Full-scale modeling of plasma-based accelerators using ponderomotive guiding center solver in OSIRIS

Anton Helm[1]

ahelm@ipfn.tecnico.ulisboa.pt

T. Silva[1], 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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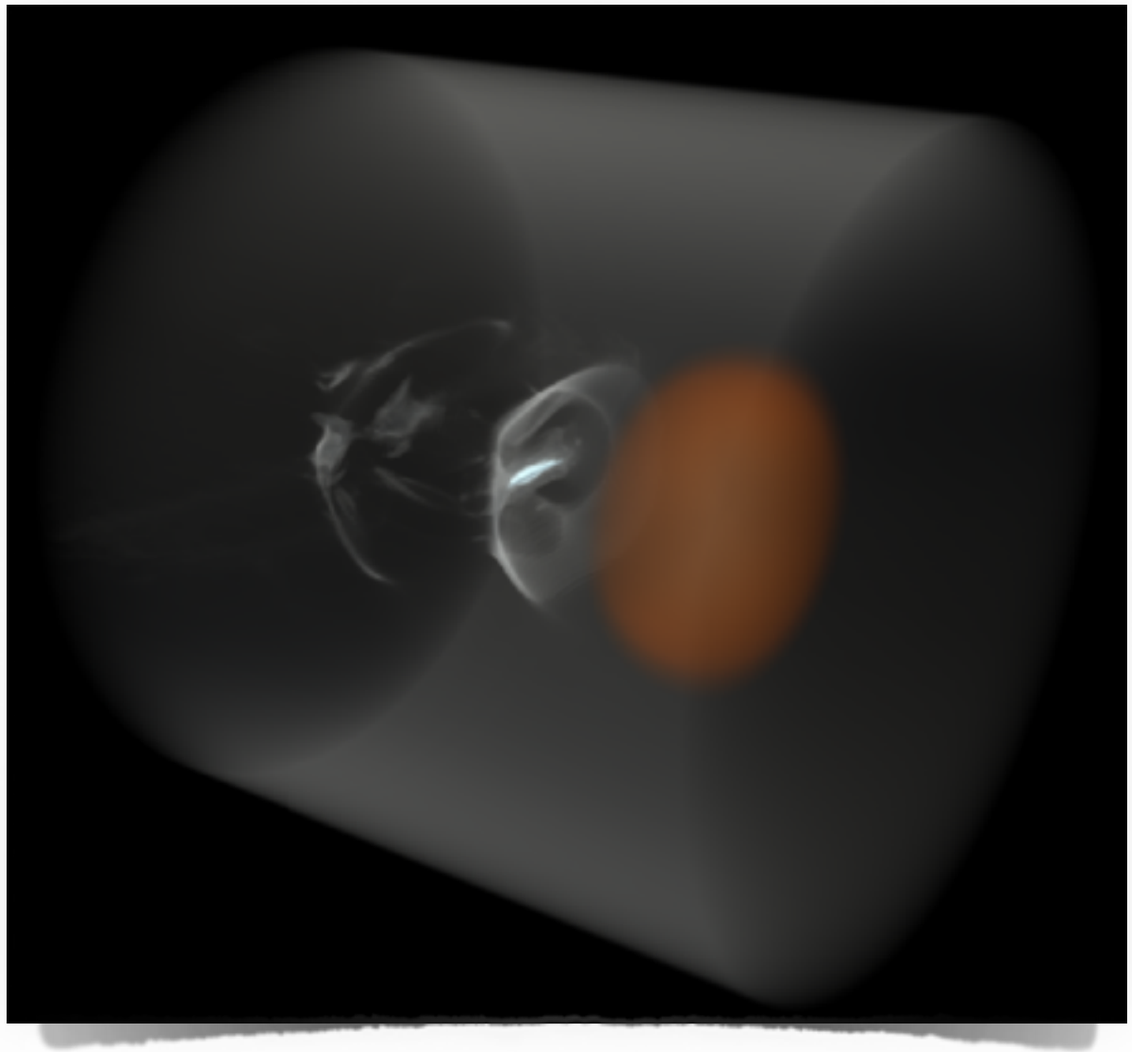
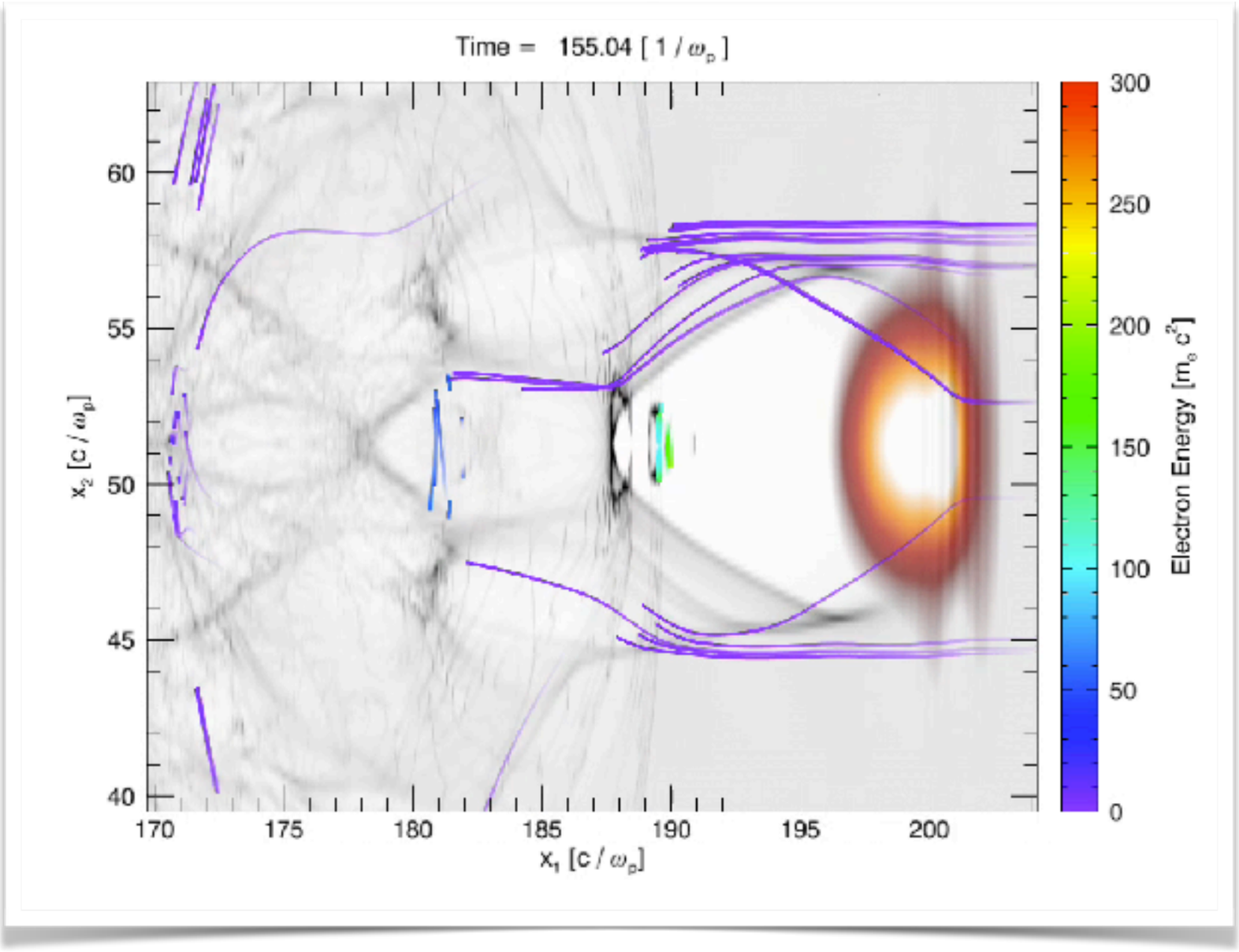
Supported by the Seventh Framework Program of the European Union



LWFA is an Exascale problem



scale disparity in modeling

multi-scale problems

- large disparity of spatial/temporal scales

sample problem: 50 GeV LWFA stage

- $\lambda_0 \sim 1\mu\text{m} \,/\, \lambda_p \sim 17\mu\text{m}$
- $L \sim 1.5$ m

computational requirements (moving window)

- $\sim 10^9$ grid cells
- $\sim 10^{10}$ particles
- $\sim 10^6 - 10^7$ iterations
- $\sim 10^{18} - 10^{19}$ operations

requirement for reduced models

Outline

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Implementation of PGC into Osiris

parallel scalability, numerical stability and control of numerical noise

Reduced modeling of down-ramp injection

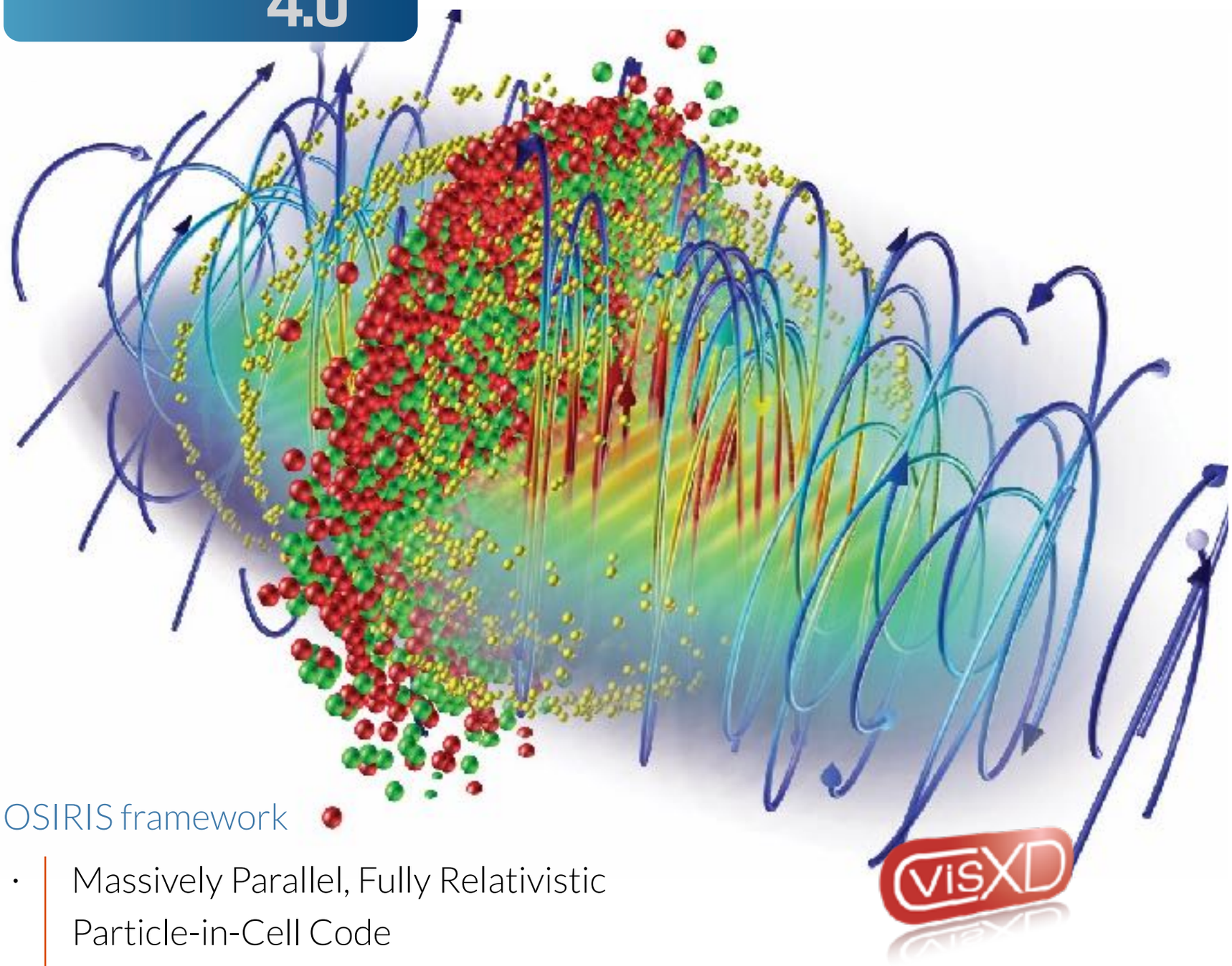
one-to-one comparison of PGC and PIC simulations

