Three dimensional modeling using ponderomotive guiding center solver

Anton Helm[1]

ahelm@ipfn.tecnico.ulisboa.pt

Ricardo Fonseca[1,2], Jorge Vieira[1], Luis 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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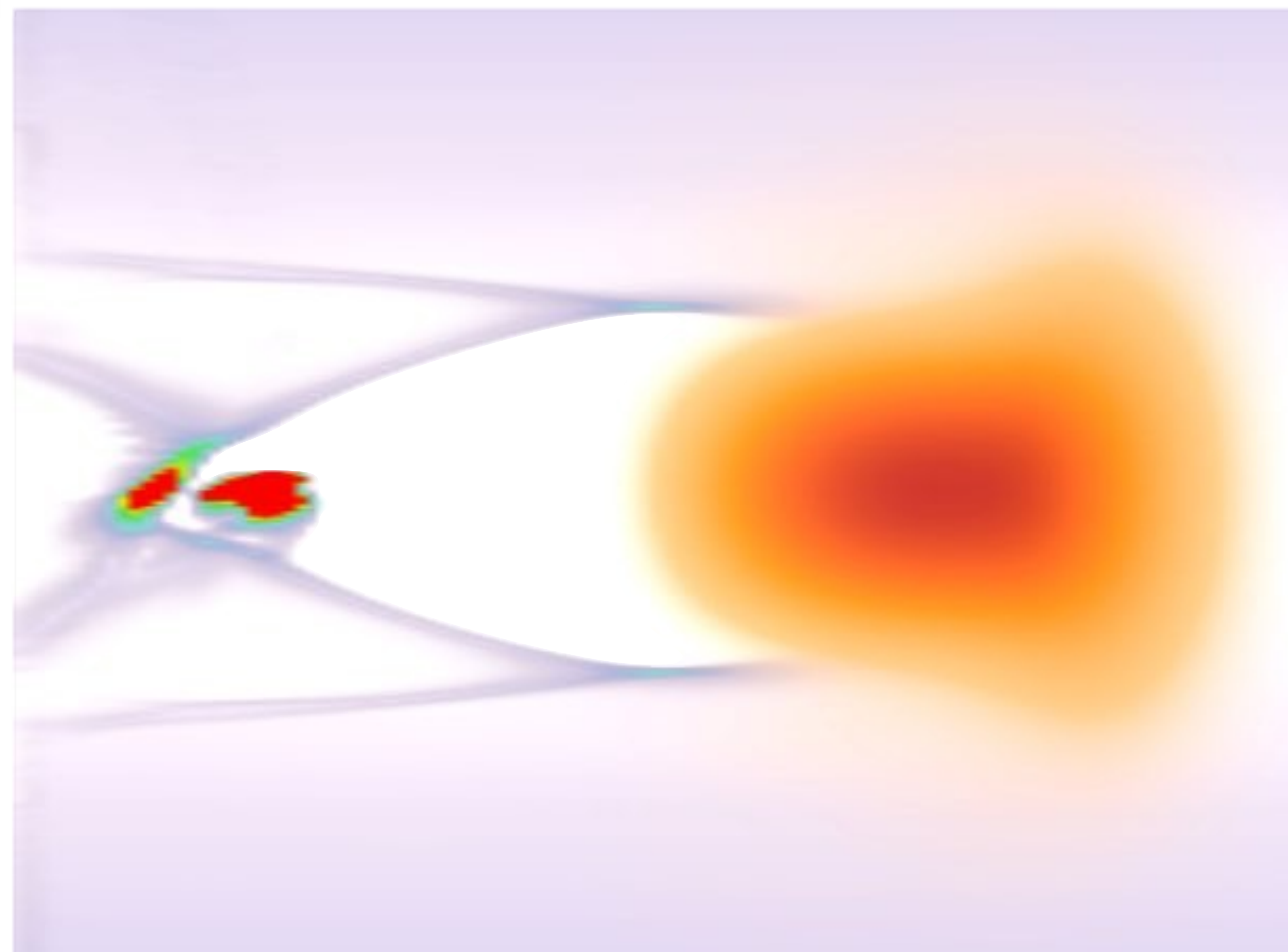

Alternatives for conventional accelerator required

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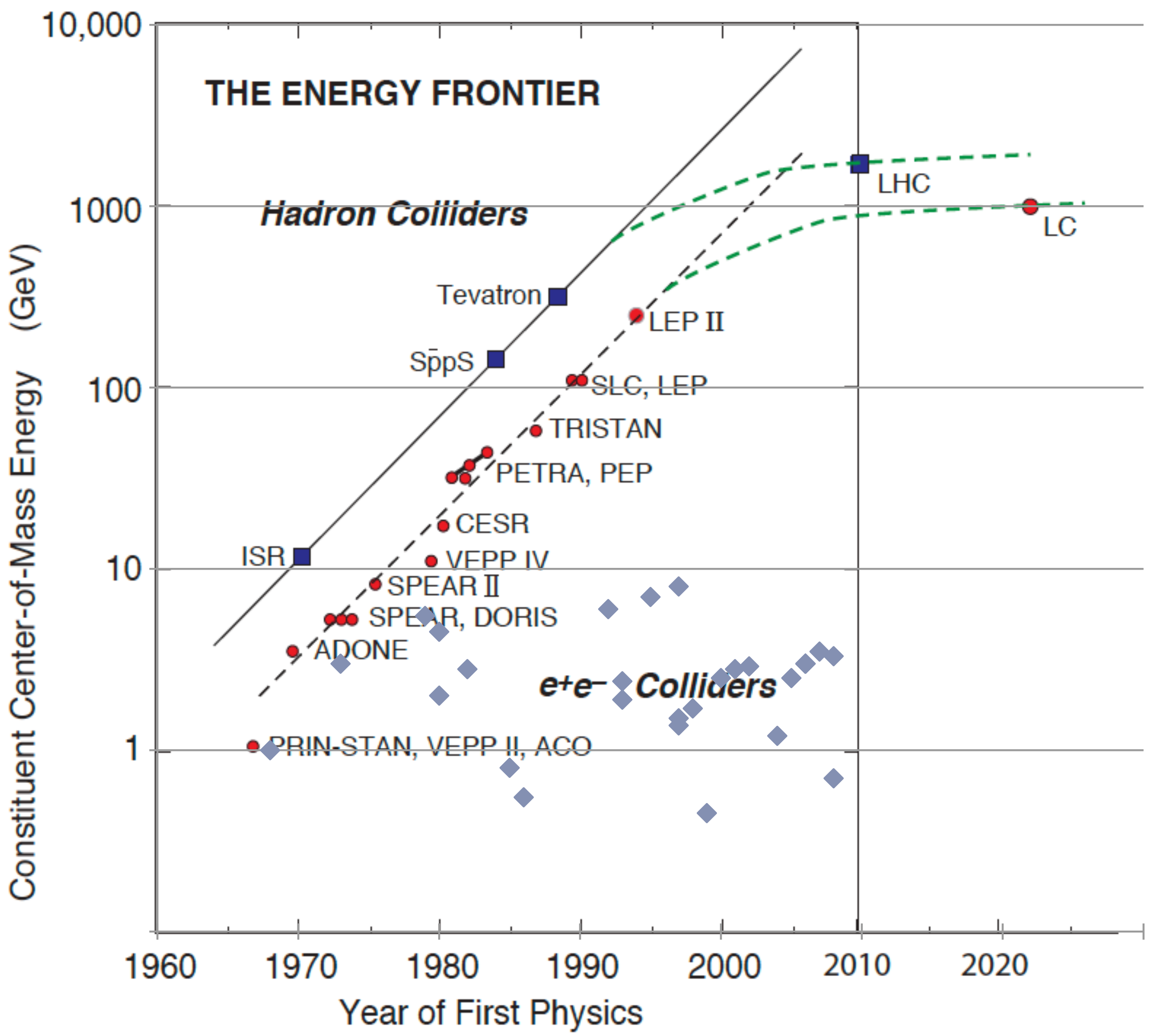
Livingston chart*



SLAC National Accelerator Laboratory

- electrons with energies up to 50 GeV (3.2 km)
- radio-frequency cavities limit: 100 MV/m

laser wakefield acceleration (LWFA)

- acceleration gradient:

$$E\left[\mathrm{V\,cm^{-1}}\right] \approx 0.96\sqrt{n_0\left[\mathrm{cm^{-3}}\right]}$$

- 1.5 m for 50 GeV electrons

$(n_0 = 10^{17}\,\mathrm{cm^{-3}})$

* J. Nash, IOP Meeting (2010)

