# Simulation modes in OSIRIS for parametric studies in 3d


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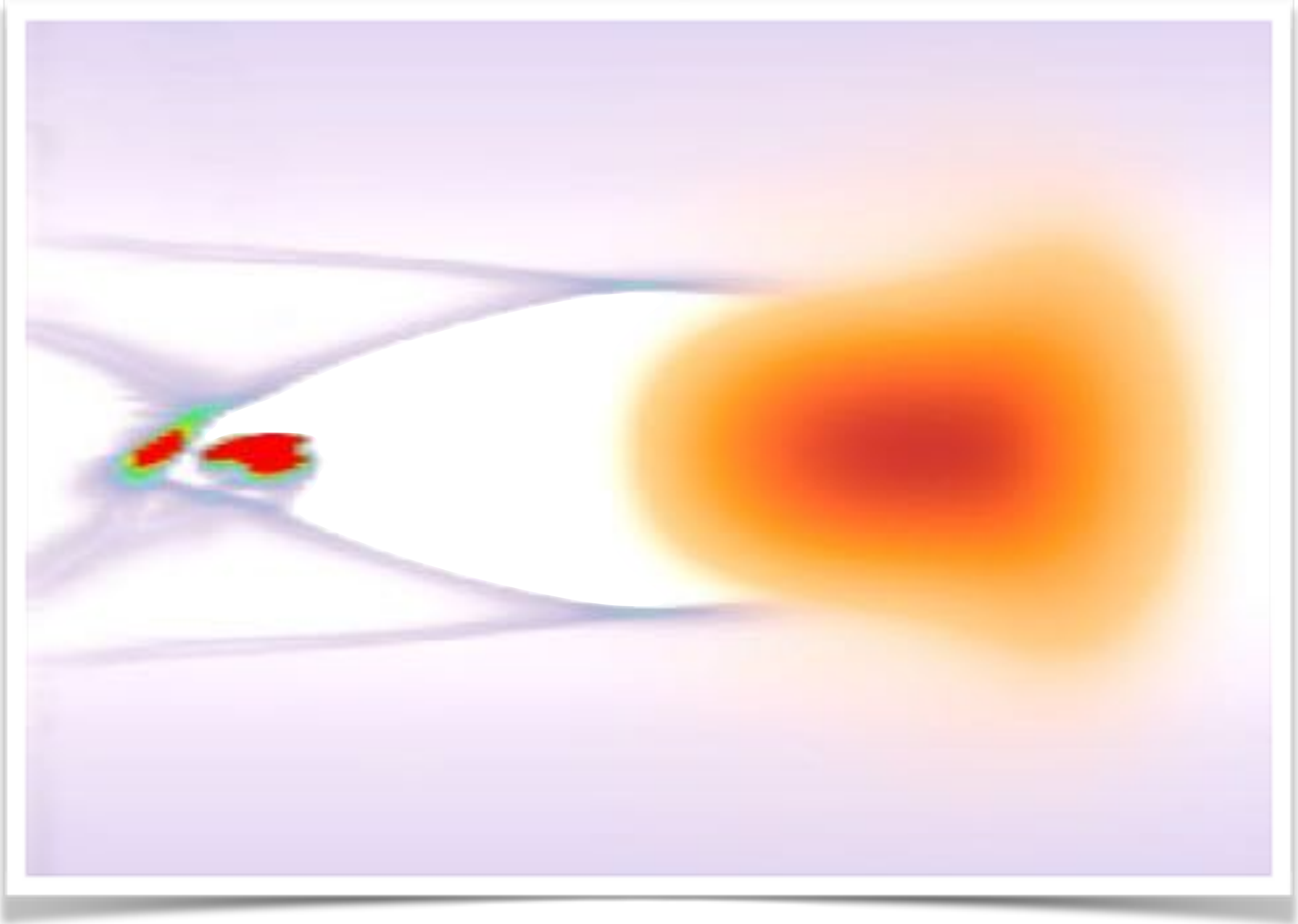


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# Outline

**Introduction**

**Reduced models for plasma-based accelerators**

Ponderomotive guiding center solver (PGC)

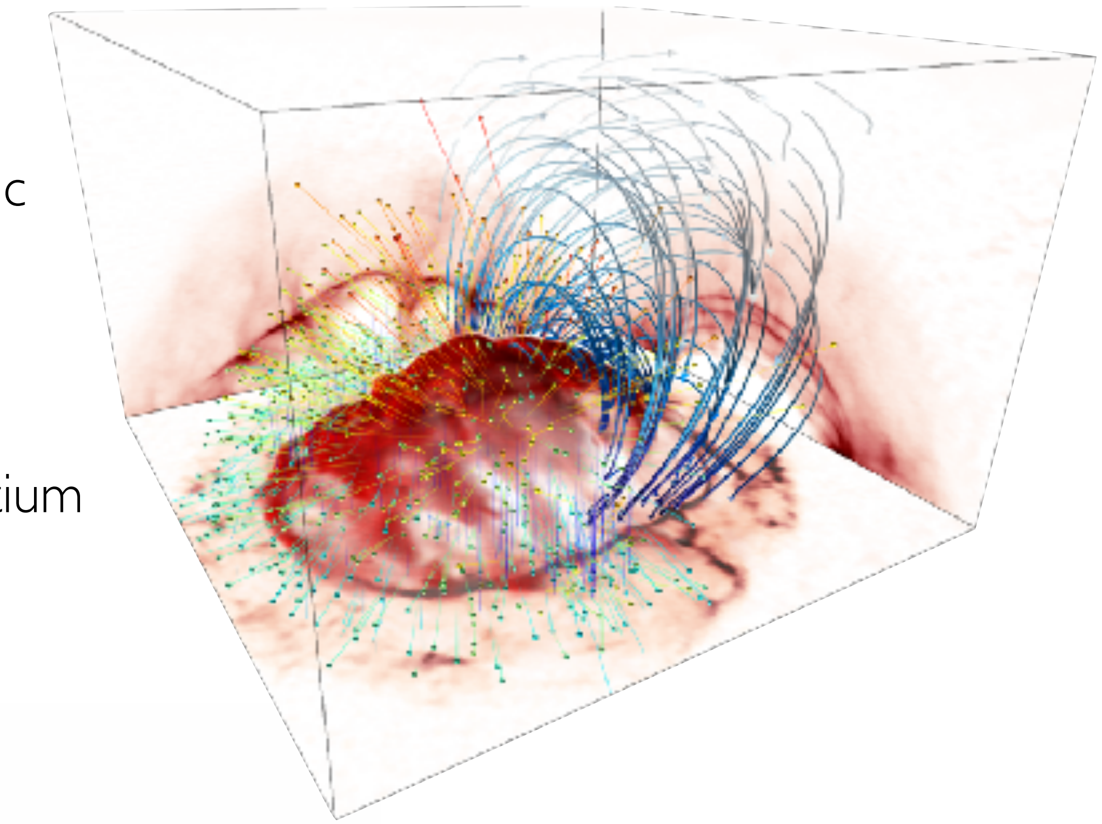
**Numerical issues in PIC based simulations**

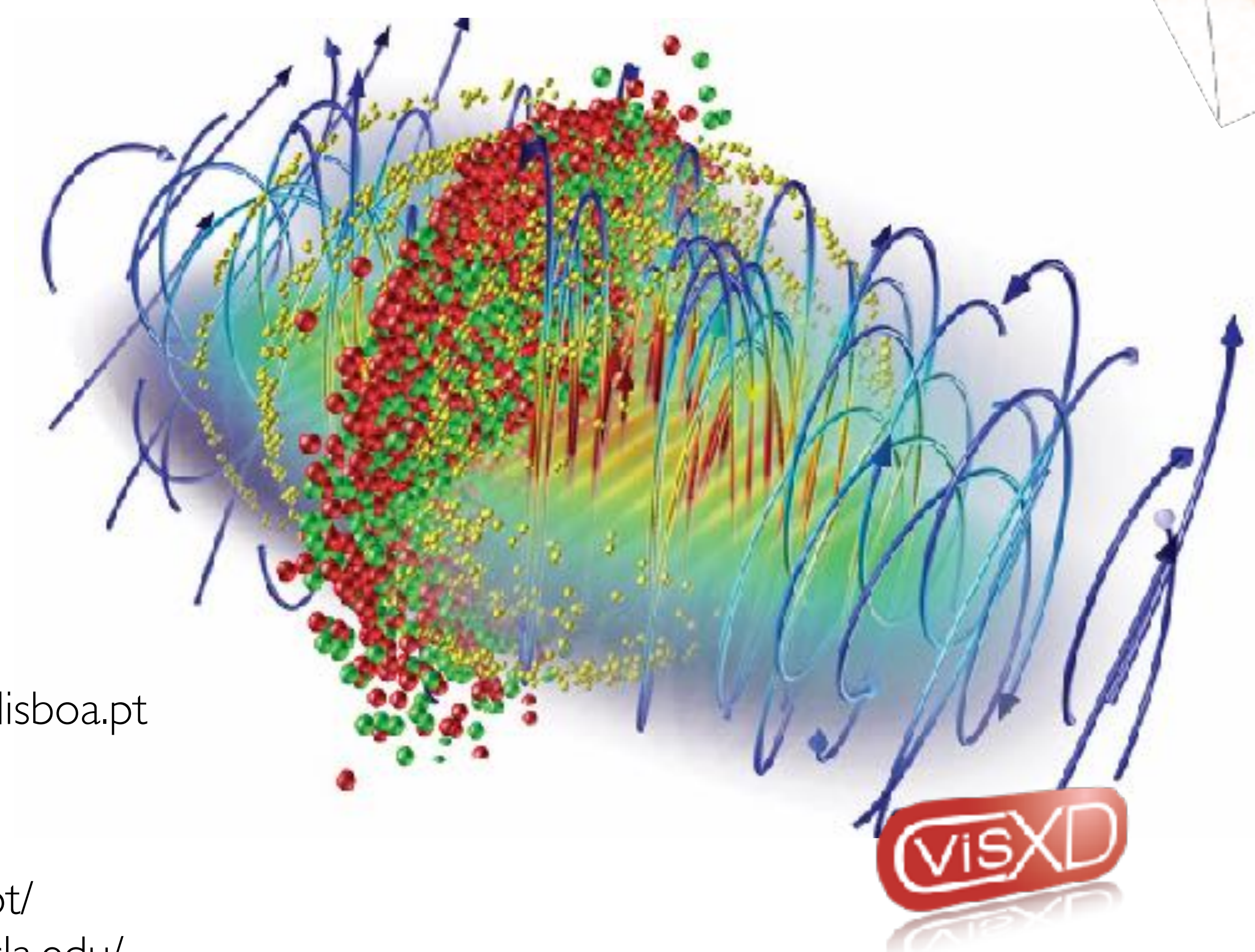
Stability of PGC and control of numerical Cherenkov instability (NCI)