Reduced modeling in the realm of AWAKE

ionization seeding for self-modulation of a long proton bunch

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

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

Scale disparity can be overcome by modeling the envelope evolution

Extensions to PIC cycle

- 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

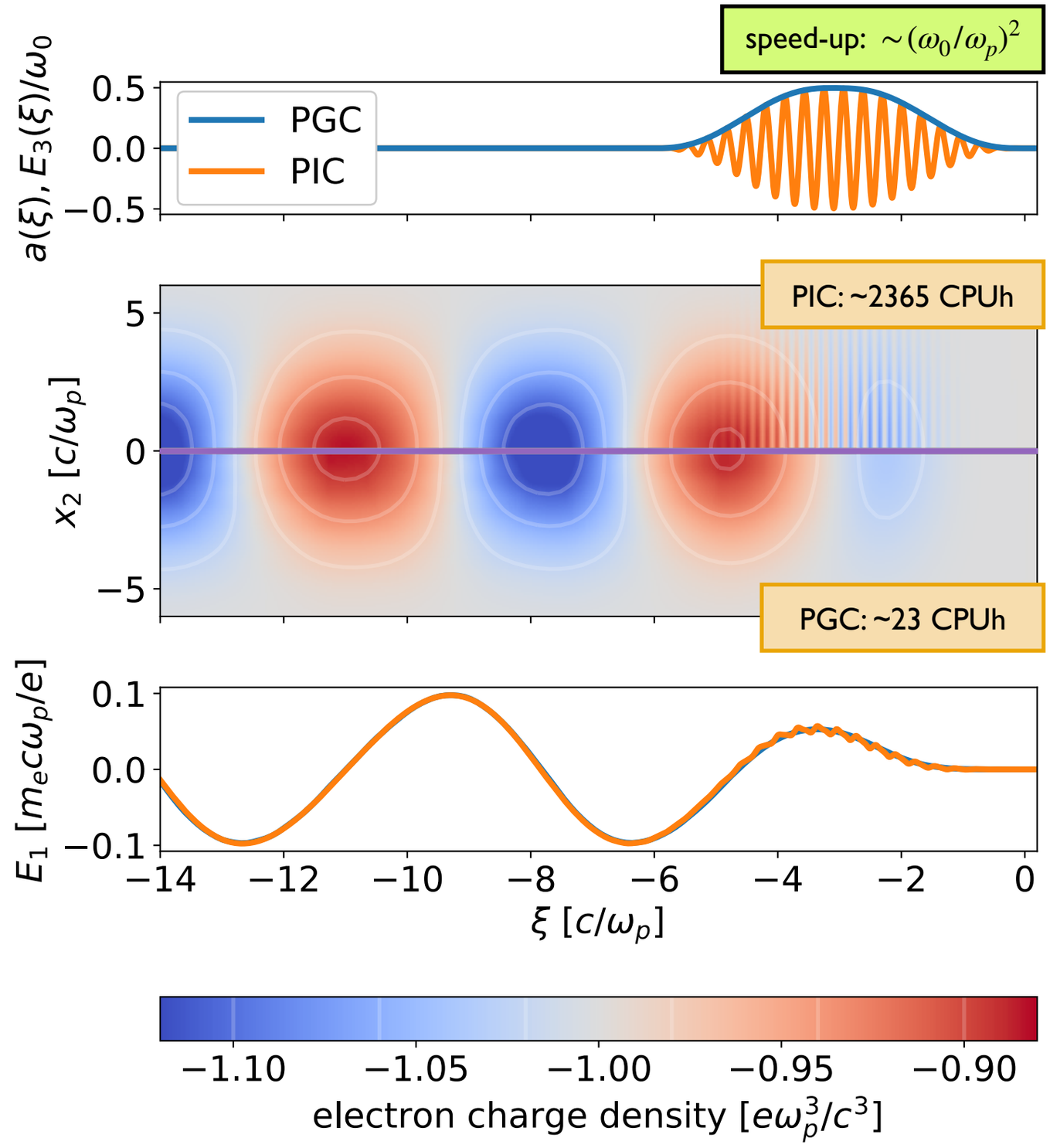
- particle advancing

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

- coupling parameters

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

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



* D. F. Gordon et al., IEEE Trans. Plasma Scii., 28(4), 1135 (2000)
** D. F. Gordon, IEEE Trans. Plasma Sci., 35, 1486–1488 (2007)

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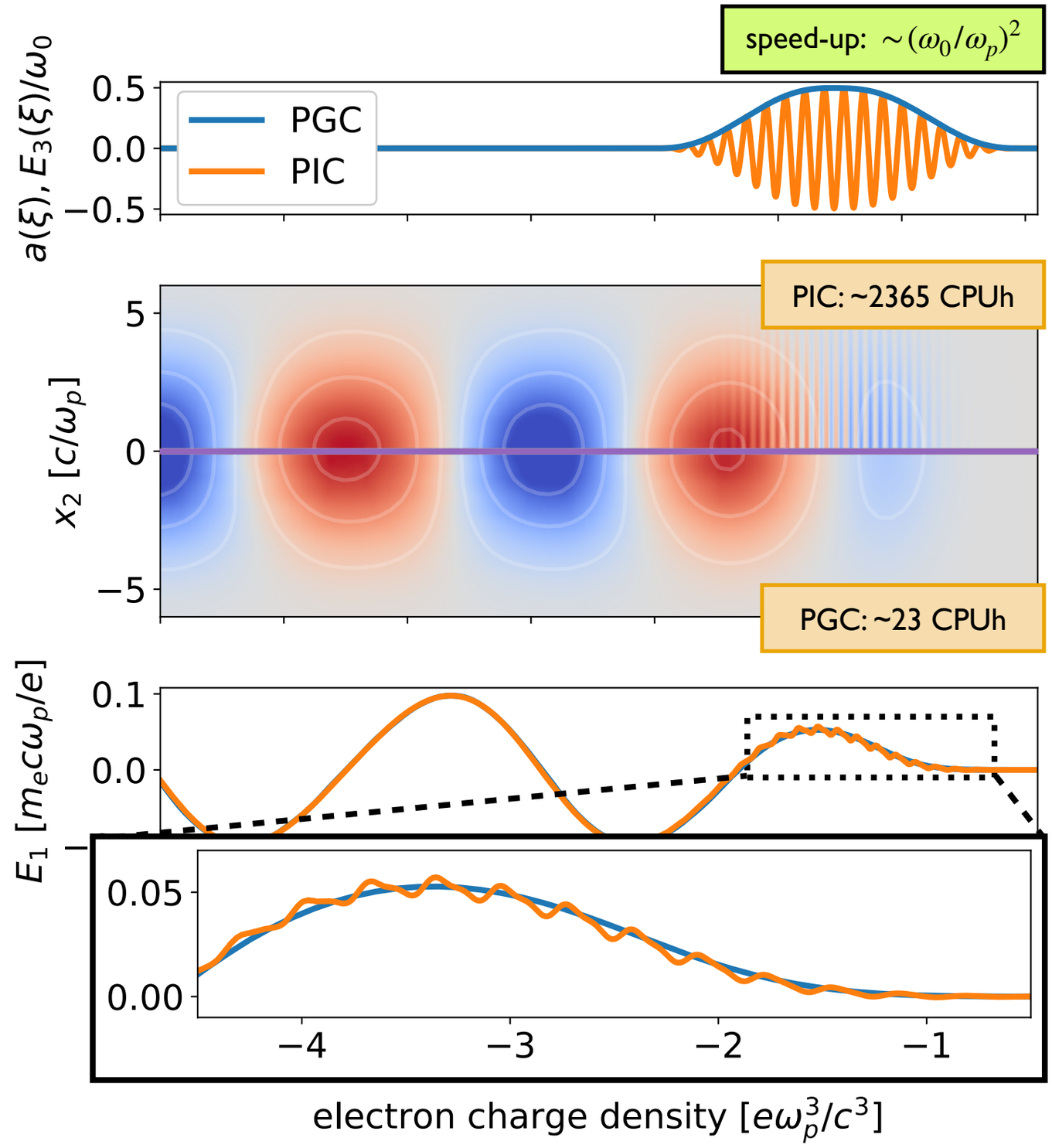

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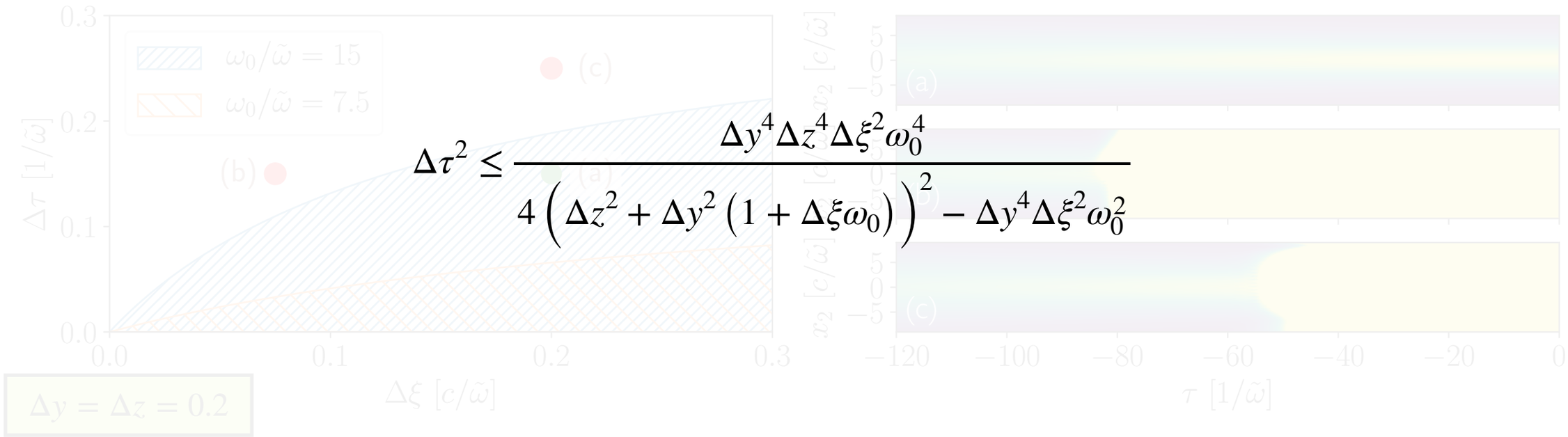
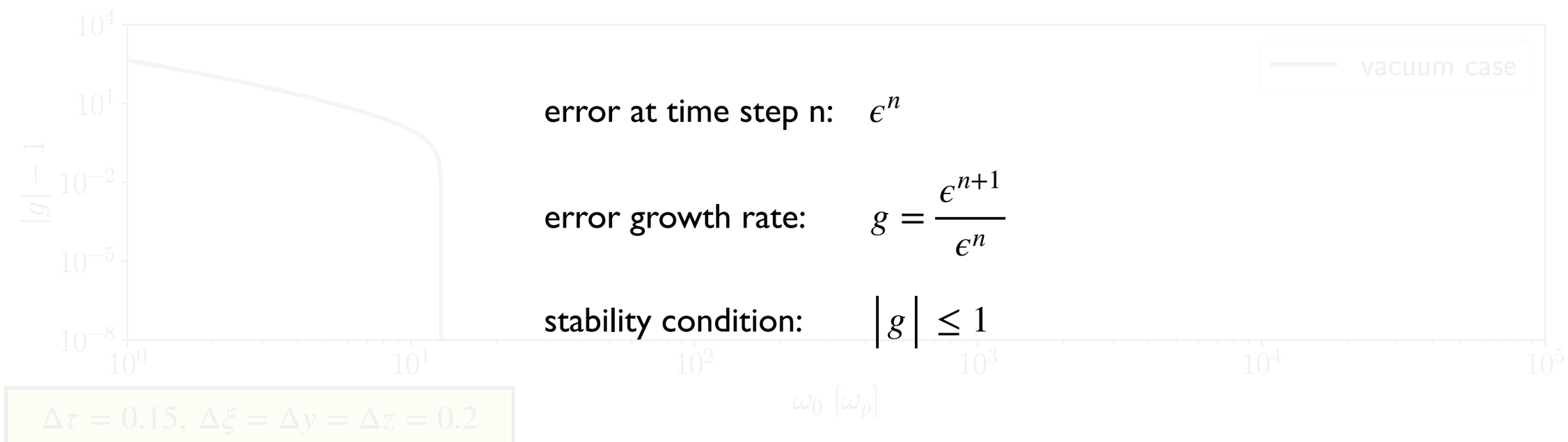
Plasma gradients lead to numerical instabilities*