Envelope approximation reduces spatial resolution

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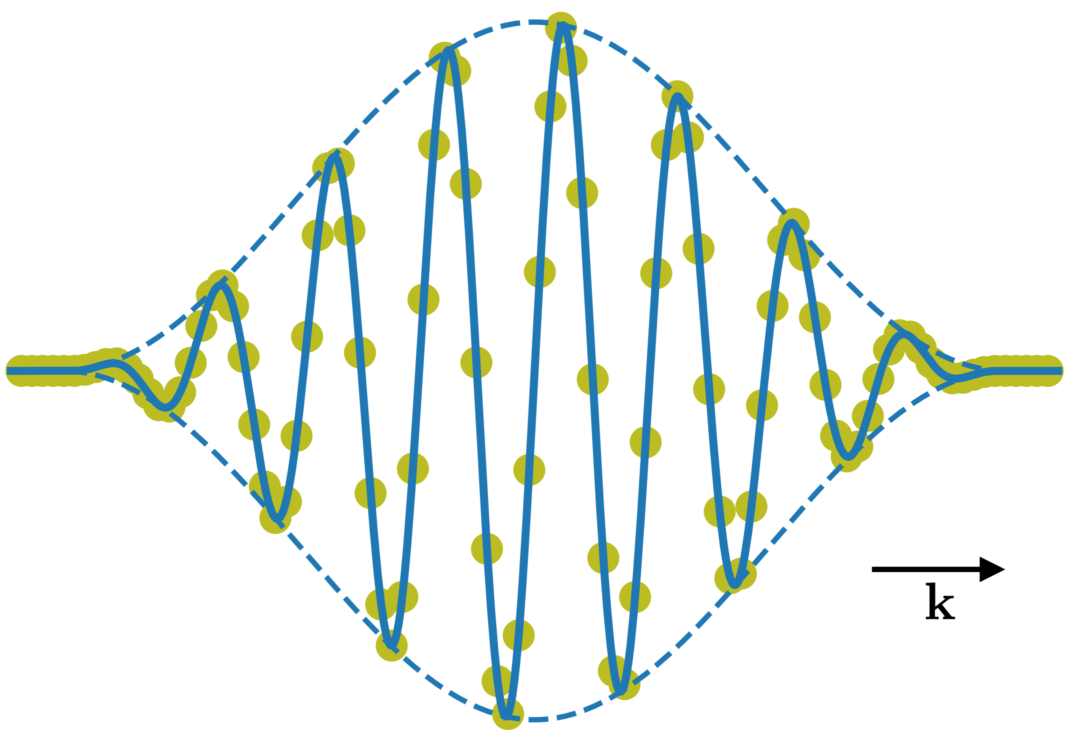
particle-in-cell (PIC)

spatial resolution:

laser wavelength

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

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

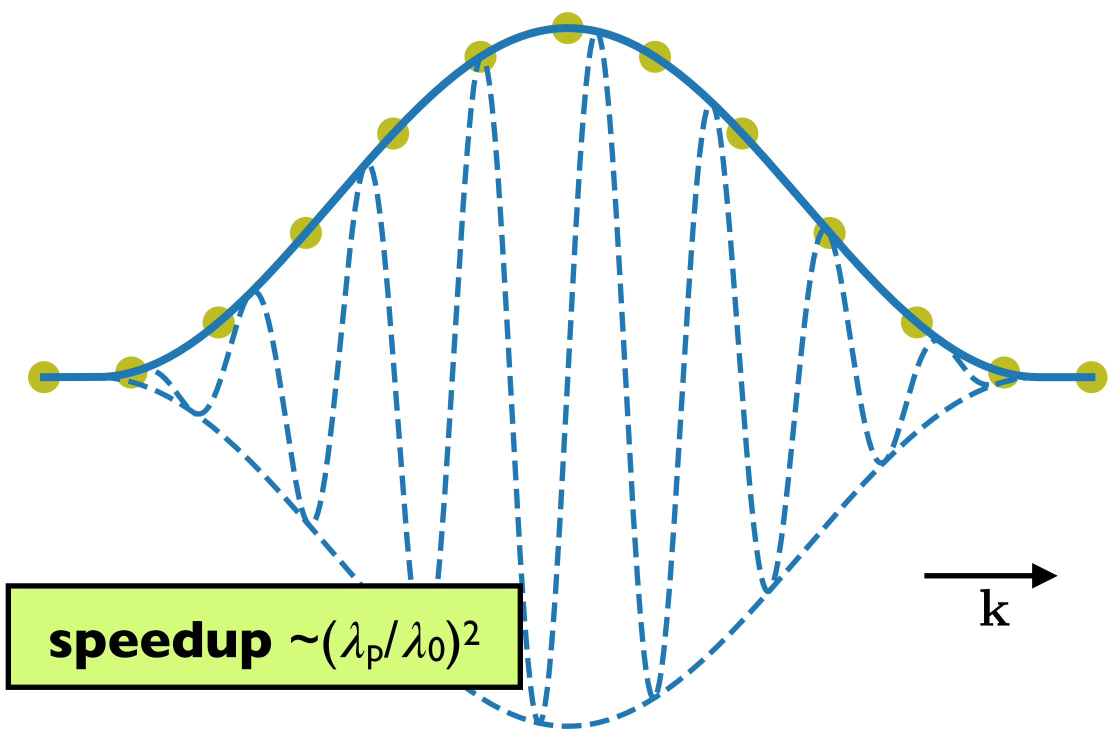


- resolve laser wavelength over propagation distance
- particle advancing is based on Lorentz force

ponderomotive guiding center (PGC)

spatial resolution:

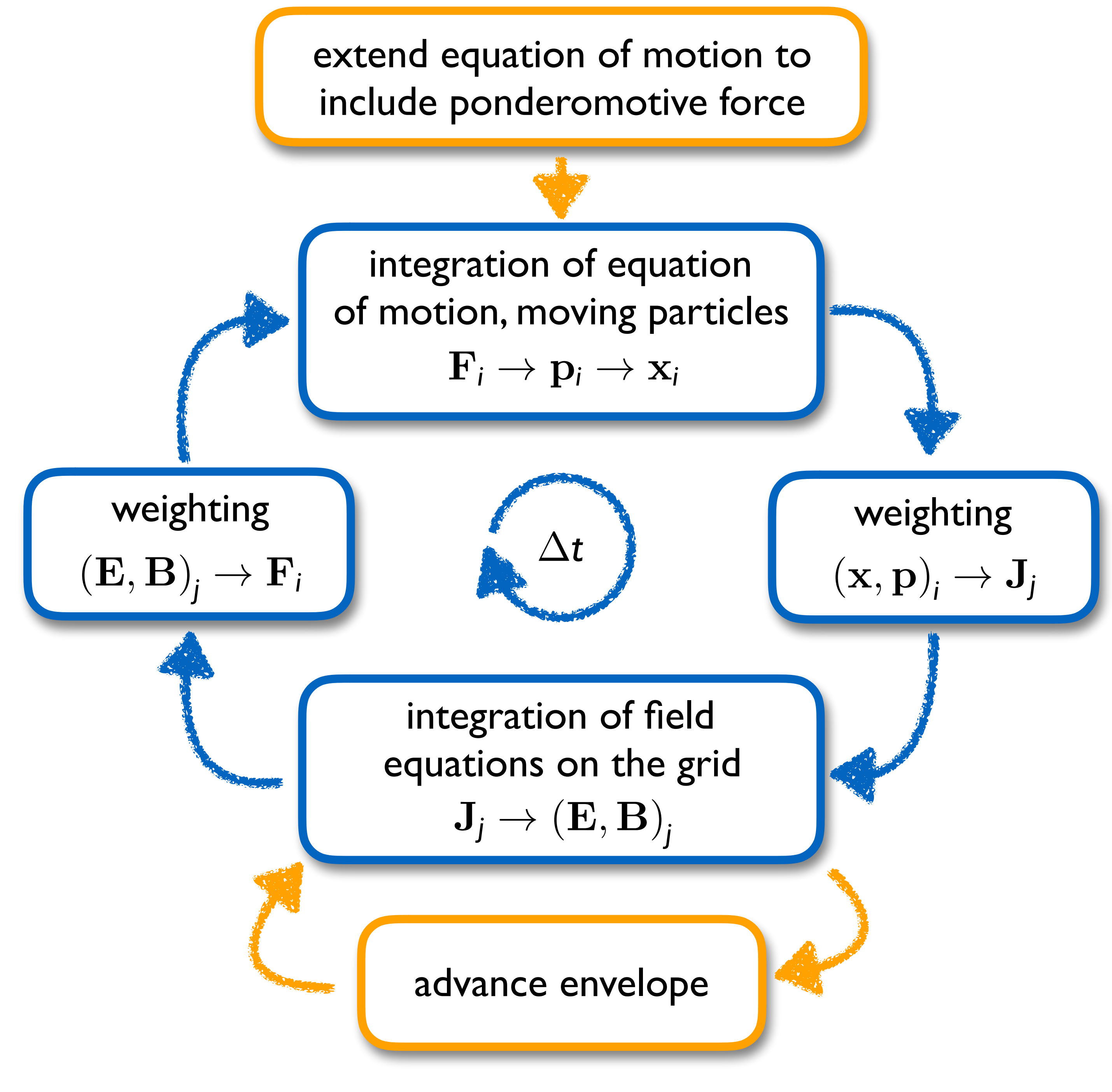
plasma skin depth



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

Incorporation of PGC into PIC cycle

extended PIC algorithm



PGC extension

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

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

laser frequency — laser envelope

- particle advancing

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

- coupling parameters

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

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

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

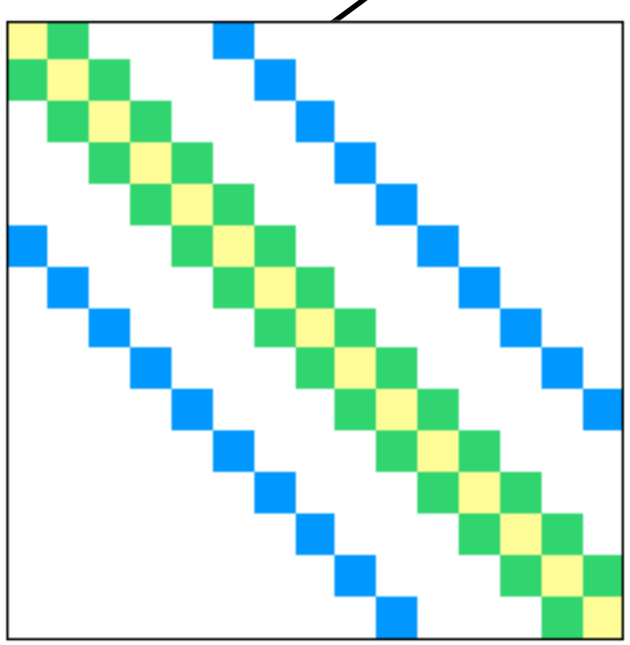
discretization of envelope equation for 3D

