A three-dimensional ponderomotive guiding center solver in Osiris

Anton Helm[1]
ahelm@ipfn.tecnico.ulisboa.pt

R. Fonseca[1,2], J. Vieira[1], L. Silva[1]

[1] GoLP / Instituto de Plasmas e Fusão Nuclear
Instituto Superior Técnico, Lisbon, Portugal

[2] ISCTE - Instituto Universitário de Lisboa, Lisbon, Portugal

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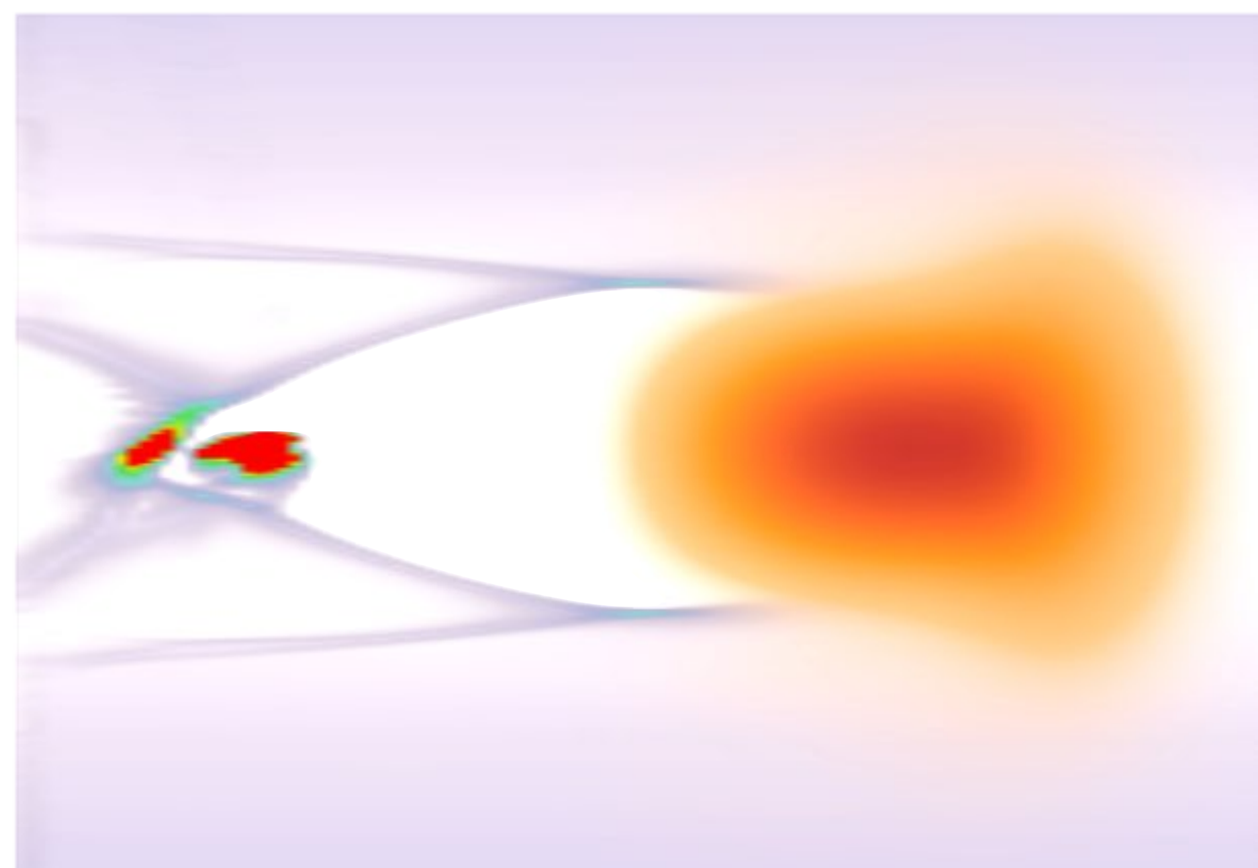

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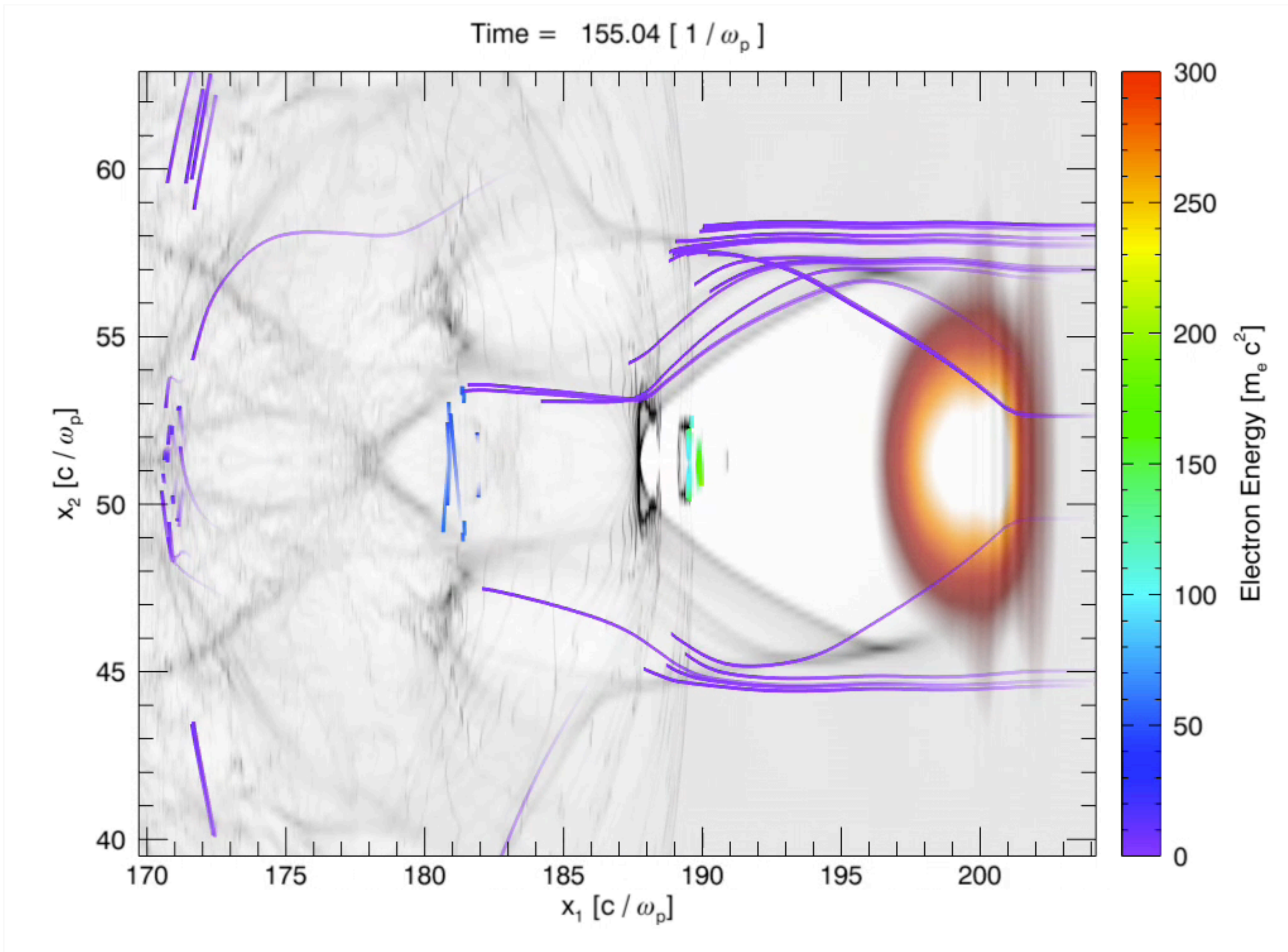
INPAIRS

Scale disparities in LWFA modeling



scale disparity in modeling

multi-scale problems

- large disparity of spatial/temporal scales

sample problem: 50 GeV LWFA stage

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

computational requirements (moving window)

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

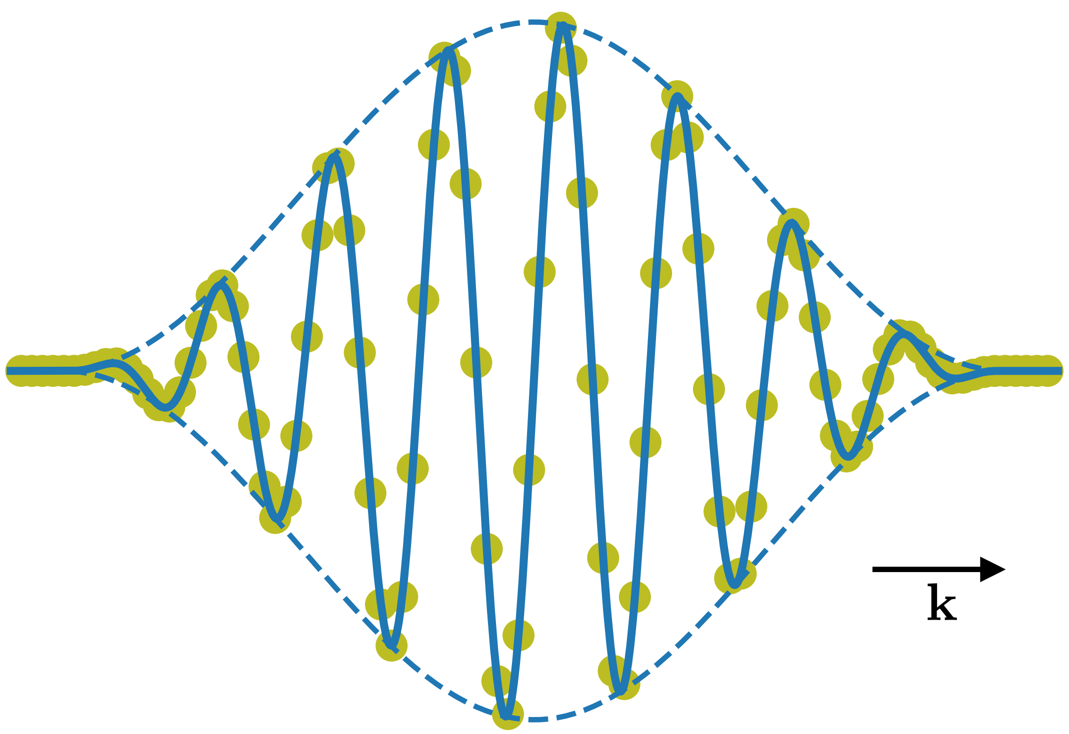
requirement for reduced models

Envelope approximation reduces spatial resolution

particle-in-cell (PIC)