# Osiris 4.0

### osiris framework

- Massively Parallel, Fully Relativistic Particle-in-Cell (PIC) Code
- Visualization and Data Analysis Infrastructure
- Developed by the osiris.consortium
  $\Rightarrow$ UCLA + IST






### code features

- **Scalability to ~ 1.6 M cores**
- SIMD hardware optimized
- Parallel I/O
- Dynamic Load Balancing
- Ionization
- **PGC support**
- **Quasi-3d support**
- QED module
- Particle merging
- Xeon Phi/GPGPU support

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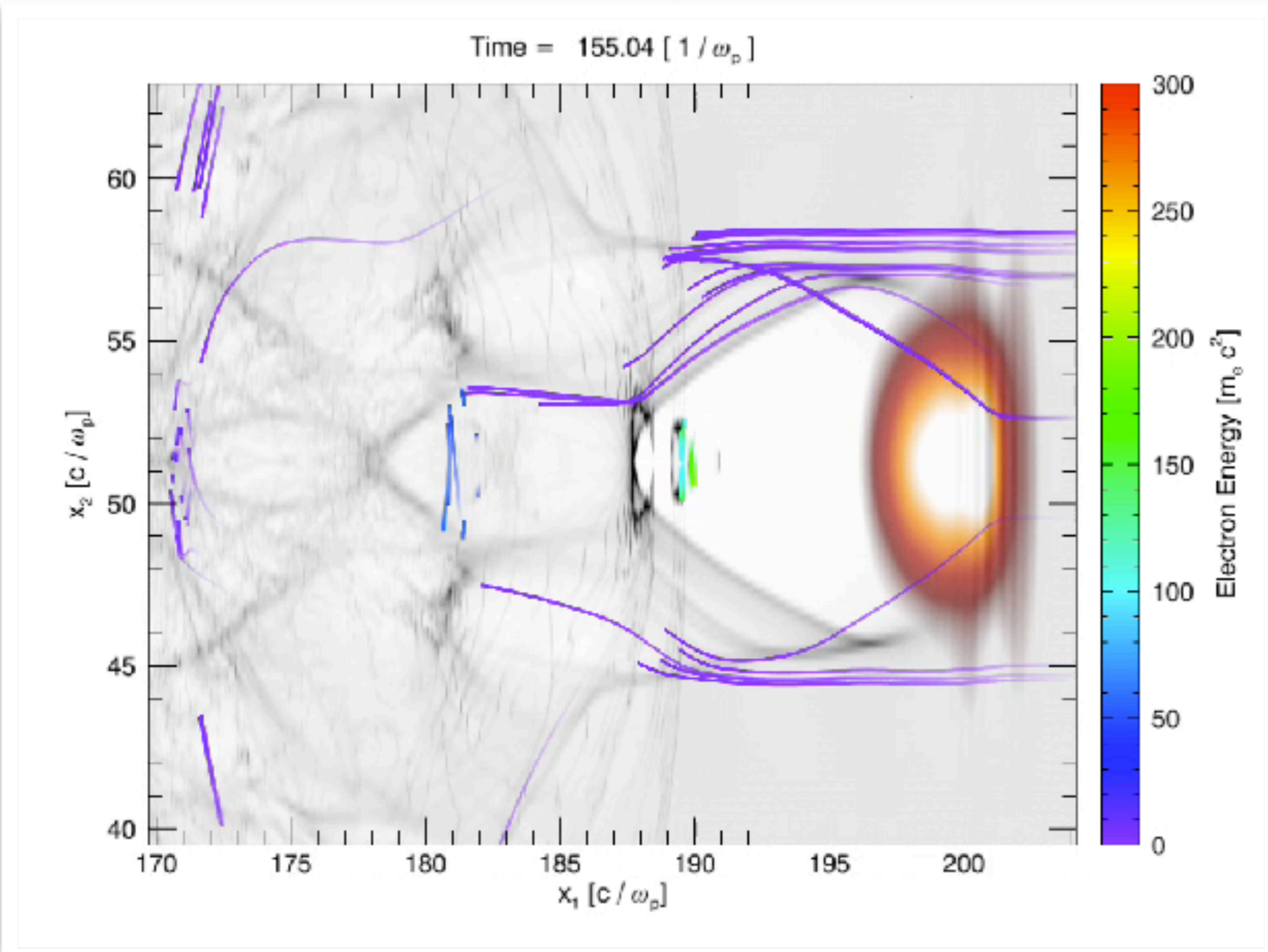
# Scale disparities in LWFA modeling




**scale disparity in modeling**

multi-scale problems

- large disparity of spatial/temporal scales

sample problem: 50 GeV LWFA stage

- $\lambda_0$ ~ 1 $\mu$m / $\lambda_p$ ~ 17 $\mu$m
- L ~ 1.5 m

computational requirements (moving window)

- ~$10^9$ grid cells
- ~$10^{10}$ particles
- ~$10^6$ - $10^7$ iterations

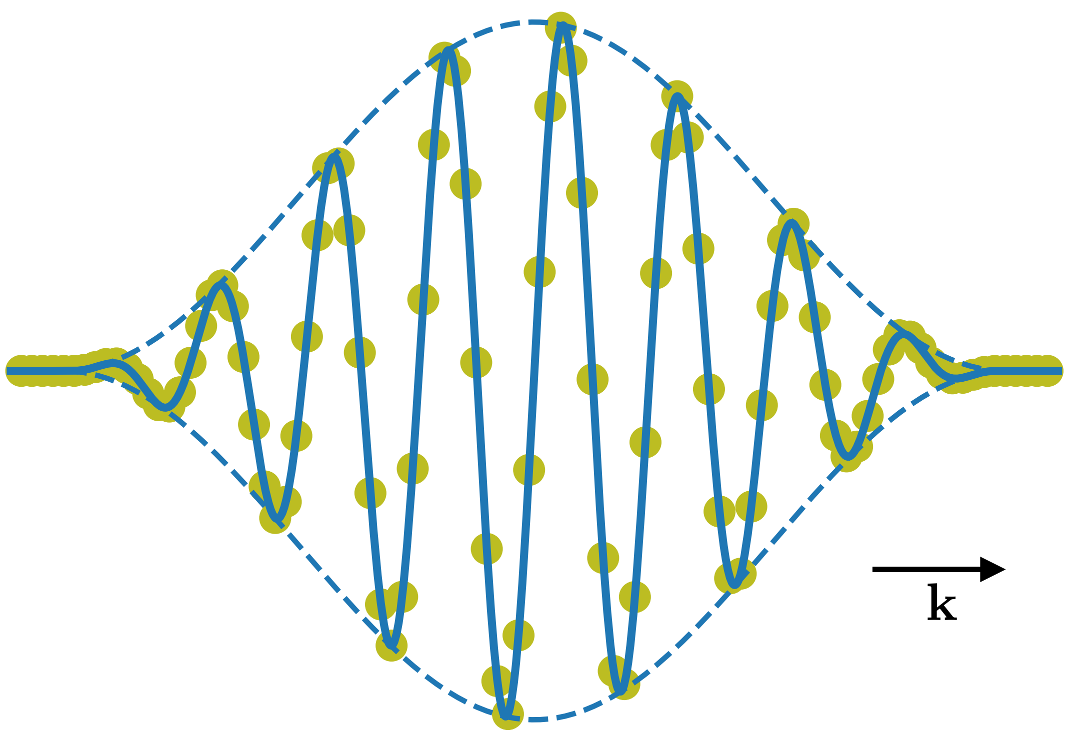
*requirement for reduced models*

# Envelope approximation reduces spatial resolution

$$\frac{\partial \mathbf{E}}{\partial \tau} = c\nabla \times \mathbf{B} - 4\pi \mathbf{j}$$
$$\frac{\partial \mathbf{B}}{\partial \tau} = -c\nabla \times \mathbf{E}$$