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

Crank-Nicolson method*,**

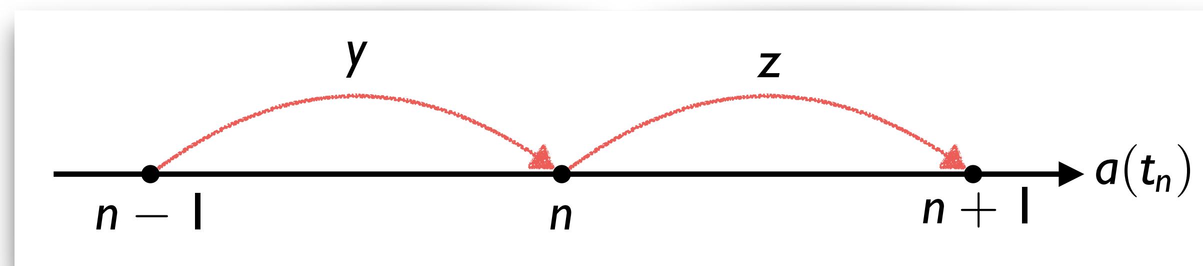
$$\left[a^{n+1} - \frac{\Delta t}{2i\omega_0}\left(\partial_y^2 + \partial_z^2\right) a^{n+1}\right]_{j,k} = S_{j,k}^{n,n-1}$$

$$\mathbf{A} \cdot a^{n+1} = S^{n,n-1}$$



- ✦ second order in time
- ✦ favorable for stability
- ✔ 2D: algebraic problem is tridiagonal
- ✘ 3D: algebraic problem is polydiagonal
- ➡ complexity for scalability and memory usage

Alternating direction implicit (ADI)



y-step:

$$\left[a^{n} - \frac{\Delta t}{2i\omega_0}\partial_y^2 a^{n}\right]_{j,k} = S_{j,k}^{n-1}$$

z-step:

$$\left[a^{n+1} - \frac{\Delta t}{2i\omega_0}\partial_z^2 a^{n+1}\right]_{j,k} = S_{j,k}^{n}$$

- ✦ second order in time
- ✔ algebraic problem is tridiagonal
- ✔ using Thomas algorithm for tridiagonal system (linear scaling)
- ✦ similarity to 2D version

* D. Gordon *et. al.*, IEEE Trans. Plasma Sci. 28, 1135 (2000)
** B. M. Cowan *et al.*, JCP 230, 61 (2011)

stability of the solver depends on resolution and laser frequency

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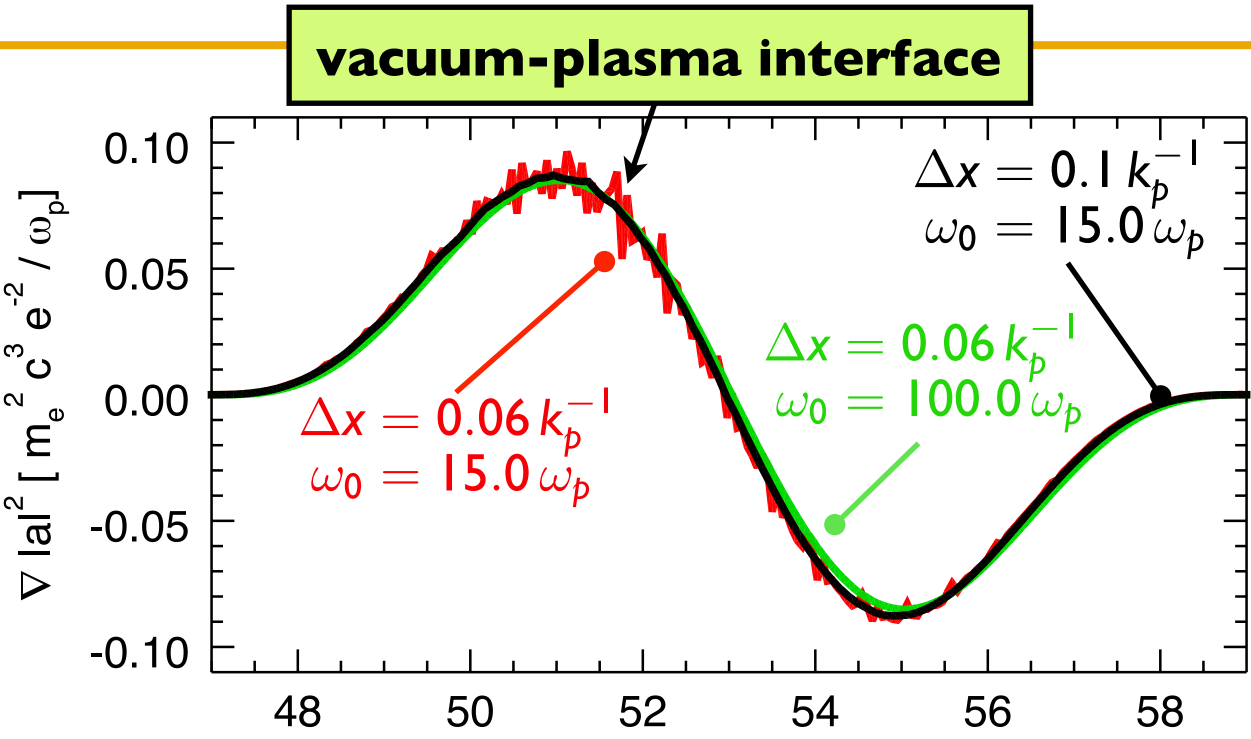
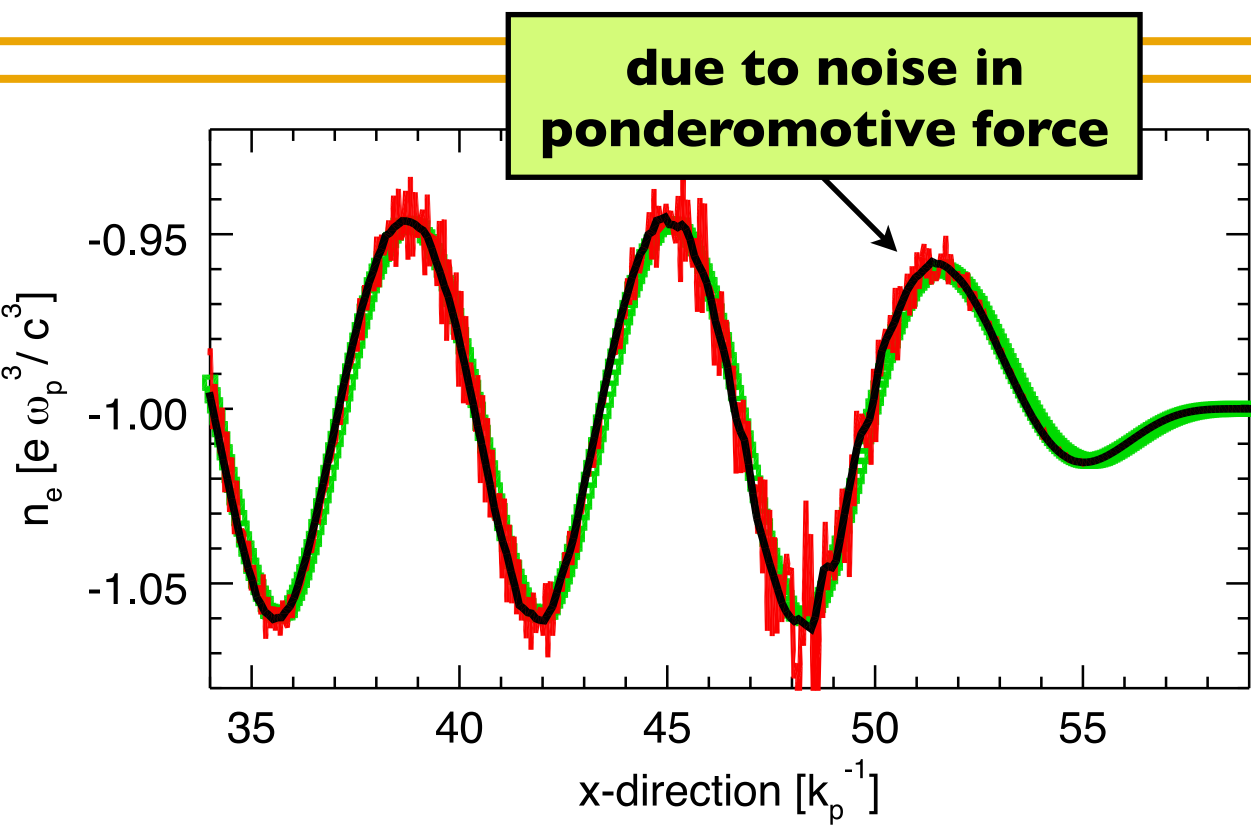
ponderomotive force