vacuum case



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

ambient plasma



error at time step n: ϵ^n

error growth rate: $g = \dfrac{\epsilon^{n+1}}{\epsilon^n}$

stability condition: $\left|g\right| \leq 1$

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

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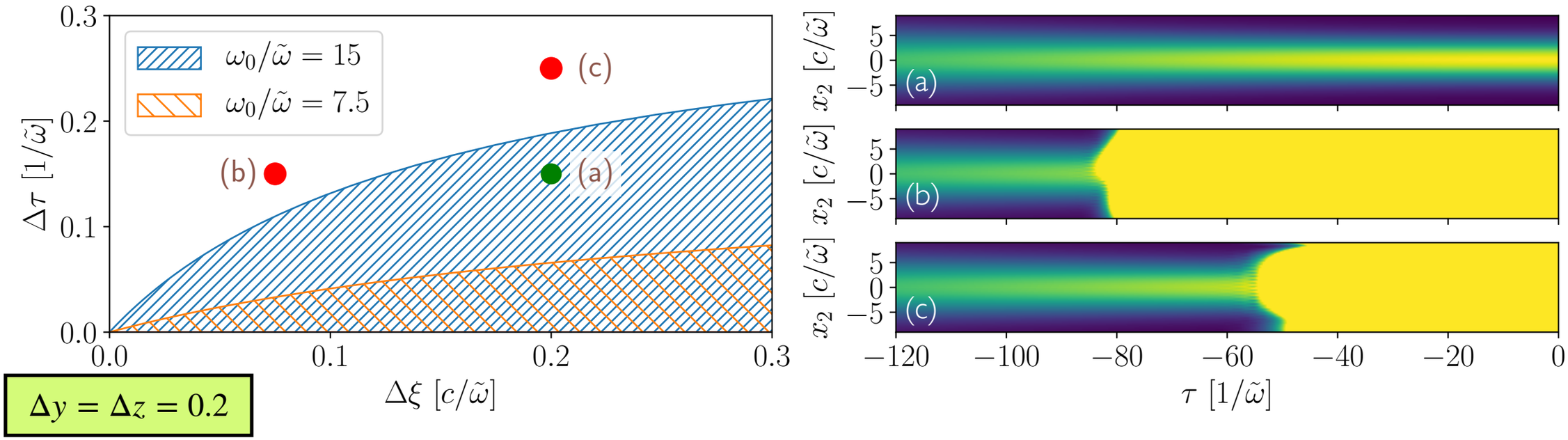
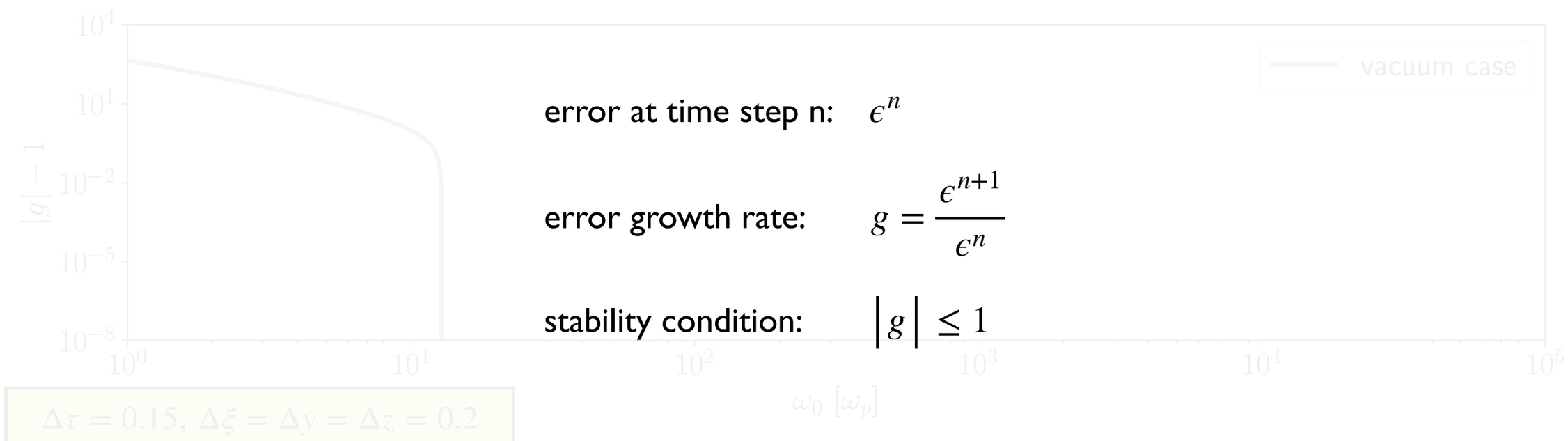


ambient plasma



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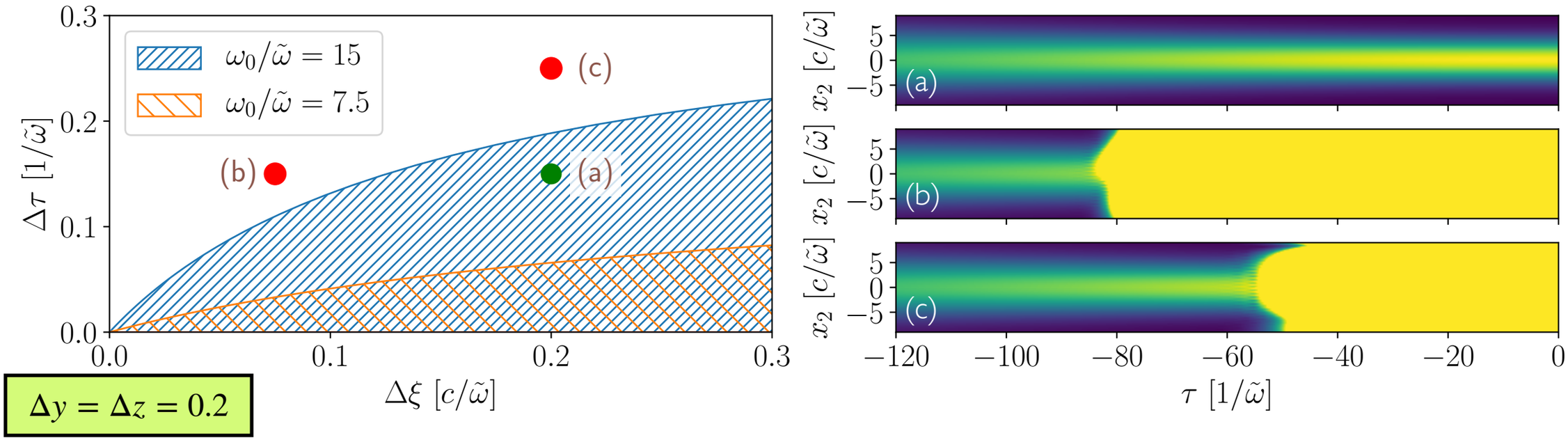

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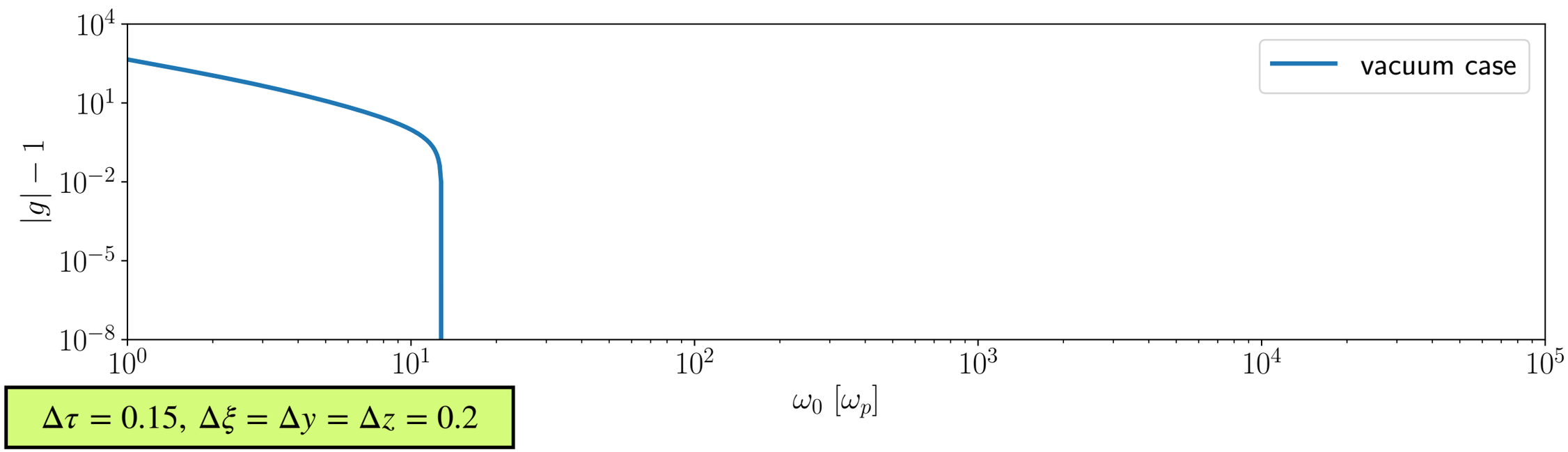

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Plasma gradients lead to numerical instabilities*