## particle-in-cell (PIC)

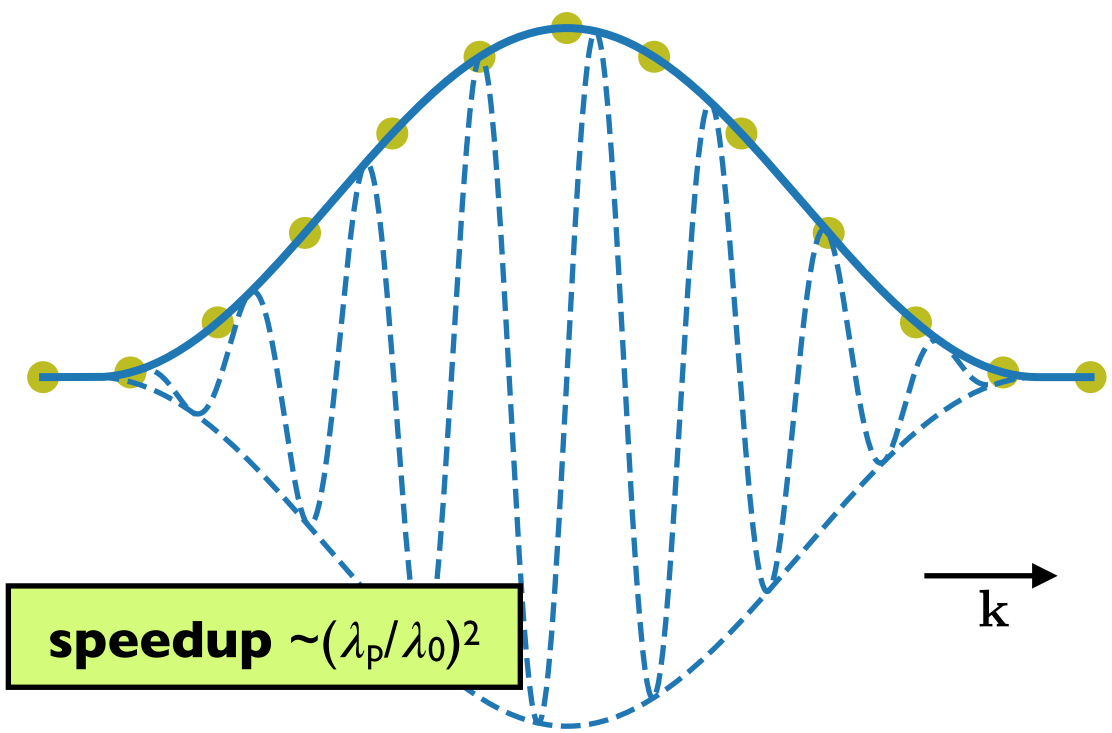
*spatial resolution:*
laser wavelength




- resolve laser wavelength over propagation distance
- particle advancing is based on Lorentz force

## ponderomotive guiding center (PGC)

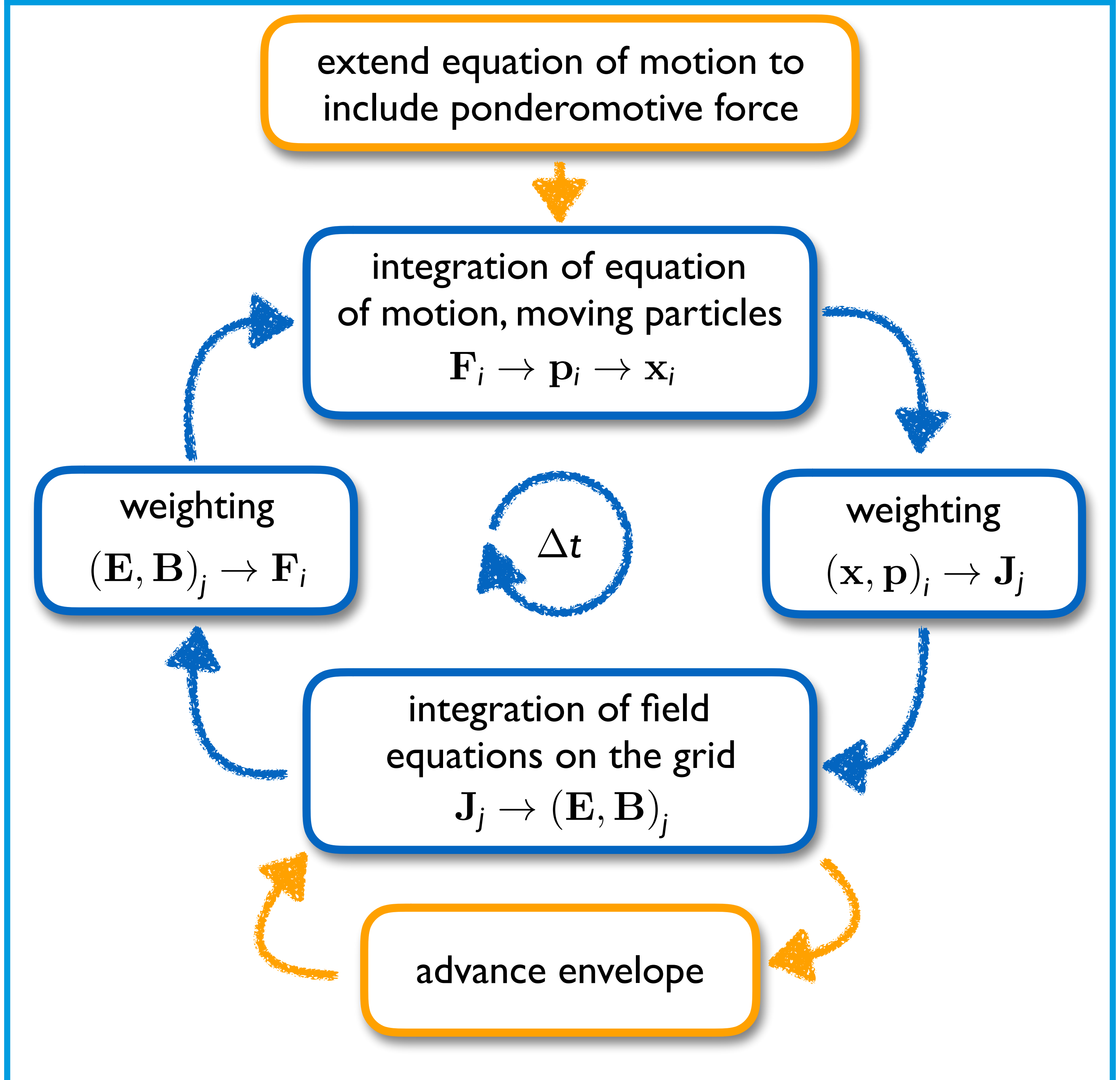
*spatial resolution:*
plasma skin depth




- requires model for laser envelope propagation
- push particles using self consistent plasma fields and ponderomotive force

# Incorporation of PGC into PIC cycle

## extended PIC algorithm




## PGC extension

- time-averaged equation for laser evolution*,** in a co-moving frame

$$\partial_\tau a = \frac{1}{2i\omega_0}\left(1 + \frac{\partial_\xi}{I\omega_0}\right)(\chi a + \Delta_T a)$$

laser frequency — laser envelope

- particle advancing

$$\mathbf{F}_p = -\frac{1}{4}\frac{q^2}{\langle m \rangle}\nabla |a|^2$$

- coupling parameters

$$\chi = -\sum_i \frac{q_i \rho_i}{\langle m_i \rangle}$$

$$\langle m \rangle = \sqrt{m_0^2 + \mathbf{p}^2 + (q|a|)^2 / 2}$$

* P. Mora and T. M, Antonsen, PRL 53, R2068 (1996)
** P. Mora and T. M, Antonsen, AIP 4, 217 (1997)

# Comparison of PGC with full PIC

## laser envelope

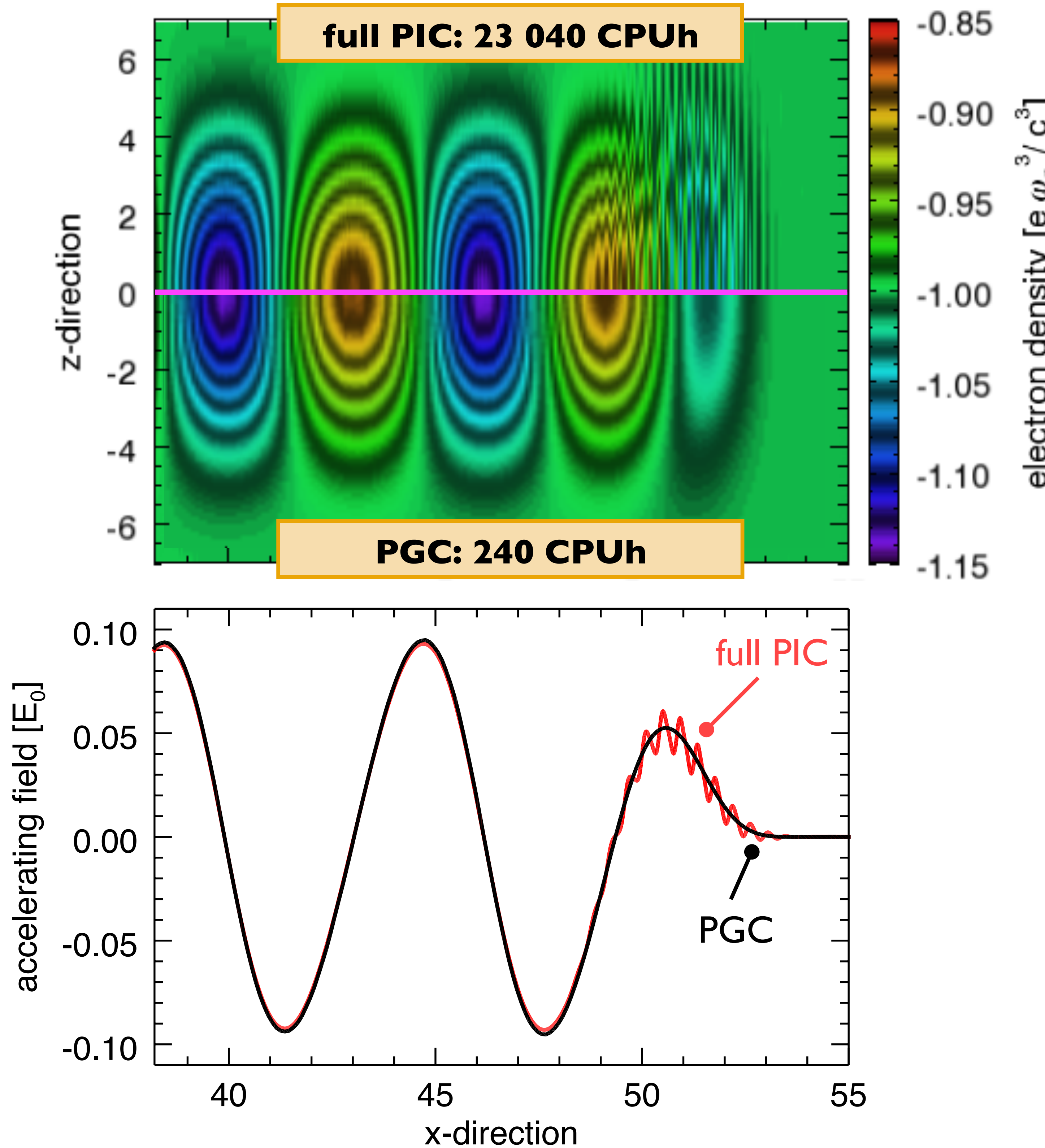
- sin² / gaussian beam profile
- pulse length = 12.0 $k_p^{-1}$
- laser frequency = 15.0$\omega_p$
- spot size = 5.0 $k_p^{-1}$
- driver amplitude = 0.5