electron density



stability of PGC solver

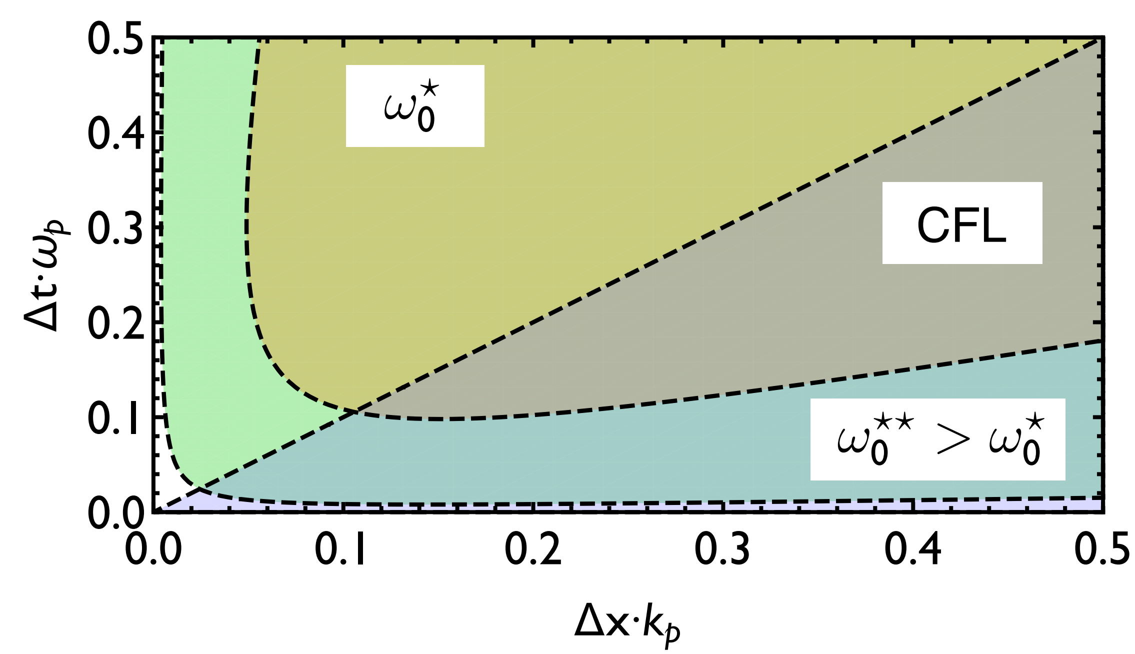
- assume 1D envelope equation

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

- stability condition after discretization

$$\left(1 - \underbrace{\frac{\chi_{i+1} - \chi_{i-1}}{2\omega_0 \Delta\xi \Delta\tau}}_{\text{density gradient}}\right)^2 + \left(\underbrace{\frac{\chi_i}{\omega_0 \Delta\tau} + \frac{\chi_i}{2\omega_0 \Delta\xi}}_{\text{density}}\right)^2 \leq 1$$

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



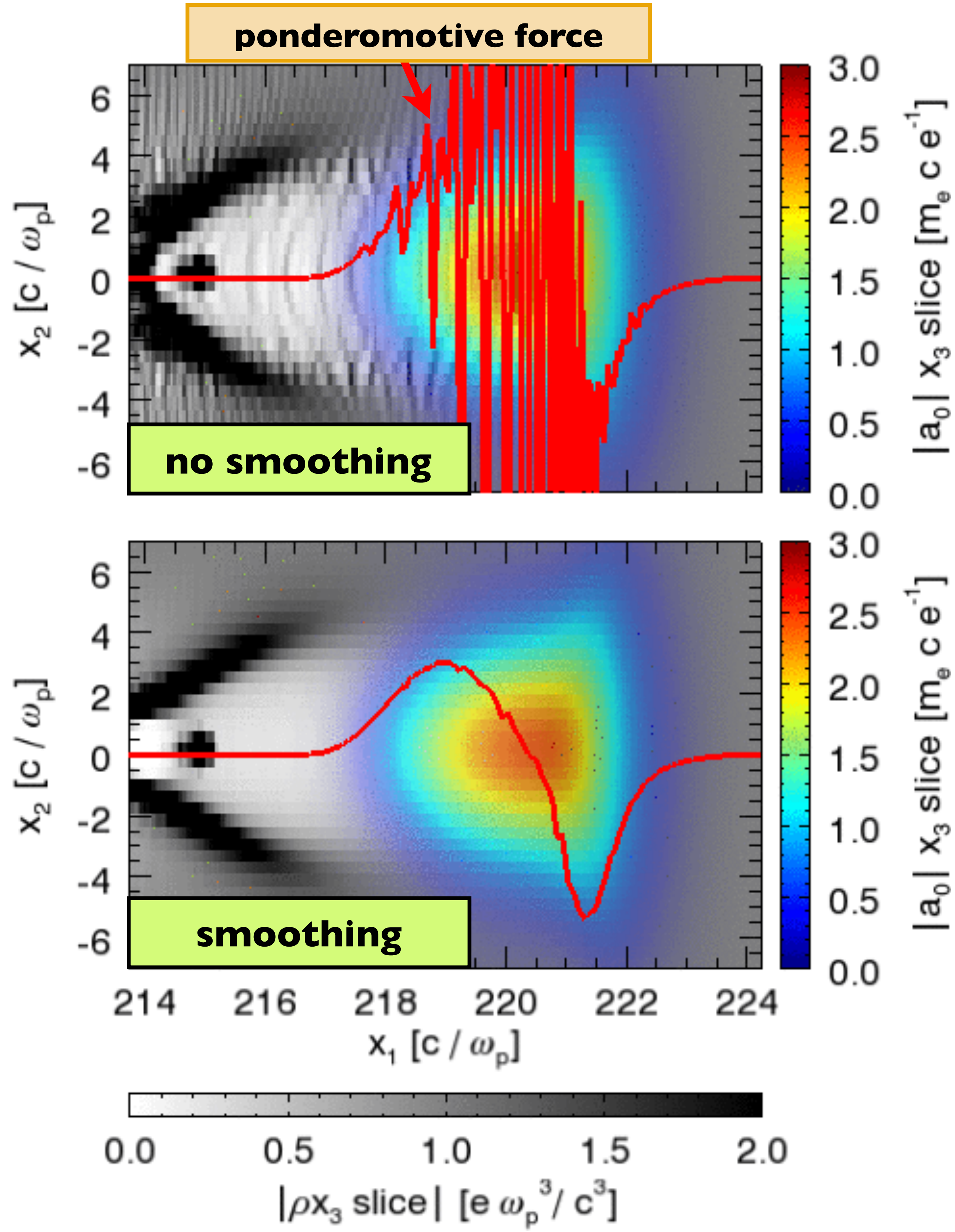
stability control for PGC

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



comparison of PGC with full PIC

laser envelope

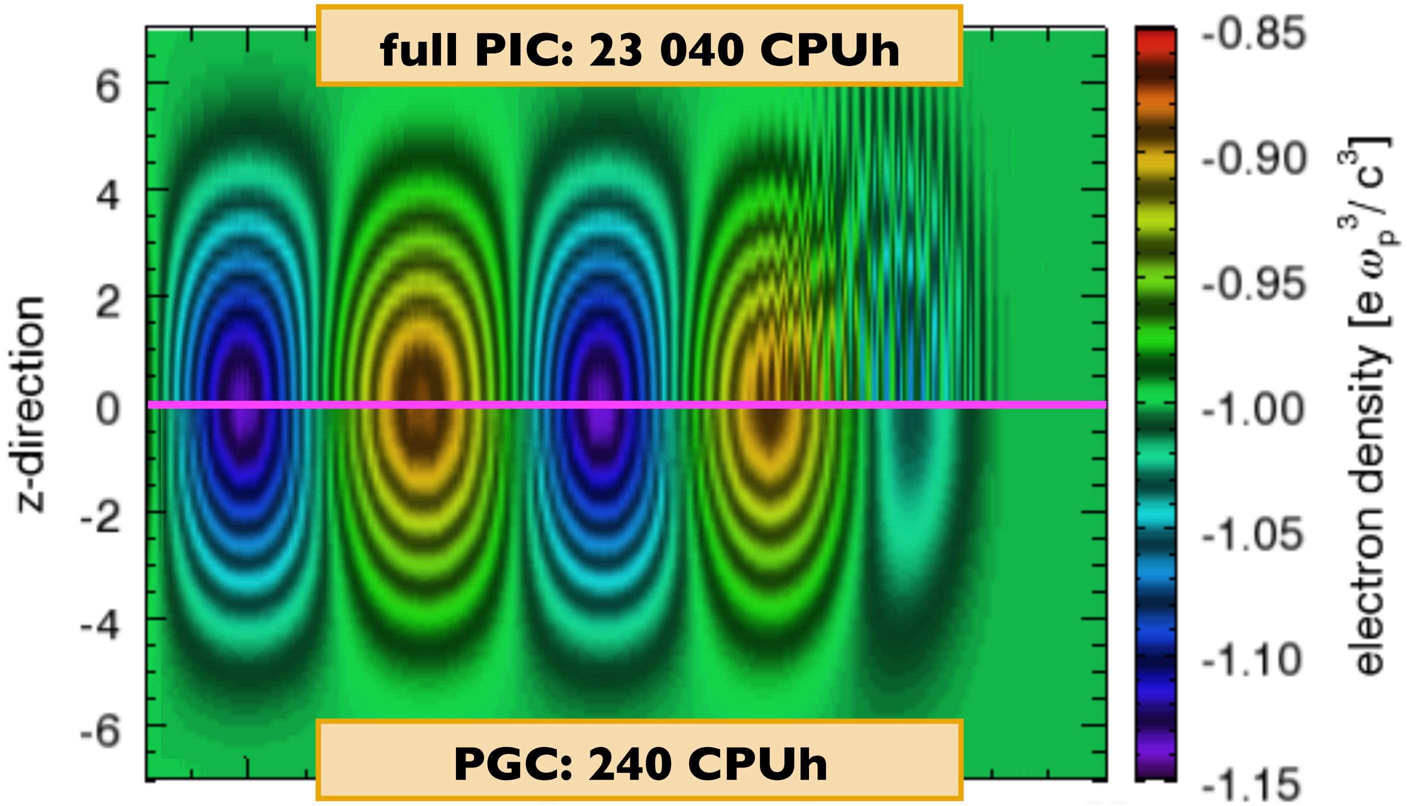
- $\sin^2$ / gaussian beam profile
- pulse length = 12.0 k_p^{-1}
- laser frequency = $15.0\omega_p$
- spot size = 5.0 k_p^{-1}
- driver amplitude = 0.5