spatial resolution:
laser wavelength

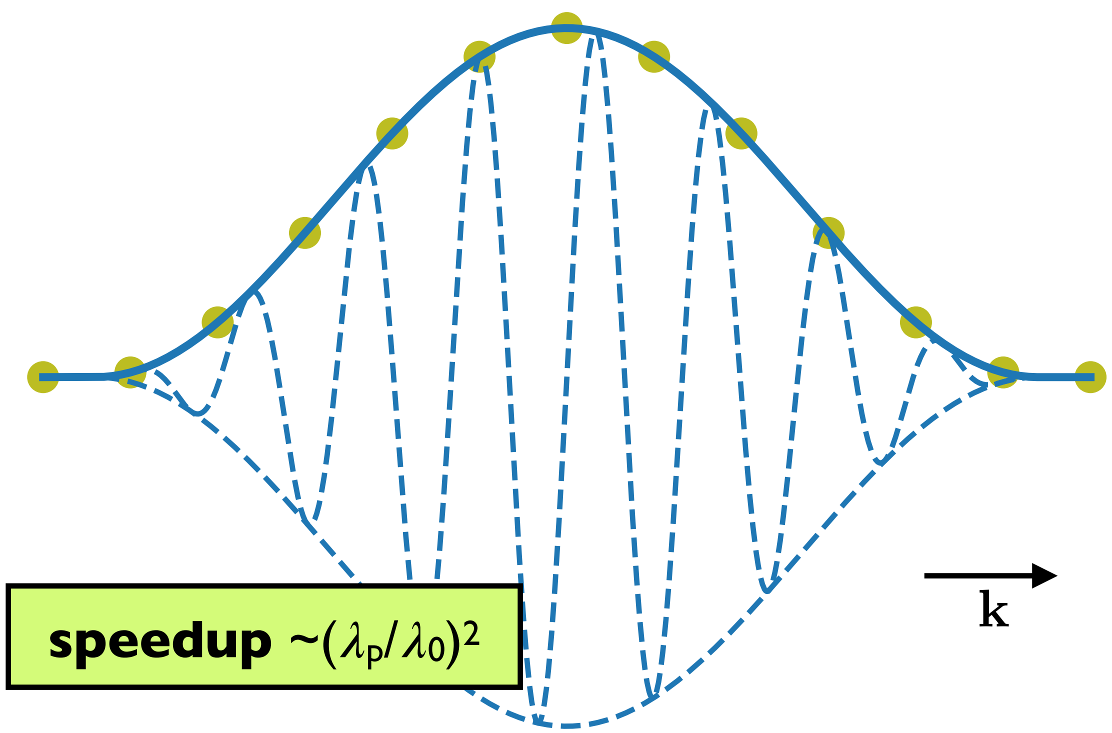
$$\frac{\partial \mathbf{E}}{\partial \tau} = c\nabla \times \mathbf{B} - 4\pi \mathbf{j}$$
$$\frac{\partial \mathbf{B}}{\partial \tau} = -c\nabla \times \mathbf{E}$$



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

ponderomotive guiding center (PGC)

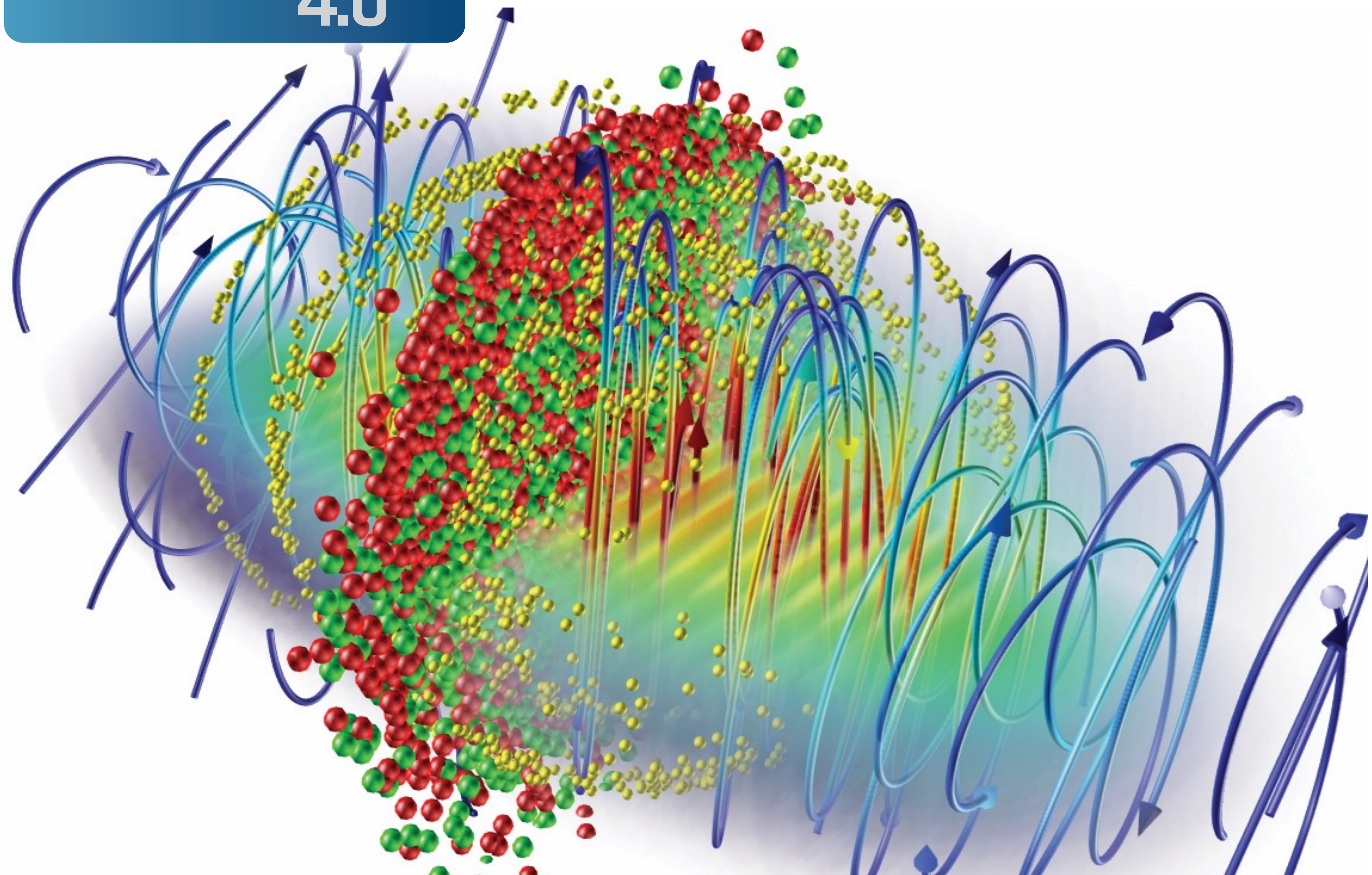
spatial resolution:
plasma skin depth



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

Osiris 4.0

Committed to open science



Open-access model

- 40+ research groups worldwide are using OSIRIS
- 300+ publications in leading scientific journals
- Large developer and user community
- Detailed documentation and sample inputs files available

Using OSIRIS 4.0

- The code can be used freely by research institutions after signing an MoU
- Find out more at:

http://epp.tecnico.ulisboa.pt/osiris

OSIRIS framework

- Massively Parallel, Fully Relativistic Particle-in-Cell Code
- Parallel scalability to 2 M cores
- Explicit SSE / AVX / QPX / Xeon Phi / CUDA support
- Extended simulation/physics models

visXD

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Ricardo Fonseca: ricardo.fonseca@tecnico.ulisboa.pt

Major features of PGC in OSIRIS

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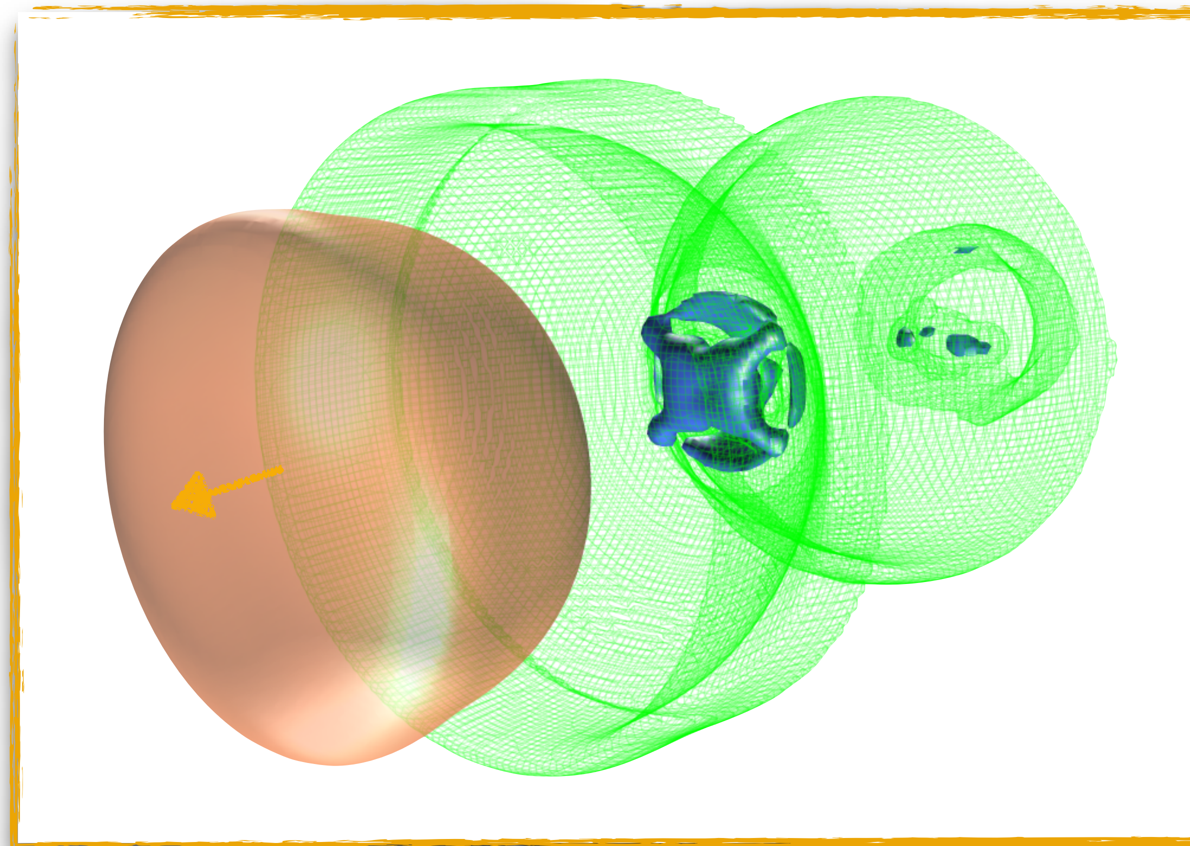
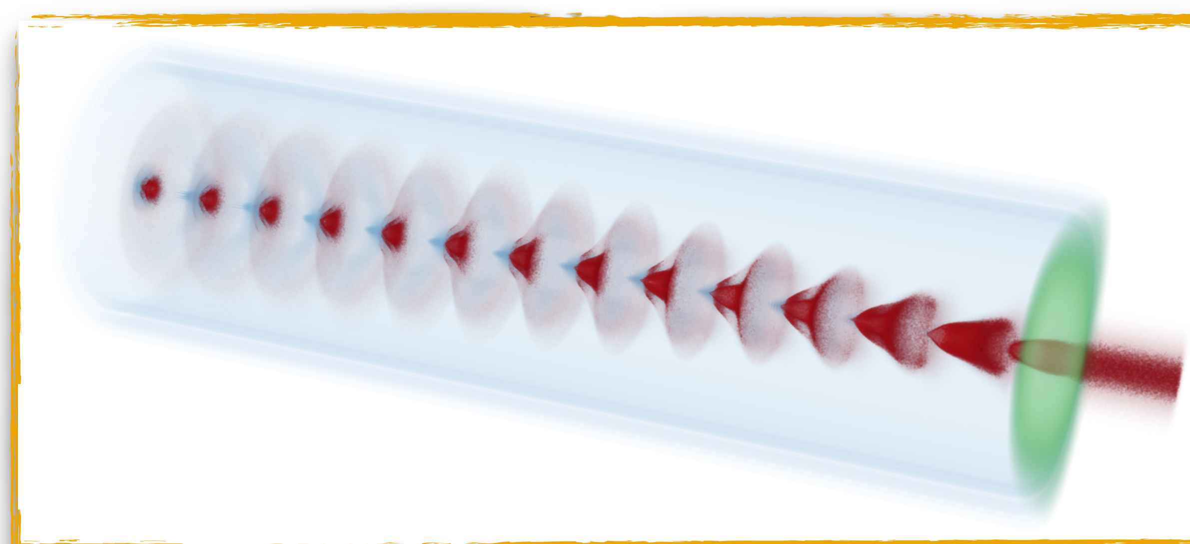
Physical features:

- moving window frame
- 2d cartesian
- 2d cylindrical cartesian
- 3d cartesian
- different laser pulse shapes
- different boundary conditions for transversal direction
- field ionization based on ADK model



Numerical stability and stability control:

- stability condition for envelope equation
- up to 4th order interpolation and deposition schemes
- smoothing for stability control



Parallel performance:

- shared memory parallelization
- distributed memory parallelization
- scalable up to 10^5 cores

Outline

Incorporation of PGC into Osiris

numerical stability and control of numerical noise

Parallel scalability of PGC

incorporation of shared and distributed memory parallelization

Physical applicability for PGC

down-ramp injection with PGC and full scale modeling of self-modulation instability

Incorporation of PGC into PIC cycle

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PGC extension

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

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

laser frequency — laser envelope

- particle advancing

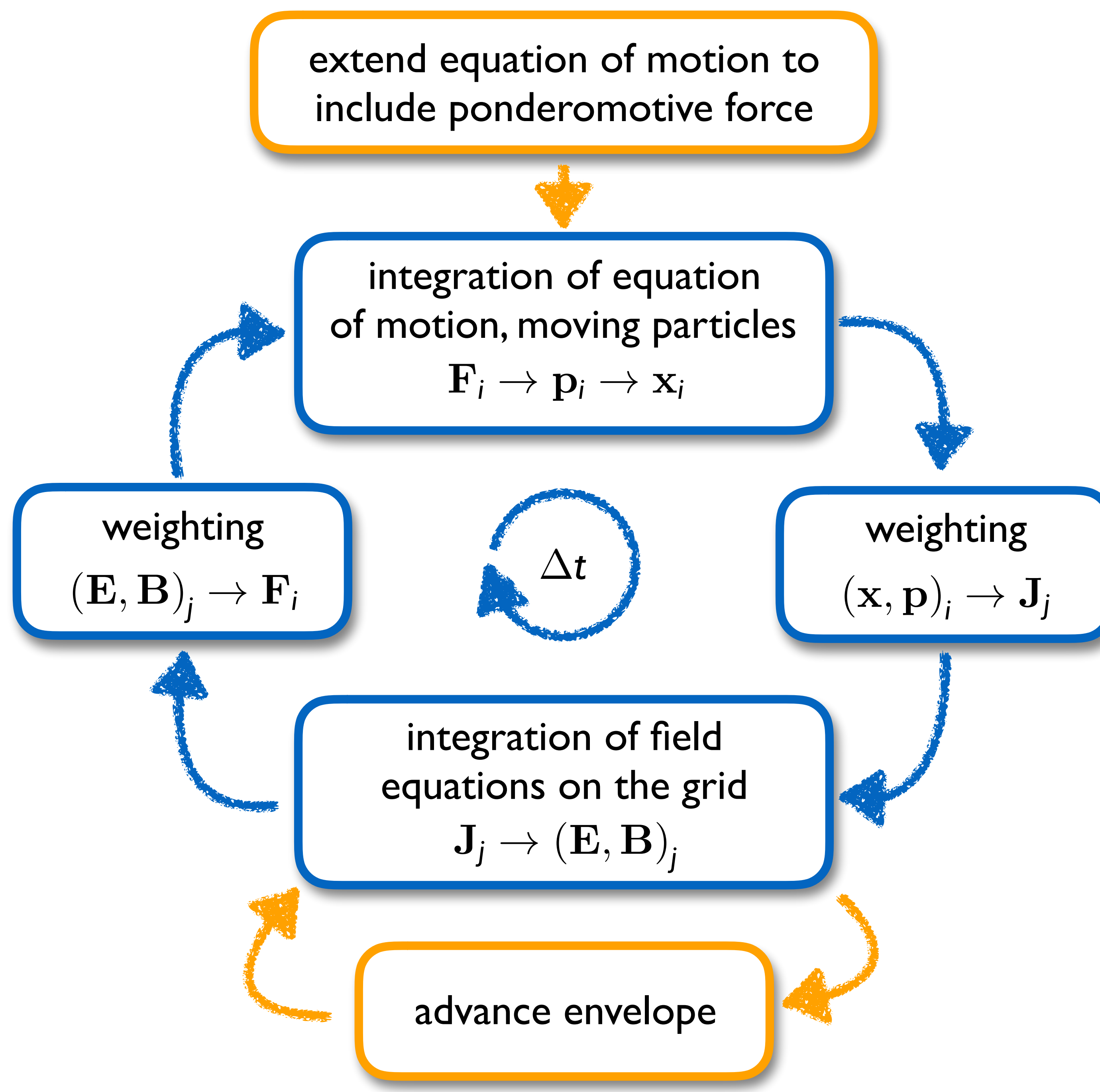
$$\mathbf{F}_p = -\frac{1}{4}\frac{q^2}{\langle m \rangle}\nabla |a|^2$$

- coupling parameters

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

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

extended PIC algorithm



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

Incorporation of PGC into PIC cycle

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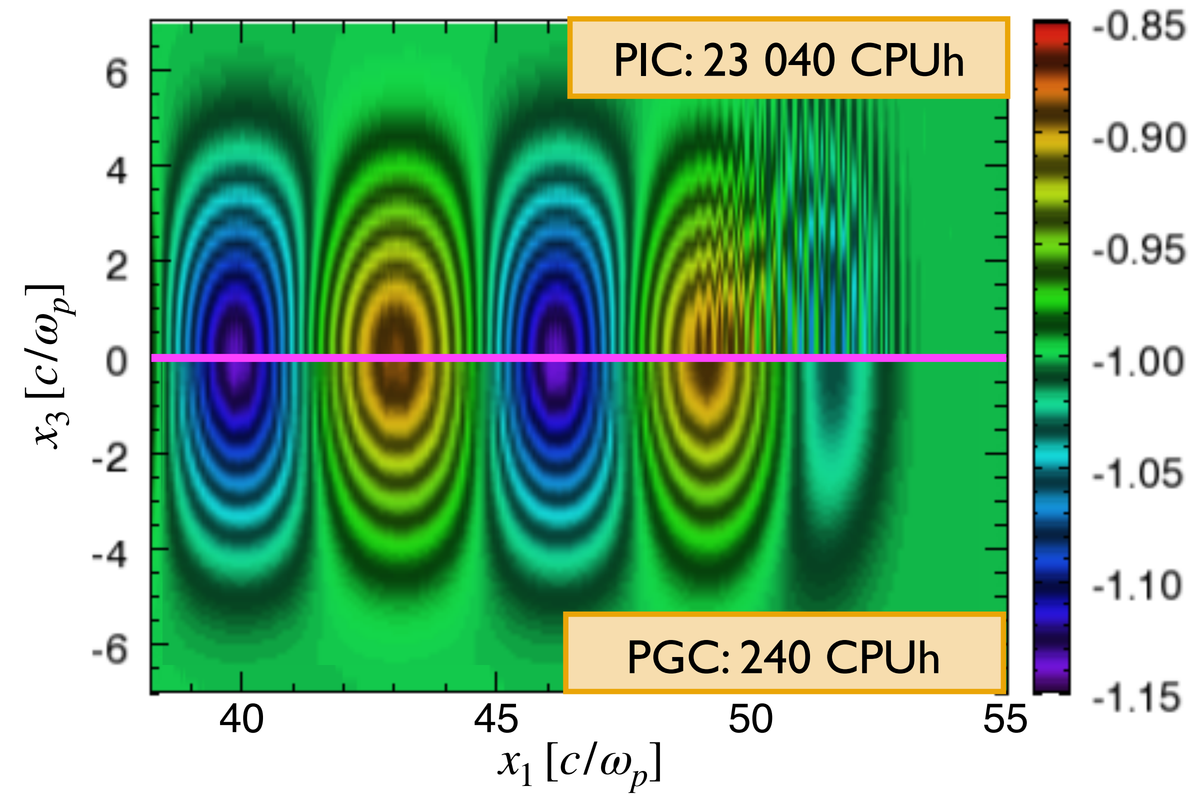
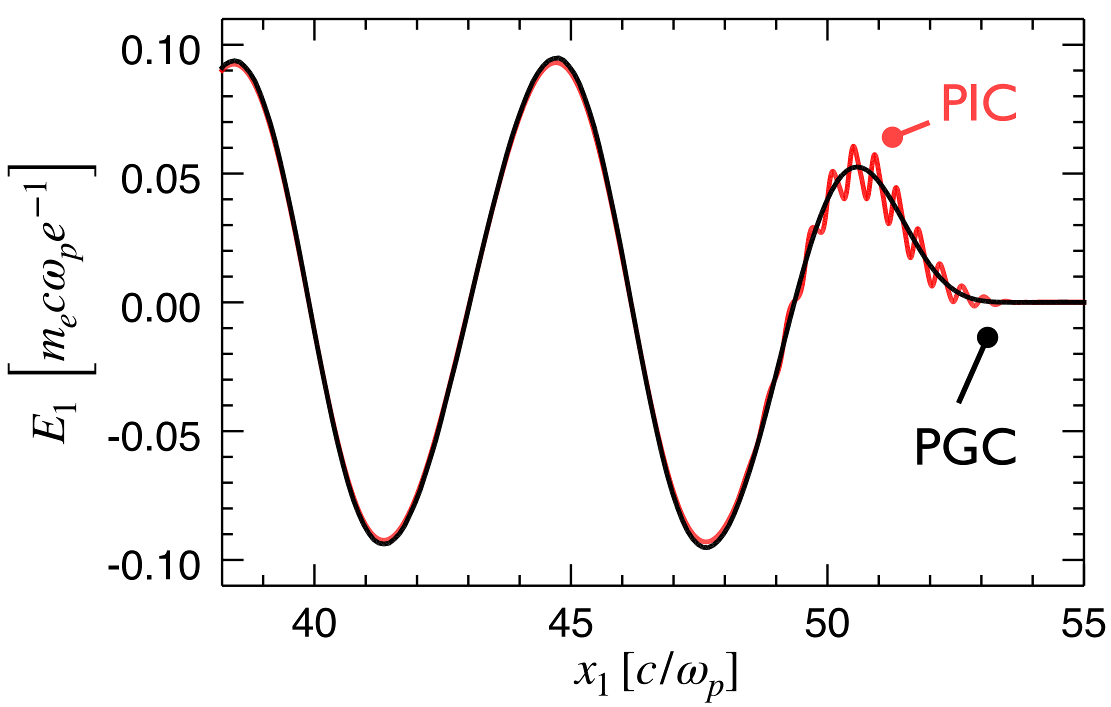
electron density (slice)