## simulation setup

- $\Delta x$ = 0.1 $k_p^{-1}$ (PGC)
- $\Delta x$ = 0.004 $k_p^{-1}$ (full PIC)
- $\Delta y = \Delta z$ = 0.1 $k_p^{-1}$
- propagation distance = 28.0 $k_p^{-1}$
- quadratic interpolation (ppc = 8)

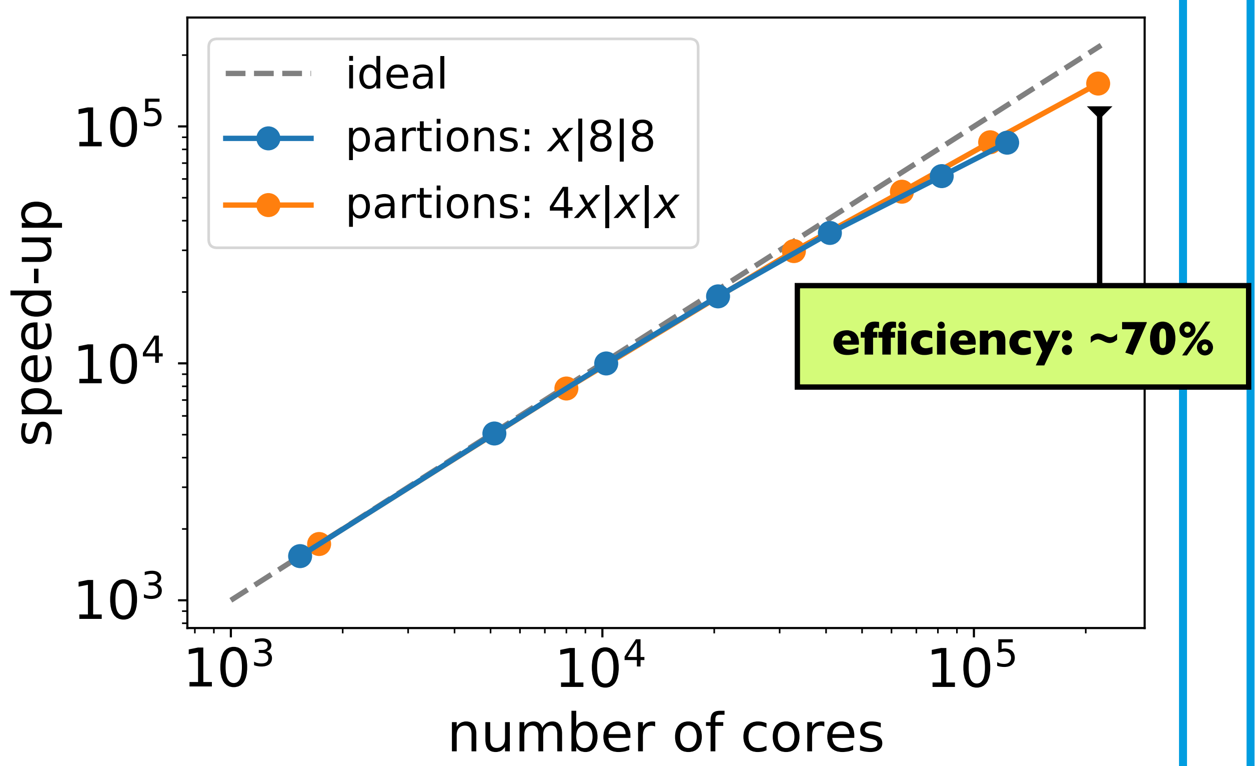
## computational reduction

- full PIC: 18 h on 1280 cores
- PGC: 4 h on 60 cores
- **speedup: 96x**



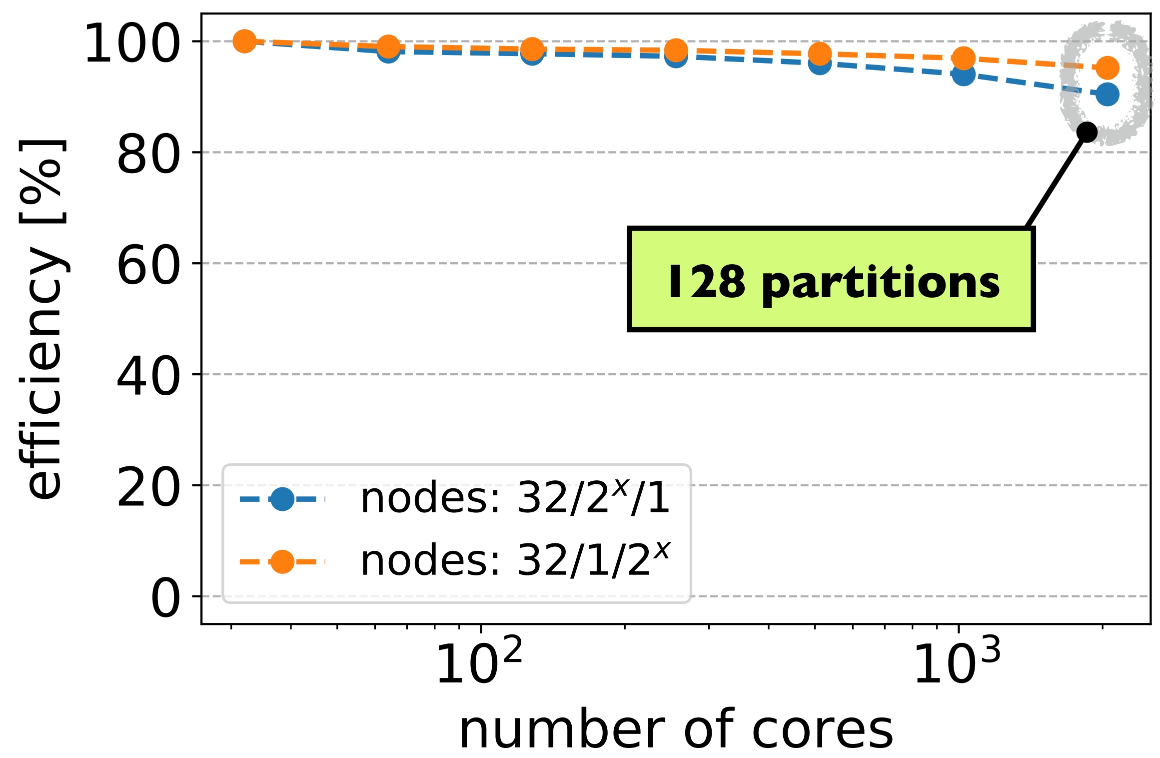
# Parallelization is scalable over thousands of cores

