Presentation of advanced methods for EM PIC

Outline

- **Spectral solvers**
  - Finite-difference vs pseudo-spectral analytical algorithms
  - Parallelization
  - Pseudo-spectral cylindrical algorithm

- **Some challenges in electro-magnetic PIC simulations**
  - Spurious numerical dispersion
  - Cancelation of E + v x B
  - Boosted-frame simulations and Cherenkov instability

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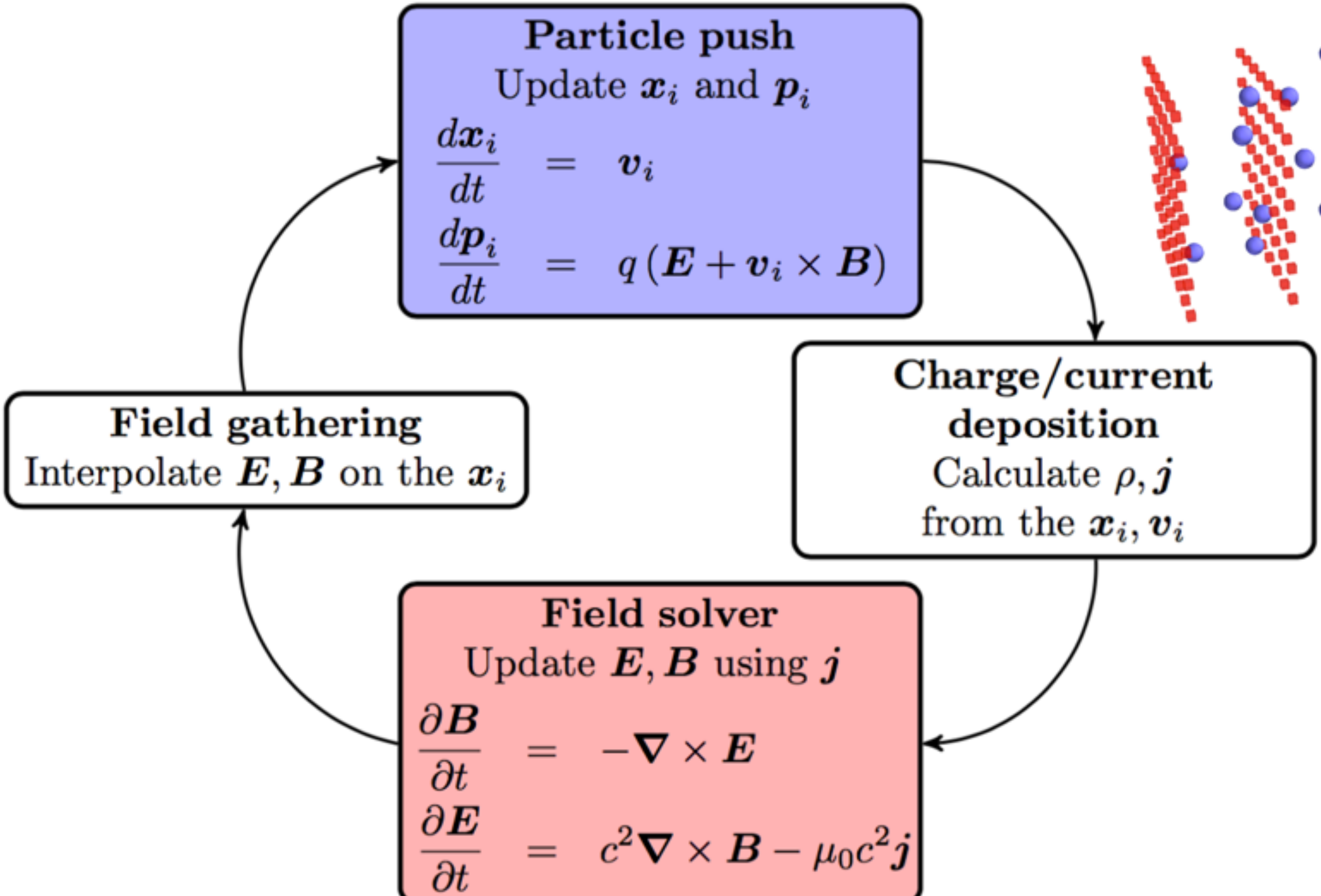
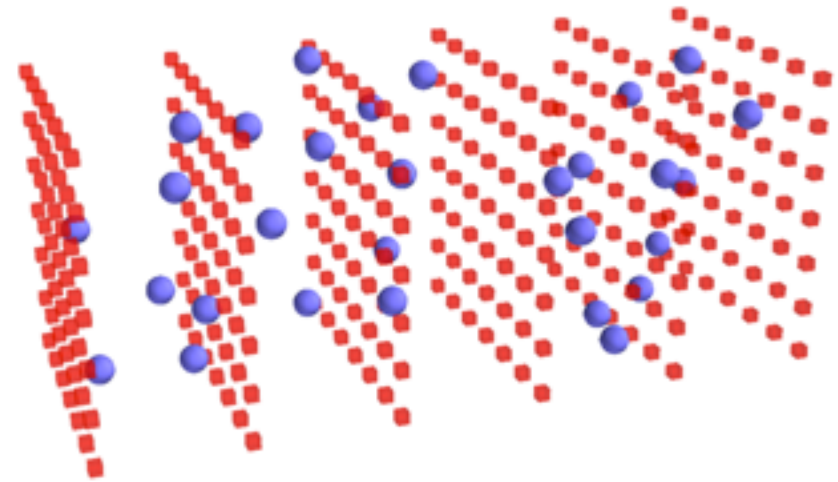
Electromagnetic Particle-In-Cell method





Finite-difference algorithms (FDTD)

Continuous equations

$$\frac{1}{c^2}\partial_t \boldsymbol{E} = \boldsymbol{\nabla} \times \boldsymbol{B} - \mu_0 \boldsymbol{J}$$

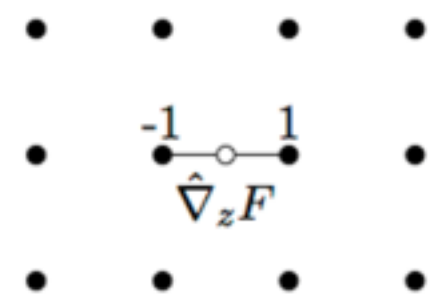
$$\partial_t \boldsymbol{B} = -\boldsymbol{\nabla} \times \boldsymbol{E}$$

Discretization →

Discrete derivatives
on a spatial grid

$$\frac{1}{c^2}\hat{\partial}_t \boldsymbol{E} = \hat{\boldsymbol{\nabla}} \times \boldsymbol{B} - \mu_0 \boldsymbol{J}$$

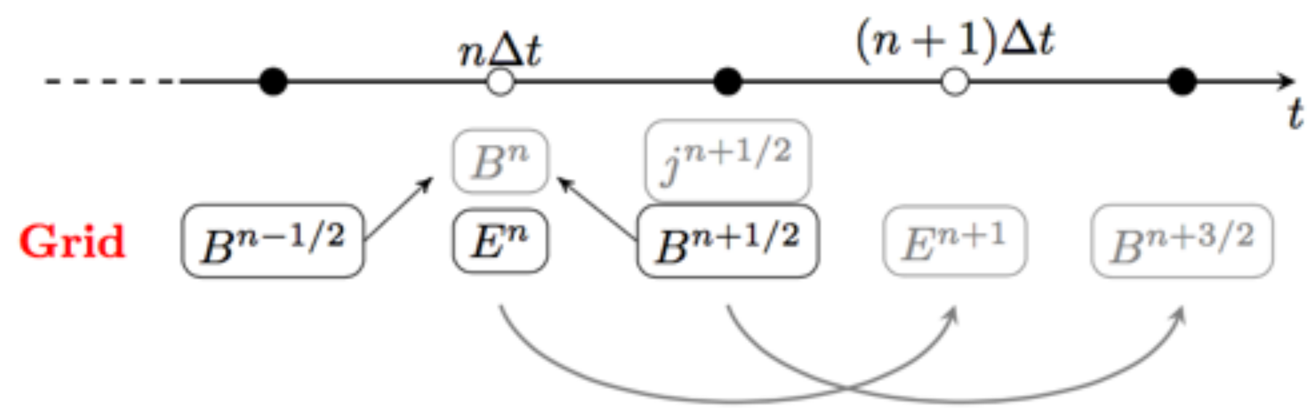
$$\hat{\partial}_t \boldsymbol{B} = -\hat{\boldsymbol{\nabla}} \times \boldsymbol{E}$$



Pros and cons

- Can be efficiently parallelized (thus very commonly used)
- But the discretization introduces **staggering in time** and **spurious numerical dispersion**

\+ Advance the fields using **finite-difference in time** (leap-frog)



Pseudo-spectral analytical algorithms (PSATD)

Continuous equations

$$\frac{1}{c^2}\partial_t \boldsymbol{E} = \boldsymbol{\nabla} \times \boldsymbol{B} - \mu_0 \boldsymbol{J}$$

$$\hat{\partial}_t \boldsymbol{B} = -\boldsymbol{\nabla} \times \boldsymbol{E}$$

Fourier transform →

Discrete grid in **k space**

$$\frac{1}{c^2}\partial_t \hat{\boldsymbol{\mathcal{E}}} = i\boldsymbol{k} \times \hat{\boldsymbol{\mathcal{B}}} - \mu_0 \hat{\boldsymbol{\mathcal{J}}}$$

$$\partial_t \hat{\boldsymbol{\mathcal{B}}} = -i\boldsymbol{k} \times \hat{\boldsymbol{\mathcal{E}}}$$

↕ FFT

Discrete **spatial** grid

$$\boldsymbol{E},\ \boldsymbol{B}$$

+ Advance the fields using **analytical integration in time**

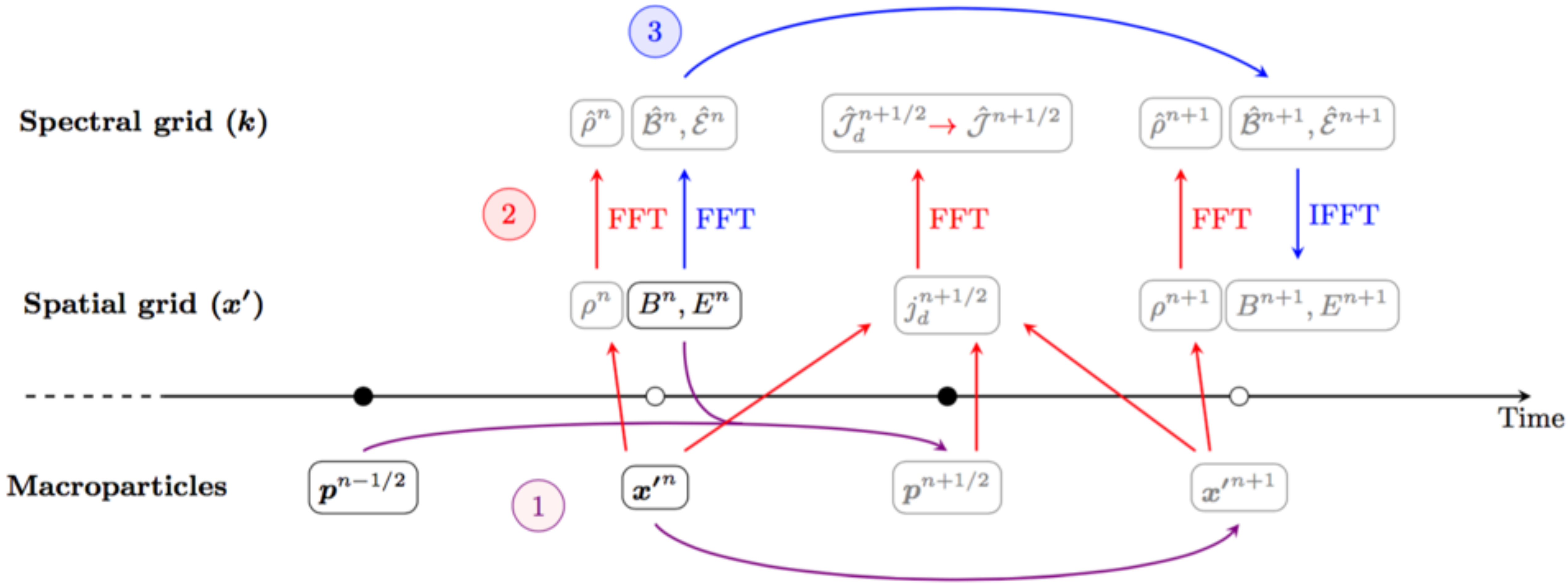
Pros and cons

- Efficient **parallelization** is challenging.
- But the fields are **centered in time** and there is **no spurious numerical dispersion**

Pseudo-spectral analytical time domaine (PSATD)

Haber et al., Advances in electromagnetic simulation techniques (1973)

Pseudo-spectral analytical algorithm



1: Field gathering + Particle push

2: Charge/Current deposition

3: Field advance in spectral space (analytical integration in time)