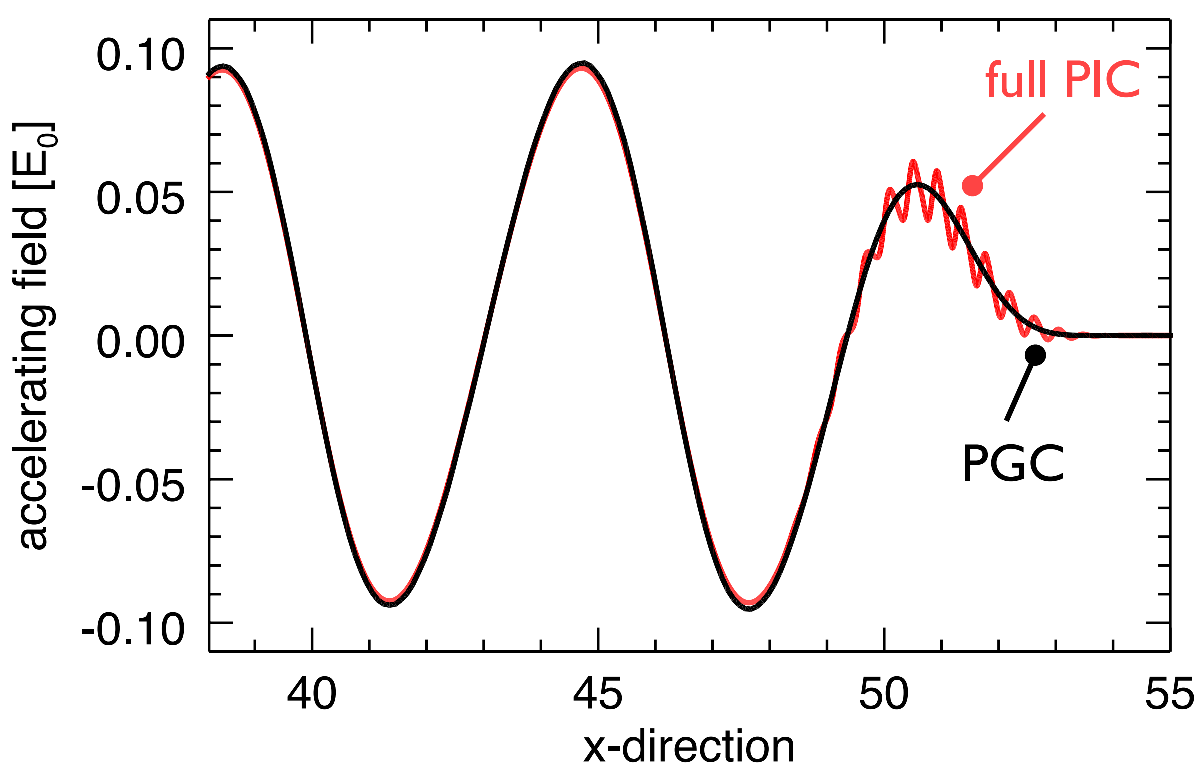
simulation setup

- $\Delta x = 0.1\ k_p^{-1}$ (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

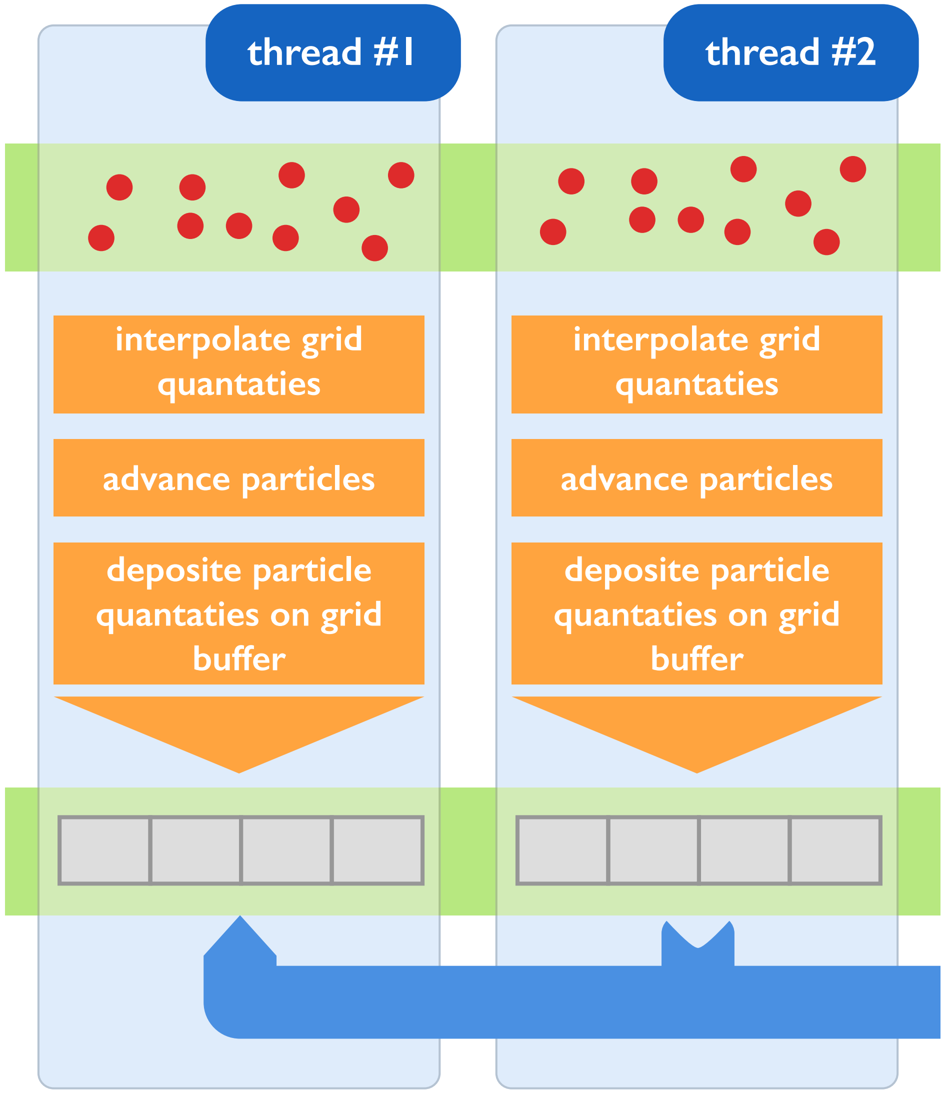
- full PIC: 18 h on 1280 cores
- PGC: 4 h on 60 cores
- **speedup: 96x**





shared memory parallelization for PGC

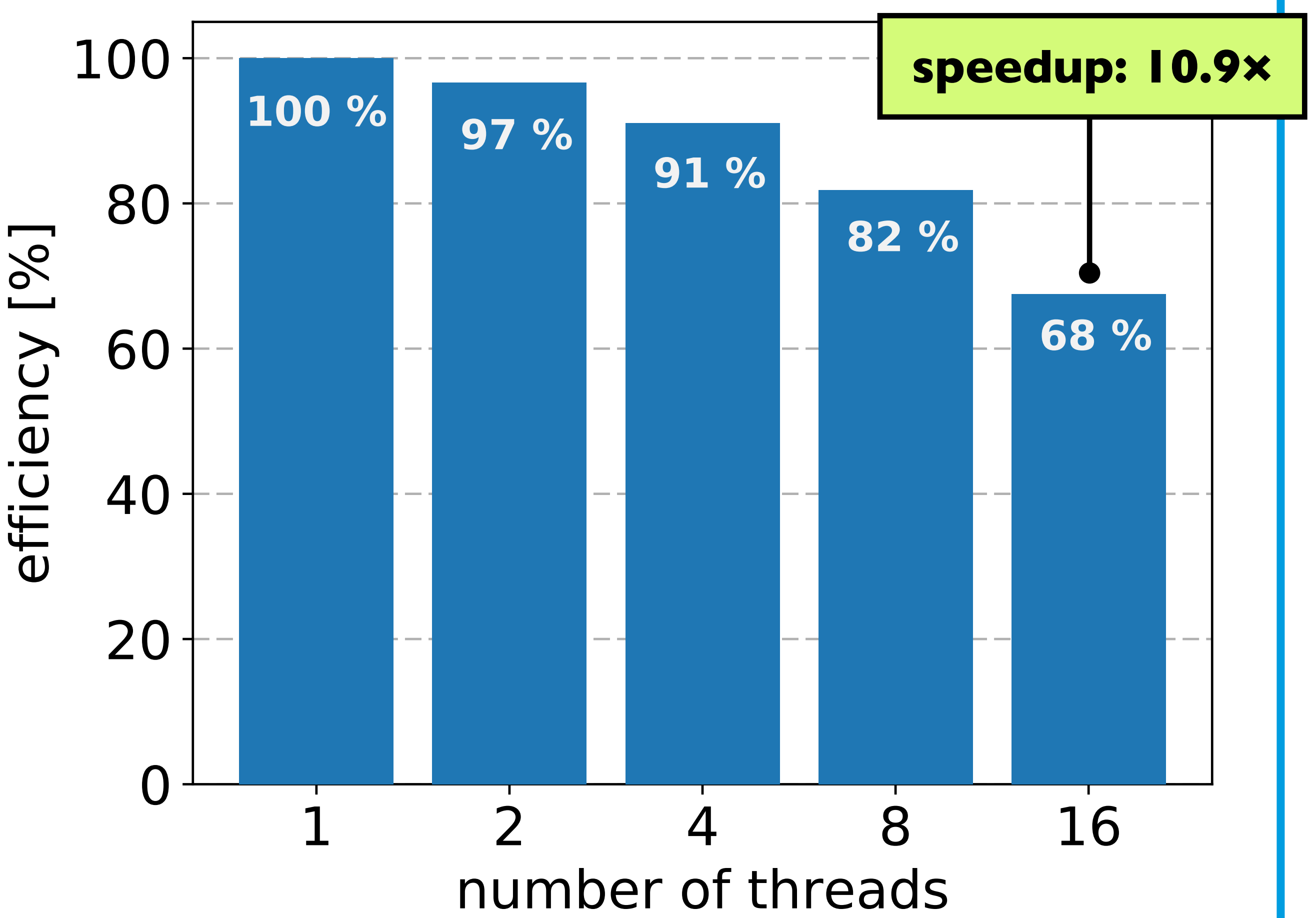
shared memory parallelization



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

distributed parallelization for PGC requires different parallelization approach compared to PIC