## strong scaling



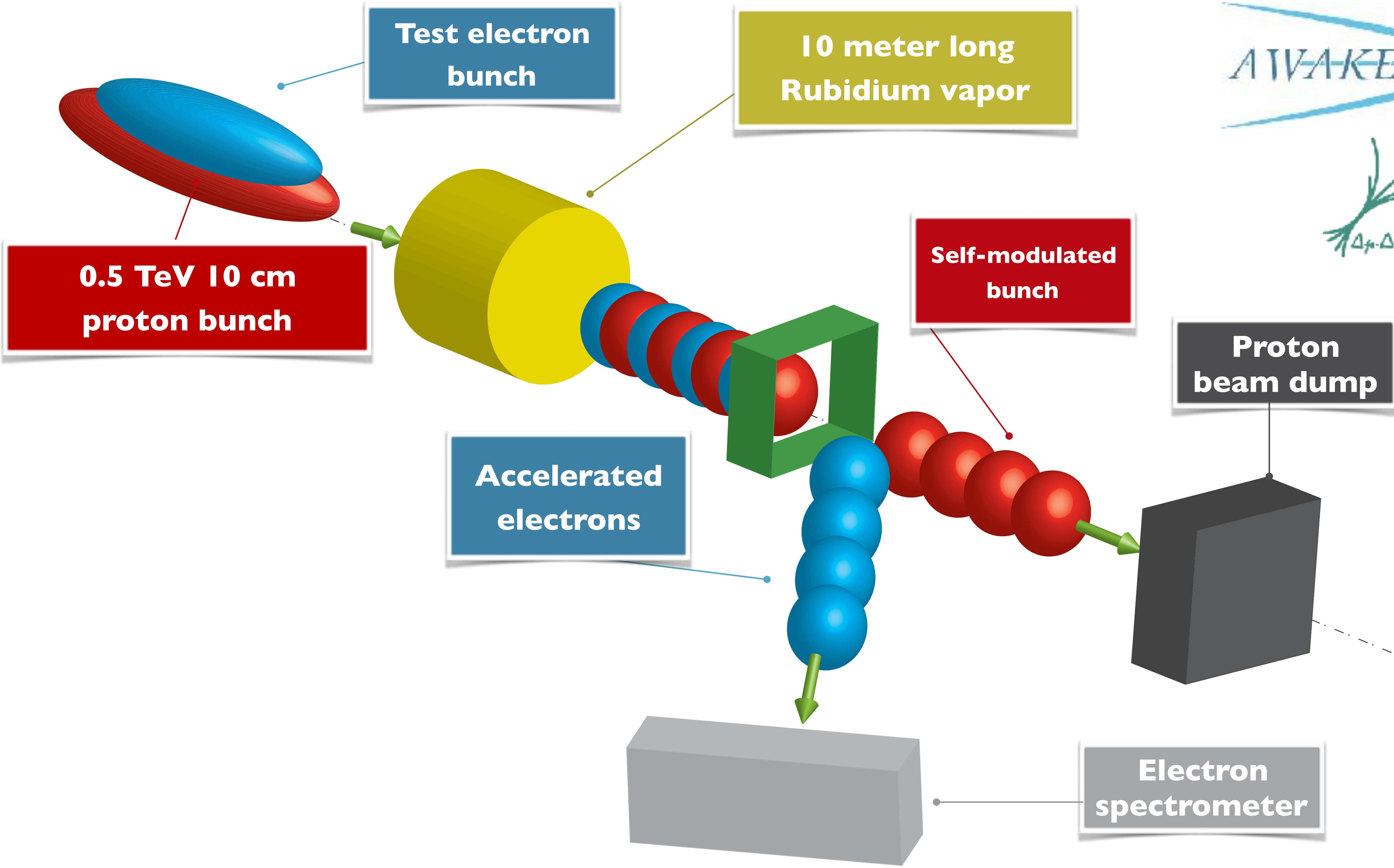

- JUQUEEN (IBM BlueGene/Q)
  - 16 cores per node / no threading
- 15360×240×240 cells and 8 ppc (500 iterations)
- periodic boundaries in transversal direction
- fixed and various number of parallel domains in transversal direction
- ✔ PGC scales from 1536 to 216000 with an efficiency drop by 30%

## weak scaling in transversal direction




- weak scaling for transversal parallelization with a custom parallelization scheme for envelope
- initial setup: 2048×10×50 cells and 8 ppc
- ✔ transpose algorithm for parallelization presents an efficiency above 90% (most scenarios <128 transversal partitions)
- ✔ bigger message sizes increase efficiency of algorithm

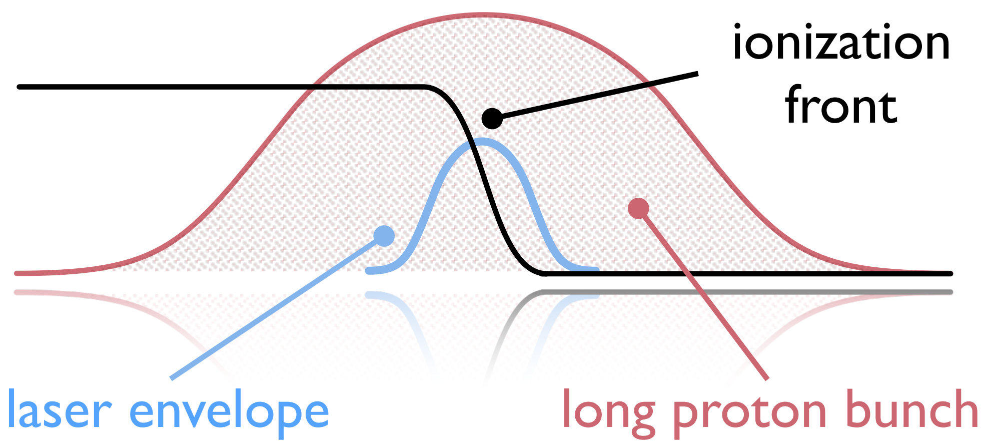
# Experimental layout of planned self-modulation proton driven wakefield acceleration experiments at CERN.




A. Caldwell *et al.*, Nat. Phys. 5, 363 (2009)
N. Kumar *et al.*, PRL 104, 255003 (2010)

# Creating plasma to cut proton bunch simultaneously

## laser pulse on top of proton bunch



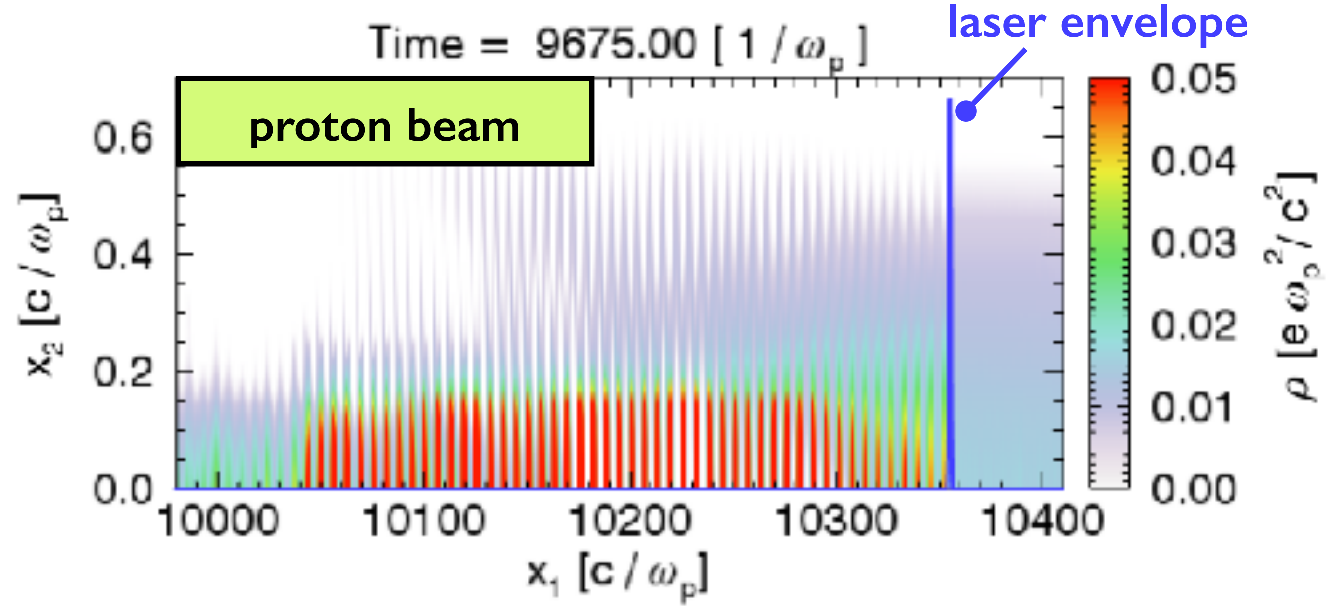

- laser pulse generates ionization front
- ionization front cuts long proton bunch sharply
- pulse excites wakes to directly seed the instability*

## full run (PGC vs full PIC)

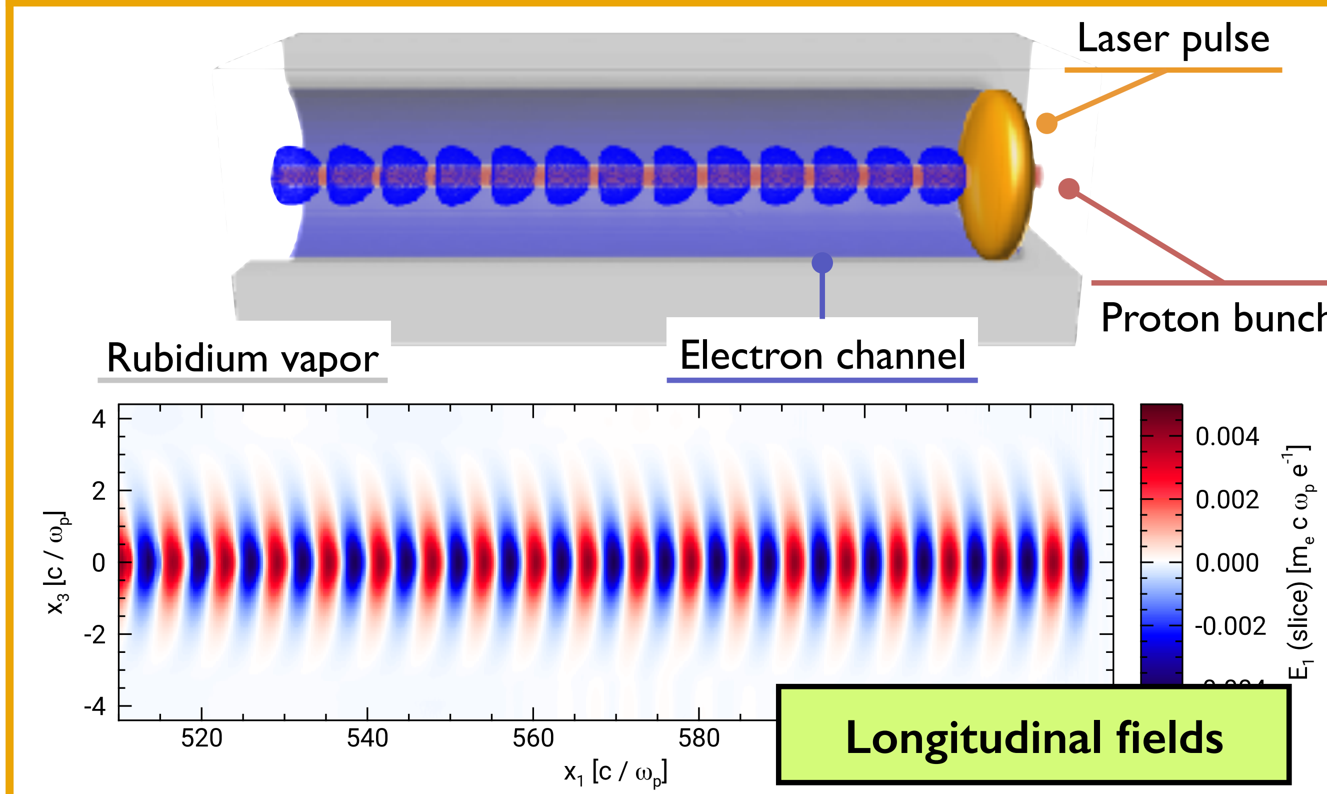
- minimalistic setup around laser ($\omega_0/\omega_p = 4000$)