accelerating field



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Stability of the envelope solver depends on laser frequency

Courant-Friedrichs-Lewy (CFL)

$$\Delta t \leq \sqrt{1/(1/\Delta x)^2 + (1/\Delta y)^2 + (1/\Delta z)^2}$$

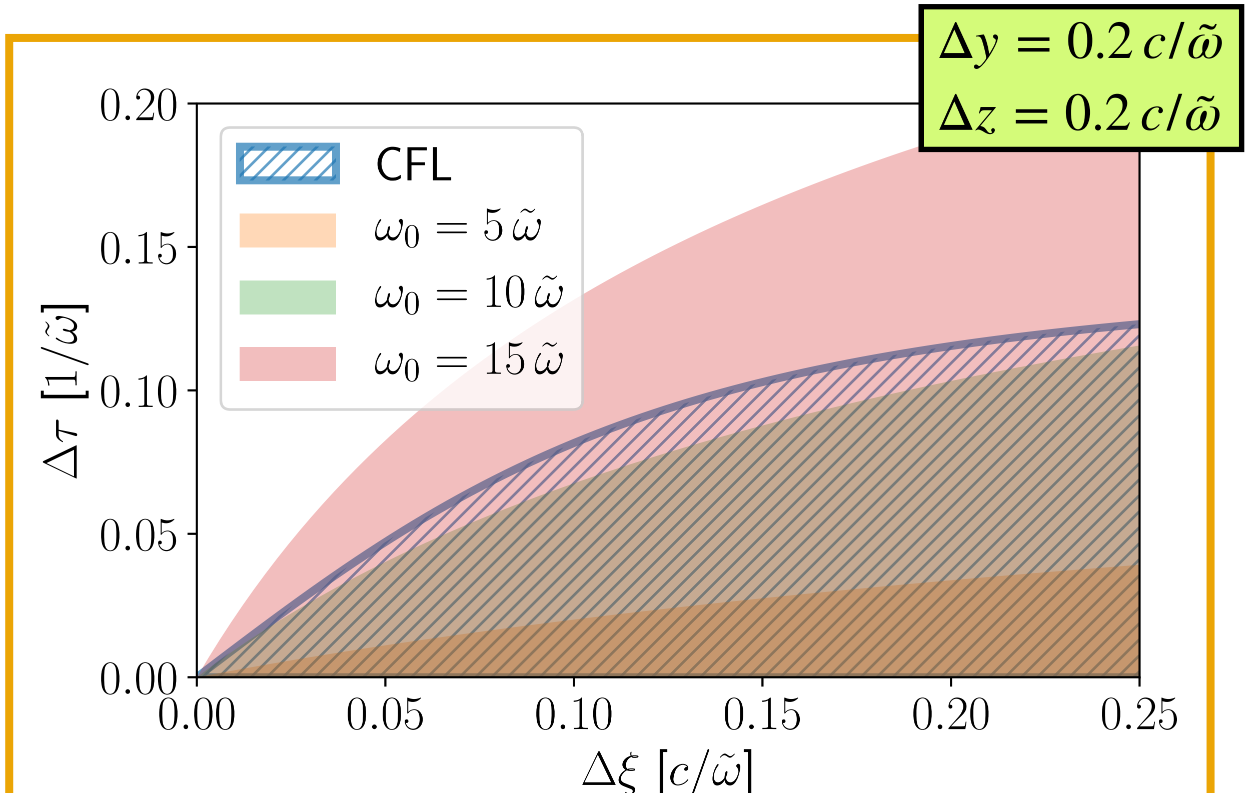
- necessary condition for stability of Maxwell solver
- does not depend on physical parameters

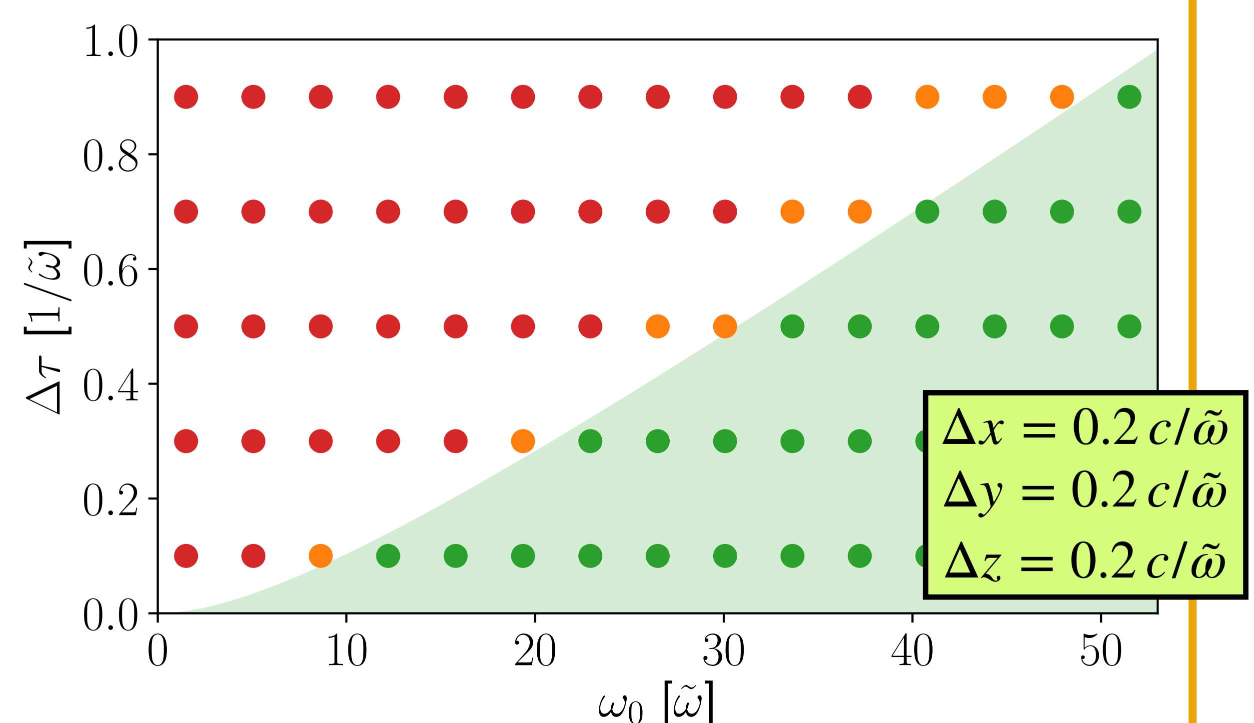
vacuum stability condition

- implicit solver for advancing of the envelope
- von-Neumann analysis for stability condition
- stability condition for the vacuum case

$$\Delta\tau^2 \leq \frac{\Delta y^4 \Delta z^4 \Delta\xi^2 \omega_0^4}{4\left(\Delta z^2 + \Delta y^2(1+\Delta\xi\omega_0)\right)^2 - \Delta y^4 \Delta\xi^2 \omega_0^2}$$

- stability depends on the laser frequency
- for higher frequencies the envelope equation becomes "more stable"





Plasma gradients lead to numerical instabilities*

numerical error

$$2i\omega_0\partial_\tau\epsilon^n_{ijk} = \left(1 + \frac{\partial_\xi}{i\omega_0}\right)\left(\chi\epsilon^n_{ijk} + \nabla^2_\perp\epsilon^n_{ijk}\right)$$