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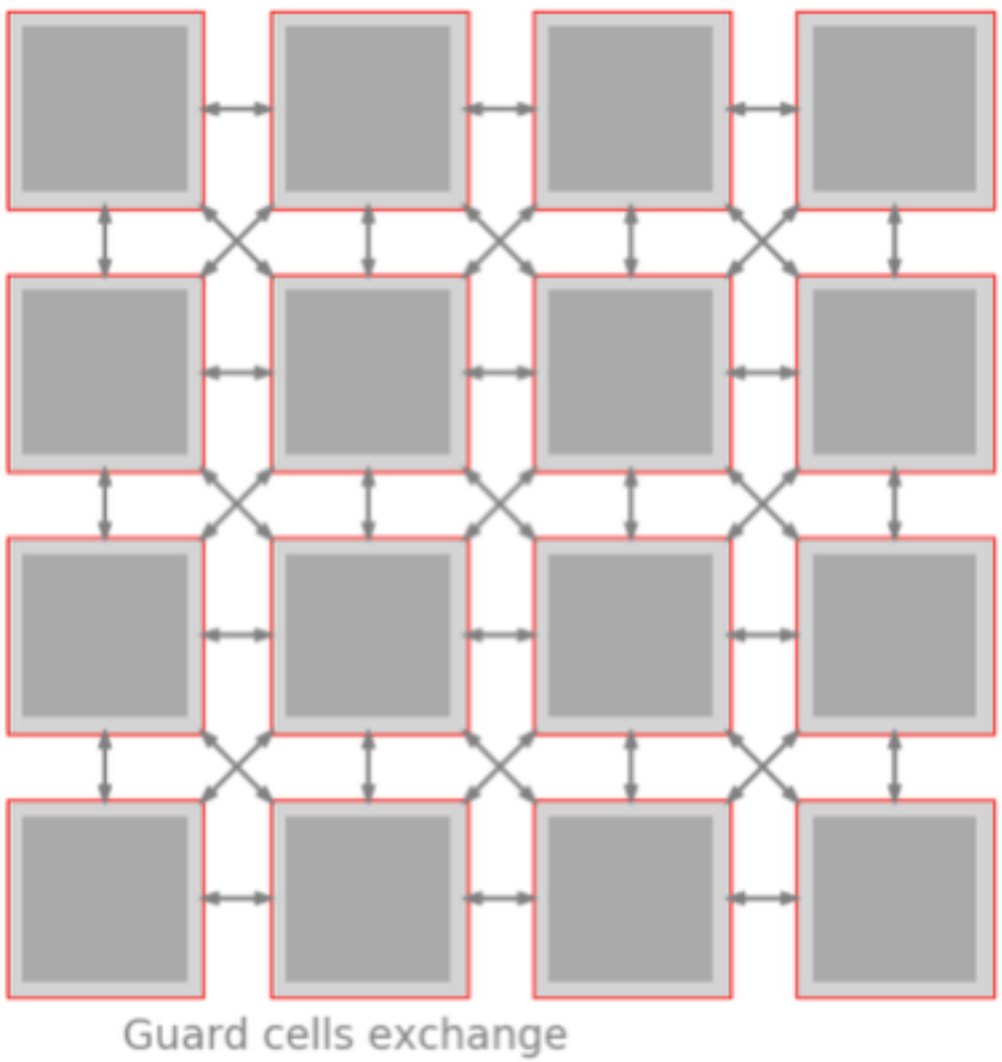
Parallelization with distributed memory (MPI)

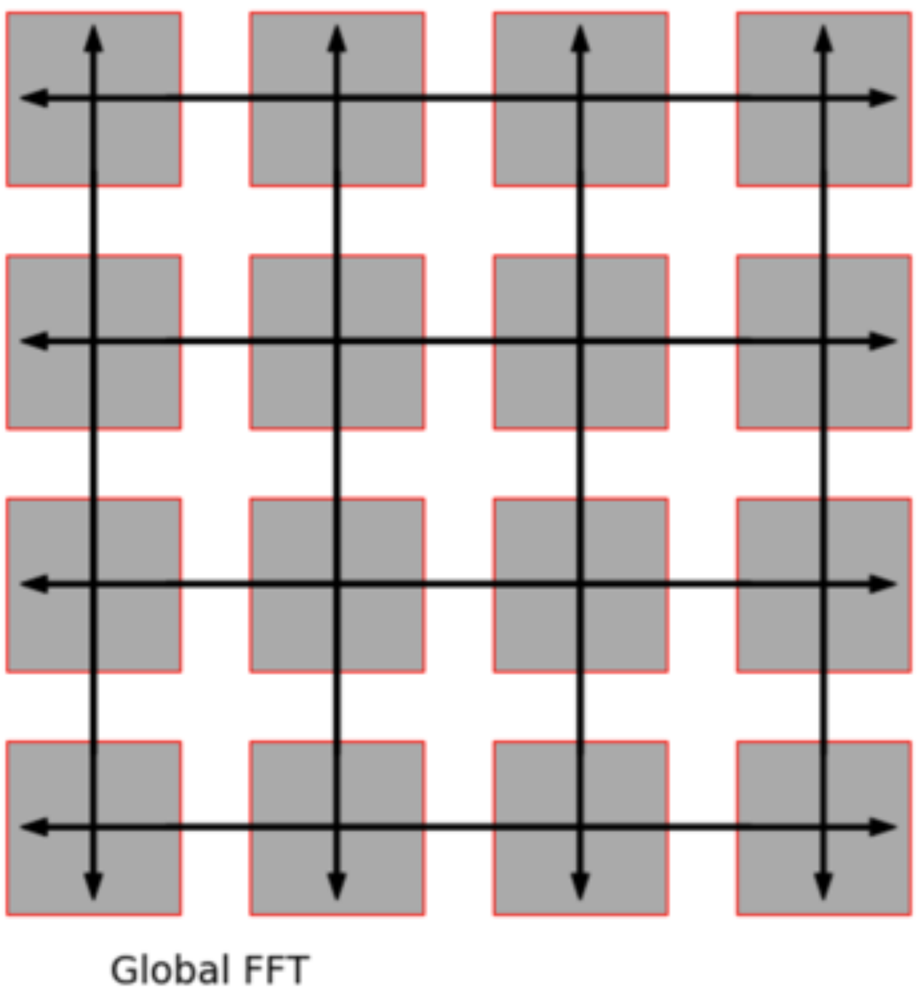
$$\frac{1}{c^2}\partial_t \boldsymbol{E} = \boldsymbol{\nabla} \times \boldsymbol{B} - \mu_0 \boldsymbol{J}$$

$$\hat{\partial}_t \boldsymbol{B} = -\boldsymbol{\nabla} \times \boldsymbol{E}$$

Finite-difference:
Exchange guard cell after field update



Spectral ("naive" implementation)
Global FFT before and after the field update in Fourier space

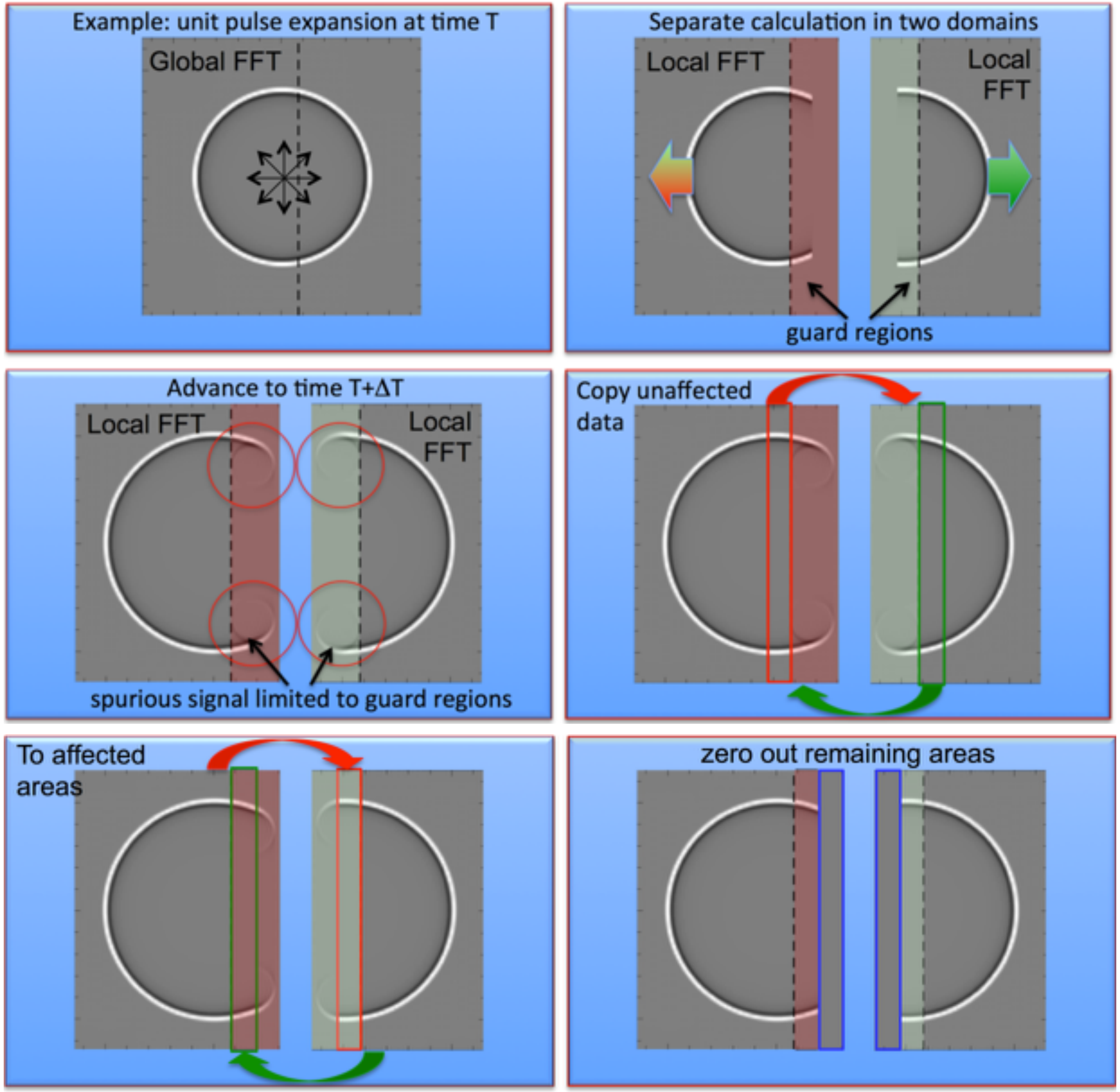


Parallelization with local FFT

Parallelization

- In theory: PSATD require **global FFT**, which does not scale well to multiple nodes
- But for the Maxwell equations, **local FFT** can be used provided that there are **enough guard cell**
- The key idea is that the error only propagates over a finite distance over a given tilmestep

First proposed by Jean-Luc
J.L.Vay, CPC (2016)



How many guard cells are needed?

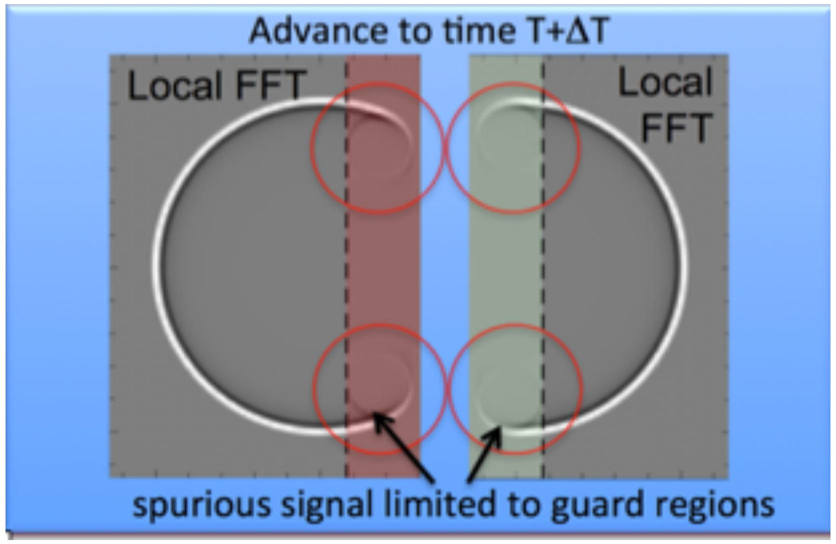
Instead of using infinite-order equation

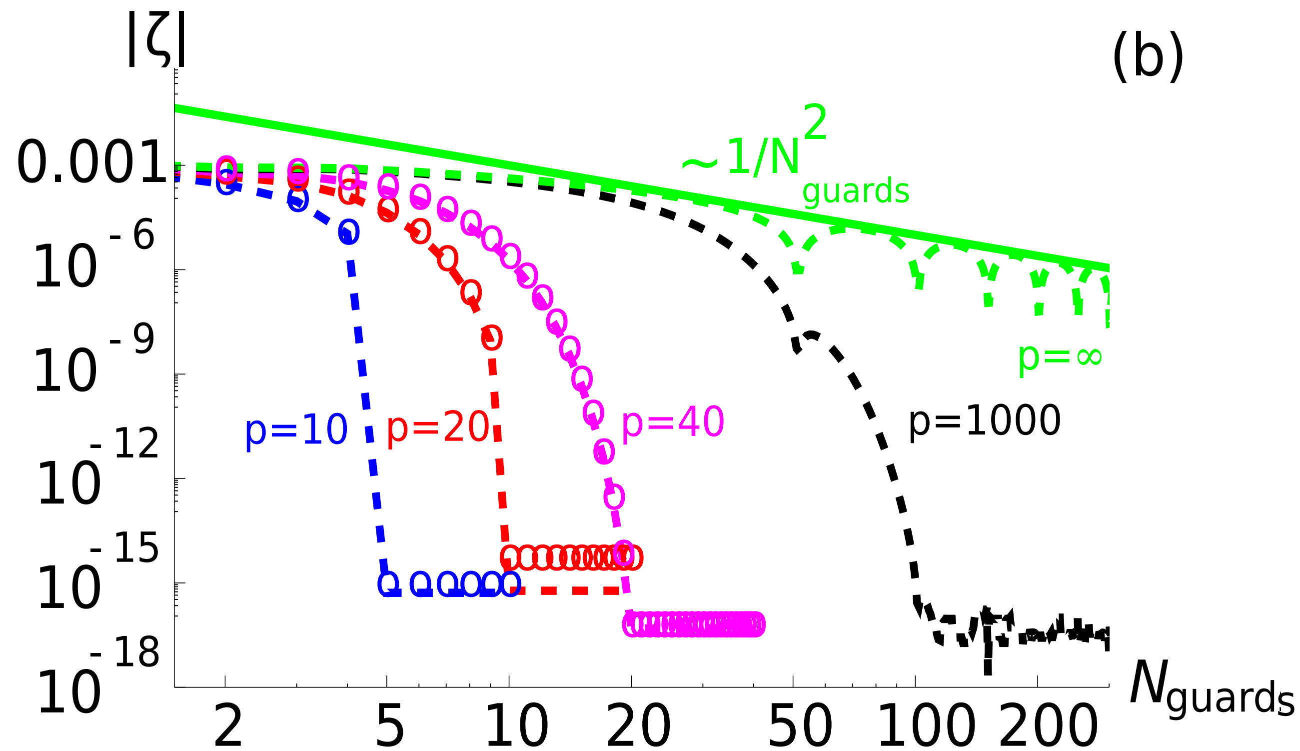
$$\frac{1}{c^2}\partial_t \hat{\boldsymbol{\mathcal{E}}} = i\boldsymbol{k} \times \hat{\boldsymbol{\mathcal{B}}} - \mu_0 \hat{\boldsymbol{\mathcal{J}}}$$
$$\partial_t \hat{\boldsymbol{\mathcal{B}}} = -i\boldsymbol{k} \times \hat{\boldsymbol{\mathcal{E}}}$$

use finite-order approximation

$$\frac{1}{c^2}\partial_t \hat{\boldsymbol{\mathcal{E}}} = i[\boldsymbol{k}] \times \hat{\boldsymbol{\mathcal{B}}} - \mu_0 \hat{\boldsymbol{\mathcal{J}}}$$
$$\partial_t \hat{\boldsymbol{\mathcal{B}}} = -i[\boldsymbol{k}] \times \hat{\boldsymbol{\mathcal{E}}}$$

where *[k]* is a p-order approximation of *k* (which is known to involve only local points)