| 0.01 €/CPUh | 2D | 3D |
|---|---|---|
| | CPU yr / cost | CPU yr / cost |
| PGC | 0.05 / 4.00 € | 17.12 / 1.50 k€ |
| PIC | 0.45 M / 40.00 M€ | 171.2 M / 15.00 B€ |

## 2d cylindrical (full propagation)




## 3d experimental setup (20 cm propagation)




* D. Gordon *et al.*, PRE 64, 046404 (2001)

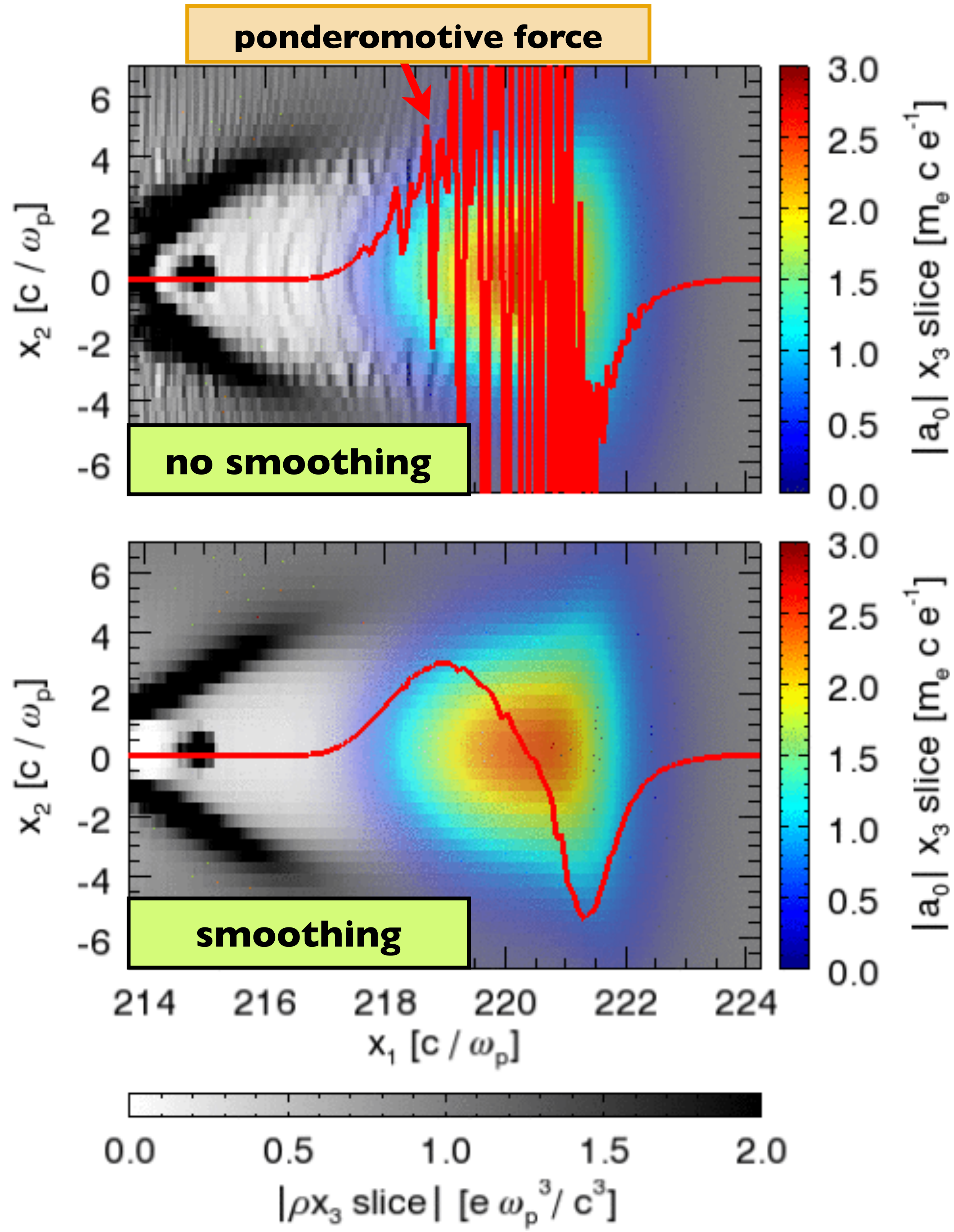
# Stability control for PGC

## particle interpolation order

- current implementation matches interpolation order of PIC cycle (up to **4th order**)
- field interpolation increases preciseness of ponderomotive force influence
- chi deposition increases stability especially in longitudinal direction

## smoothing of PGC quantities

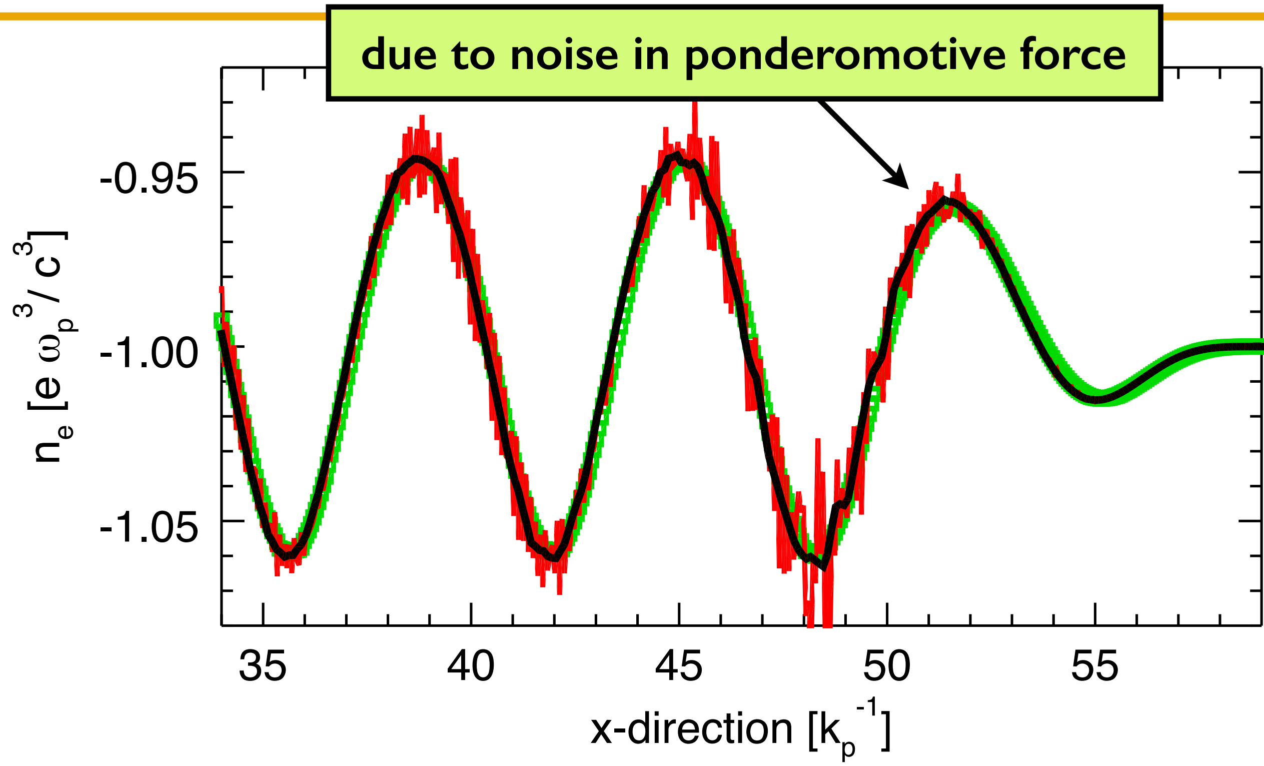
- allows explicit control of numerical noise
- includes several filters to control the noise level and cutoff of the noise
- smoothable quantities:
  - plasma parameter chi
  - ponderomotive force
  - laser envelope