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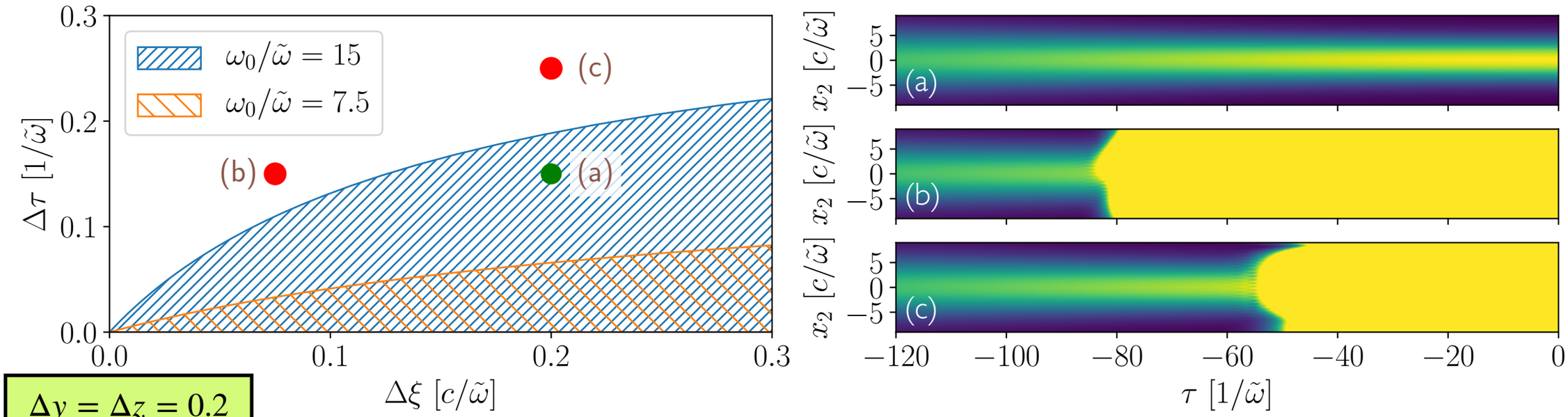
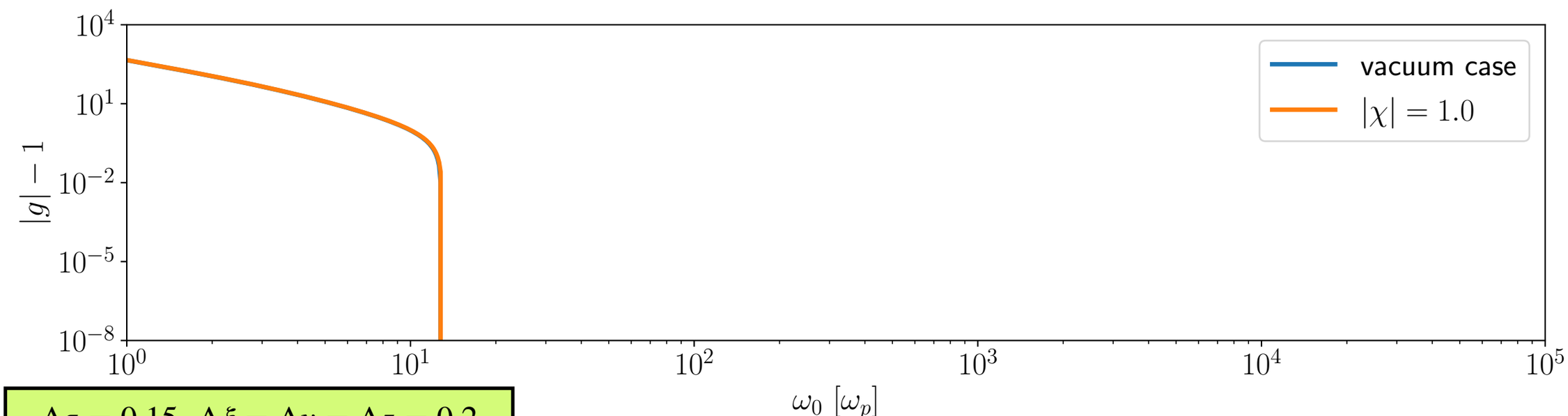
vacuum case



$\Delta y = \Delta z = 0.2$

ambient plasma



$\Delta\tau = 0.15,\ \Delta\xi = \Delta y = \Delta z = 0.2$

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

Plasma gradients lead to numerical instabilities*

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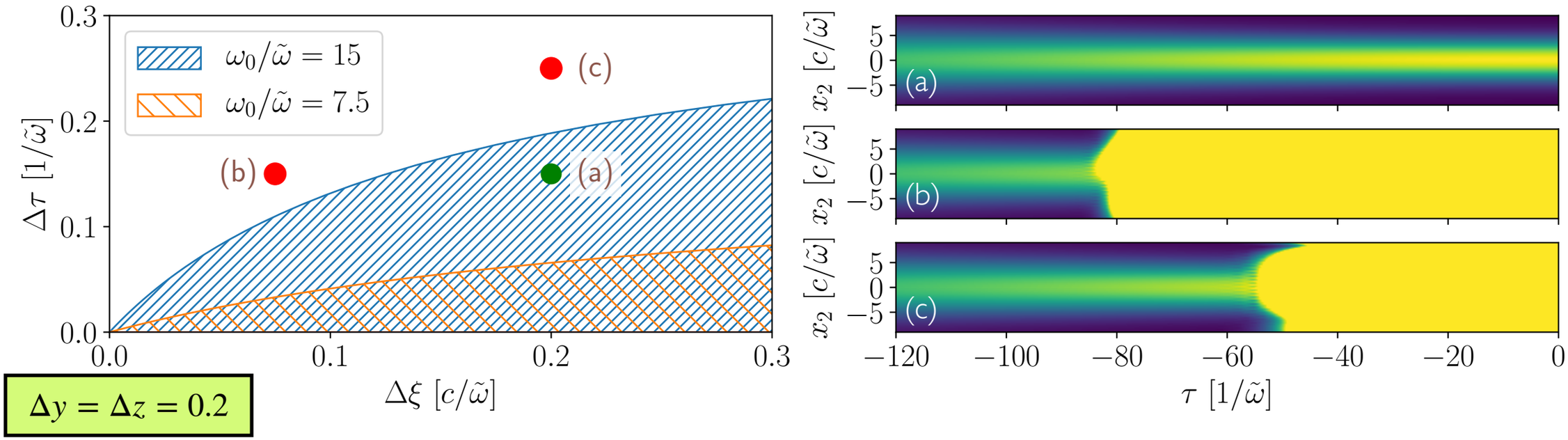
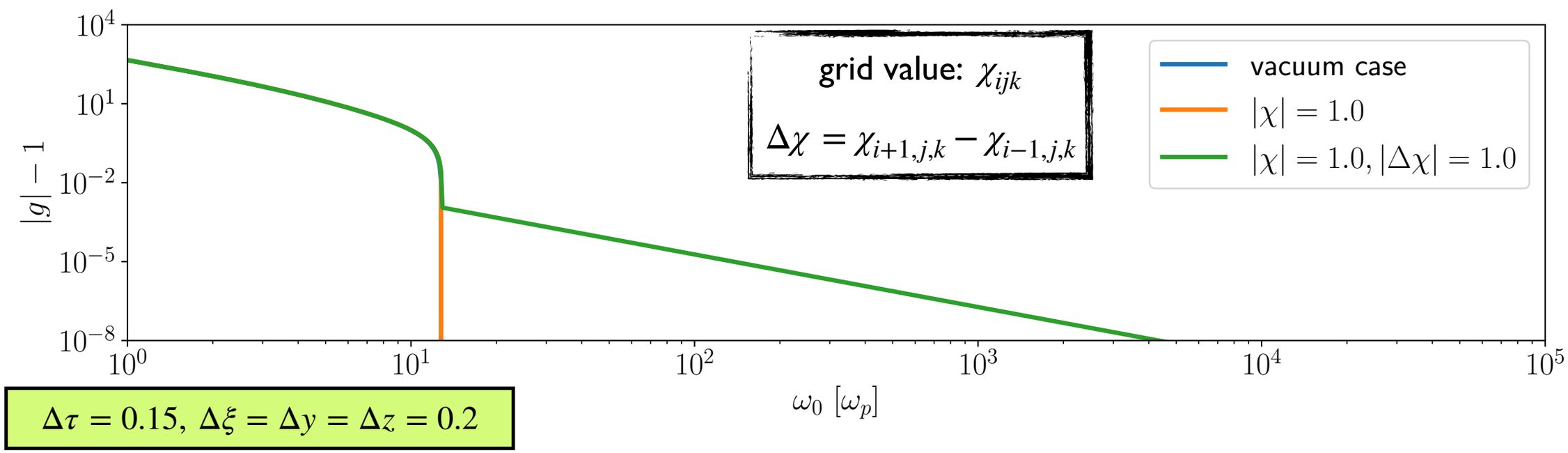
vacuum case



ambient plasma



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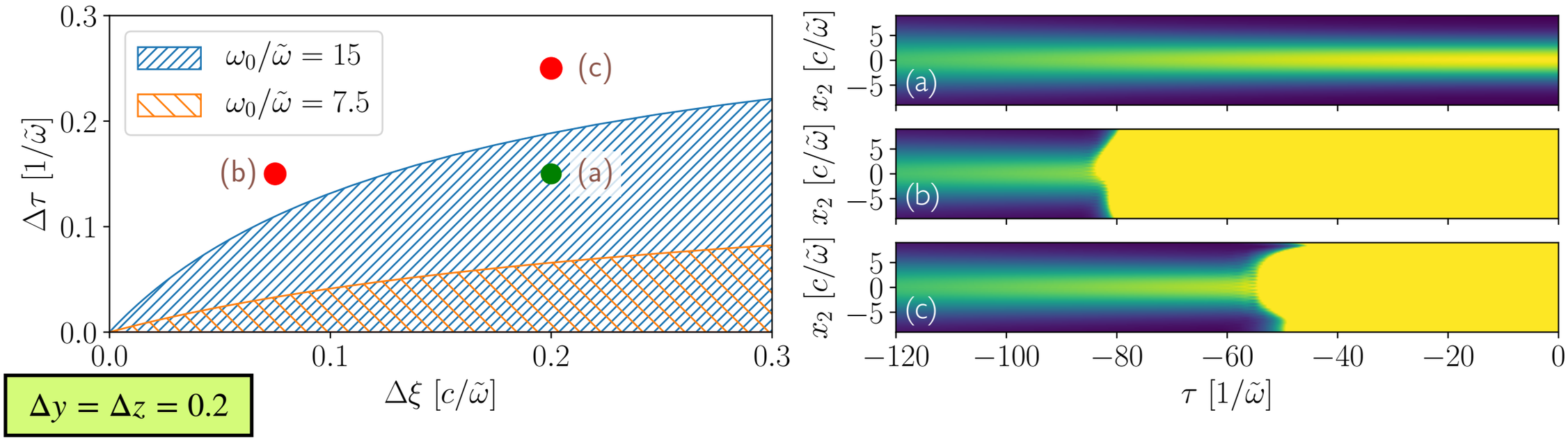
vacuum case



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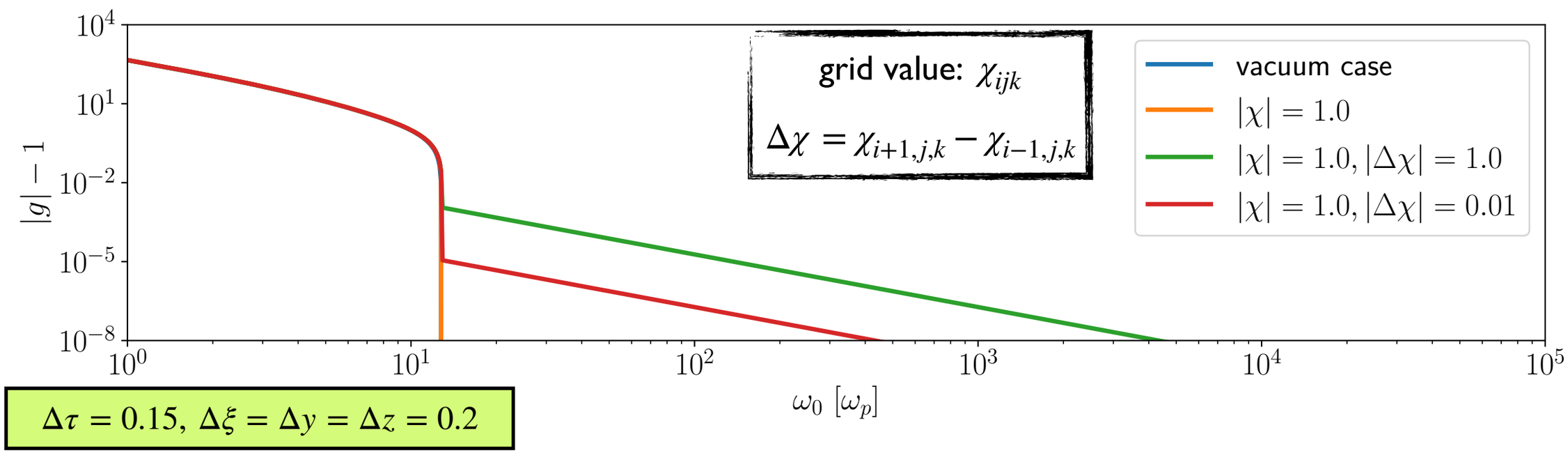