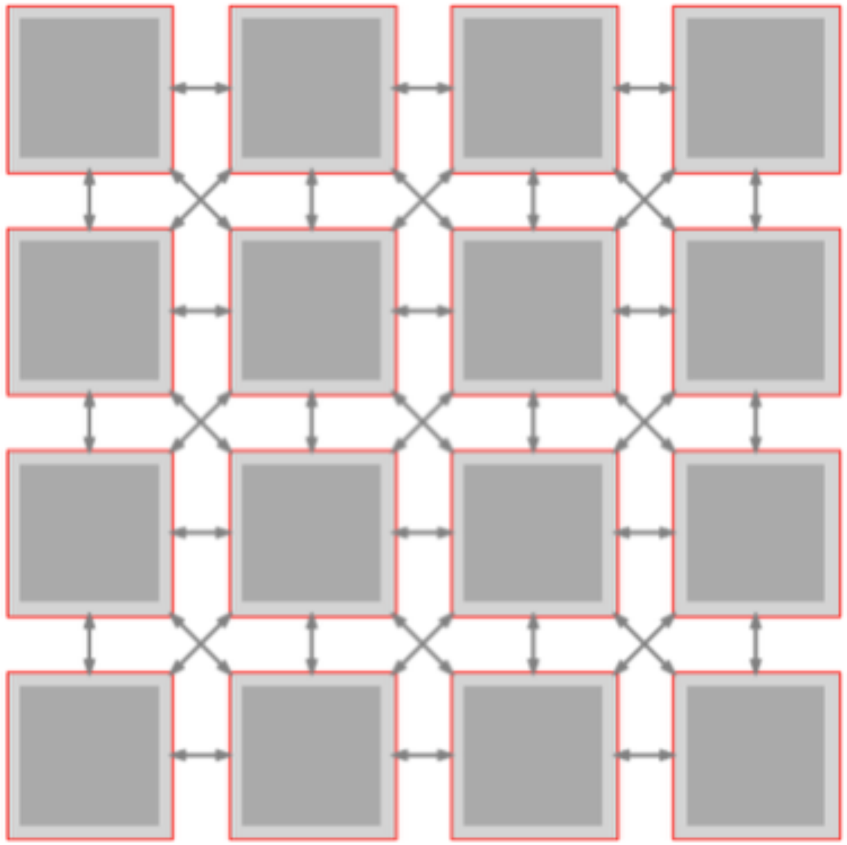




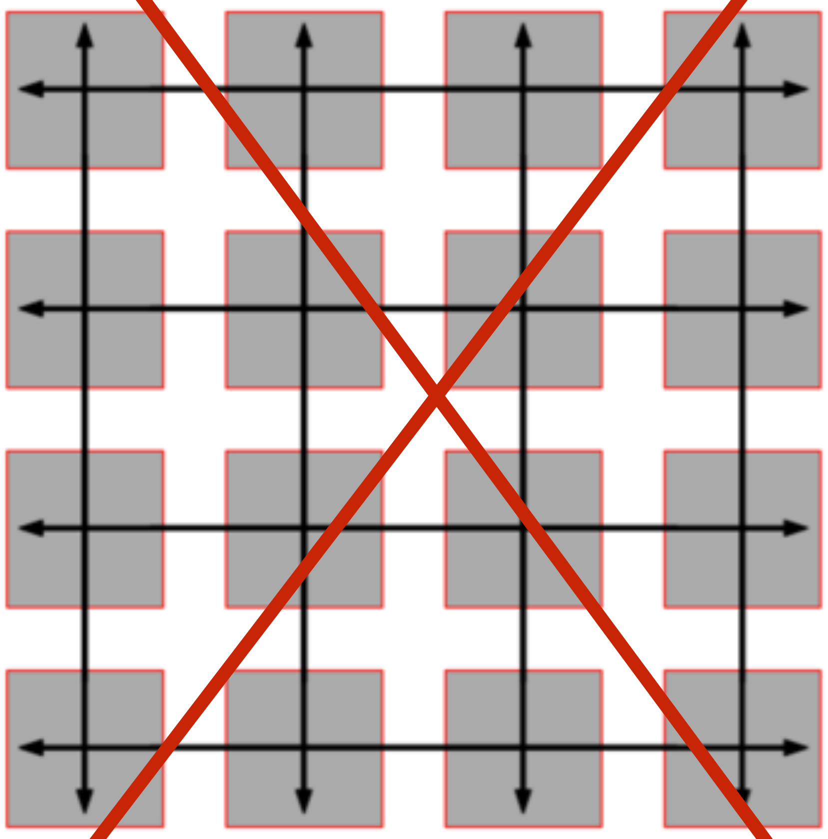
H. Vincenti and J-L Vay, *CPC* **200**, 147 (2016)

Parallelization with distributed memory (MPI)

Finite-difference:
Exchange guard cell after field update

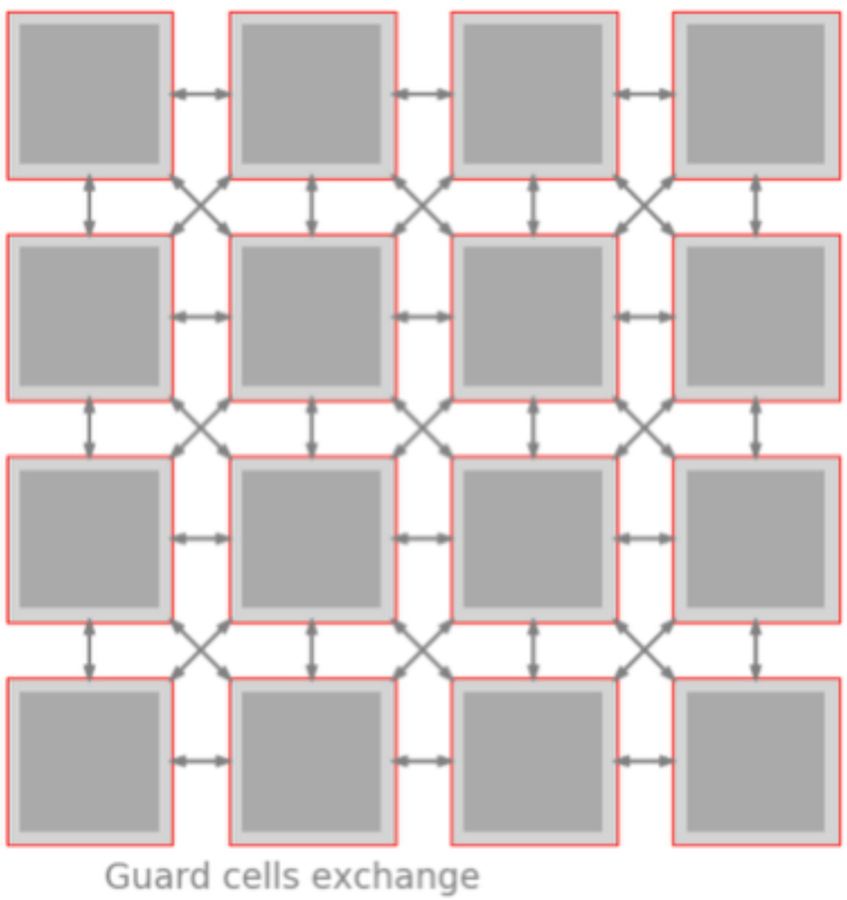


~~**Spectral ("naive" implementation)**
Global FFT before and after the field update in Fourier space~~

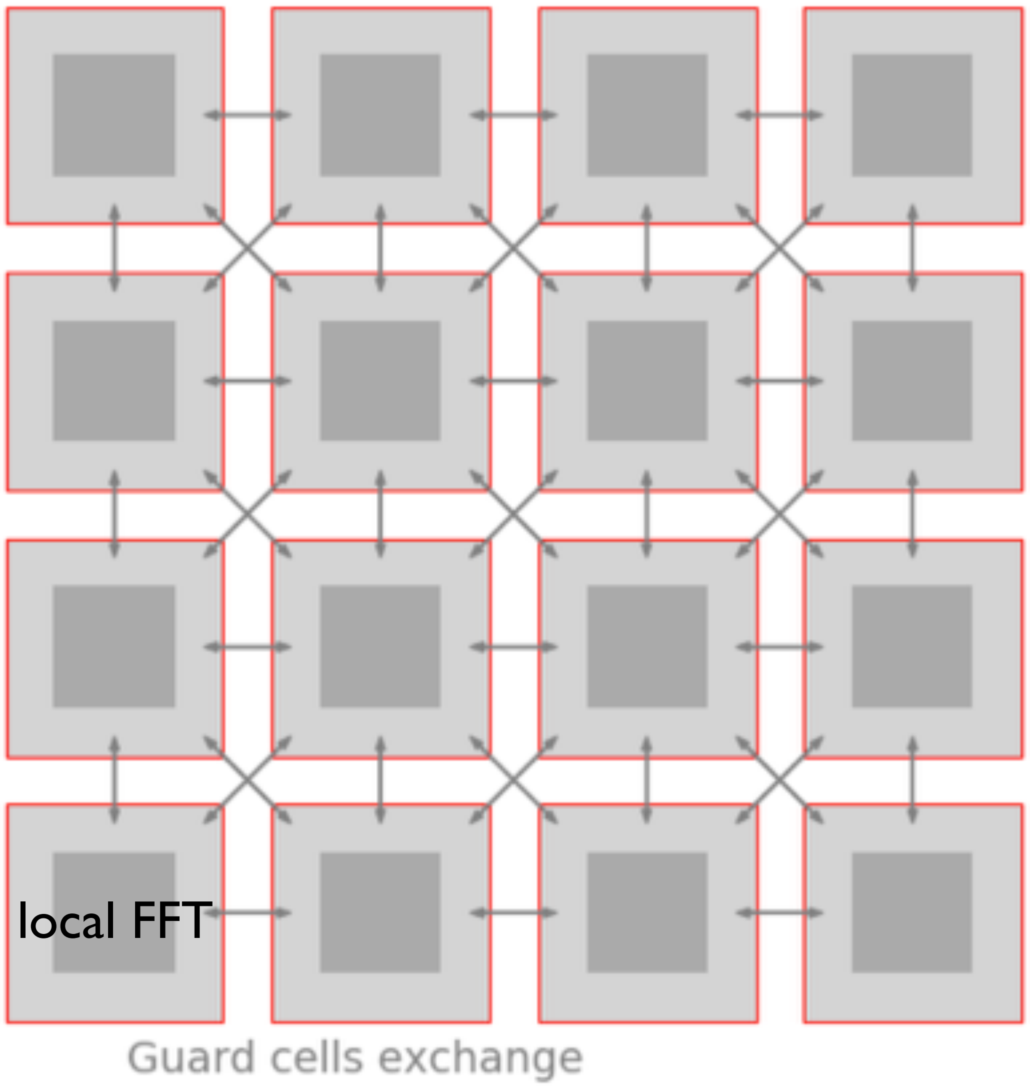


Parallelization with distributed memory (MPI)