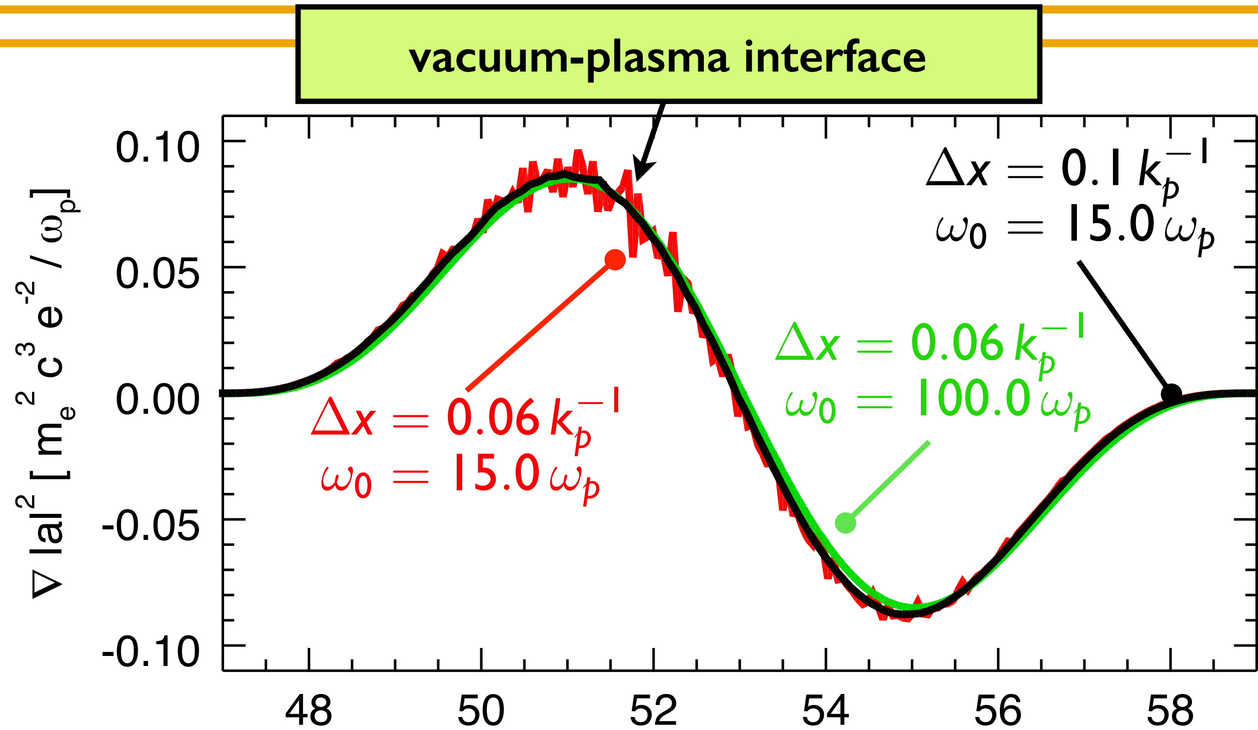
# Stability of the solver depends on resolution and laser frequency

TÉCNICO LISBOA

**electron density**




**ponderomotive force**




## stability of PGC solver

- assume 1D envelope equation

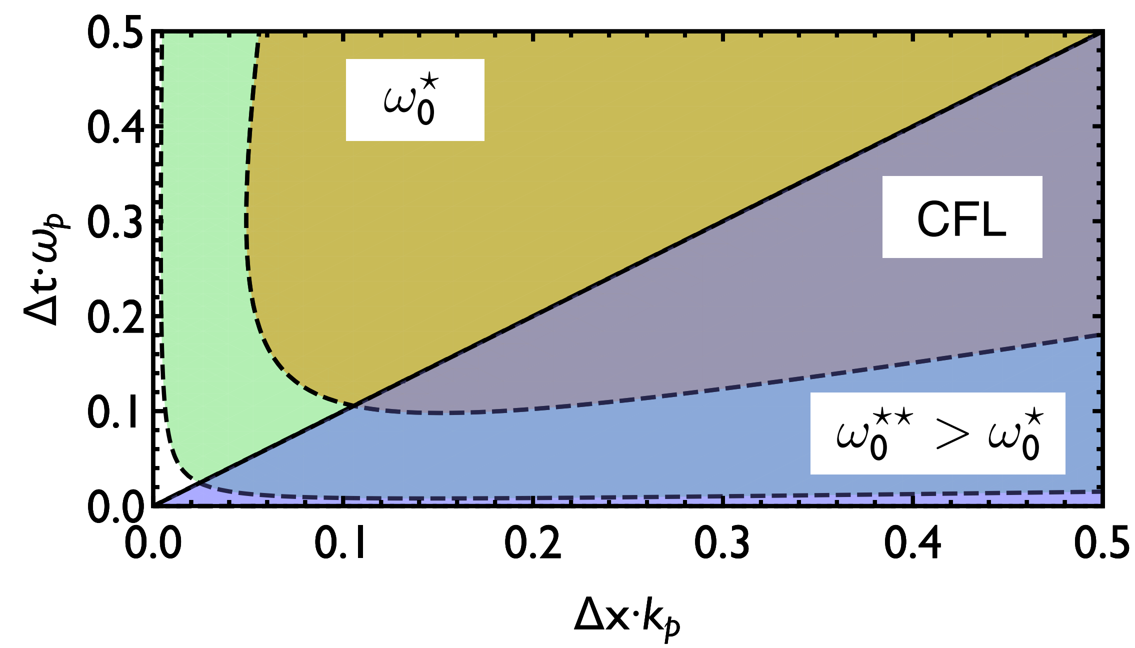
$$\partial_\tau a = \frac{1}{2i\omega_0}\hat{D}p = \frac{1}{2i\omega_0}\left[\left(1+\frac{\partial_\xi}{i\omega_0}\right)(\chi a)\right]$$

- stability condition after discretization

density gradient — density

$$\left(1-\frac{\chi_{i+1}-\chi_{i-1}}{2\omega_0\Delta\xi\Delta\tau}\right)^2+\left(\frac{\chi_i}{\omega_0\Delta\tau}+\frac{\chi_i}{2\omega_0\Delta\xi}\right)^2\le 1$$

- additional condition to Courant-Friedrichs-Lewy
- check only at runtime possible

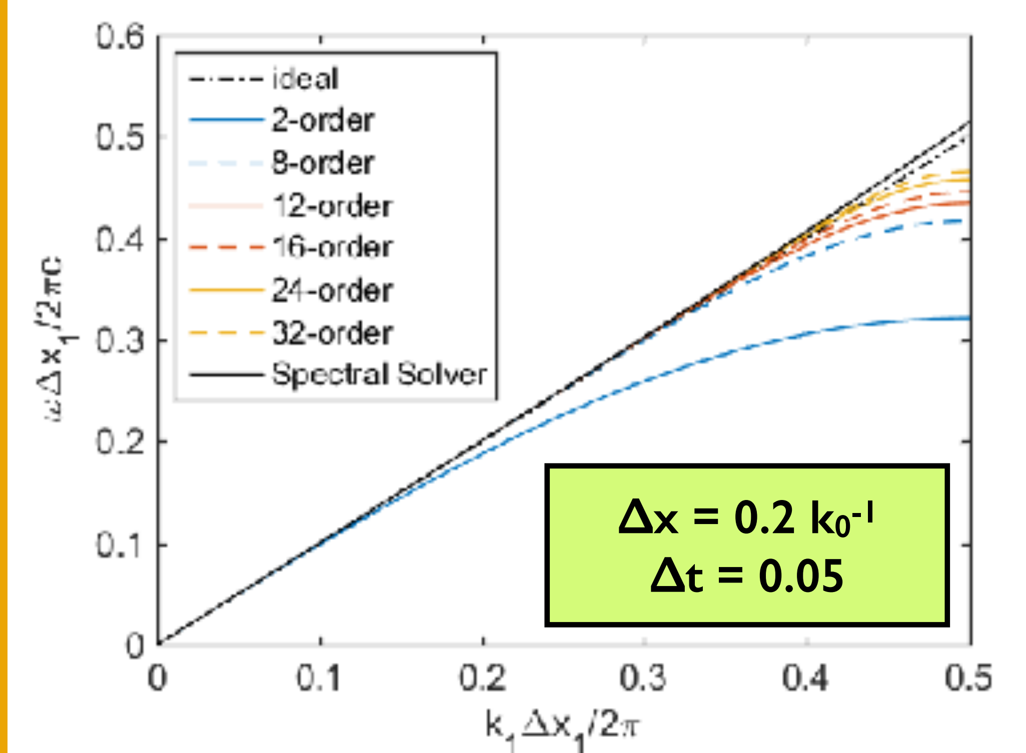


# Numerical Cherenkov instability (NCI)

## artificial numerical issues for PIC

- PIC results based on FDTD are prone to numerical Cherenkov radiation and NCI
- spectral based method mitigates numerical Cherenkov radiation but NCI is still present
- NCI observable in multi-dimensional PIC simulations with relativistic beams due to discretization*
  - LWFA in boosted Lorentz frame
  - relativistic plasmas

