Plasma channel, $n_0 \approx 3\times10^{17}$ e/cm^3

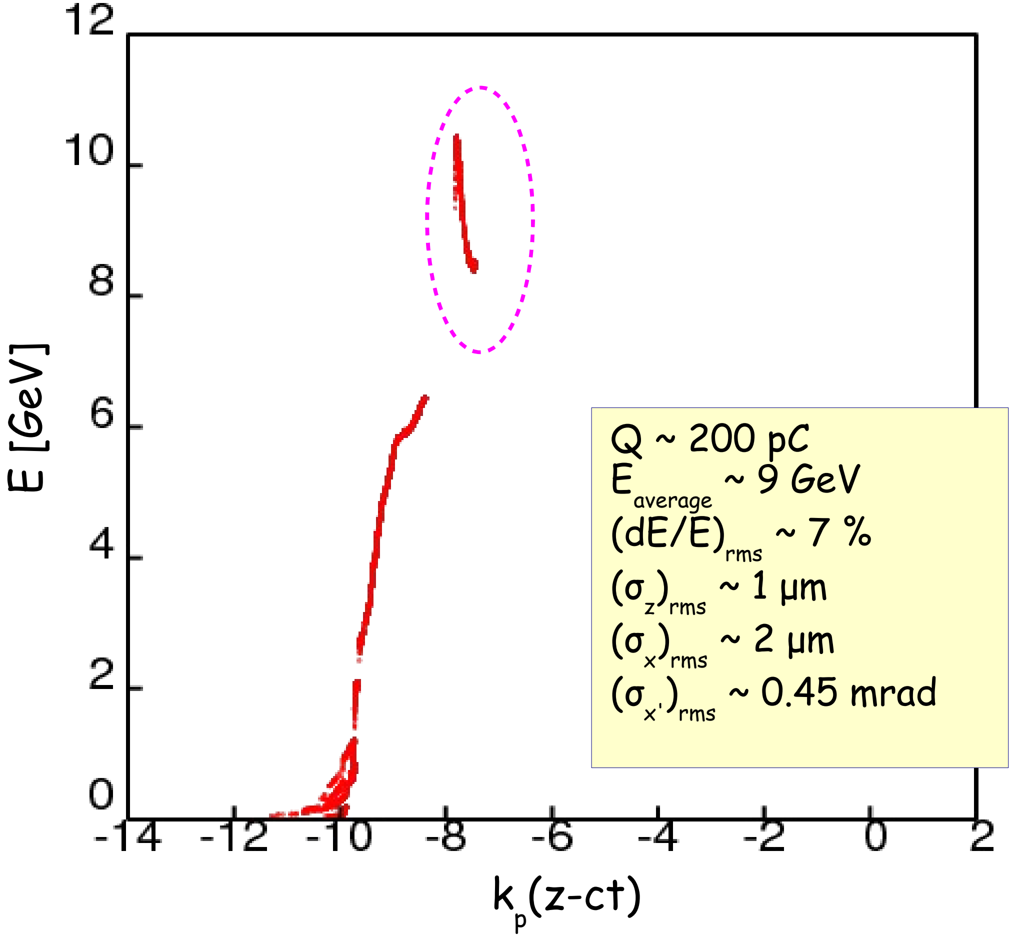




Simulation cost: < 10^5 kCPUh (gain ~ 10^3) [NERSC]

10 GeV-class quasi-monoenergetic beams can be obtained in ~ 10 cm capillary

longitudinal phase space @ z = 10 cm



Q ~ 200 pC

$E_{average}$ ~ 9 GeV

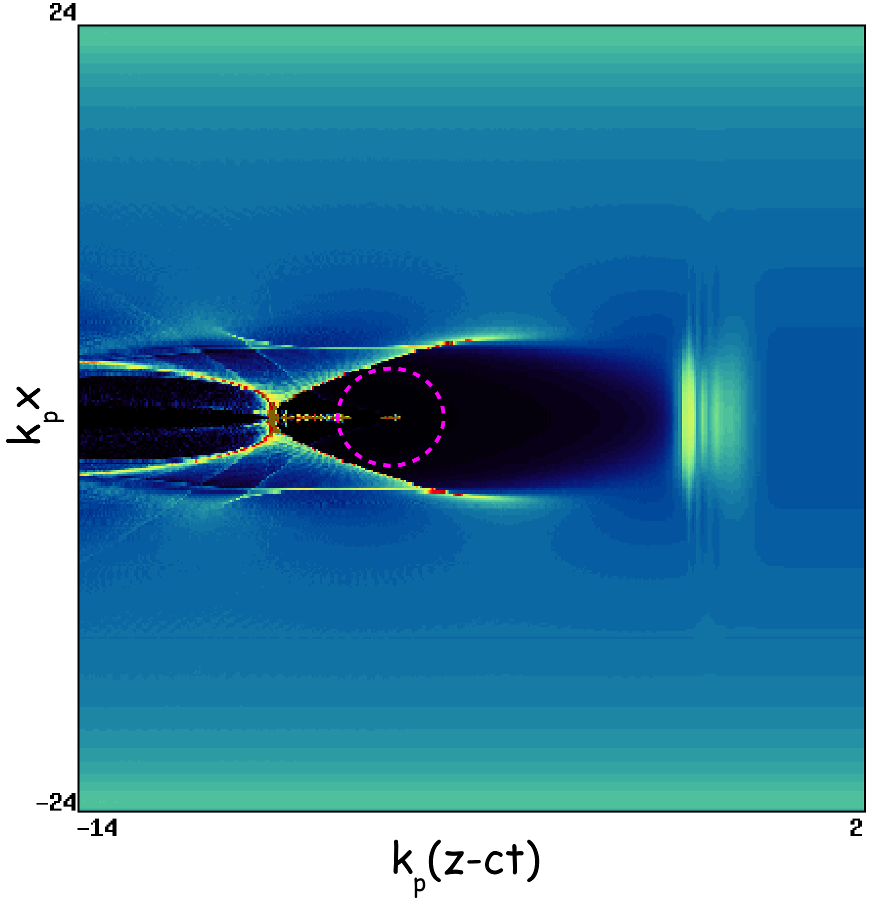
$(dE/E)_{rms}$ ~ 7 %

$(\sigma_z)_{rms}$ ~ 1 μm

$(\sigma_x)_{rms}$ ~ 2 μm

$(\sigma_{x'})_{rms}$ ~ 0.45 mrad

plasma density @ z =10 cm



Conclusions

The INF&RNO computational framework has been presented

- ✓ features: envelope, ponderomotive, 2D cylindrical, PIC/Fluid integrated, LBF, parallel
- ✓ the code is **several orders of magnitude faster compared to "full" PIC**, while still retaining physical fidelity
- ✓ the code has been **widely benchmarked and validated**
- ✓ modeling of future BELLA experiments show 10 GeV-class beams in ~ 10 cm

Plasma density