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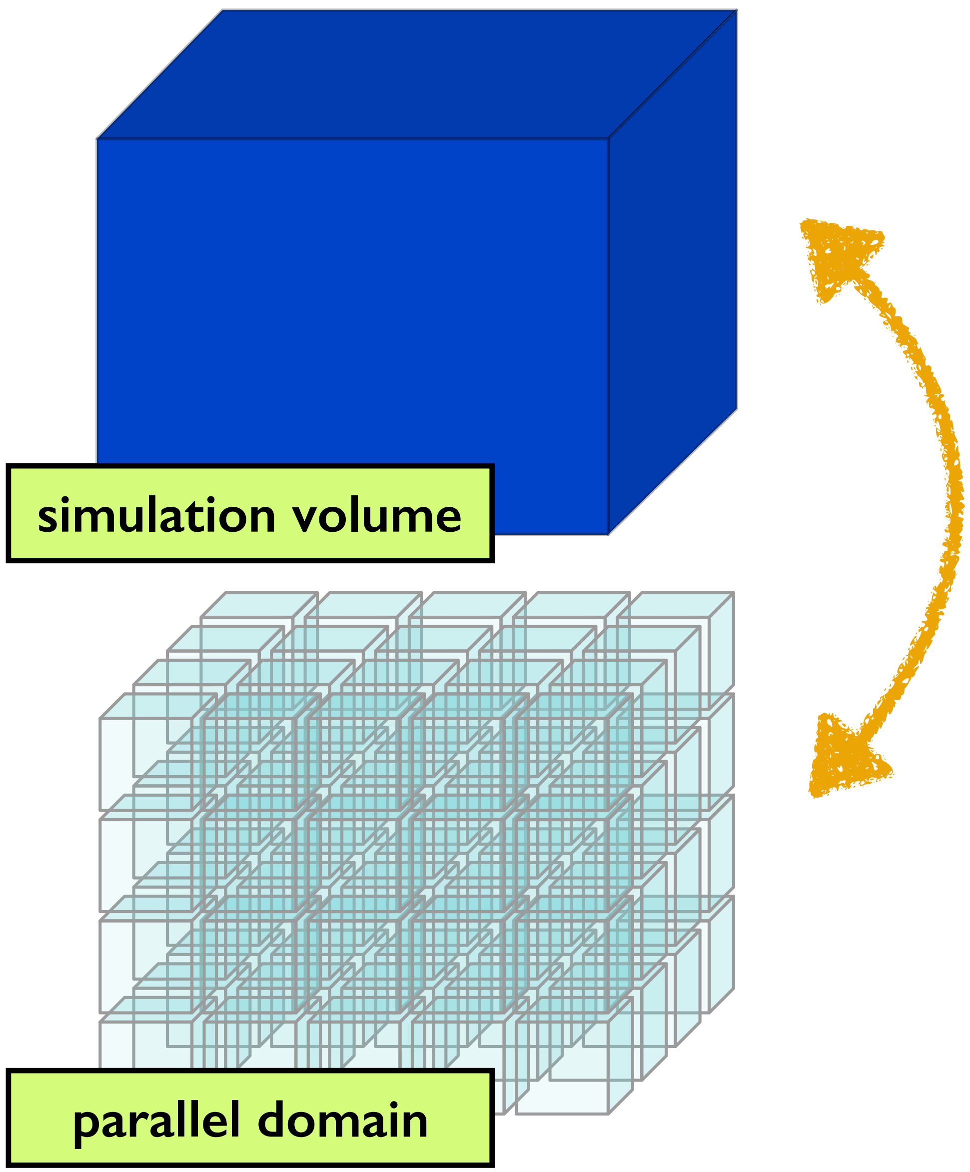
distributed memory parallelization



spatial domain decomposition

- ✔ memory is scalable with number of cores
- ✘ non-localized memory access - data on remote node needs to be send

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- ✦ advancing of grid quantities in PIC is commonly based on explicit numerical schemes
- ✦ explicit schemes allow to decompose simulation volume spatially in parallel domains
- ✦ communication between domains is based on nearest neighbour

explicit

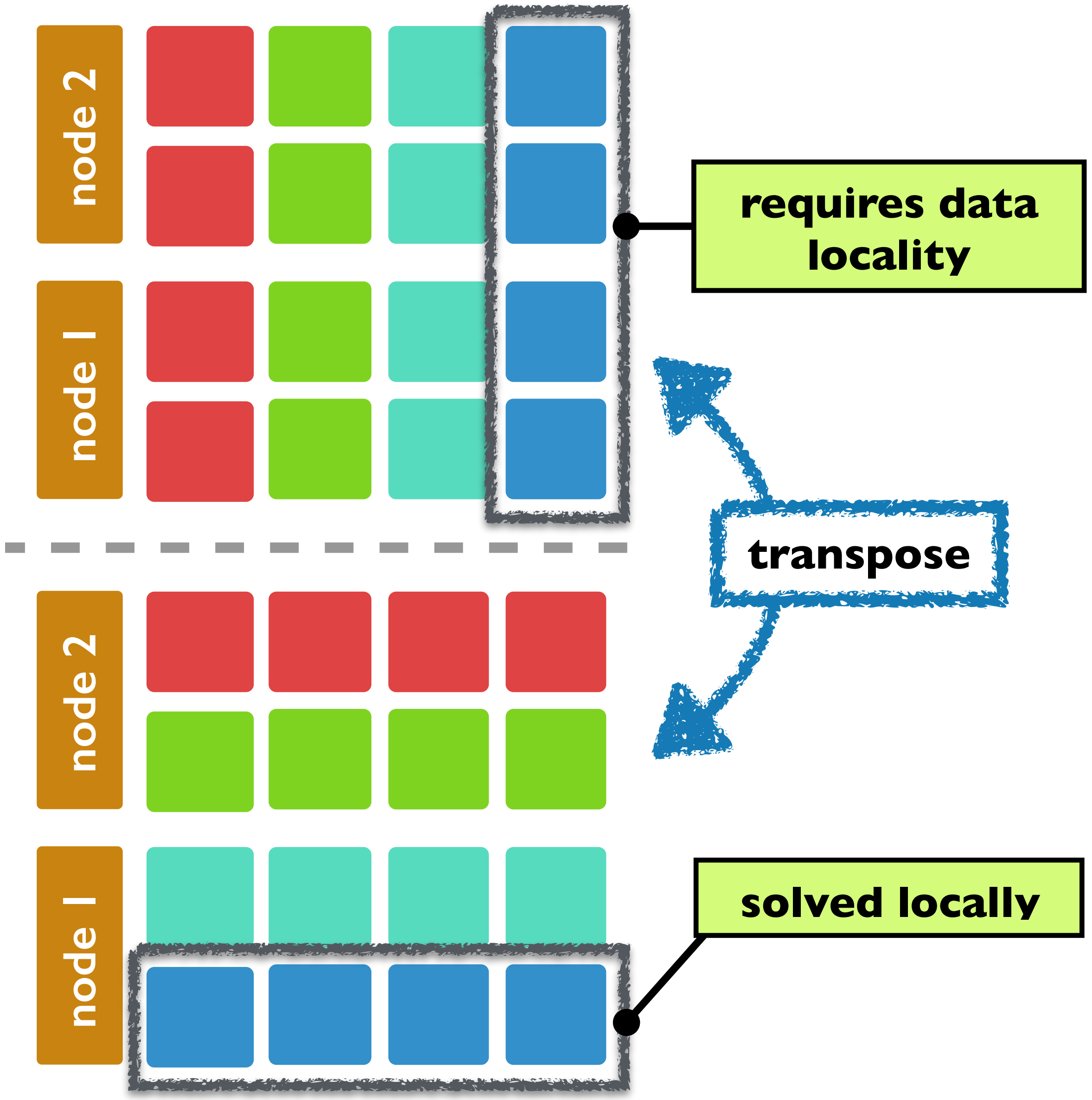
$$\partial_\tau a = \frac{1}{2i\omega_0}\left(\hat{D}p + \Delta_T a\right)$$

implicit

- ✦ envelope equation is advanced by an explicit scheme in longitudinal direction and by an implicit scheme in transversal
- ✔ for longitudinal direction spatial domain decomposition can be adopted
- ✘ implicit scheme for transversal direction requires data locality for slice in transversal direction

parallel transpose of envelope equation in transversal direction for distributed memory parallelization

transversal parallelization



✔ allows parallel decomposition in transversal direction

✘ requires node to node communication for each transversal direction

- spatial domain decomposition without further adaptation will lead to single-node computation with other nodes being idle
- due to data locality requirement, a transpose operation is used
- a subsection of local grid is send to other node and a subsection of non-local grid is received from other node
- transpose operation requires node to node communication in transversal direction
- after parallel transpose operation, advancing of an envelope slice can be performed locally
- after local advancing performing second parallel transpose operation for gathering local envelope values