**dispersion relation**



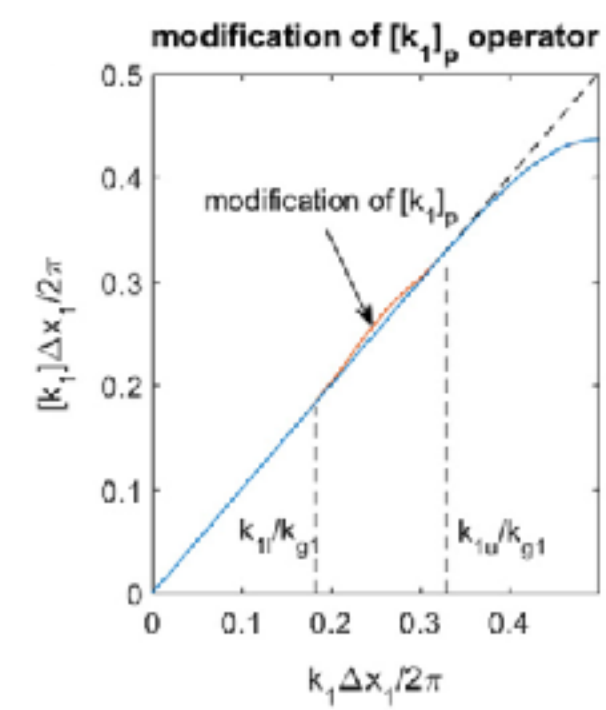

**customized solver****

- using a 32-order stencil with controlled coefficients
- coefficients are given by:

$$\partial^{+}_{p^*,x_1} f_{i_1,i_2} = 1/\Delta x_1 \sum_{l=1}^{M} \hat{C}_l^p \left(f_{i_1+l,i_2} - f_{i_1-l+1,i_2}\right)$$

$$\partial^{-}_{p^*,x_1} f_{i_1,i_2} = 1/\Delta x_1 \sum_{l=1}^{M} \hat{C}_l^p \left(f_{i_1+l-1,i_2} - f_{i_1-l,i_2}\right)$$

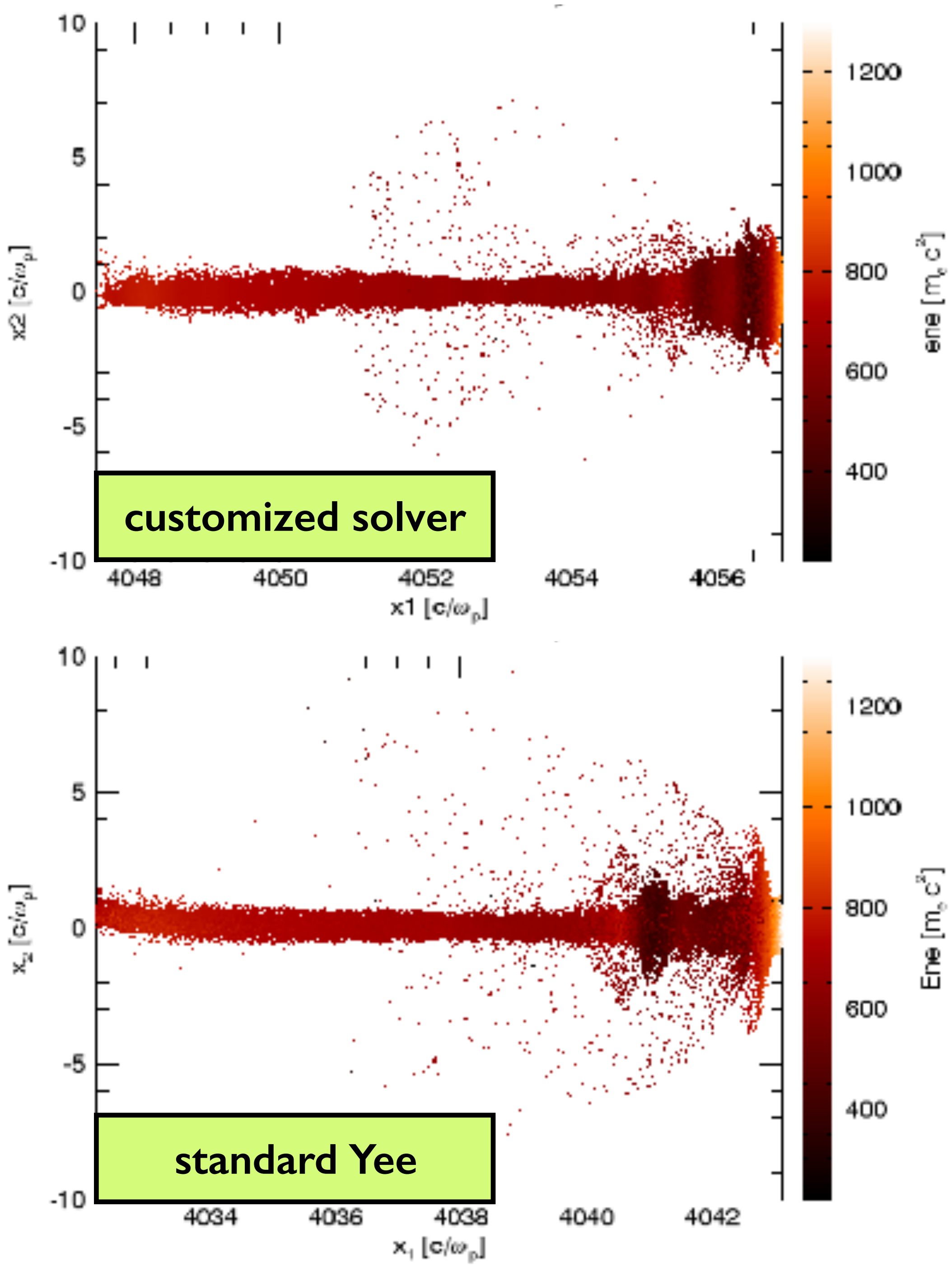
- requires current correction to satisfy continuity equation (Gauss's law)



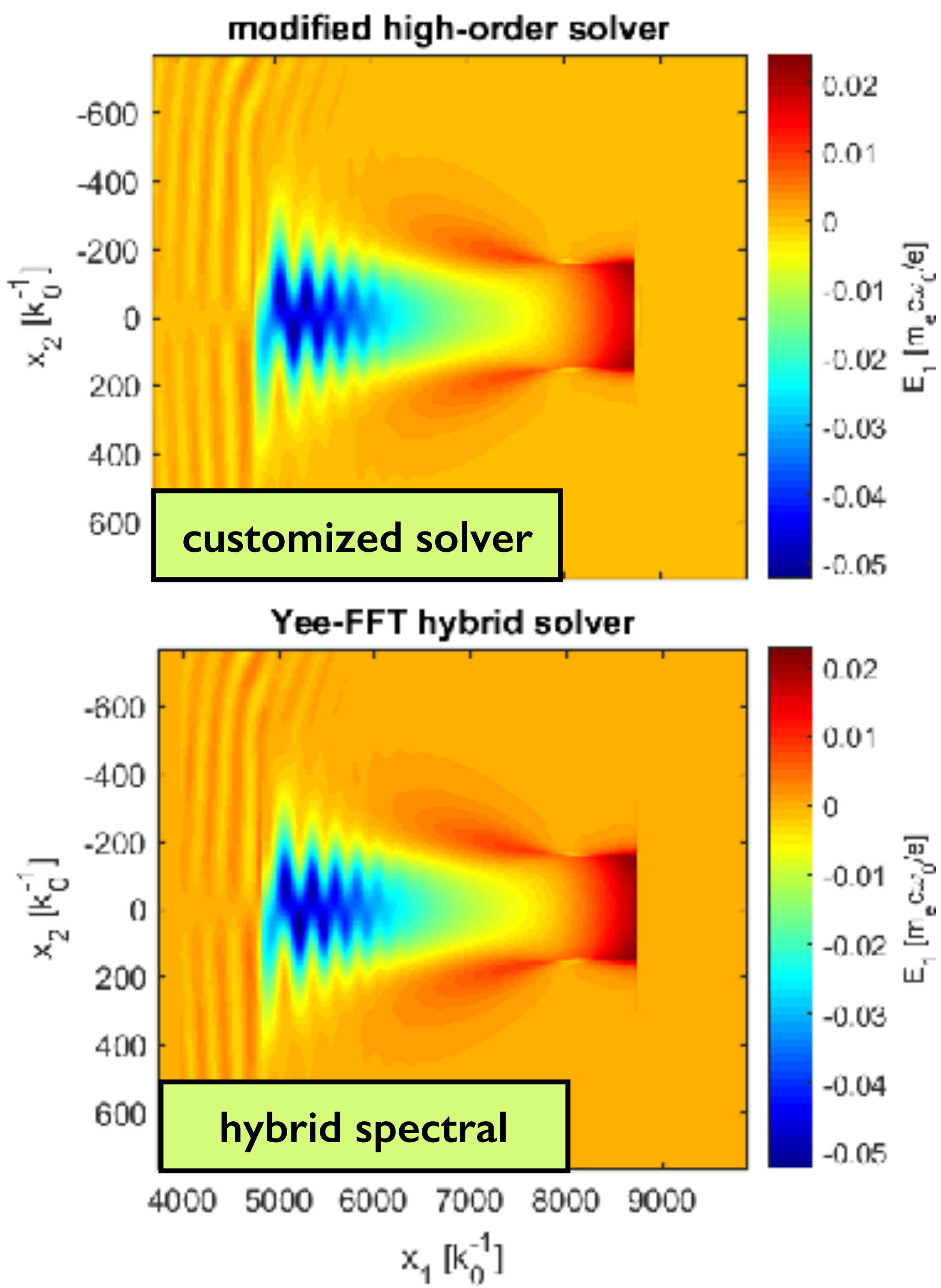

* X. Xu *et al.*, Comput. Phys. Commun. 184, 2503 (2013)
** F. Li *et al.*, Comput. Phys. Commun. 214, 6-17 (2017)

# Customized solver for two examples

## beam loading and injection




## boosted frame simulations



# conclusions & acknowledgement

**Scale disparity can be overcome with reduced models**

- reduced computational resources and time
- implementation and stability of ponderomotive guiding center for 3D

**Applications benefit from reduced models**

- massive parameter studies for different scenarios are feasible with reduced models
- full propagation for high $\omega_0/\omega_p$-cases can be studied

**Stability of numerical schemes**

- stability requires to be well discussed for PIC simulations to aim for the right physical parameters
- customized solver can be used to mitigate NCI

Simulation results obtained at Accelerates cluster (IST), JUQUEEN (JSC) and Cori (NERSC/LBNL)

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