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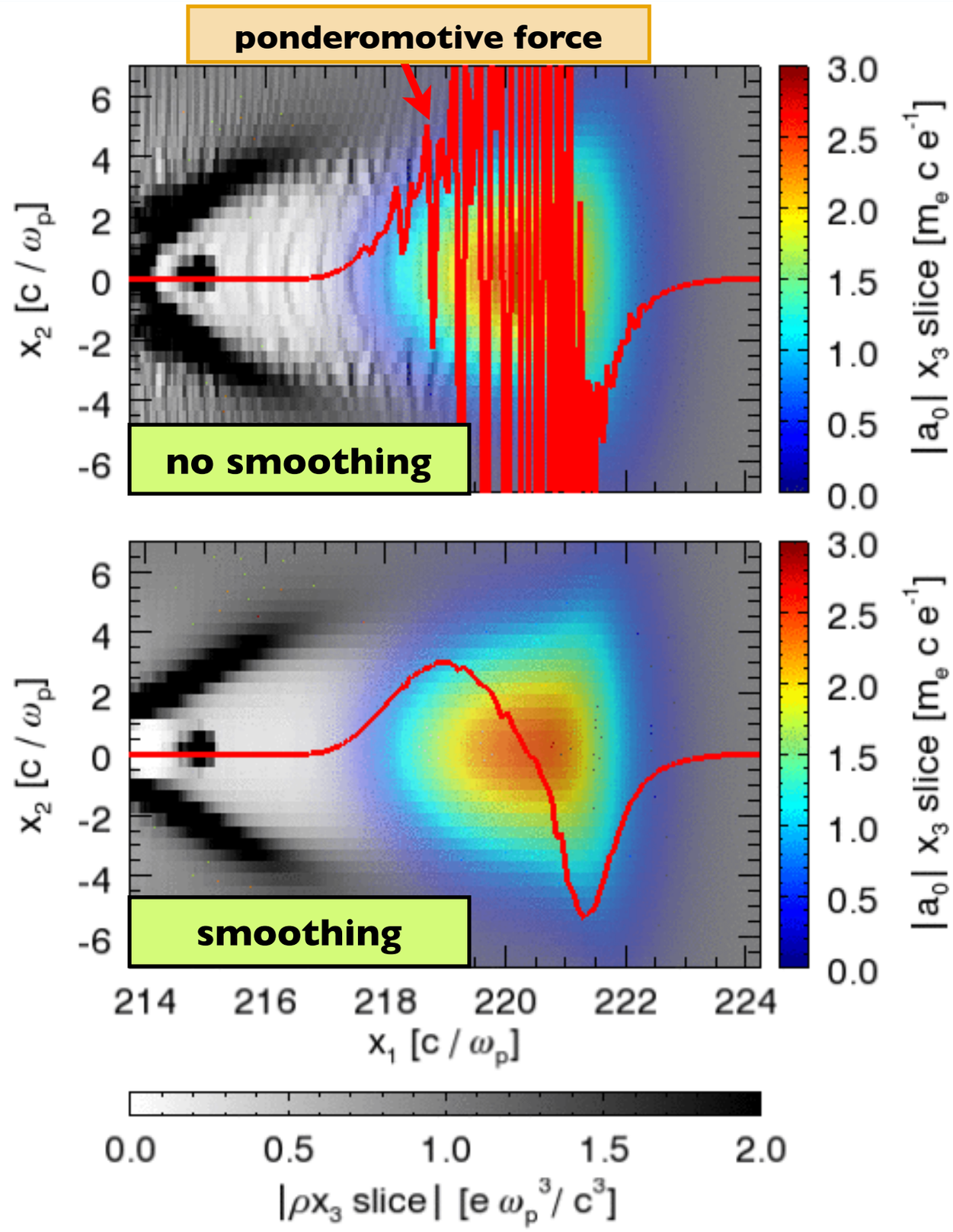
Stability control for PGC

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

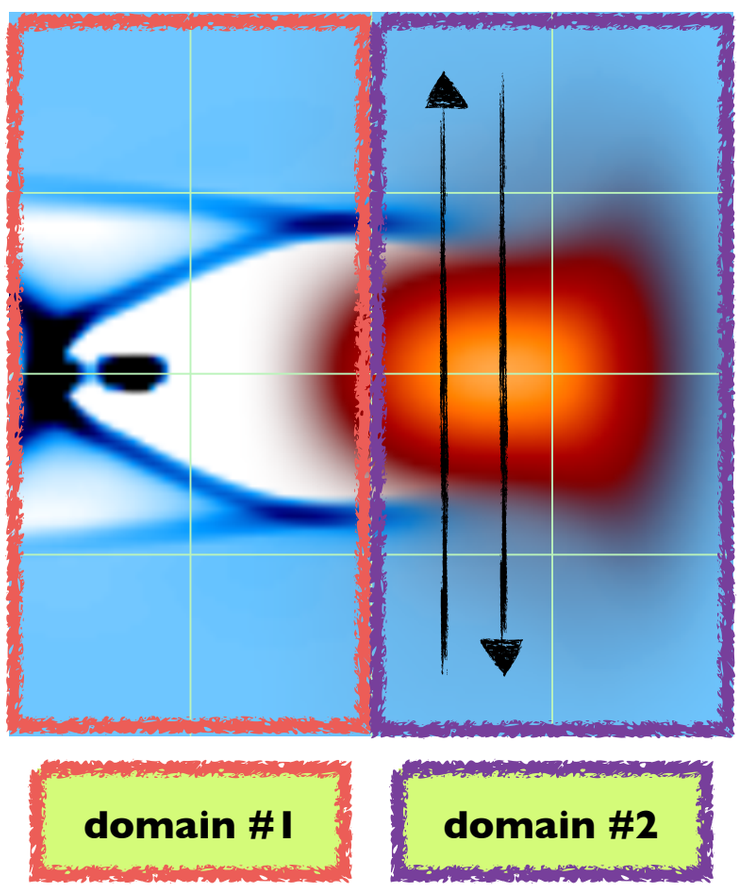
- allows explicit control of numerical noise
- includes several filters to control the noise level and cutoff of the noise
- smoothable quantities:
  - plasma parameter chi
  - ponderomotive force
  - laser envelope