- two communications communications per node per time step required
- non-blocking MPI send/recv for reducing communication bottleneck
- communication between nodes is based on MPI

parallelization is scalable over thousands of cores

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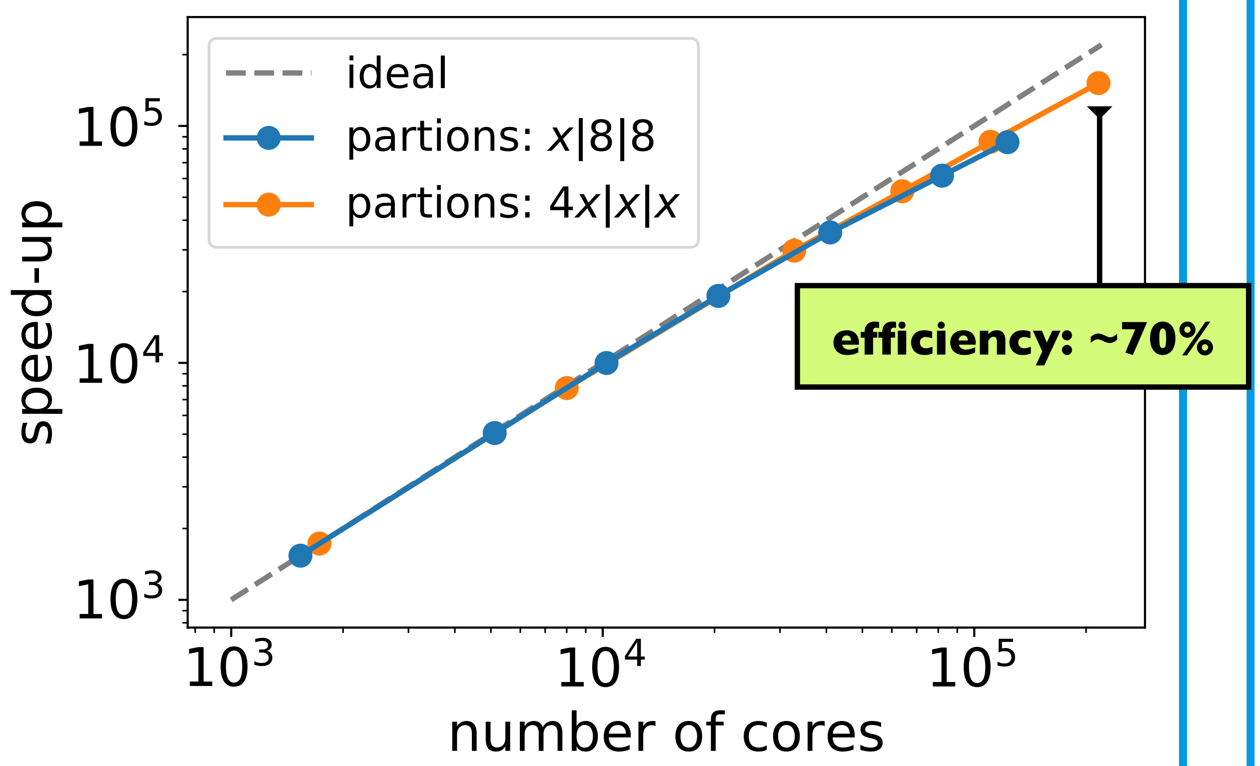
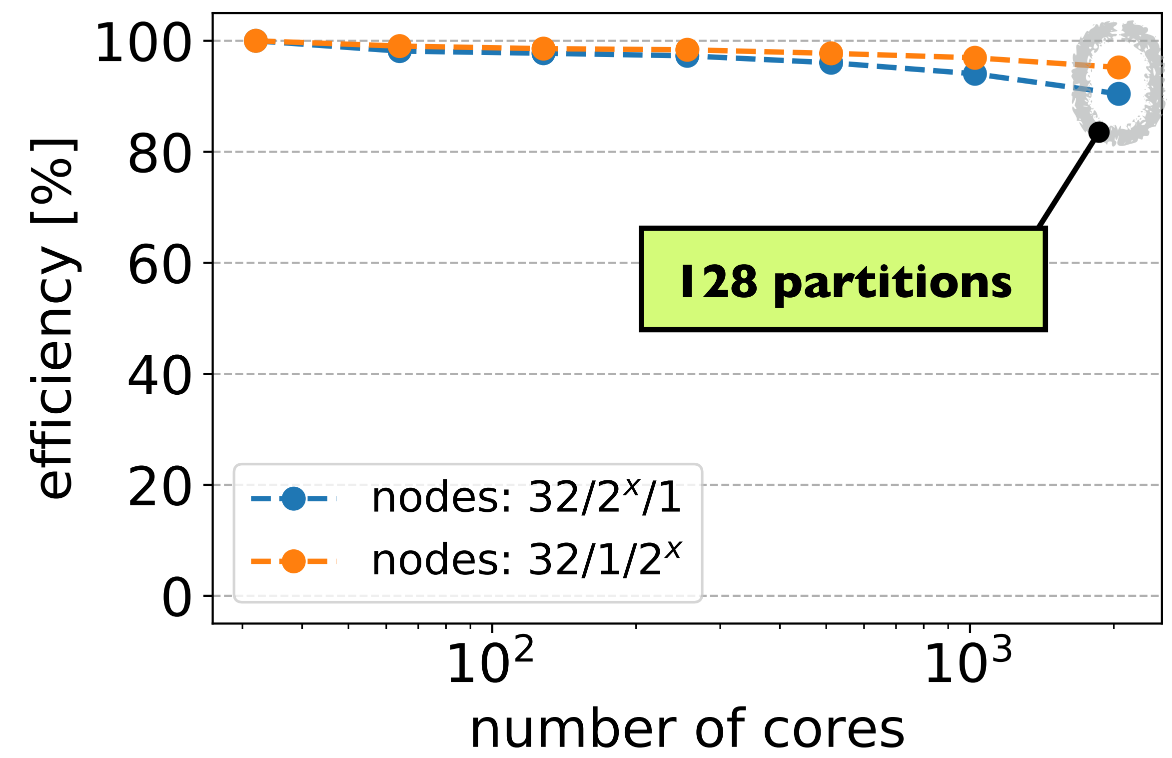
strong scaling



- 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
- initial setup: 2048×10×50 cells and 8 ppc
- periodic boundaries in transversal direction
- ✔ 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.

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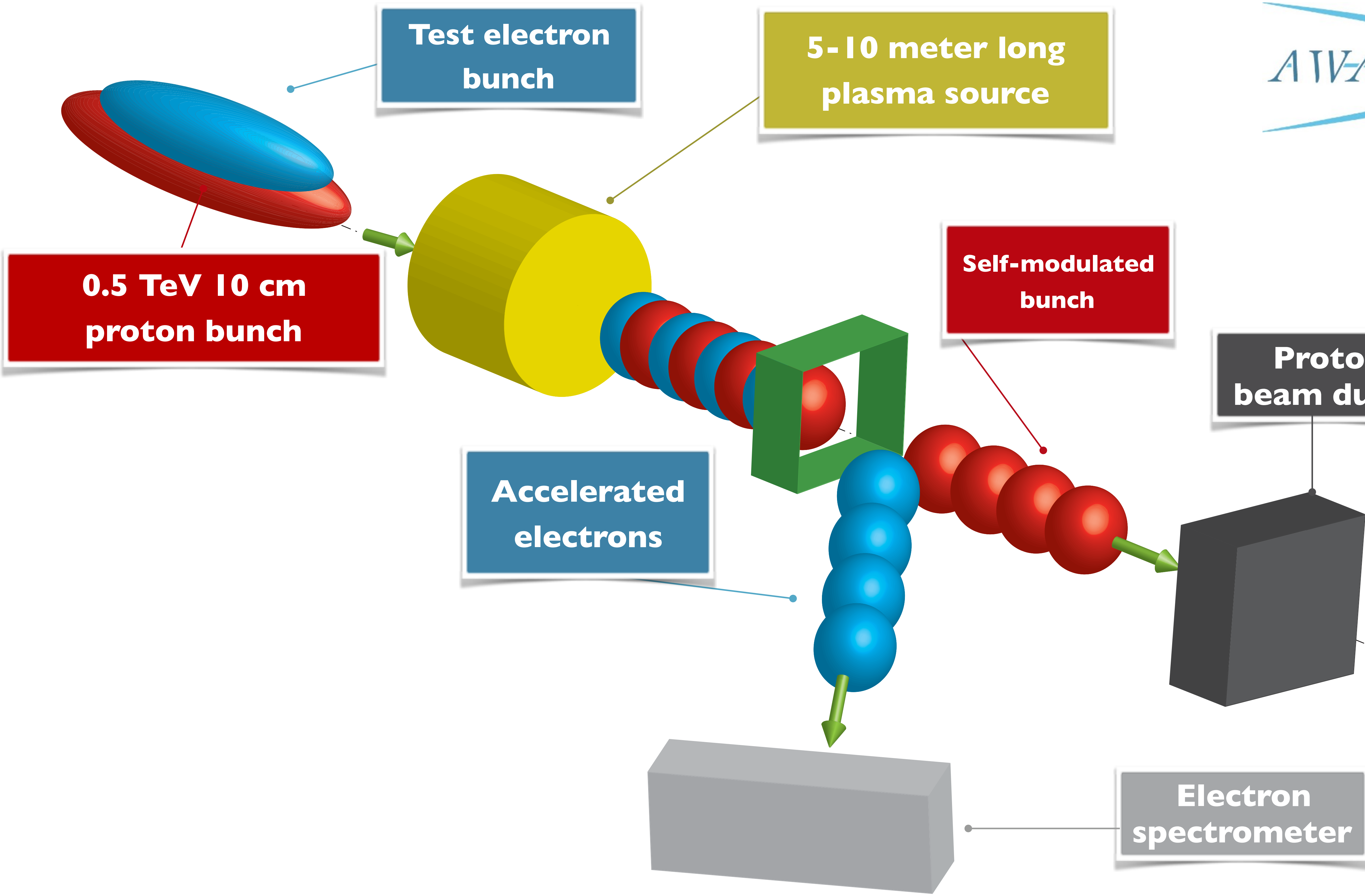