- numerical stable:

$$|g| = |\epsilon^{n+1}/\epsilon^n| \leq 1$$

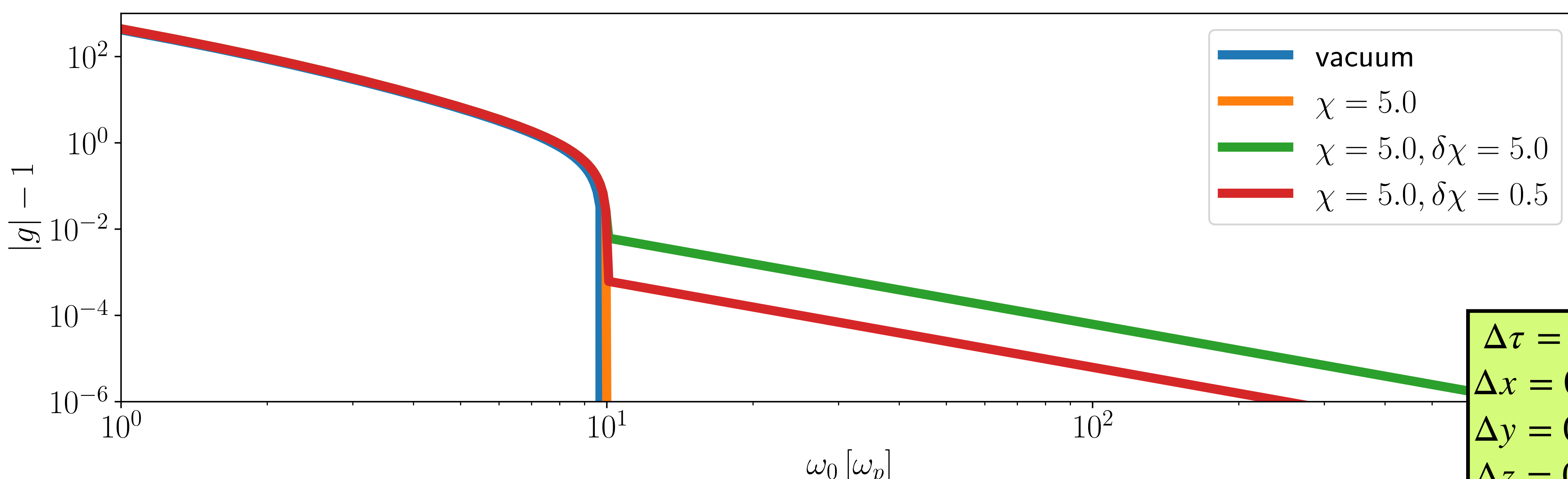
- plasma parameter:

$$\chi \equiv \chi_{ijk} \sim \mathcal{O}(\rho)$$

- plasma gradients:

$$\delta\chi \equiv \chi_{(i+1),j,k} - \chi_{(i-1),j,k}$$

numerical error growth rate for PGC



$\Delta\tau = 0.1\omega_p^{-1}$
$\Delta x = 0.2\ c/\omega_p$
$\Delta y = 0.2\ c/\omega_p$
$\Delta z = 0.2\ c/\omega_p$

* A. Helm et al., to be submitted (2019)

Stability control for PGC

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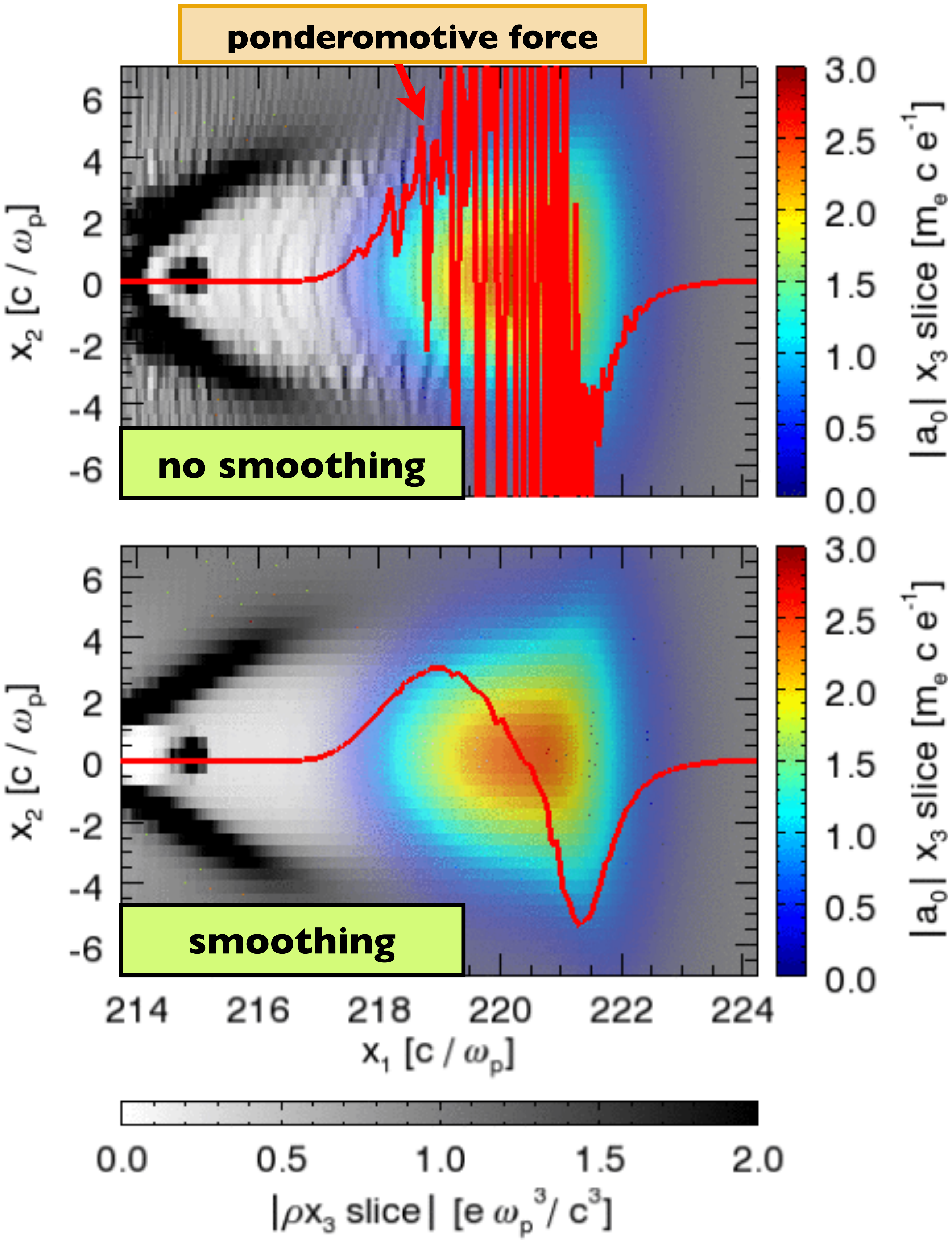
particle interpolation order