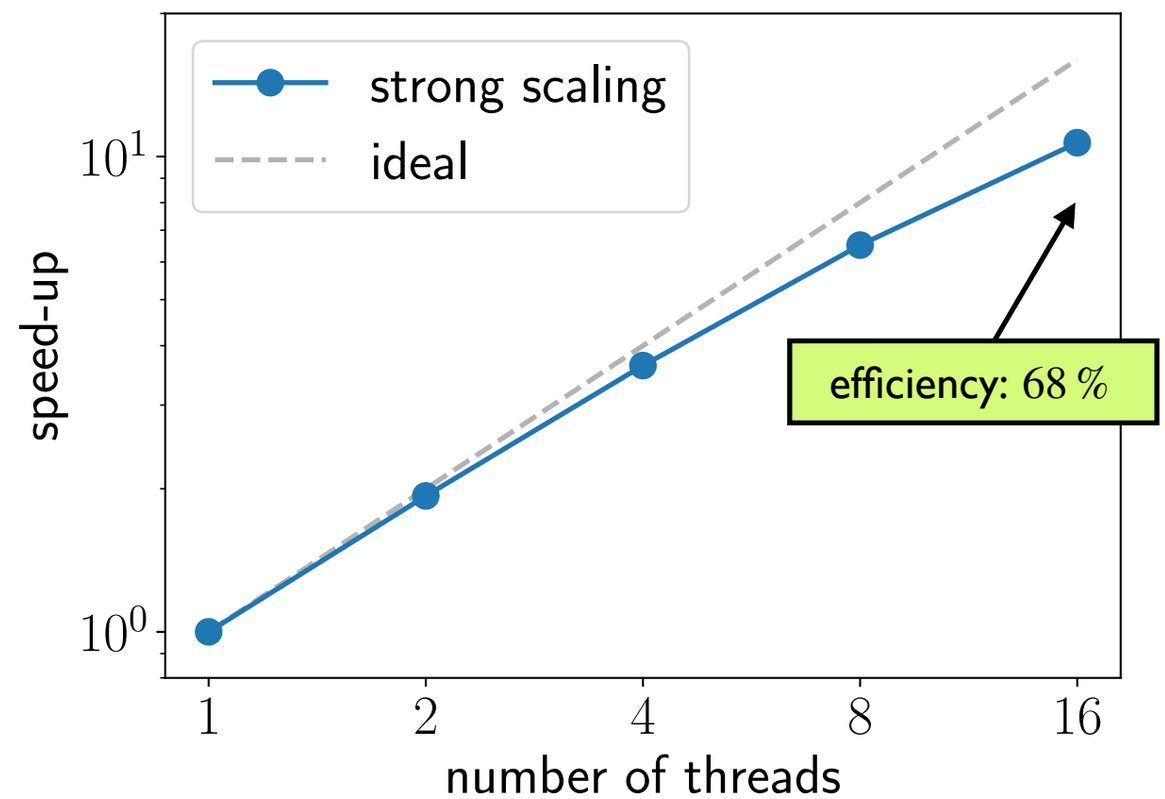
Shared memory parallelization

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

enforces data locality in transverse plane

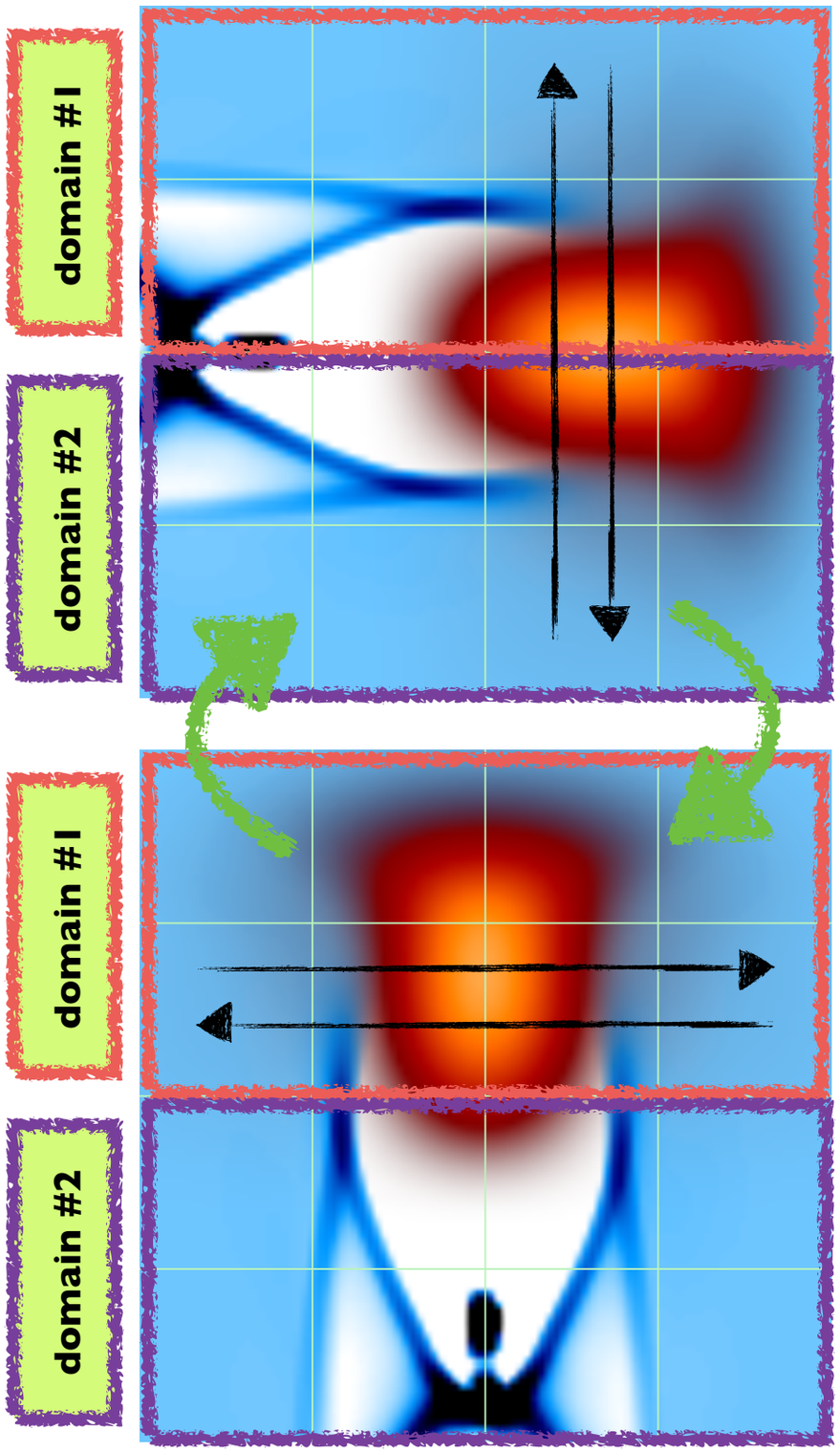


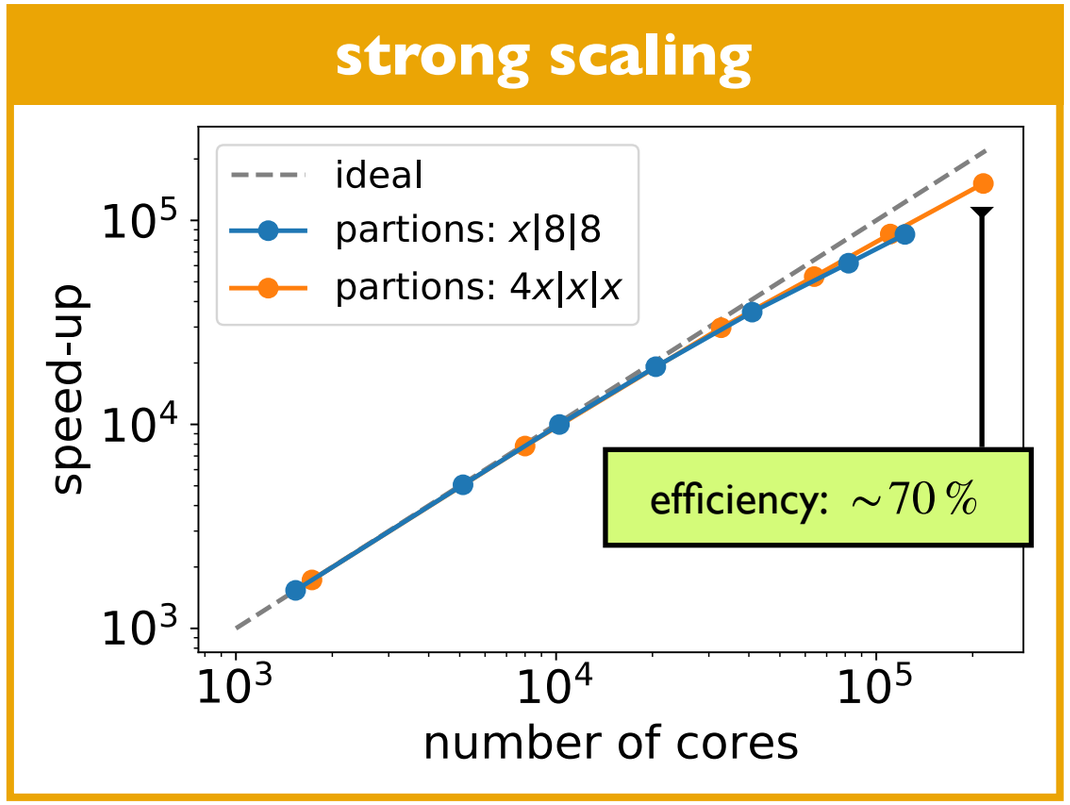
thread-based strong scaling

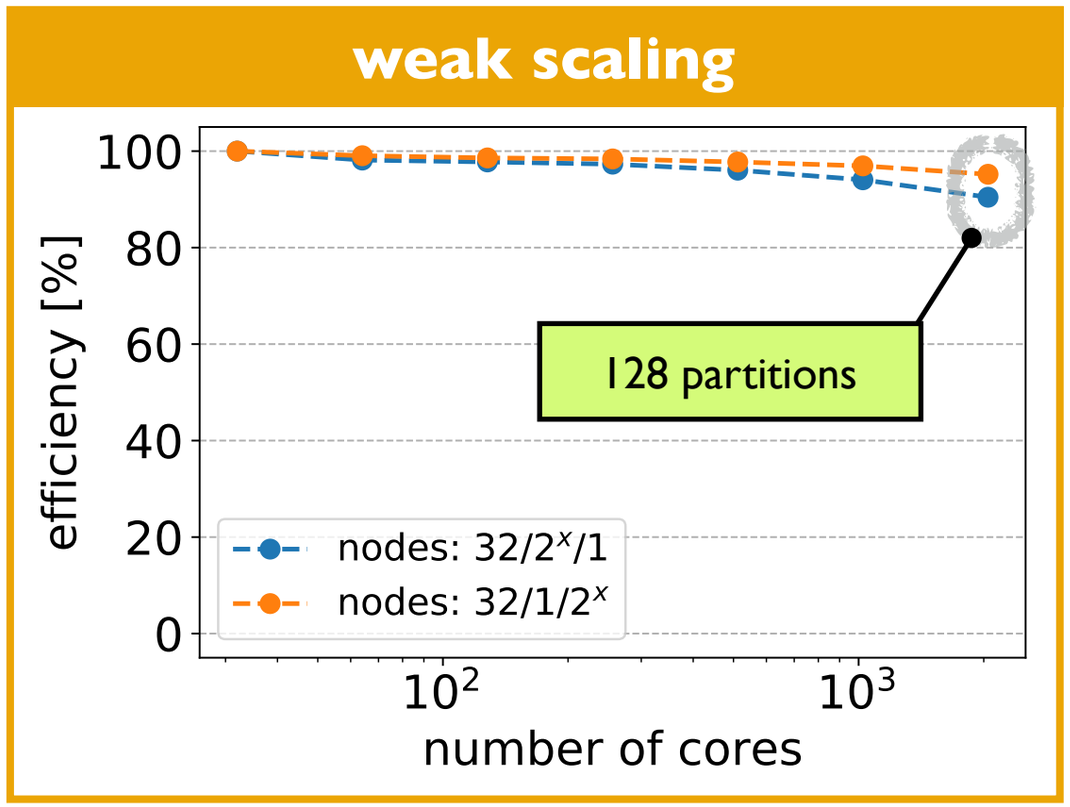


- ✦ JUQUEEN (IBM BlueGene/Q) - 16 cores per node
- ✦ number of cores: 32 / 64 / 128 / 256 / 512
- ✦ 500 time steps - 608x152x152 cells and 8 ppc
- ✦ using distributed parallelization in longitudinal direction
- ✔ scaling over one order of cores using shared memory parallelization

Shared memory parallelization for PGC







Reduced modeling of down-ramp injection*

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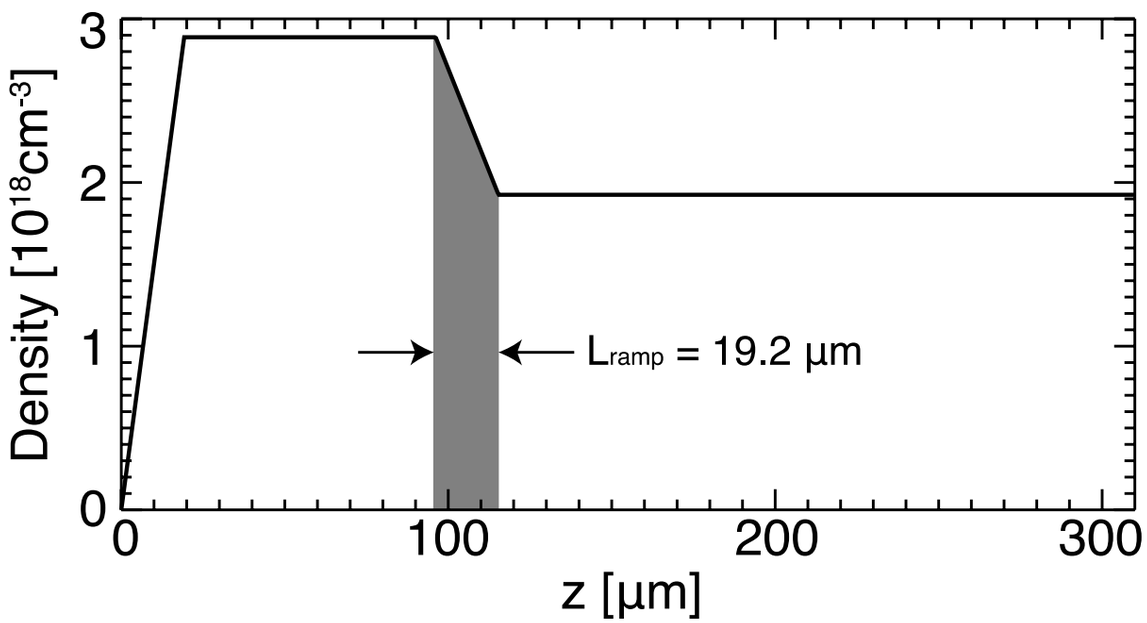
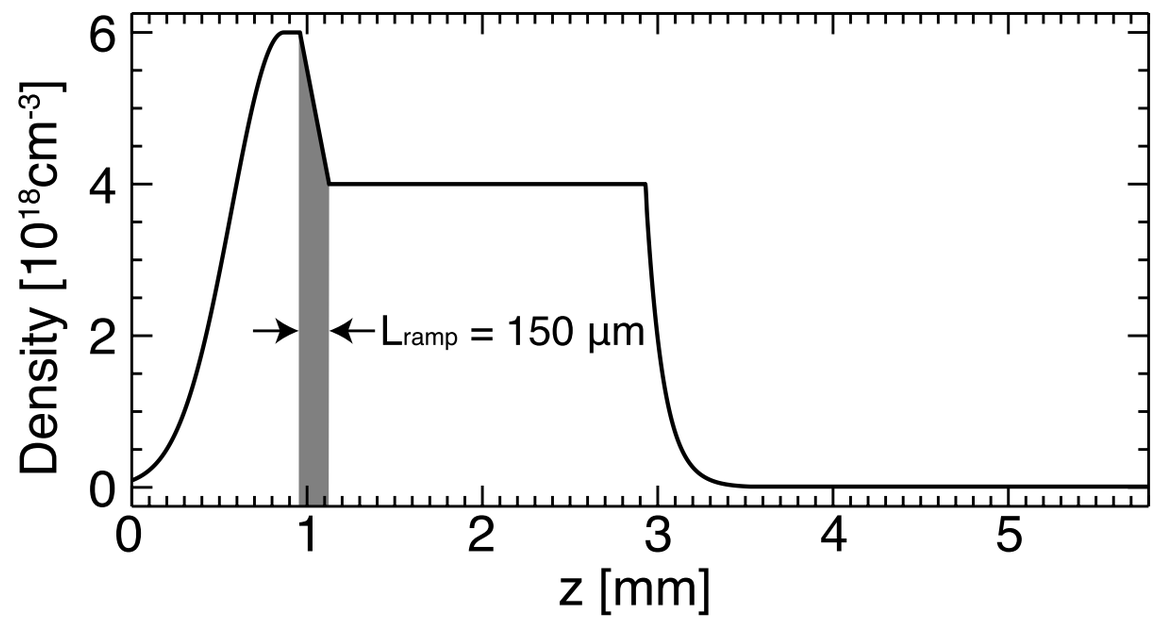
short down-ramp transition