Finite-difference:
Exchange guard cell after field update



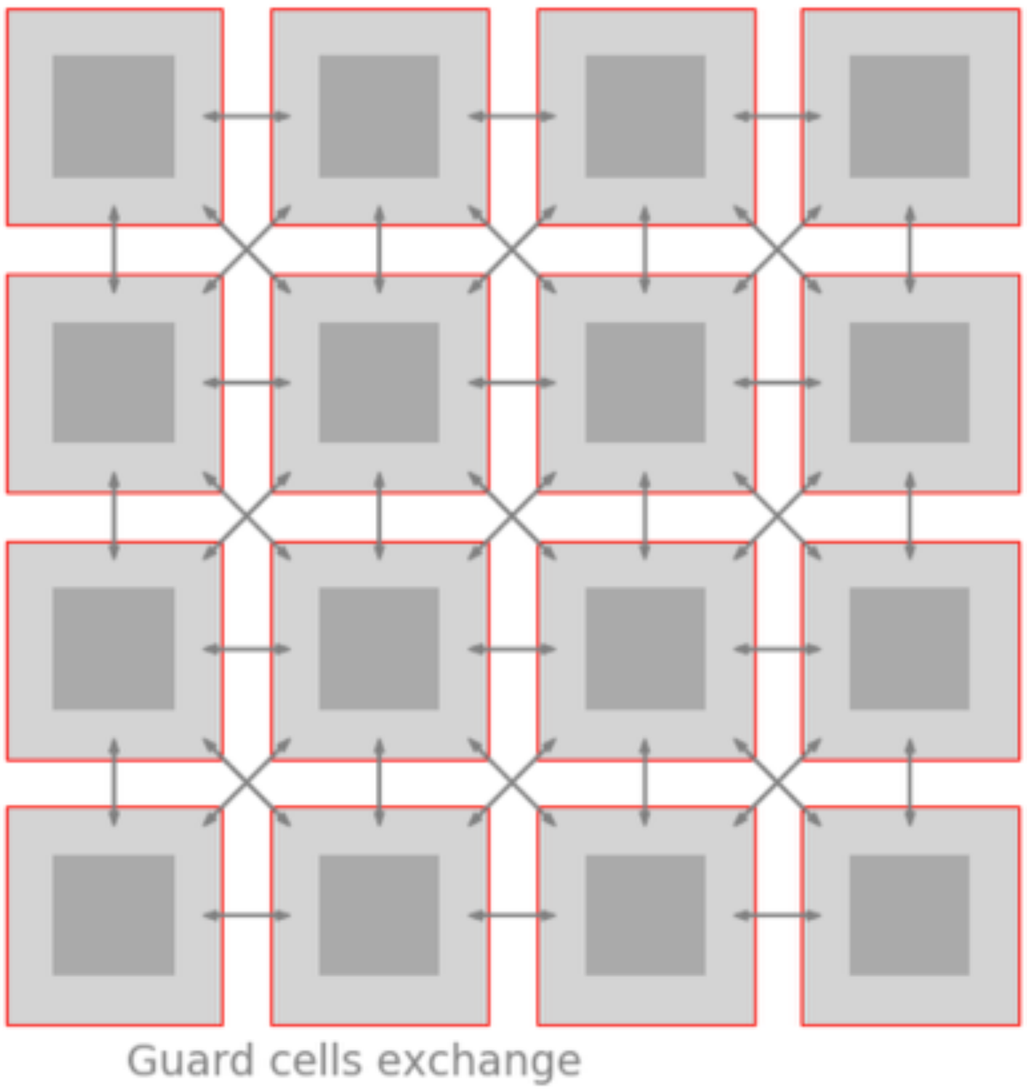
Spectral:
Exchange (many) guard cell after field update



Allows good scaling to many nodes: H.Vincenti, J.-L.Vay, ArXiv: 1707.08500. **(2018)**

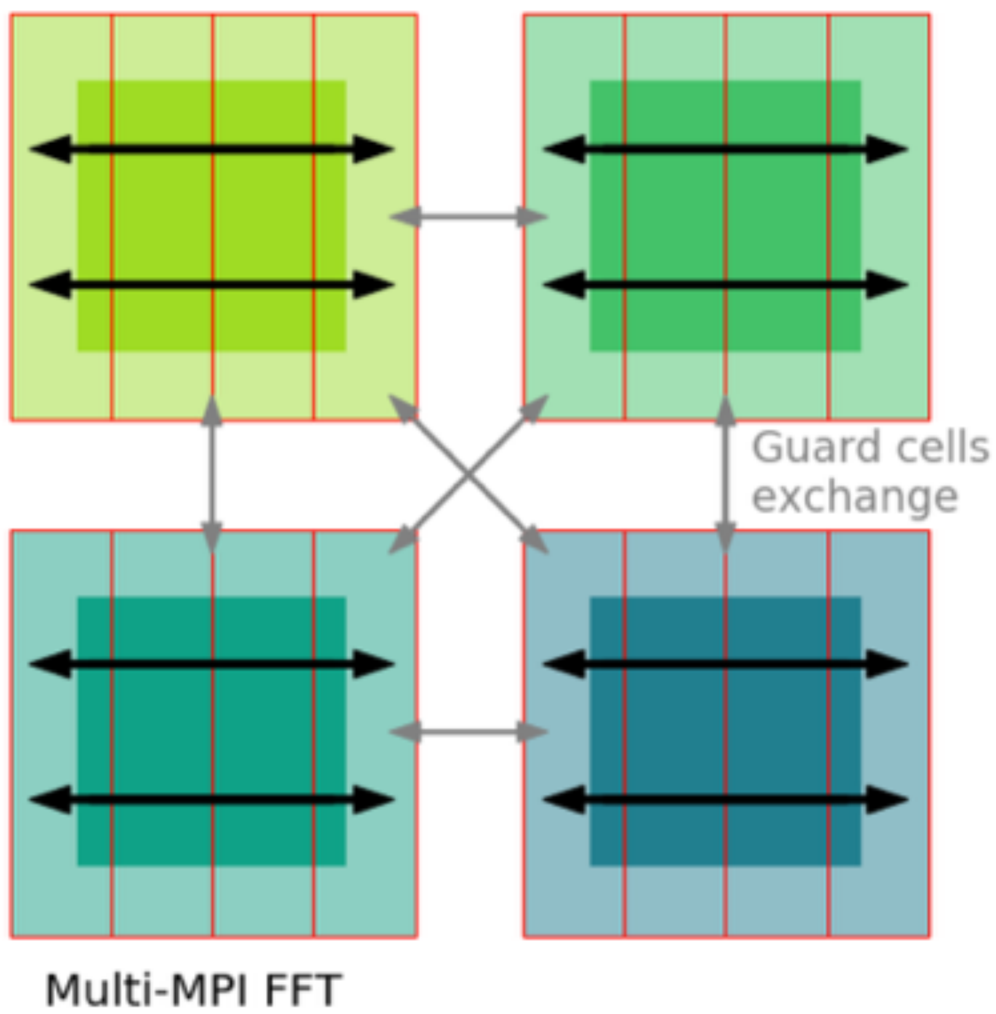
Hybrid FFT approach allows even better scaling

Spectral:
Exchange (many) guard cell after field update



→

Spectral:
Use global FFT within MPI groups,
and guard cell exchange between MPI groups



Implemented in PICSAR and WarpX
(See H. Kallala's talk from Tuesday)

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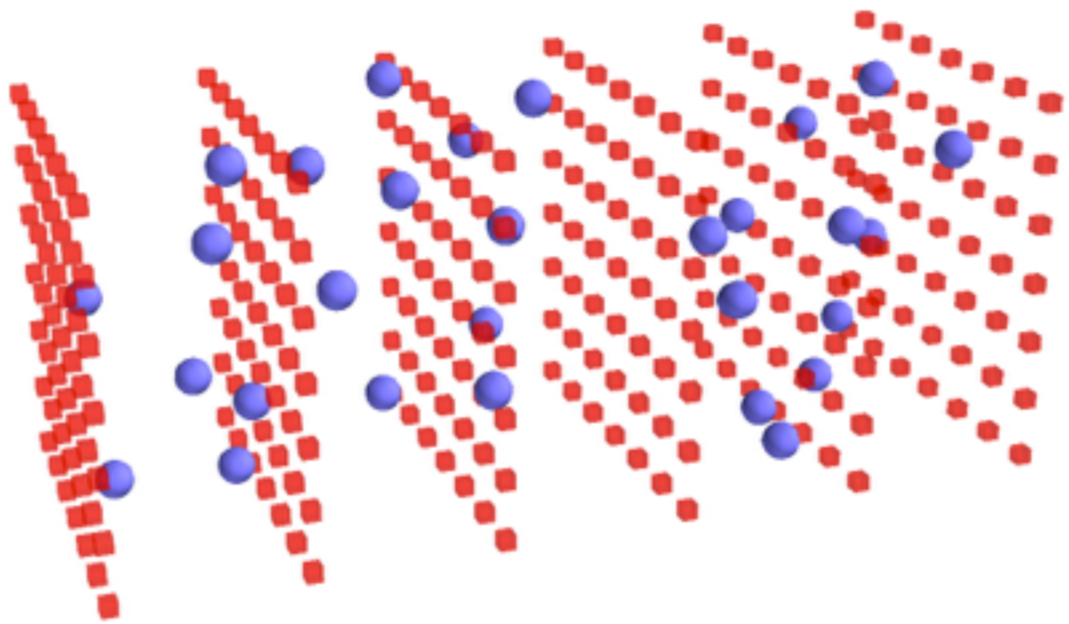
Spectral cylindrical algorithm

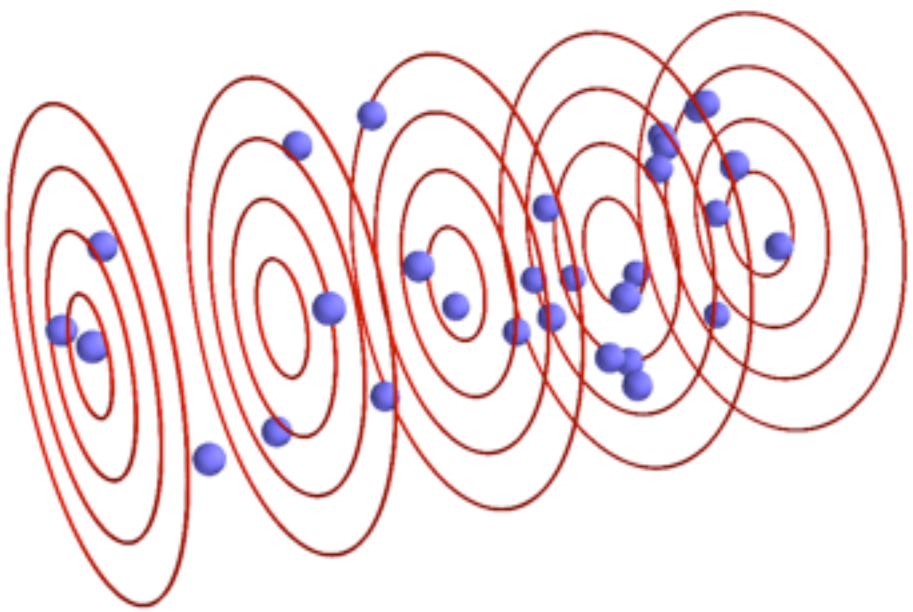
Traditional PIC codes

Use full **3D mesh**



Cylindrical PIC codes

Use a few **2D meshes** in (r, z)
(one mesh per azimuthal mode)



In the case of laser-wakefield acceleration:
Cylindrical codes use 2 azimuthal modes (m=0 and m=1),
which requires vastly less **memory & compute power** than full 3D.

Spectral cylindrical algorithm

Continuous equations in **cylindrical coordinates**

$$\partial_t B_r = -\frac{1}{r}\partial_\theta E_z + \partial_z E_\theta$$

Fourier transform

Discrete **spectral** grid

$$\frac{1}{c^2}\partial_t \boldsymbol{\mathcal{E}} = i\boldsymbol{k} \times \boldsymbol{\mathcal{B}} - \mu_0 \boldsymbol{\mathcal{J}}$$

$$\partial_t \boldsymbol{\mathcal{B}} = -i\boldsymbol{k} \times \boldsymbol{\mathcal{E}}$$

FFT

Discrete **spatial** grid

$$\boldsymbol{E},\ \boldsymbol{B}$$

\+ Advance the fields using **analytical integration in time**

Spectral cylindrical algorithm

Continuous equations in **cylindrical coordinates**

$$\partial_t B_r = -\frac{1}{r}\partial_\theta E_z + \partial_z E_\theta$$

Fourier transform in z

Hankel transform in r

Discrete **spectral** grid

$$\partial_t \mathcal{B}_{+,m} = i\frac{k_\perp}{2}\mathcal{E}_{z,m} - k_z \mathcal{E}_{+,m}$$

FFT, DHT

Discrete **spatial** grid

$$\boldsymbol{E},\ \boldsymbol{B}$$

$$F_z(\boldsymbol{r}) = \frac{1}{(2\pi)^2}\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}k_z \int_0^{\infty} k_\perp \mathrm{d}k_\perp\ \hat{\mathcal{F}}_{z,m}(k_z,k_\perp)\ J_m(k_\perp r)\, e^{-im\theta+ik_z z}$$

$$F_r(\boldsymbol{r}) = \frac{1}{(2\pi)^2}\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}k_z \int_0^{\infty} k_\perp \mathrm{d}k_\perp\ \left(\hat{\mathcal{F}}_{+,m}(k_z,k_\perp)\ J_{m+1}(k_\perp r) + \hat{\mathcal{F}}_{-,m}(k_z,k_\perp)\ J_{m-1}(k_\perp r)\right) e^{-im\theta+ik_z z}$$

$$F_\theta(\boldsymbol{r}) = \frac{1}{(2\pi)^2}\sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}k_z \int_0^{\infty} k_\perp \mathrm{d}k_\perp\ i\left(\hat{\mathcal{F}}_{+,m}(k_z,k_\perp)\ J_{m+1}(k_\perp r) - \hat{\mathcal{F}}_{-,m}(k_z,k_\perp)\ J_{m-1}(k_\perp r)\right) e^{-im\theta+ik_z z}$$