- 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

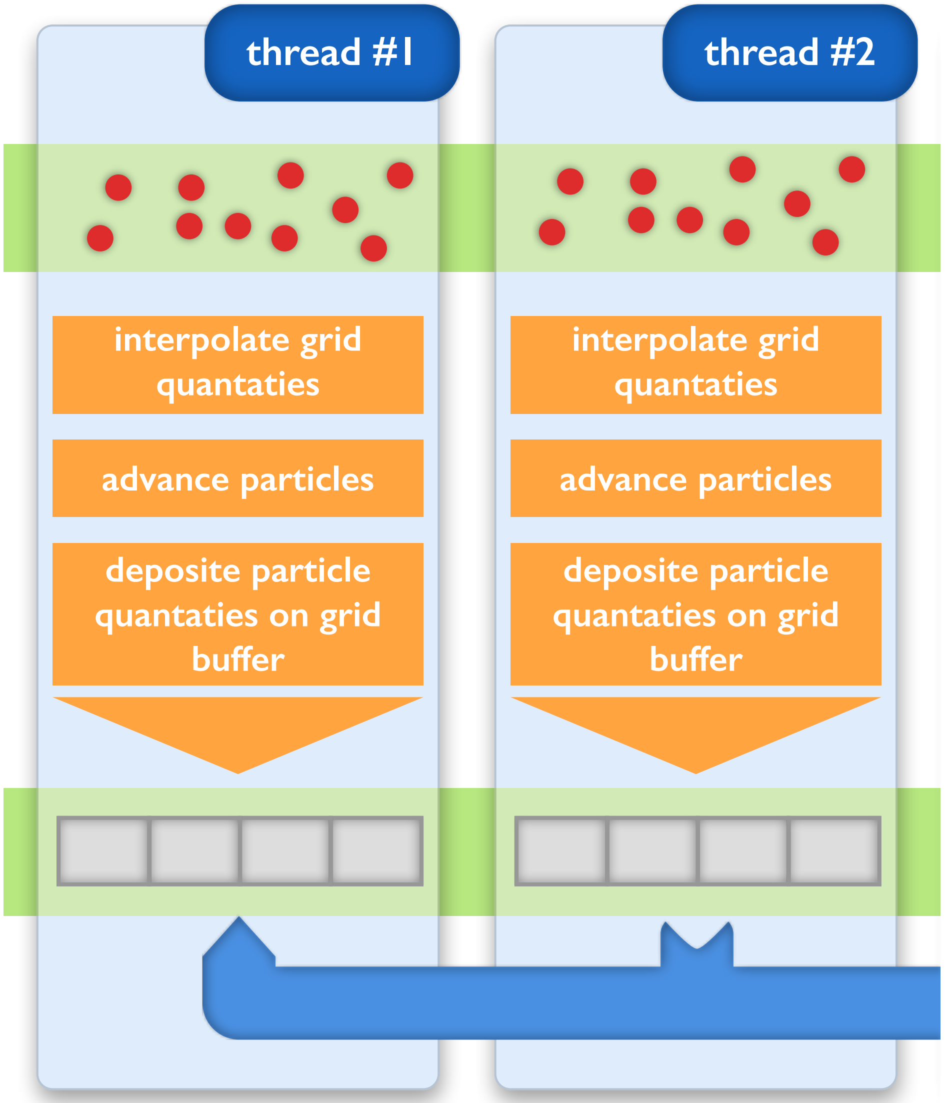
smoothing of PGC quantities

- 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



Shared memory parallelization for PGC

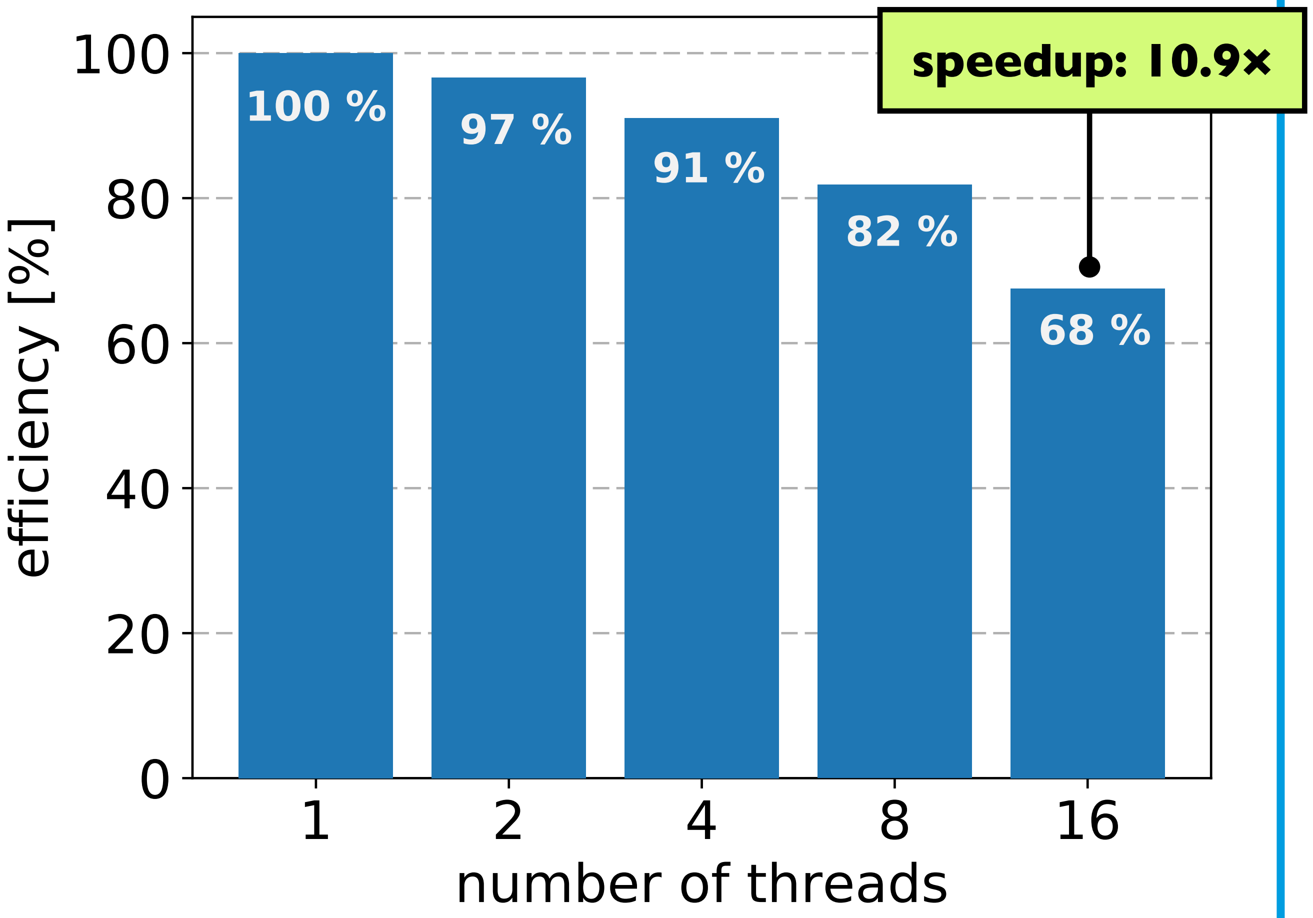
shared memory parallelization



thread-based particle advancing

- ✔ data sharing between threads is fast
- ✔ envelope solver can be parallelized easily
- ✘ lack of scalability between memory and cores
- ✘ memory is limited to cores and does not scale

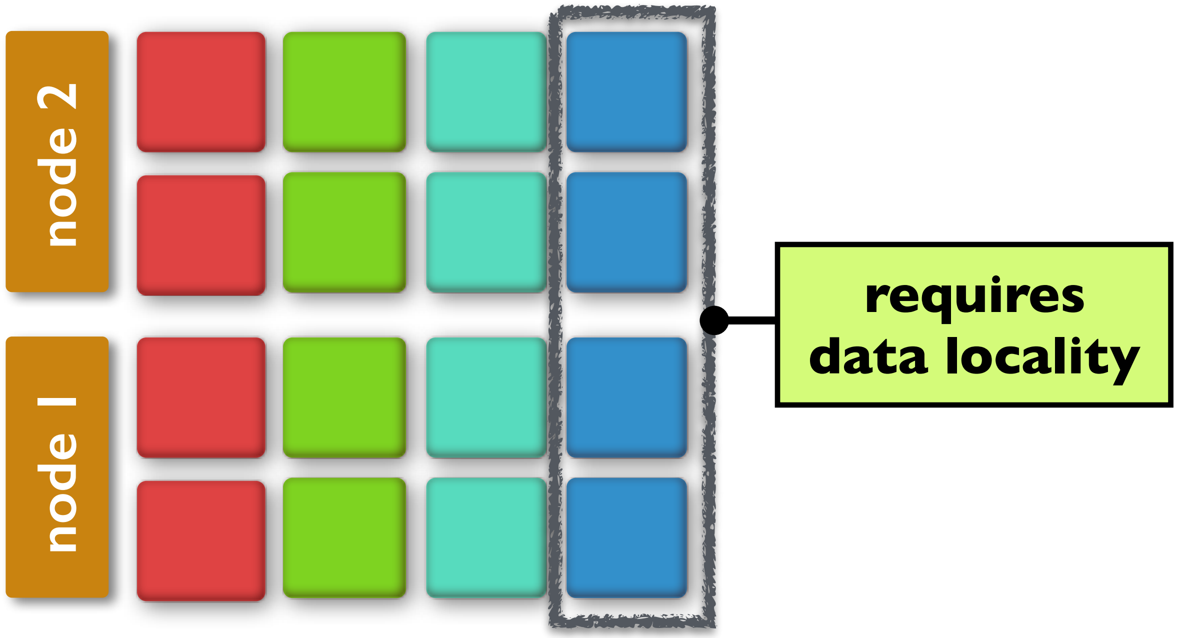
thread-based strong scaling



- ✦ JUQUEEN (IBM BlueGene/Q) - 16 cores per node
- ✦ number of cores: 32 / 64 / 128 / 256 / 512
- ✦ 500 time steps - 608x152x152 cells and 8 ppc
- ✦ using distributed parallelization in longitudinal direction
- ✔ scaling over one order of cores using shared memory parallelization

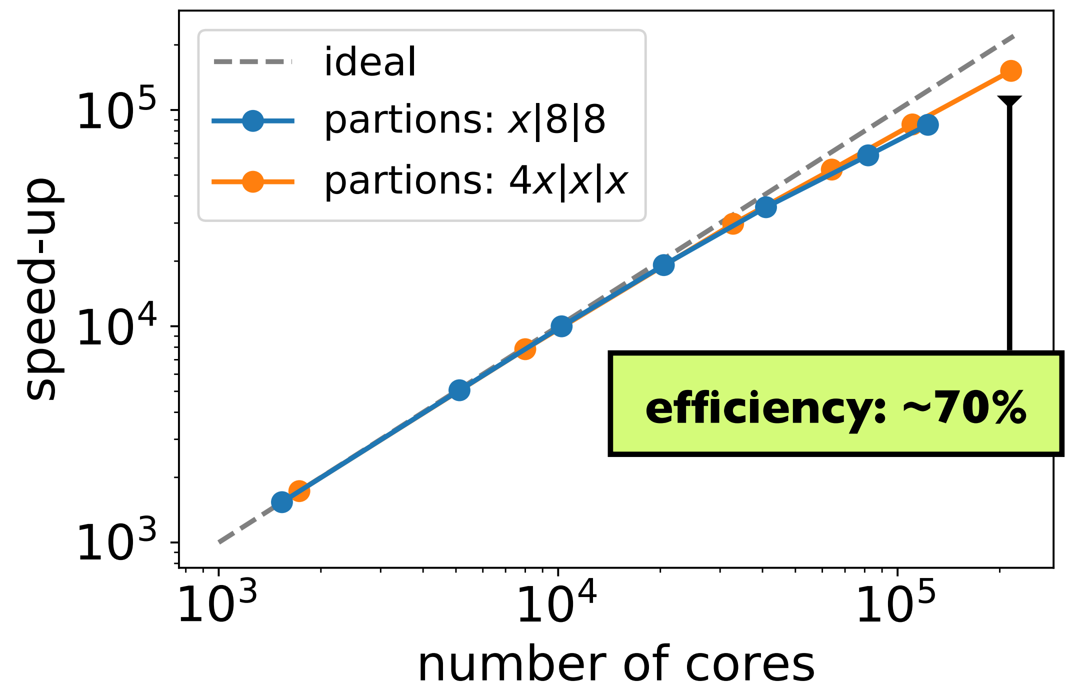
Parallelization is scalable over thousands of cores

distributed memory parallelization

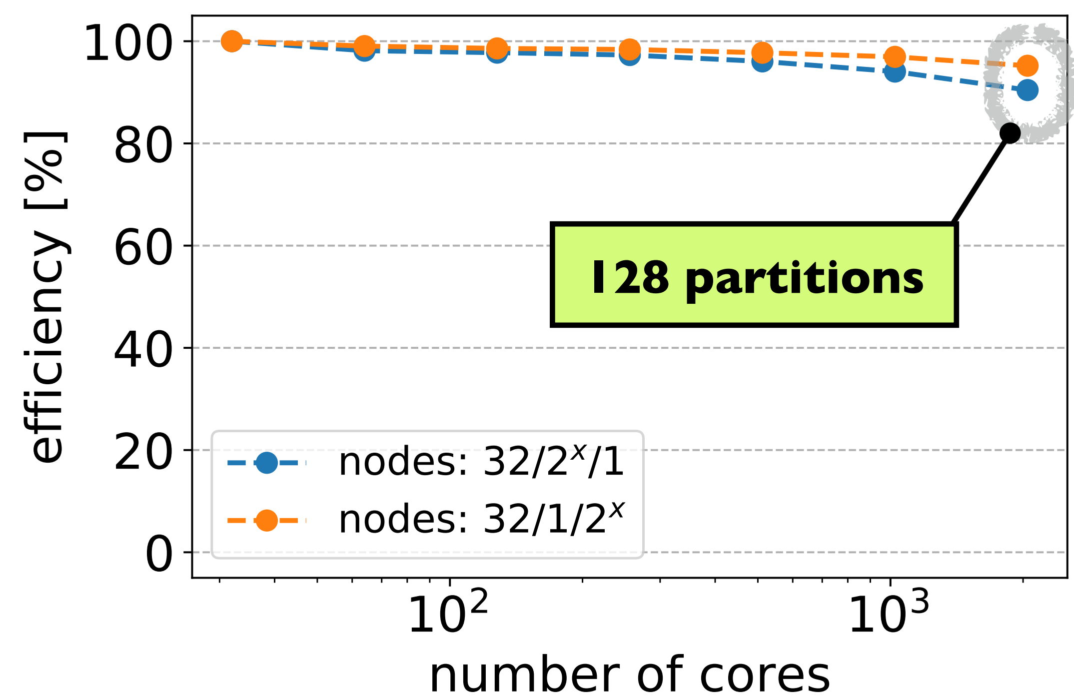


- advancing the envelope requires data locality in transversal direction due to implicit finite difference scheme
- data locality can be achieved through a transpose operation
- scaling tests were carried out on JUQUEEN
  - 16 cores per node / no threading (IBM BlueGene/Q)
- strong scaling: 15360×240×240 with 8 ppc and 500 steps
- weak scaling: 10 cells in x_2 and 50 cells in x_3
- ✔ PGC scales from 1536 to 216000 with >70% efficiency