AWAKE

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

creating plasma to cut proton bunch simultaneously

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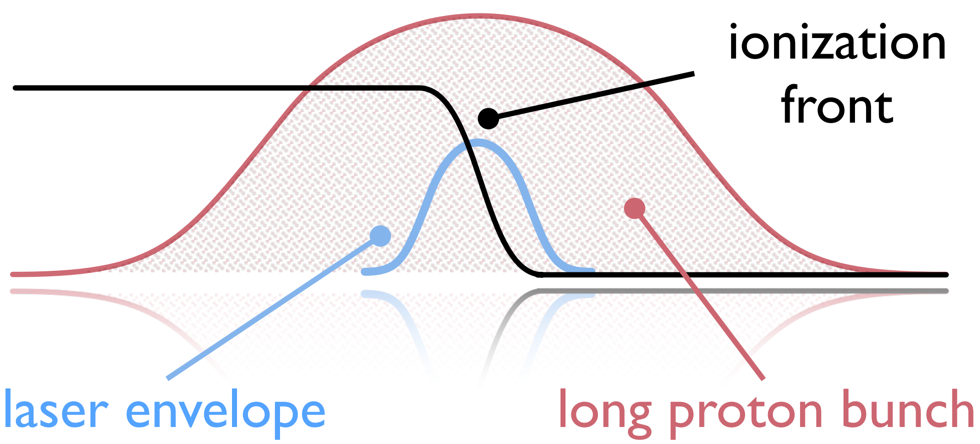
laser pulse on top of proton bunch

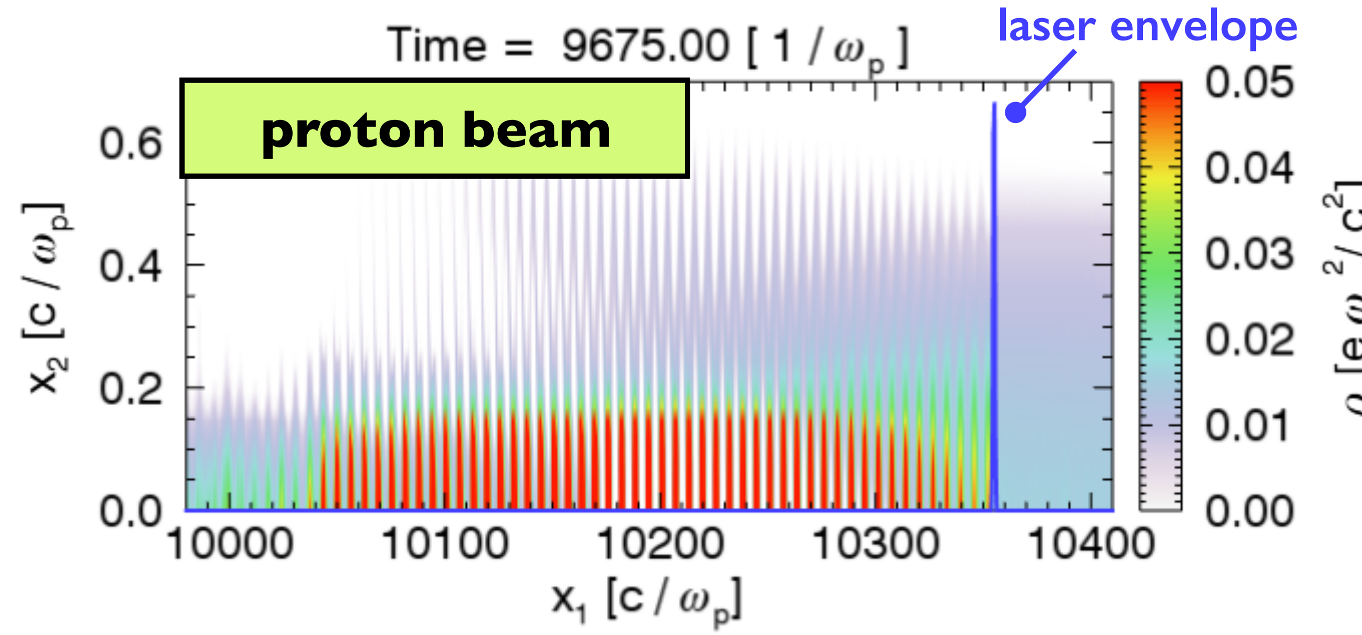


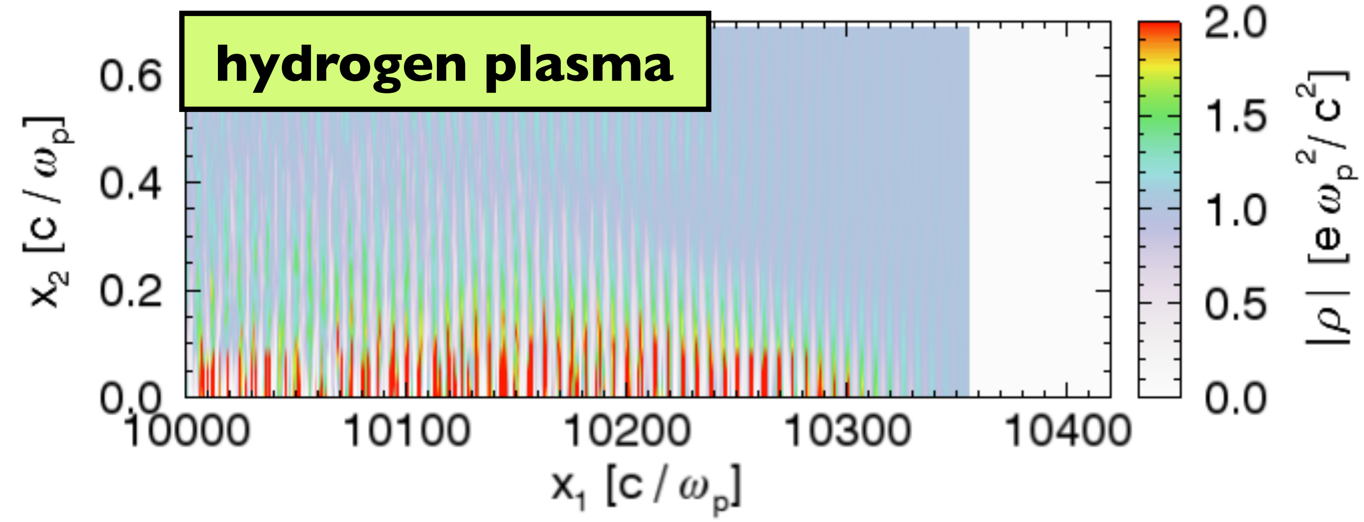
- ✦ laser pulse generates ionization front
- ✦ ionization front cuts long proton bunch sharply
- ✦ pulse excites wakes to directly seed the instability*

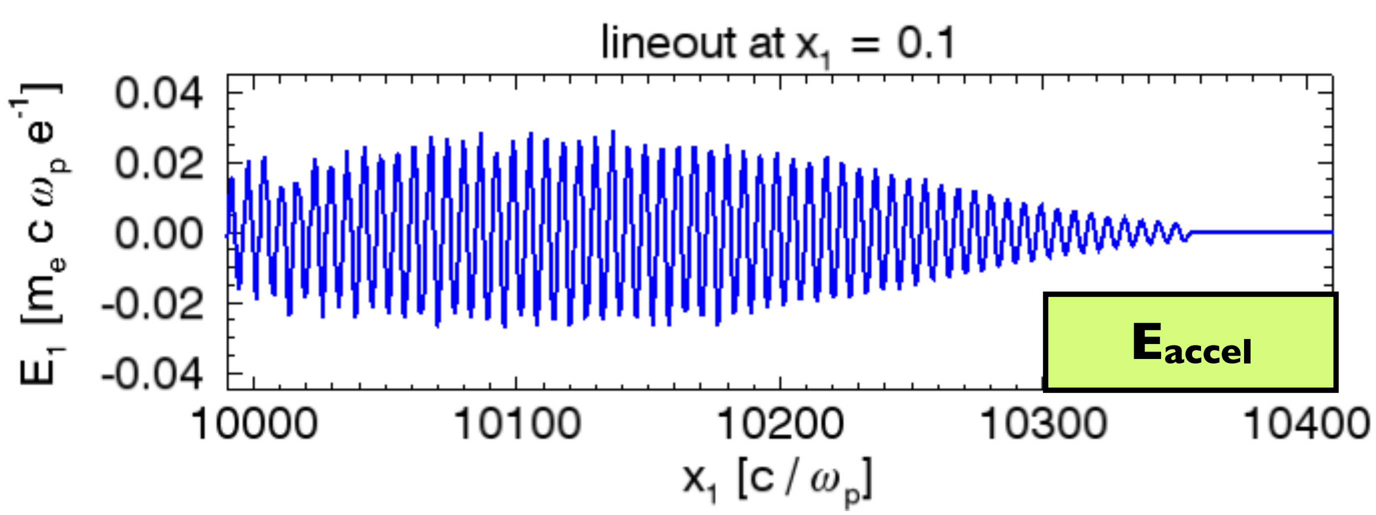
full run (PGC vs full PIC)

- ✦ 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€







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

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 $\omega_0/\omega_\mathrm{p}$-cases can be studied

Parallelization of ponderomotive guiding center

- shared memory parallelization can gain up to one order higher scalability
- ponderomotive guiding center solver can be scaled over thousands cores using shared memory parallelization

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