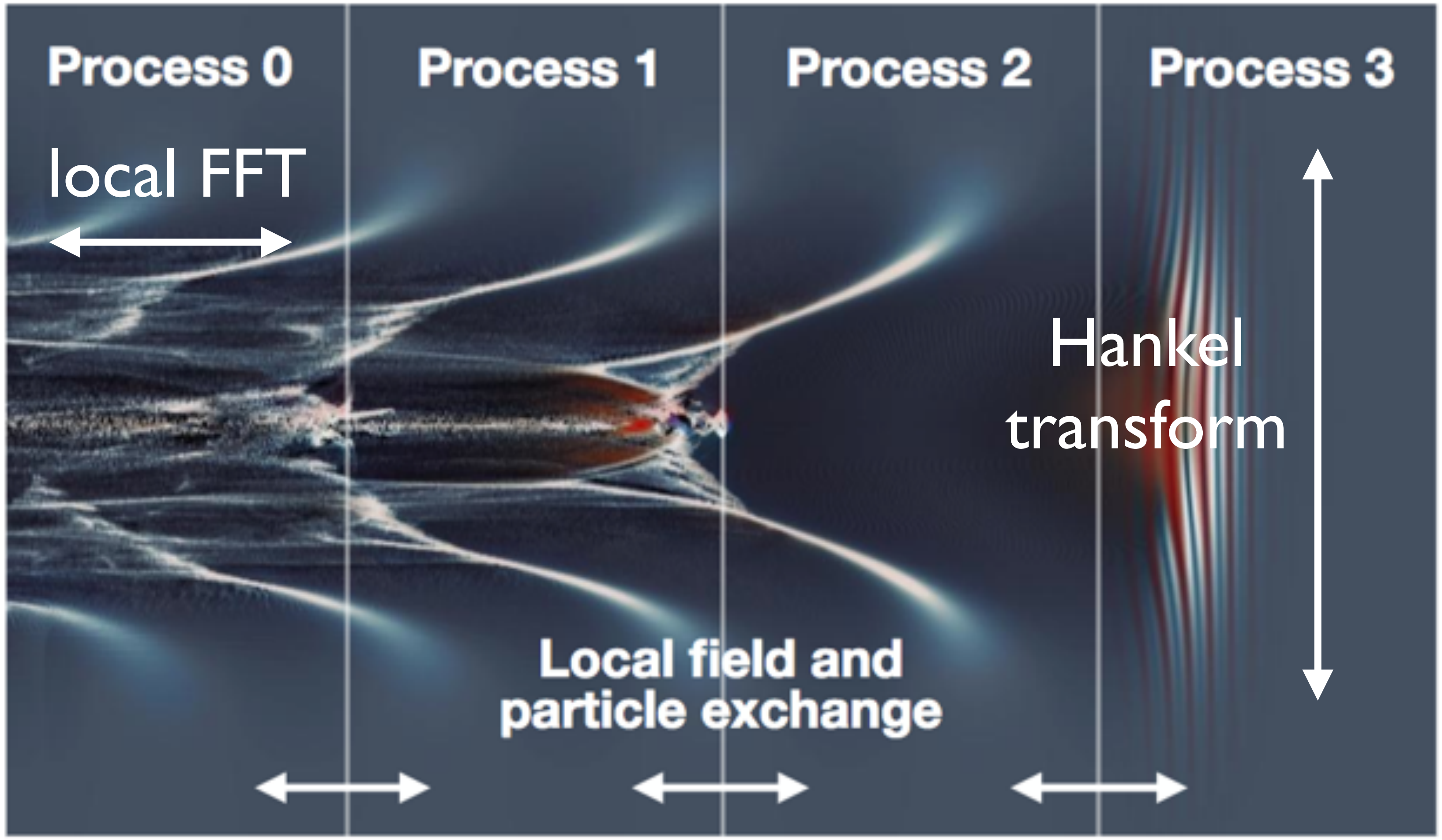
Mathematical details:
R. Lehe et al., Comp. Phys. Com., 2016

Implemented in the code FBPIC

+ Advance the fields using **analytical integration in time**

Parallelization

No similar MPI decomposition, with local Hankel transform…



But the Hankel transform is still parallelized across shared-memory hardware (multi-core node, GPU)

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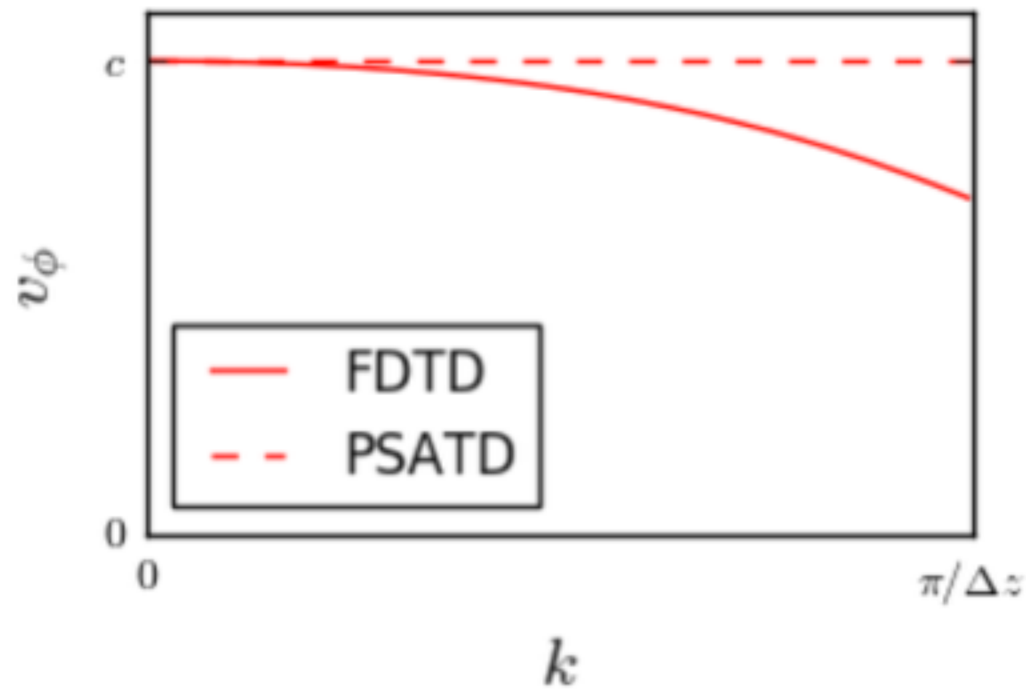
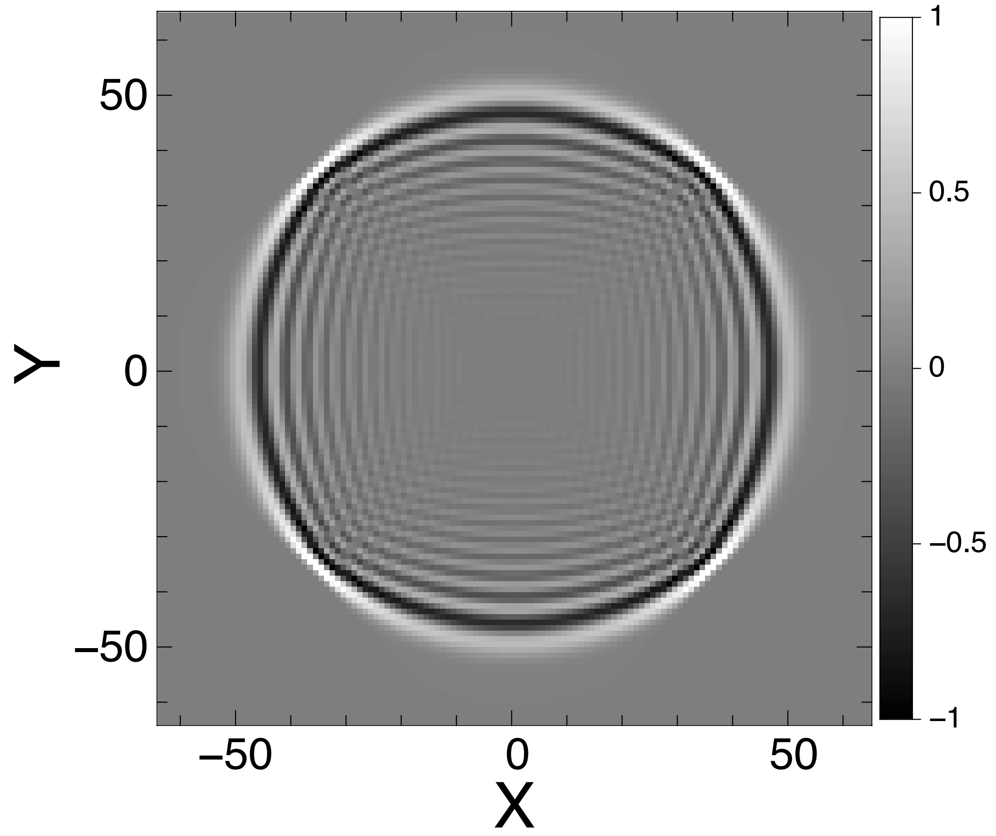
Numerical dispersion

Spurious numerical dispersion

- In (most) **finite-difference algorithms**, the electromagnetic waves propagate **slower than c,** even in vacuum.



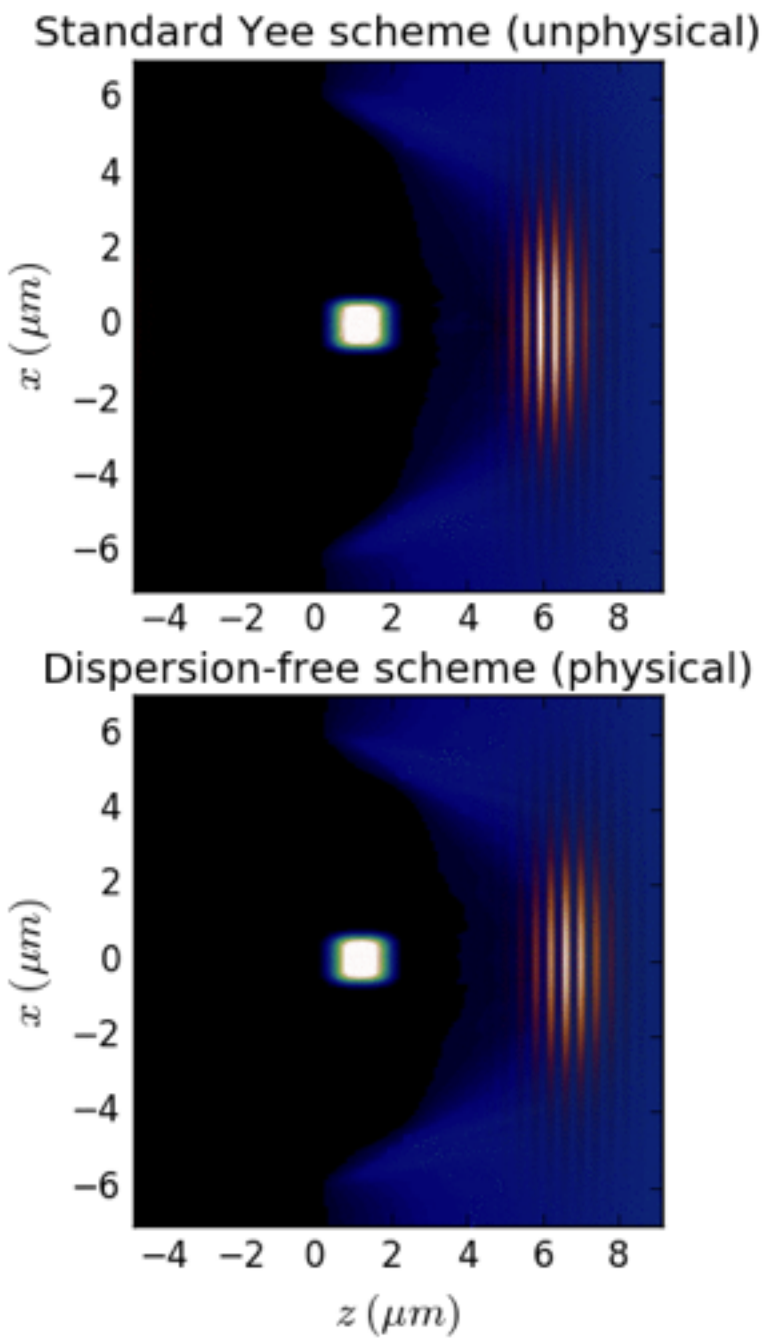
Velocity depends on the wave number k.



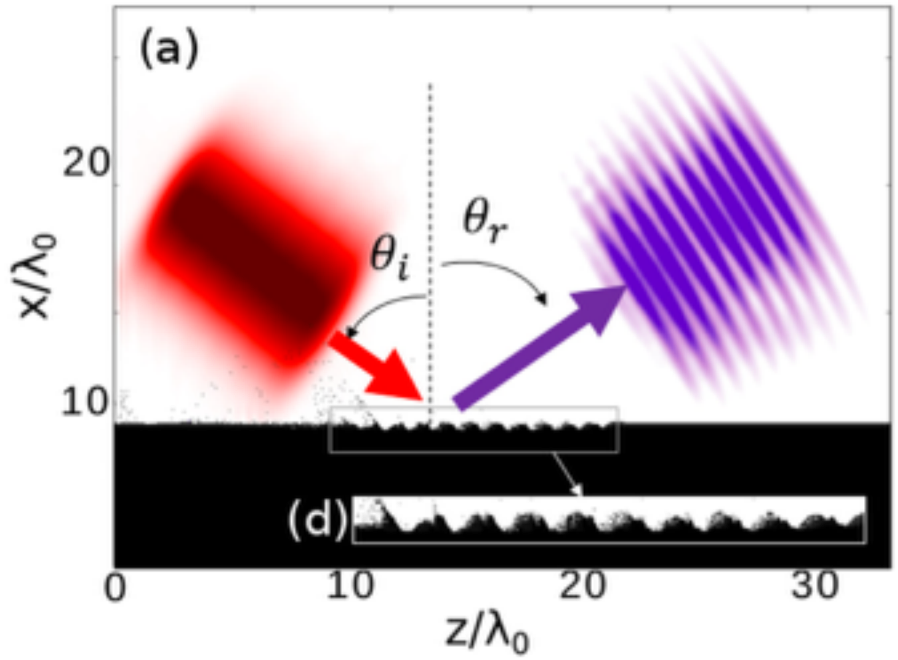
Velocity depends on the angle (anisotropy).