strong scaling



weak scaling



PGC for parametric studies for down ramp injection

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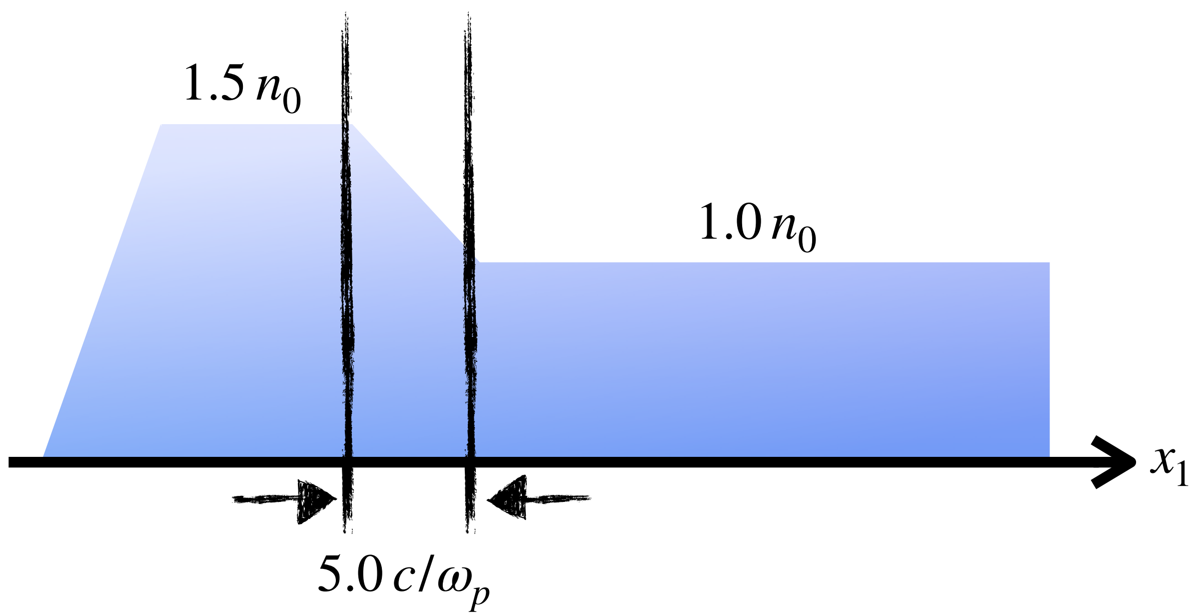
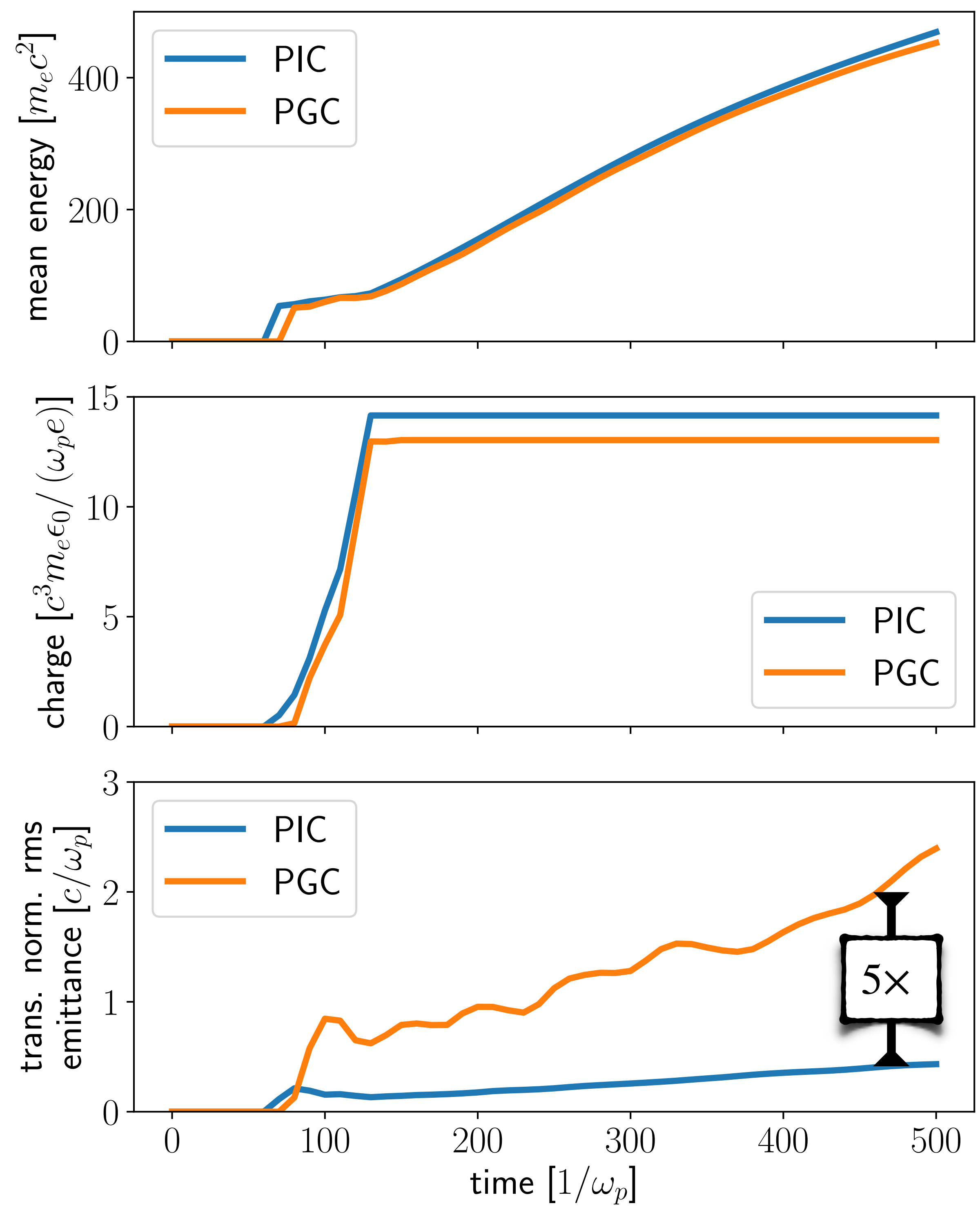
down ramp injection case

density profile:

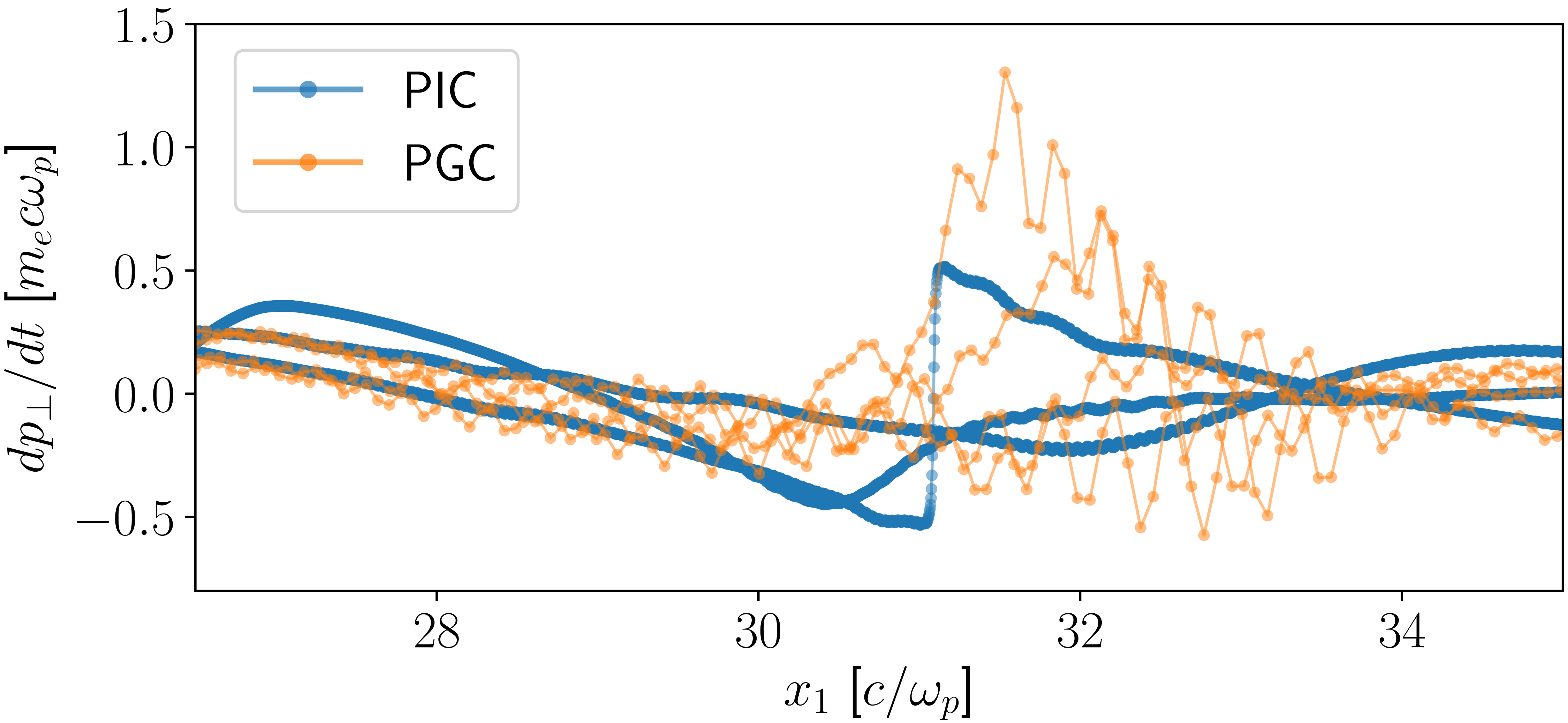


- PGC allows to perform parametric studies with a fraction of computational costs compared to PIC
- attractive tool for design studies like EuPRAXIA
- comparison of PGC vs. PIC:
  - identical transversal resolution
  - longitudinal resolution: $\Delta\xi_{\mathrm{PIC|PGC}} = \lambda_{0|p}\,/\,62$
  - injected electron bunch with $\gamma > 50$
  - mean energy and charge are in agreement
  - emittance 5x higher for PGC