Laser parameters:

- laser wavelength: $\lambda_0 = 800$ nm
- pulse duration: $\tau_l = 57.2$ fs
- normalized vector potential: $a_0 = 2.82$
- beam waist: $w_0 = 17.2\,\mu$m

long down-ramp transition

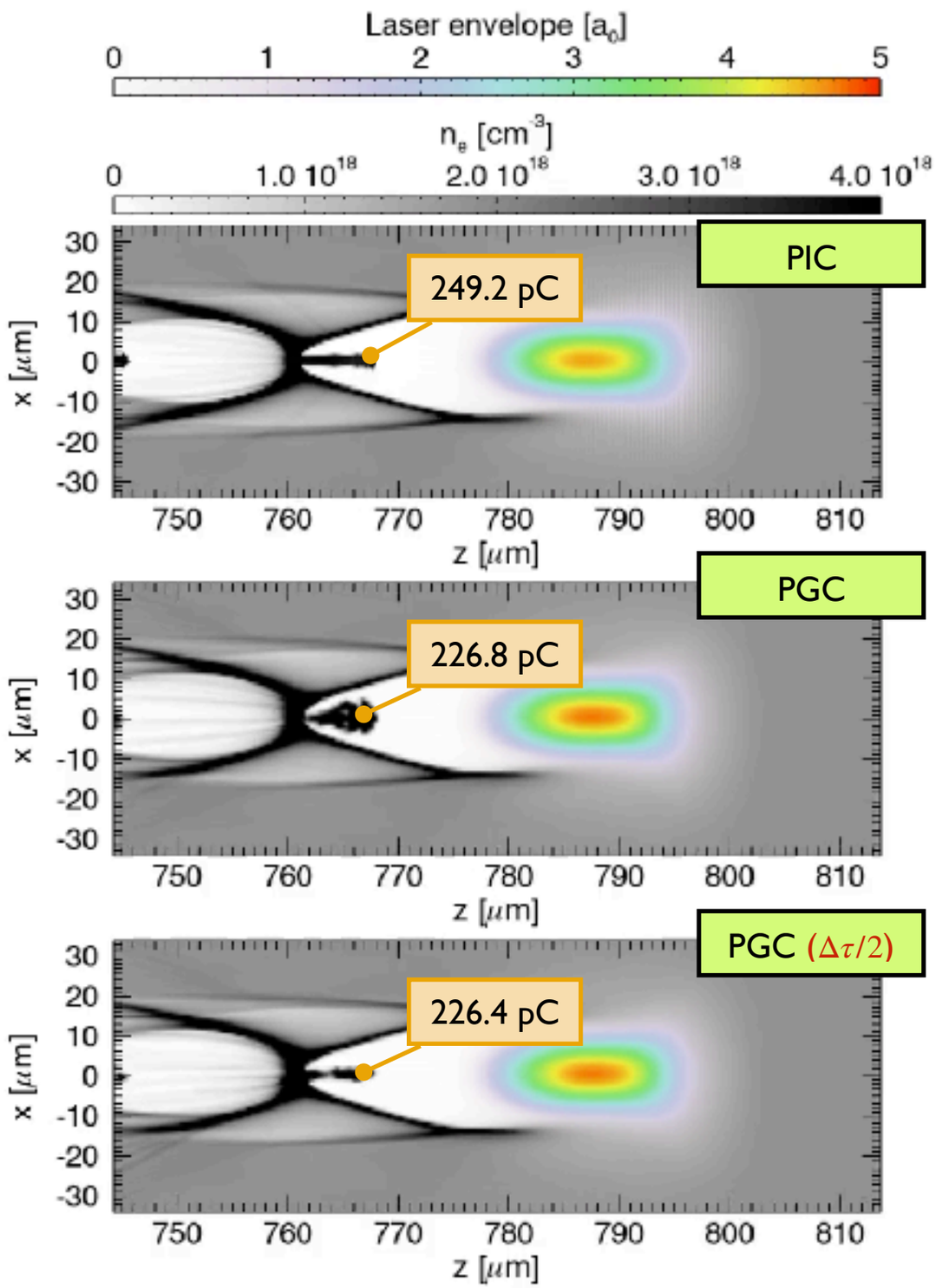


Laser parameters:

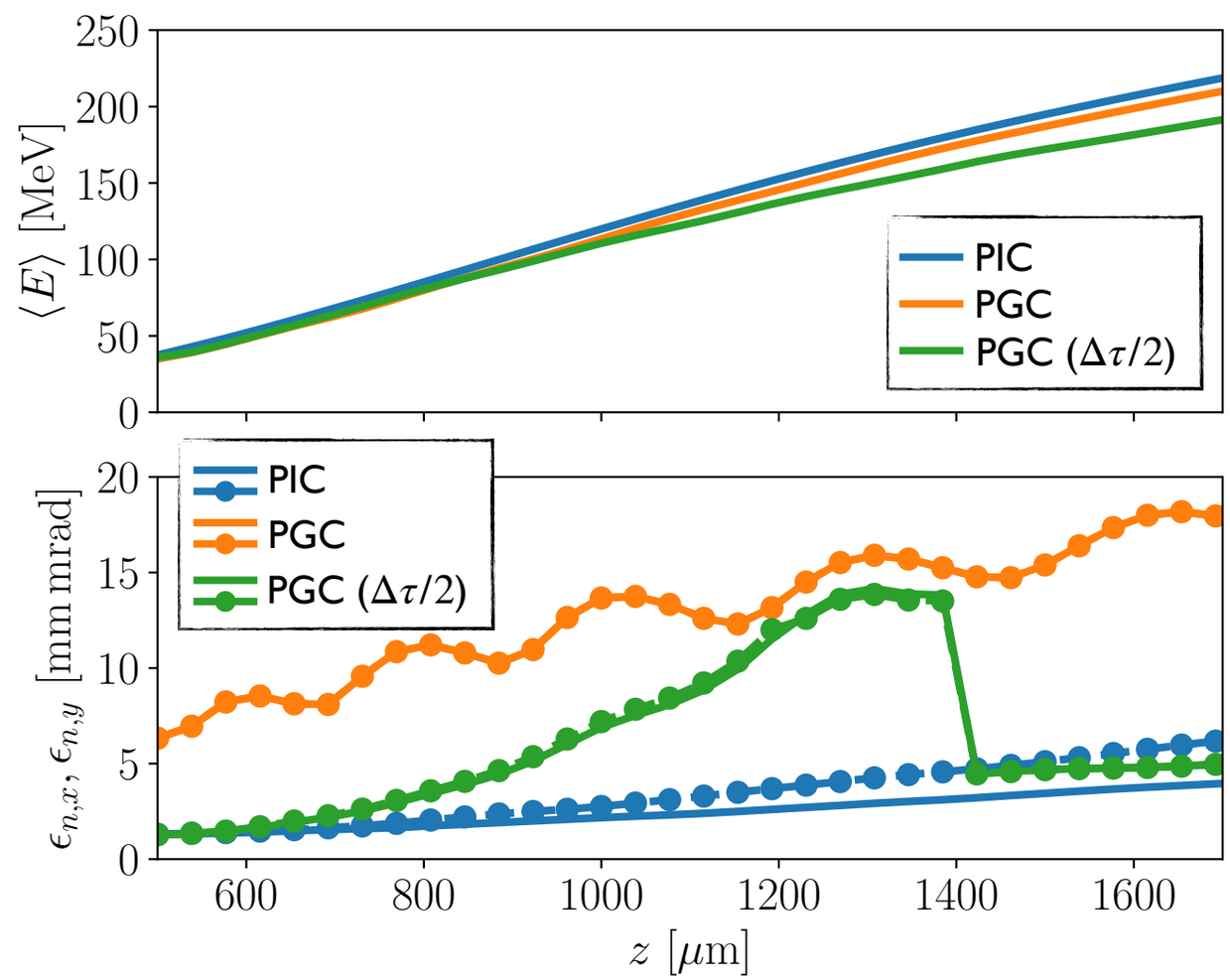
- laser wavelength: $\lambda_0 = 800$ nm
- pulse duration: $\tau_l = 30.0$ fs
- normalized vector potential: $a_0 = 1.8$
- beam waist: $w_0 = 18\,\mu$m

* S. Kalmykov *et al.*, PRL 103, 135004 (2009)

Reduced time-step affects impacts on beam emmitance



beam parameters



- charge and mean energy are in good agreement
- emittance is 5x higher for PGC case
- discrepancy in emittance arises from poor injection
- higher order pusher could lead to reduced emittance