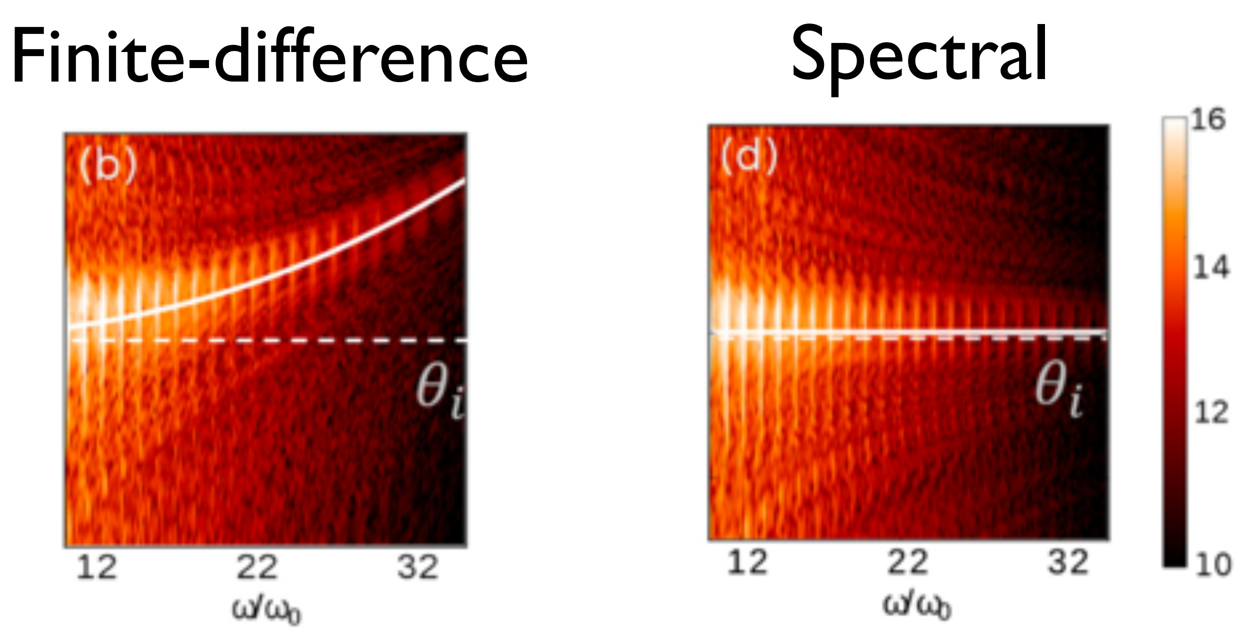
Numerical dispersion can have strong impact in simulations

Early dephasing



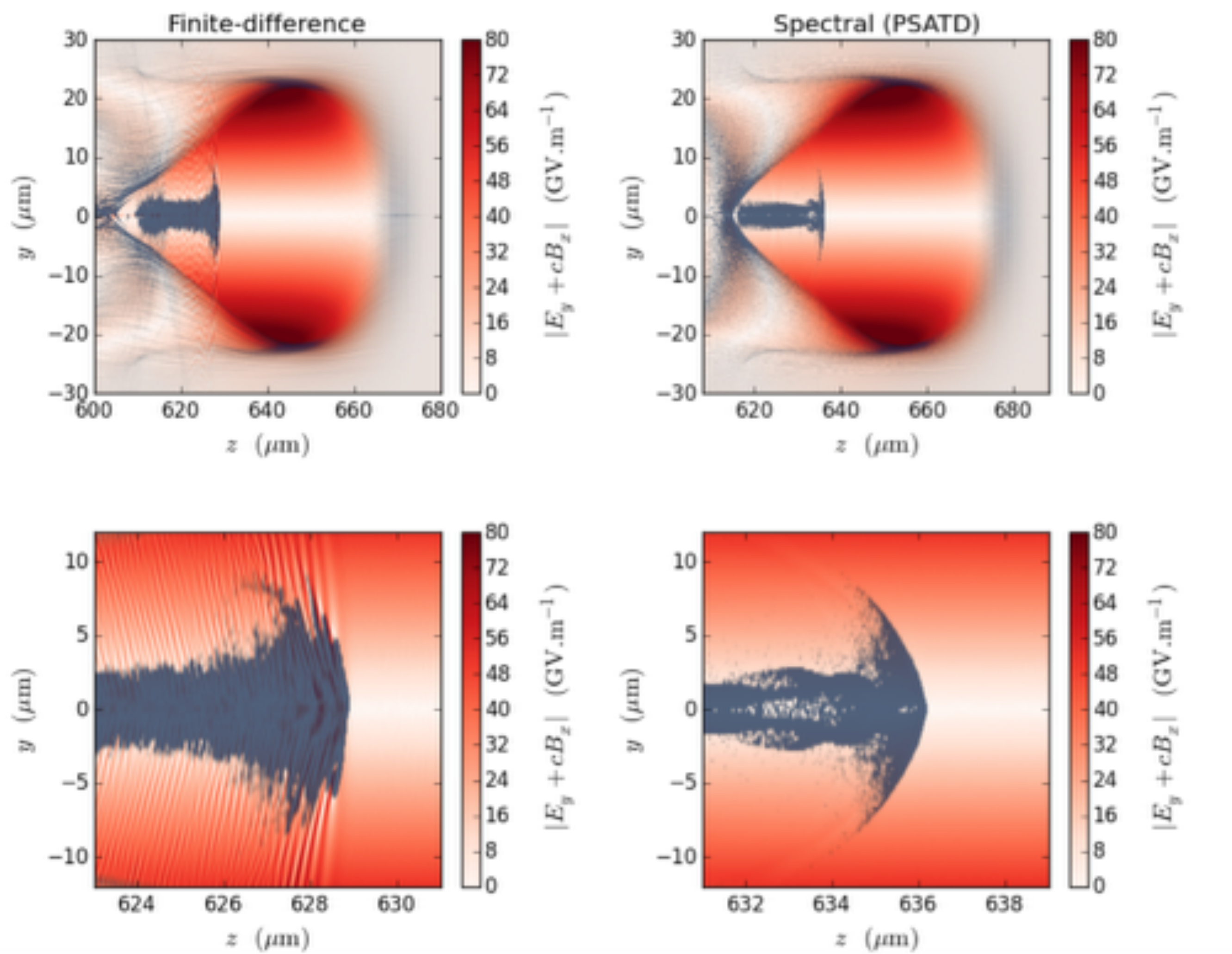
Deflection of laser-produced harmonics





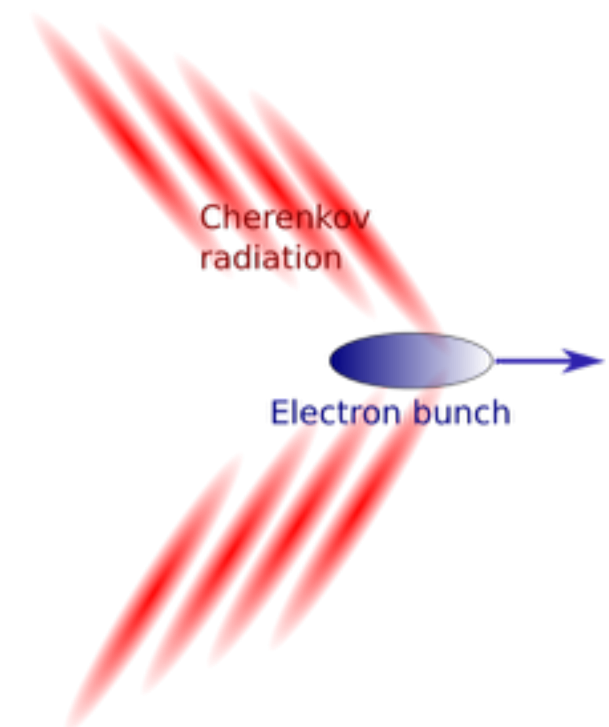
(See G. Blaclard's talk earlier)

Numerical dispersion can have strong impact in simulations



Numerical Cherenkov radiation

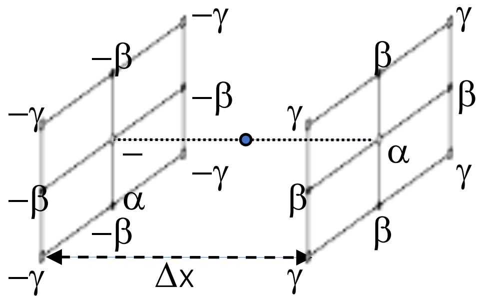
- Electron bunch travels faster than the electromagnetic waves in the simulation.
- As a consequence, it emits unphysical Cherenkov radiation.



Some existing solutions against numerical dispersion

Extended stencil

- Can reduce numerical dispersion along a given axis.
  (and avoid numerical Cherenkov)



- But has anisotropy

J. B. Cole, IEEE Trans. Microw. Theory Tech. **45** (1997)
A. Pukhov, J. Plasma Physics **61** (1999) 425
M. Karkkainen et al., Proc. ICAP, Chamonix, France (2006)
B. Cowan et al, PRST-AB **16** (2013) 041303
A. Blinne et al, ArXiv:**1710.06829** (2017)
R. Lehe et al, PRST-AB **16** (2013) 021301

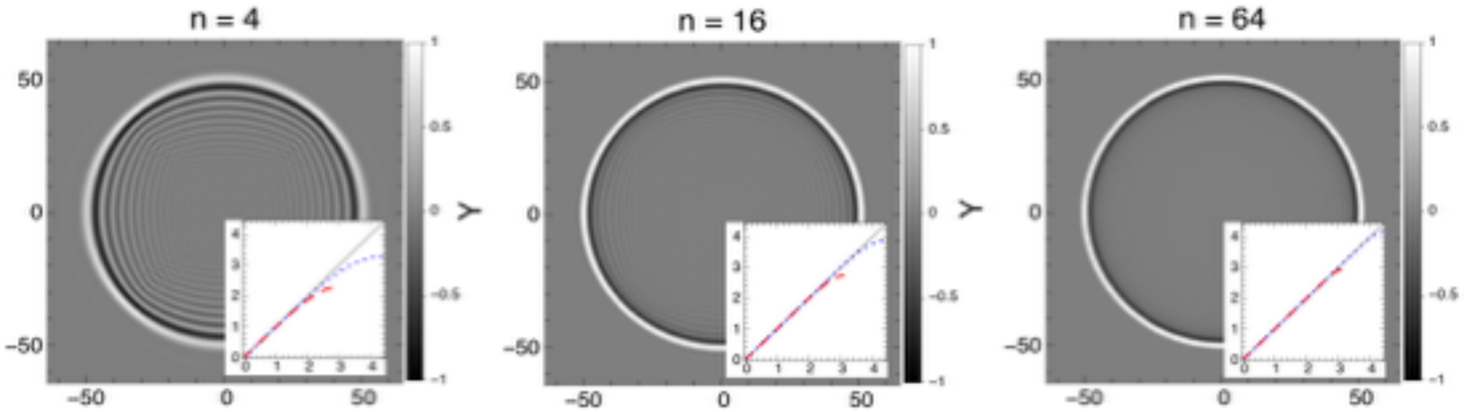
Directional splitting

- Uses collocated grid ; dispersion-free along axes
- But again, has anisotropy

R. Nuter et al, Eur. Phys. J. D **68**, 177 (2014)

Spectral (PSATD)

- Dispersion and anisotropy are reduced when increasing the order p



J.L. Vay, CPC (2016) ;
H. Vincenti and J-L Vay, *CPC* **200**, 147 (2016)

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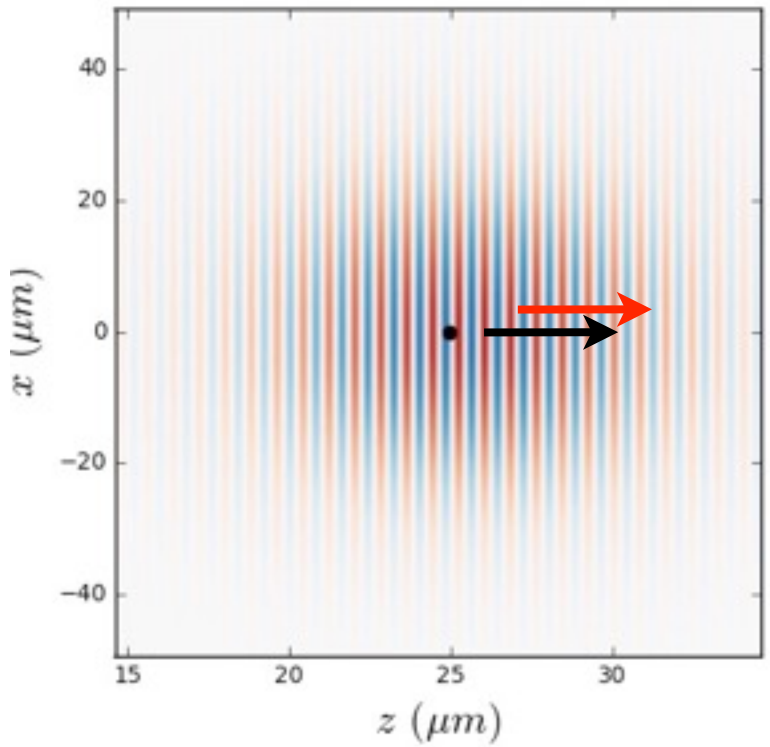
Physics sometimes involves tight cancelation in E + v x B

Example

- Copropagating relativistic electron and laser pulse



- The force on the electron is

$$\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B} \sim \frac{\boldsymbol{E}}{\gamma^2}$$

Challenges for PIC

- The gathered E and B (from mesh to particles) must have the **right amplitude and phase** to allow this tight cancelation.

- Given the gathered E and B, the particle pusher should be able to reproduce this cancelation

$$\frac{d\boldsymbol{p}}{dt} = q\left(\boldsymbol{E} + \frac{\boldsymbol{p}}{\gamma m} \times \boldsymbol{B}\right)$$

Particle pusher

Existing pushers

$$\frac{\boldsymbol{p}^{n+1/2} - \boldsymbol{p}^{n-1/2}}{\Delta t} = q\left(\boldsymbol{E}^n + \left(\frac{\boldsymbol{p}}{\gamma m}\right)^n \times \boldsymbol{B}^n\right)$$

Differ in how they treat the velocity in the right hand-side.