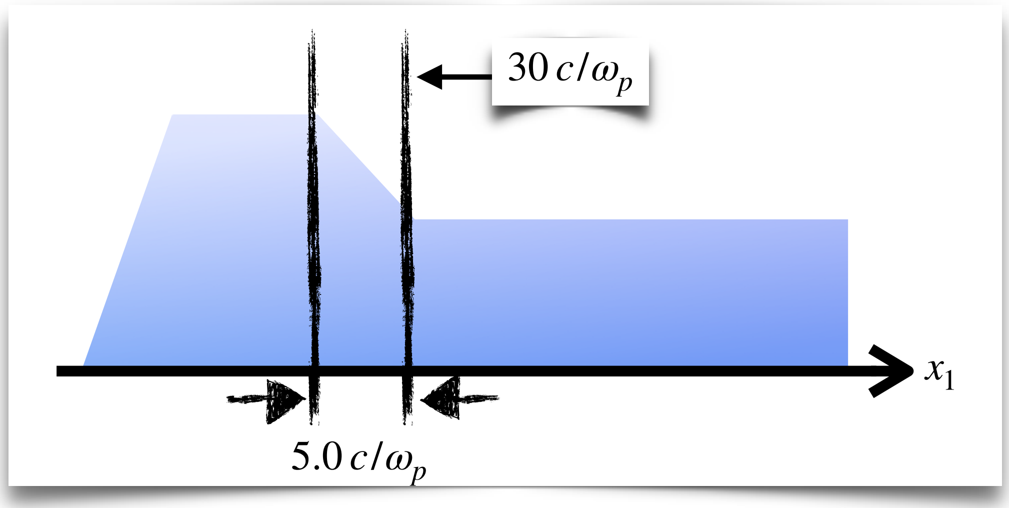
injected beam properties



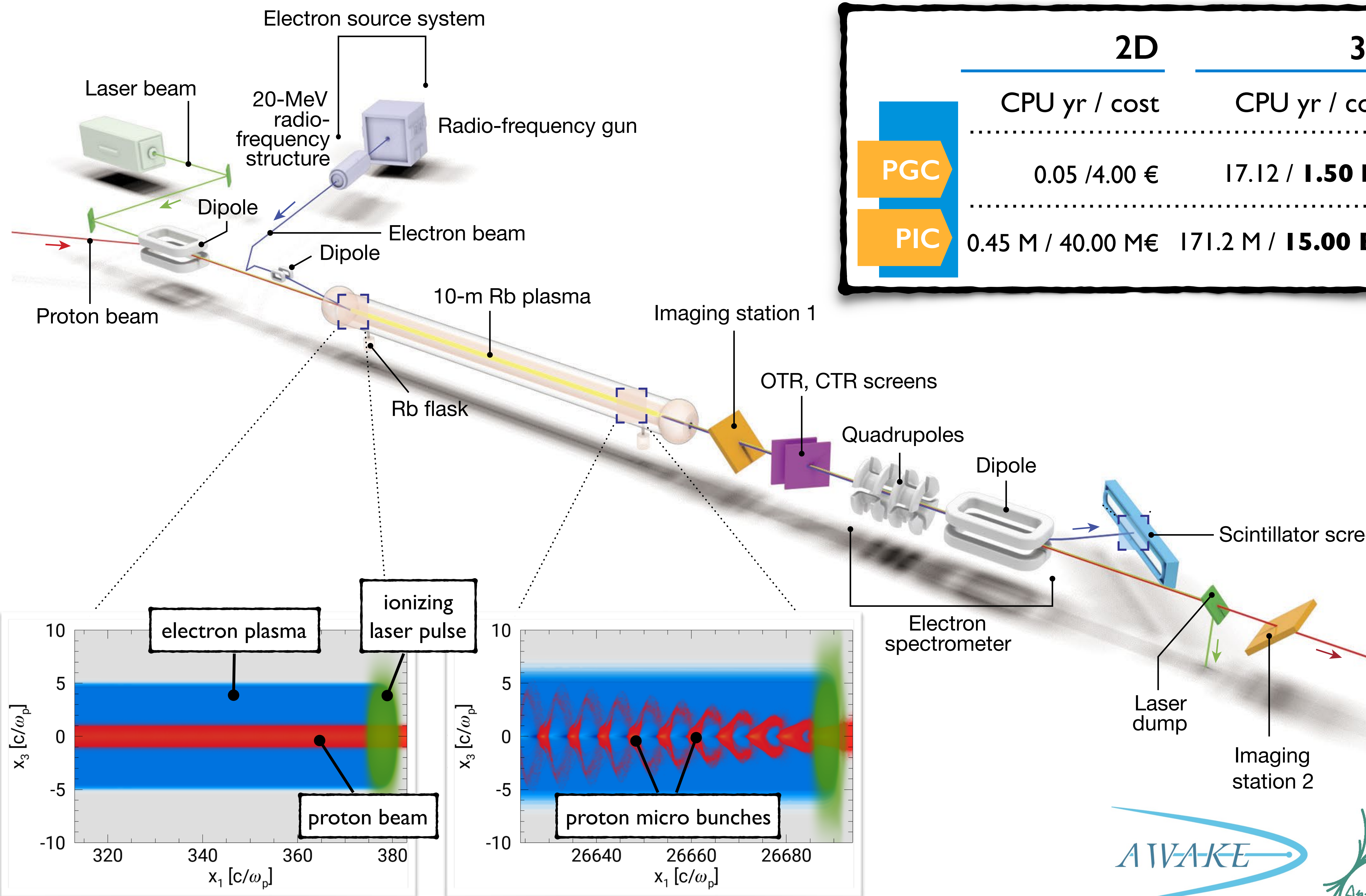
Temporal resolution leads to higher emittance



- fields structure is describe on long scales associated to plasma scales
- plasma scales are resolved by PGC
- temporal resolution for PGC case is reduced by λ_p/λ_0



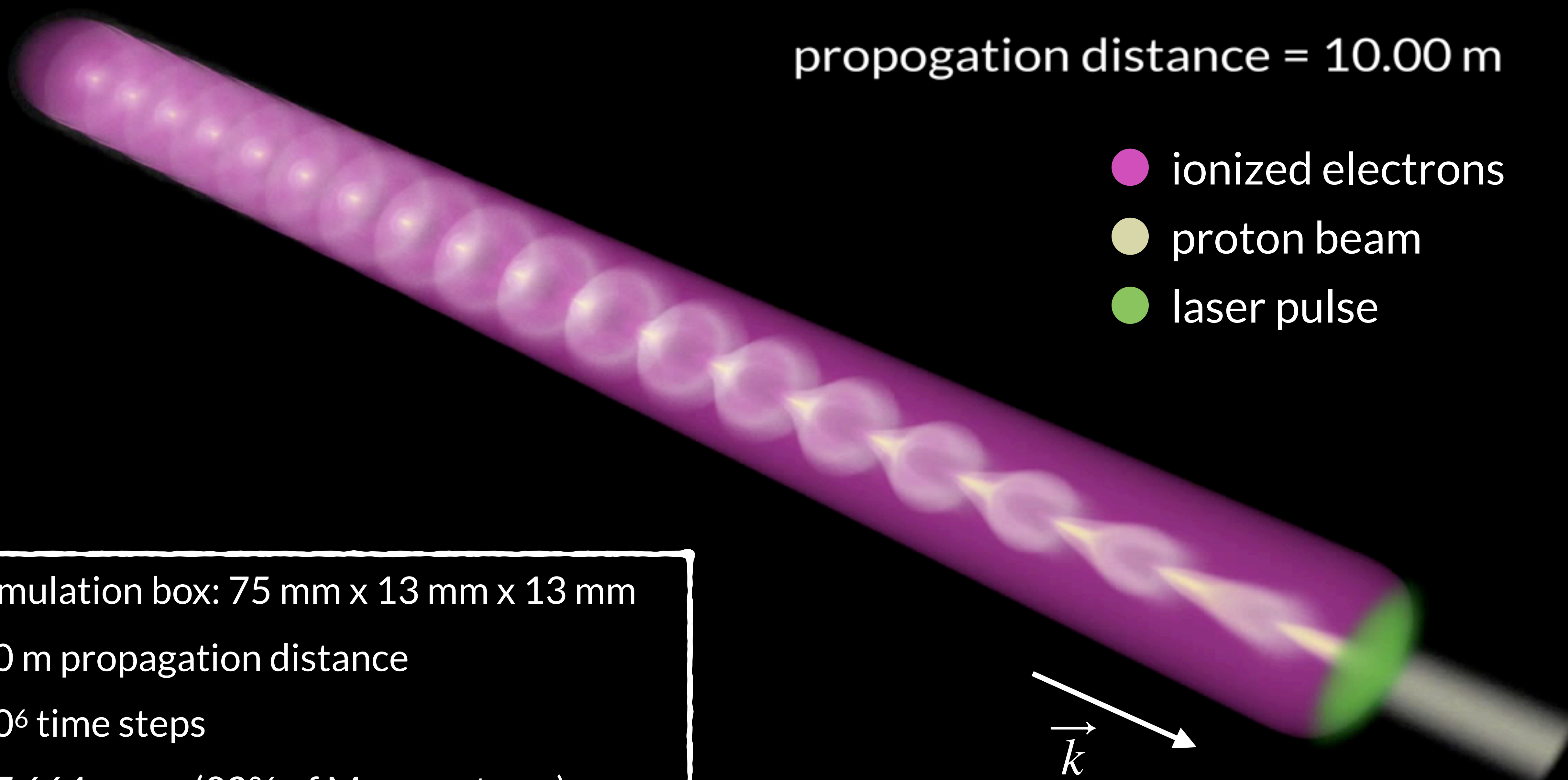
Acceleration of electrons in the plasma wakefield of a proton bunch*



	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€**

* Adli, E. et al., *Nature*, *561* (7723), 363–367 (2018)

Ionization seeding with PGC for self-modulation instability



- simulation box: 75 mm x 13 mm x 13 mm
- 10 m propagation distance
- 10^6 time steps
- 17 664 cores (92% of Marenostrum)
- ~3M CPUh

Conclusions & acknowledgement

Numerical stability and control

- in general PGC is unconditionally unstable if plasma gradients are present
- control can be provided by applying smoothing filters

Scale disparity can be overcome with reduced models for LWFA

- important for parametric studies of LWFA
- for cases where $\omega_0/\omega_p \gg 1$

Parallel scalability

- using shared memory parallelization, PGC can scaled over one order of magnitude
- using distributed memory parallelization, PGC can be scaled over 10^5 cores
- PGC and parallel scalability is required for full study of experiments like AWAKE

Simulation results obtained on JUQUEEN (JSC), Cori (NERSC/LBNL) and Marenostrum (BSC)

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