Reduced modeling for injector stage in the context of EuPRAXIA*

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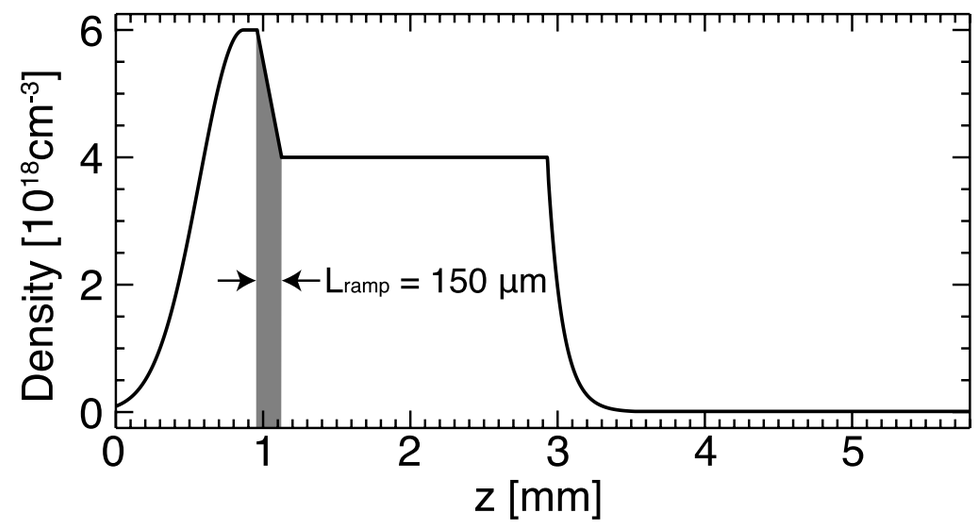
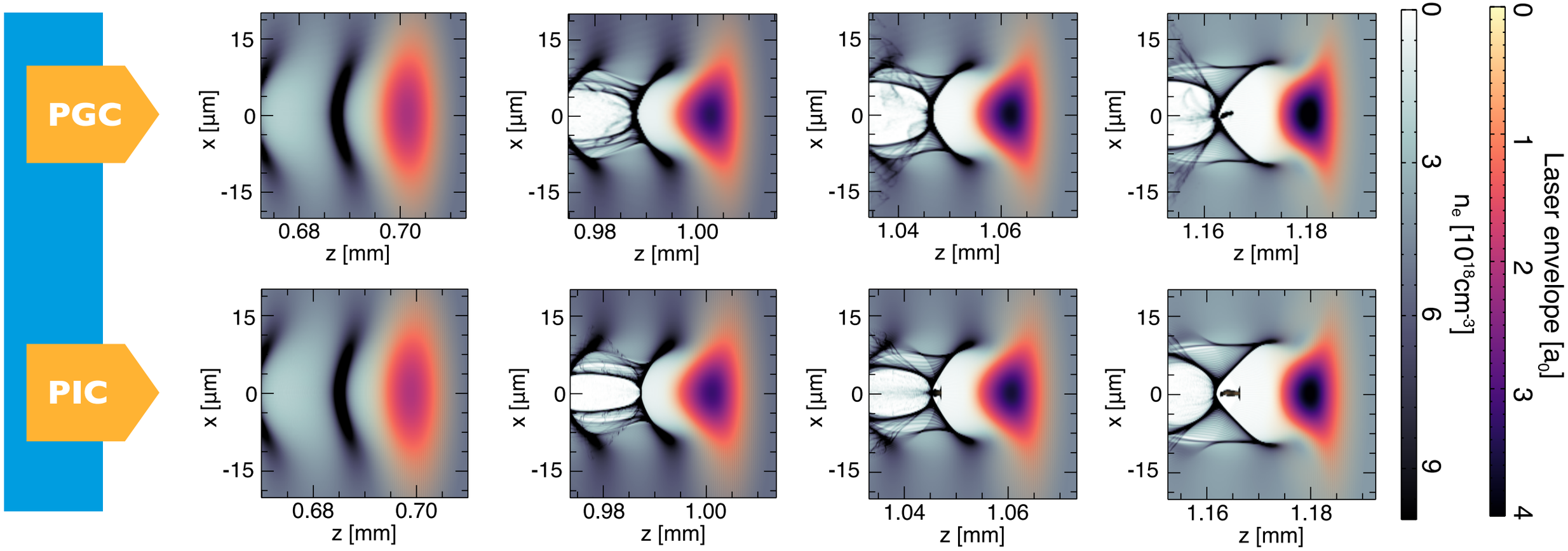
- comparison of full PIC and PGC
- strong agreement for laser evolution and plasma fields
- PGC does not model injection properly
- mitigation of numerical Cherenkov instability through Lehe-solver**
- PGC can be used for grasping laser evolution and the plasma response with the wakefield structure





* T. Silva et al., submitted (2019)

** R. Lehe et al., *PRE*, 94 (5), 053305–16 (2016)

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

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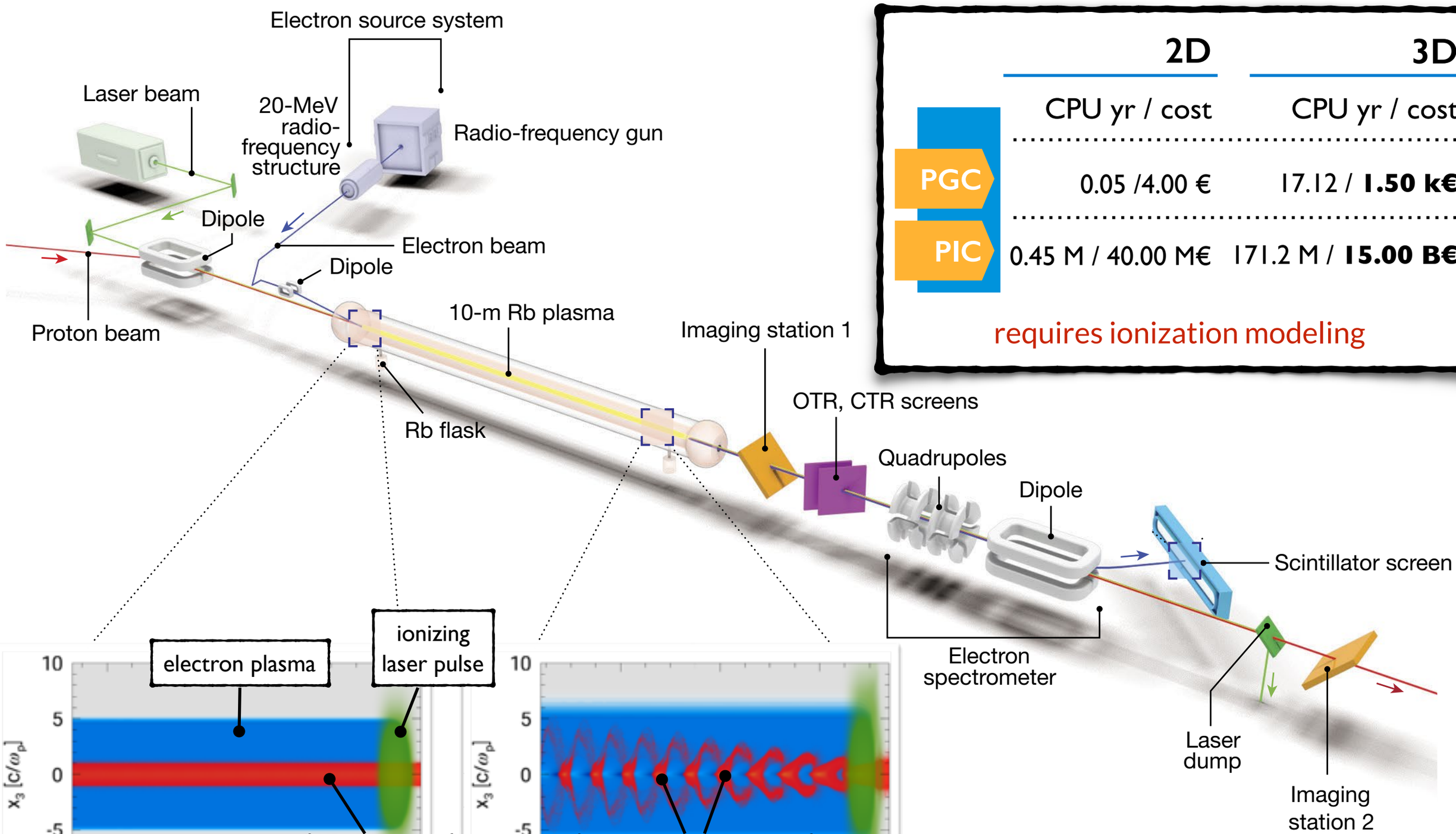
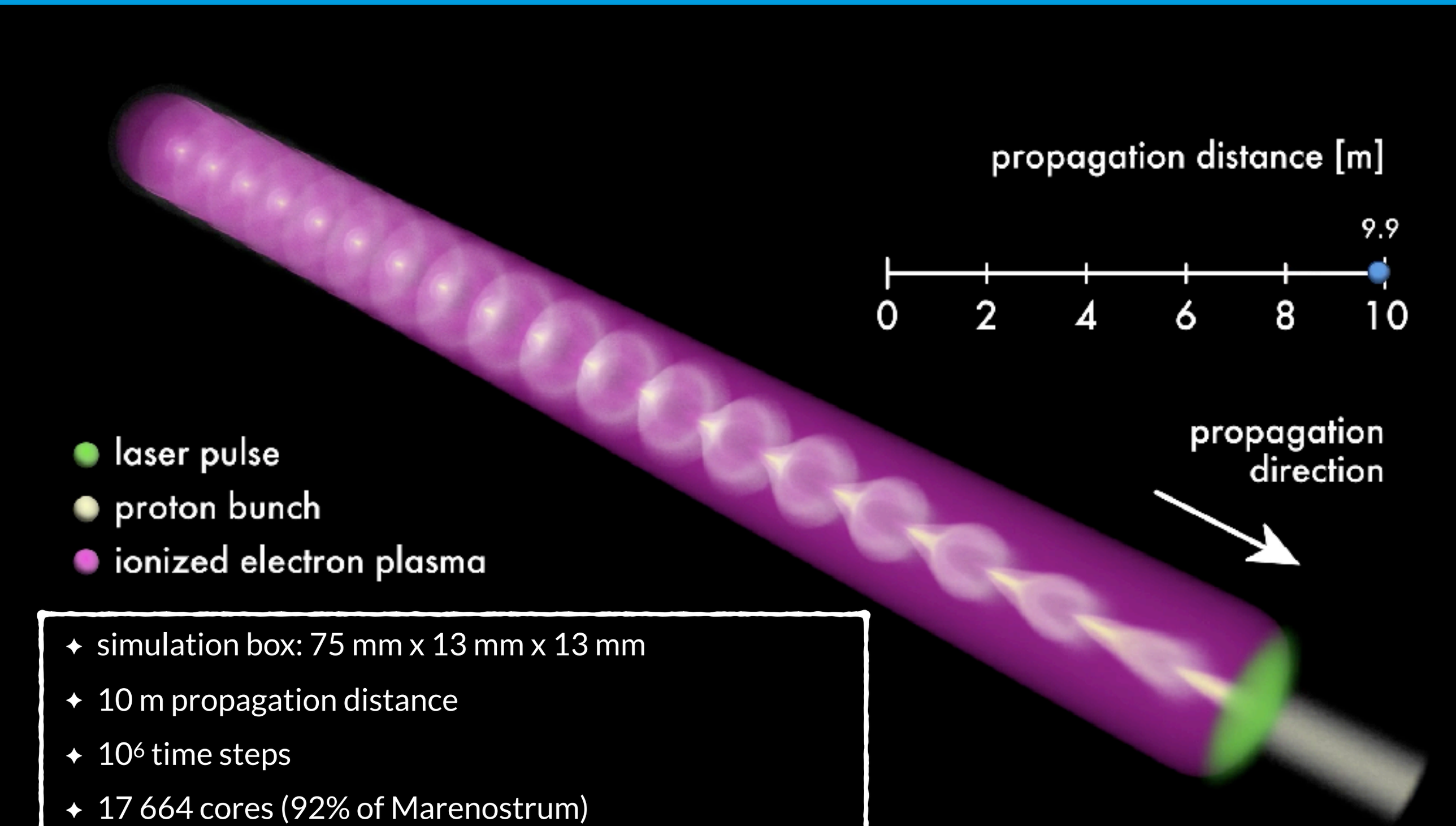
	2D	3D
	CPU yr / cost	CPU yr / cost
PGC	0.05 /4.00 €	17.12 / **1.50 k€**
PIC	0.45 M / 40.00 M€	171.2 M / **15.00 B€**

requires ionization modeling



* 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

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Reduced modeling on the plasma scale

- control of numerical instability is crucial for PGC
- parallelisation of envelope equation over thousands of cores

Reduced modeling of down-ramp injection

- PGC can be used to grasp the laser evolution and generated plasma fields
- higher order particle pusher for better modeling the particle injection

Self-consistent modeling of self-modulation instability

- ionization injection incorporated into PGC
- full 10 m AWAKE runs can be modeled with PGC

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

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