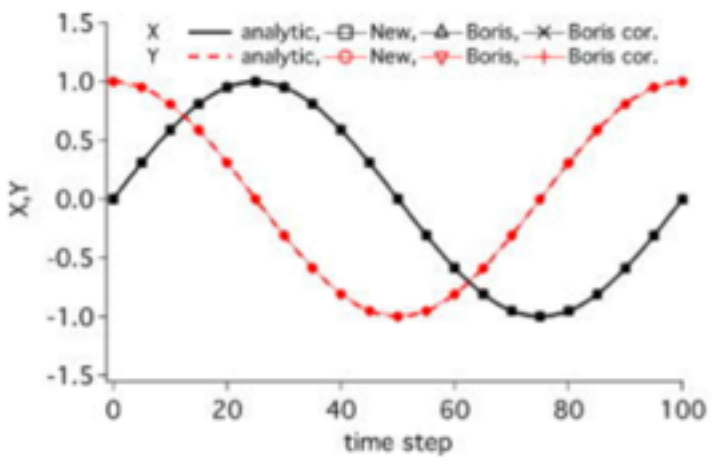
J. Boris, Proc. Fourth Conf. Num. Sim. Plasmas (1970)

J.L. Vay, Physics of Plasmas 15, 056701 (2008)

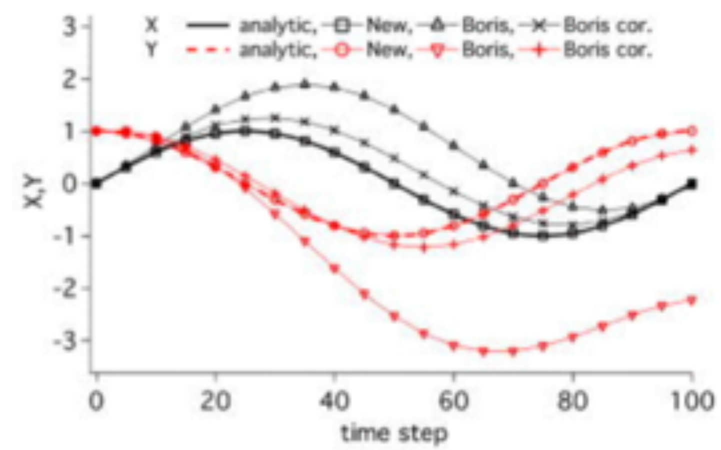
A. V. Higuera et al, arXiv:1701.05605 (2017)

Benchmark

Lab frame: pure B



Boosted frame: E and B with tight cancelation



J.L. Vay, Physics of Plasmas 15, 056701 (2008)

But in this case, the fields are uniform and constant: no problem from gathering.

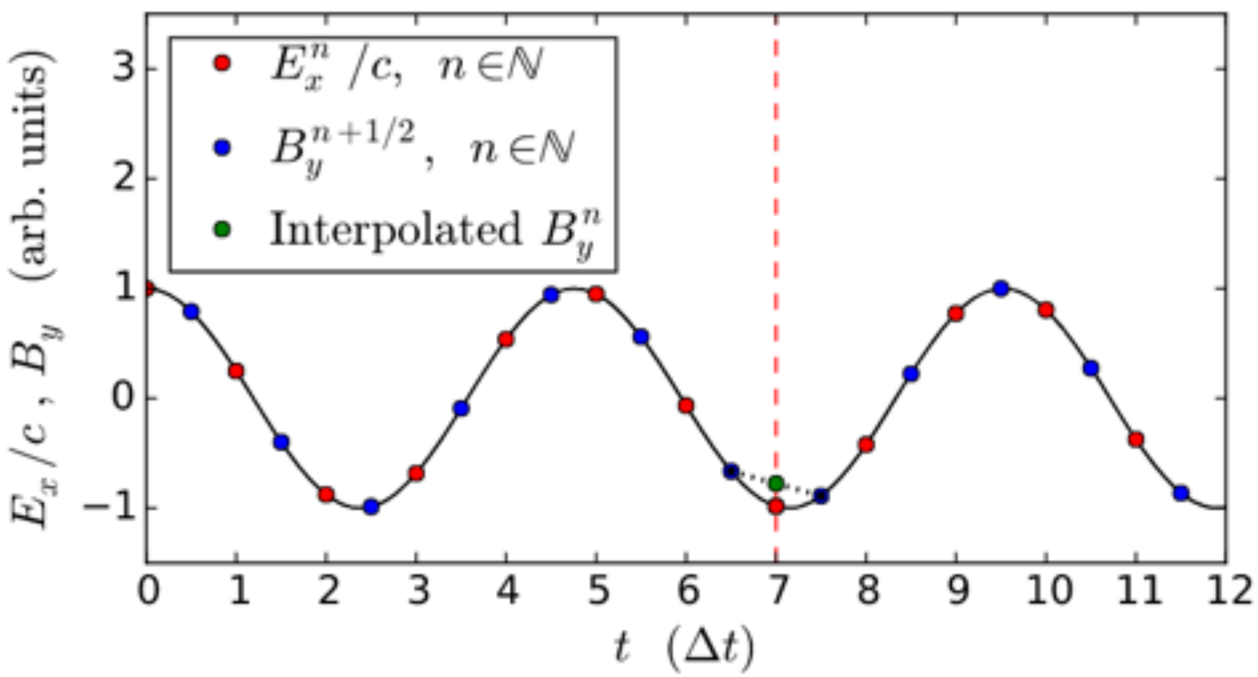
Time-varying fields: staggering issues

$$\frac{\boldsymbol{p}^{n+1/2} - \boldsymbol{p}^{n-1/2}}{\Delta t} = q\left(\boldsymbol{E}^n + \left(\frac{\boldsymbol{p}}{\gamma m}\right)^n \times \boldsymbol{B}^n\right)$$

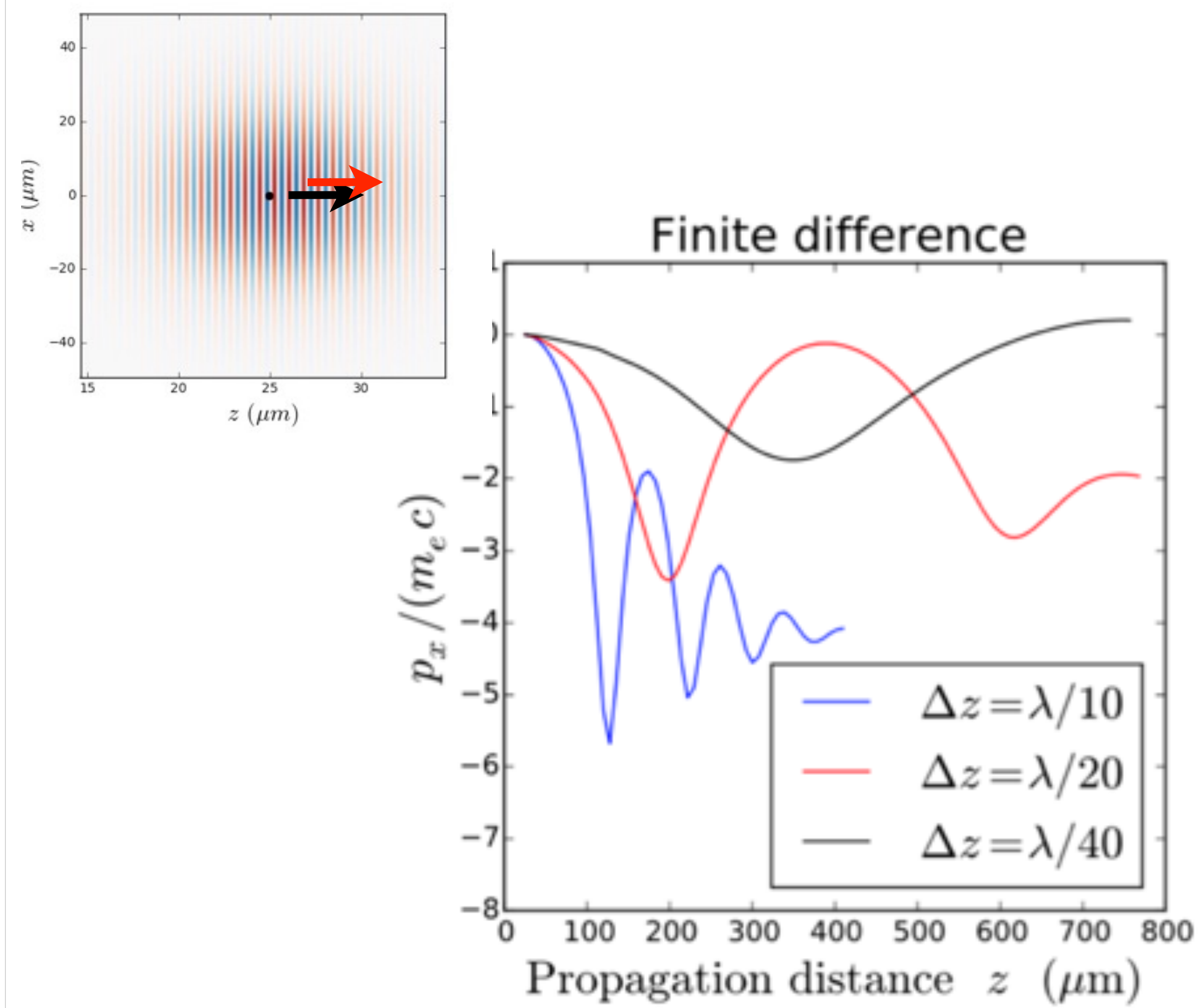
Issue

The staggering of E and B imposes that B (but not E) is averaged in time

This prevents tight cancelation.

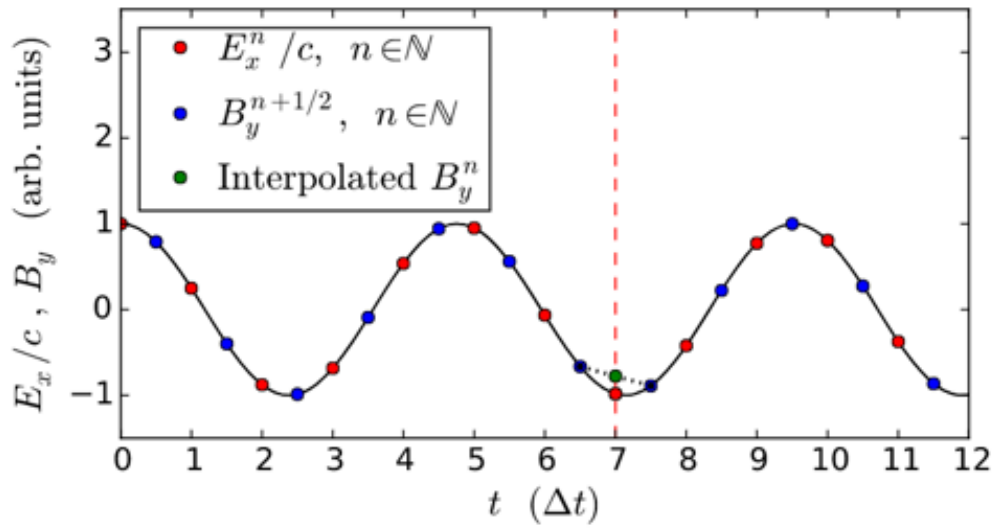


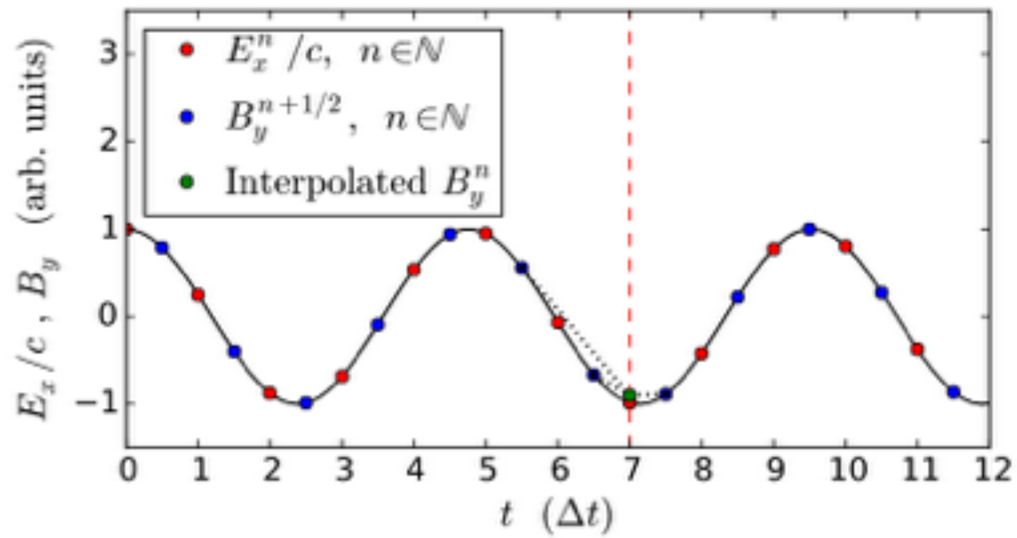
Benchmark



Some existing solutions

Higher-order interpolation

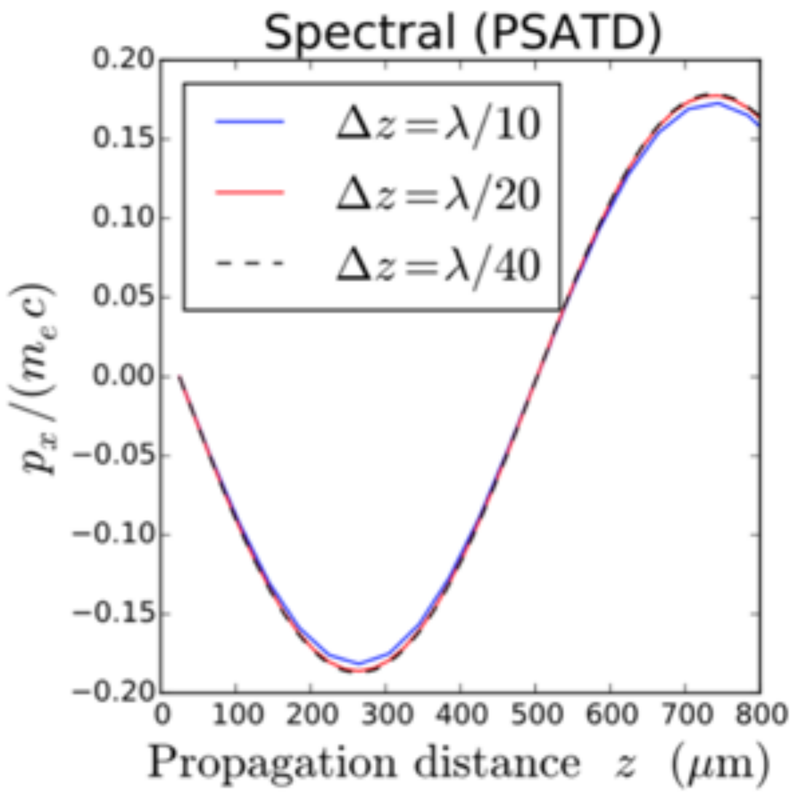




R. Lehe, PRSTAB, 2014

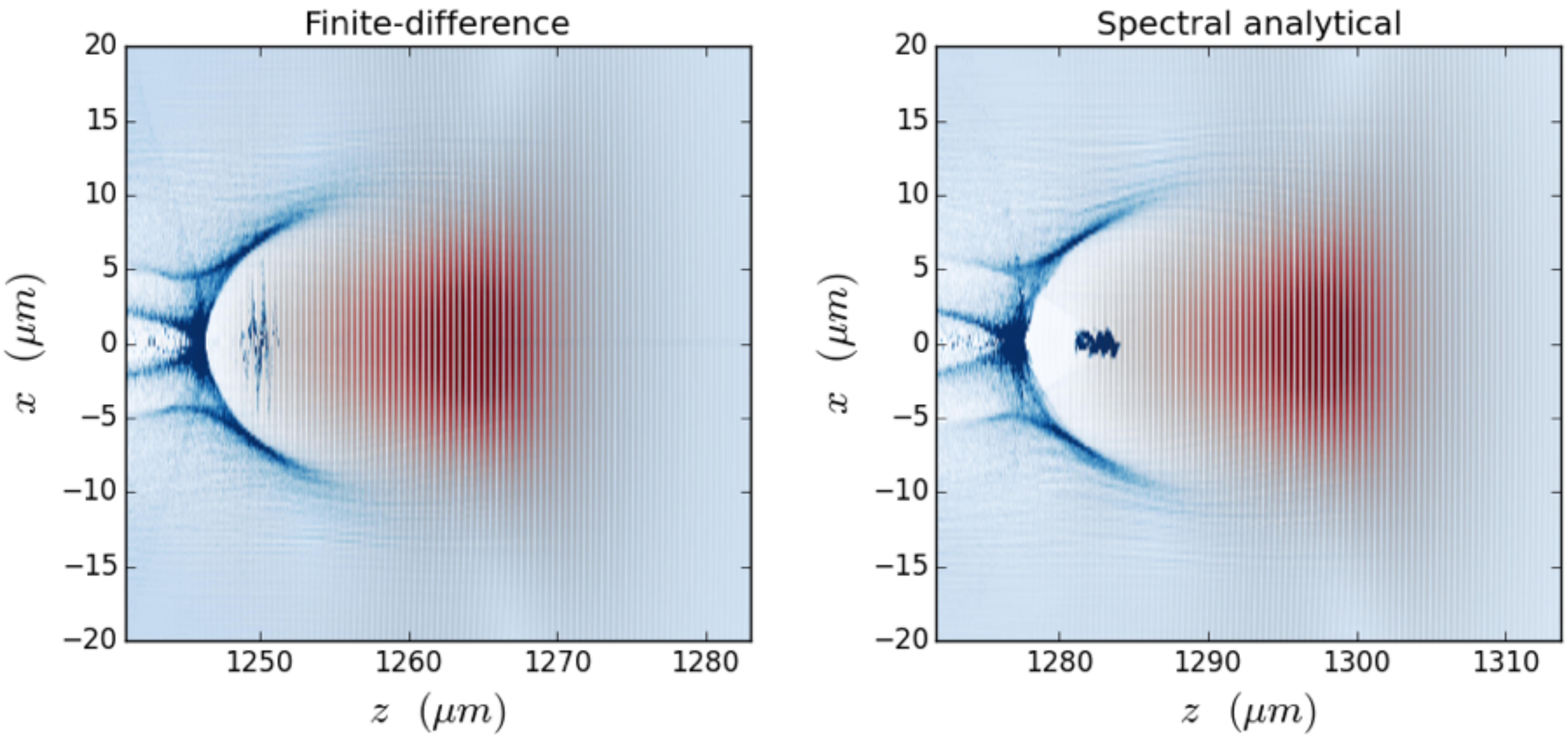
Spectral solver (PSATD)

- E and B are defined at the same time ; no need to average/interpolate B



Laser-bunch interaction

Concrete example in laser-wakefield acceleration



In the finite-difference case, the accelerated electrons feel a **spurious force** from the laser.

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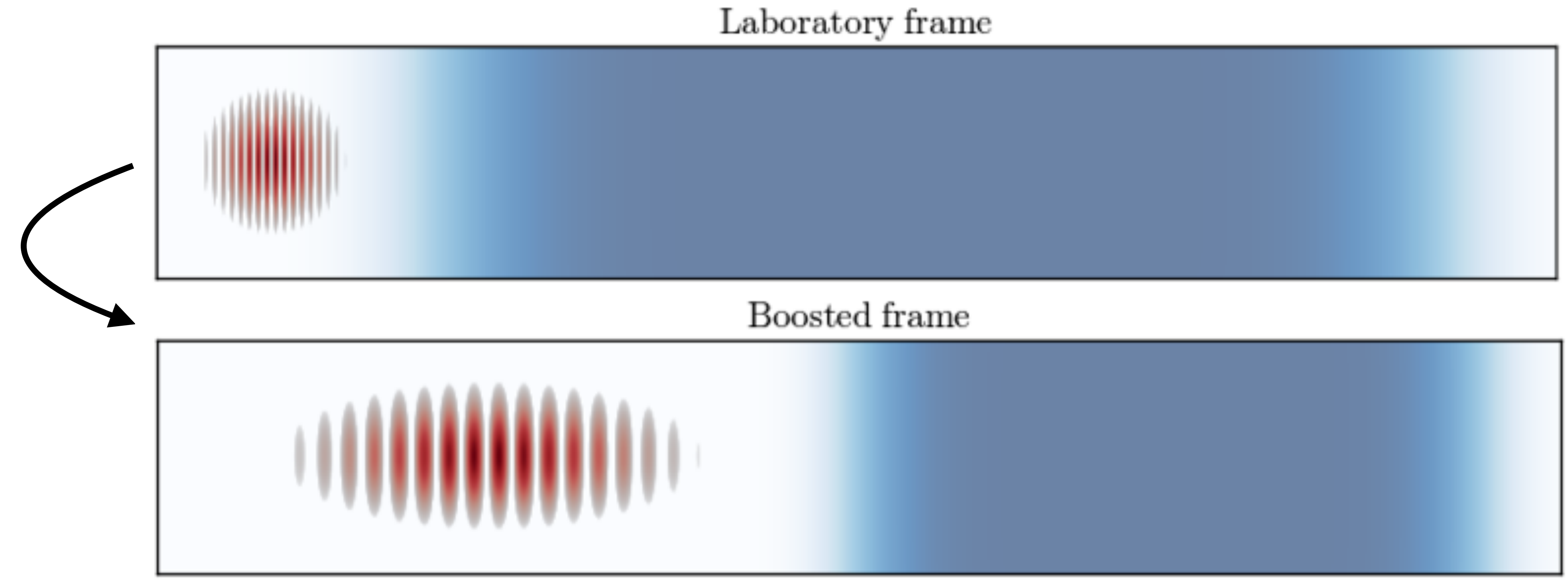
Boosted-frame can speed up Particle-In-Cell simulations.

Lorentz transform

γ_b



Lab-frame PIC simulation

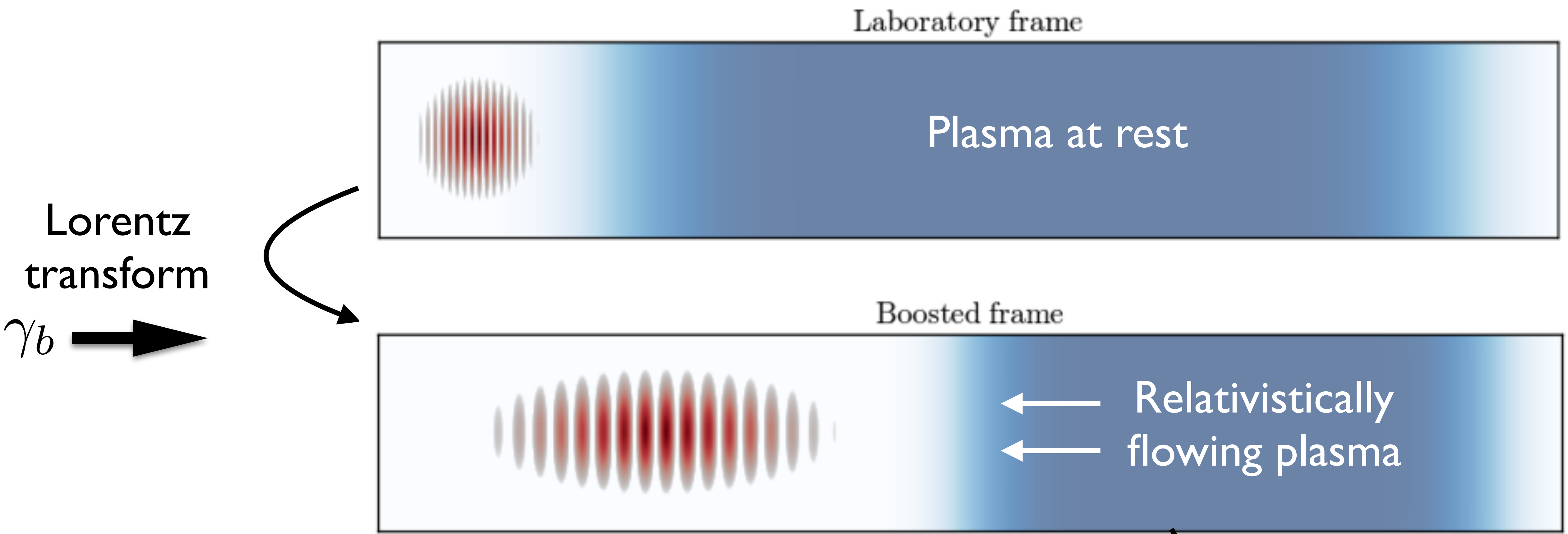
- Laser oscillations impose **small grid cells** and **small timestep**
- Propagating through the entire plasma is **computationally expensive**

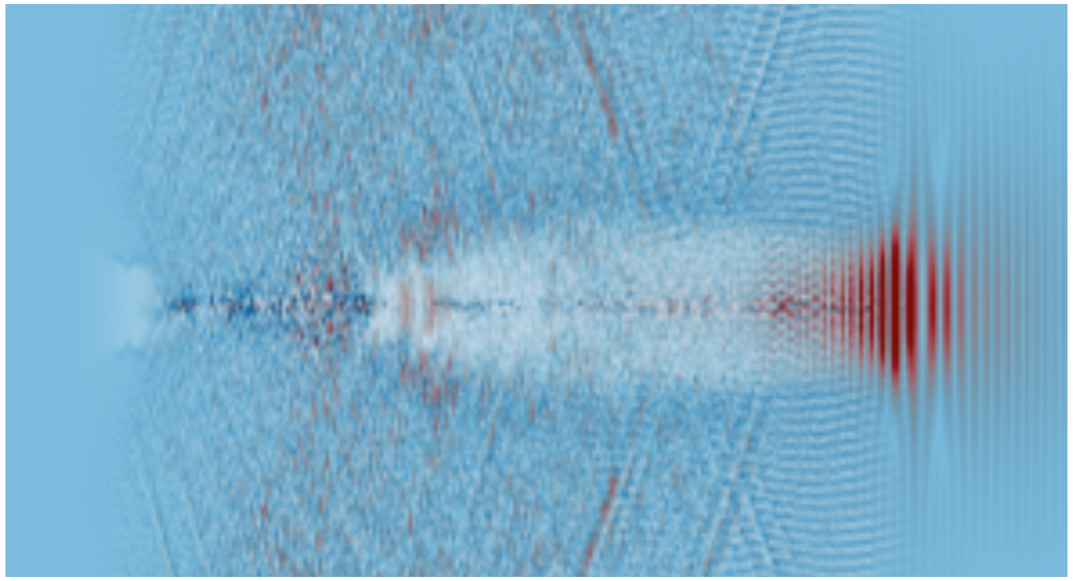
Boosted-frame PIC simulation

- Transformed laser oscillations relax constraints on grid cell and timestep.
- Computational **speed up** of the order $2\gamma_b^2$

Vay, PRL, 2007

Problem: the Numerical Cherenkov Instability





Problem

Relativistically flowing plasmas are **numerically unstable**, with the Particle-In-Cell algorithm

Existing solutions

"Magic" time step

- There is (solver-dependent) time step that minimizes the instability

J-L Vay et al, JCP, **230**, 15, (2011);
B. Godfrey and J-L Vay, JCP, **267**, 1-6 (2014)

Filtering of E and B

- Filter the gathered E and B in a particular way that suppresses the instability

B. Godfrey and J-L Vay, JCP, **267**, 1-6 (2014);
B. Godfrey and J-L Vay, CPC, **196**, 221-225 (2015)

"Bumped" dispersion

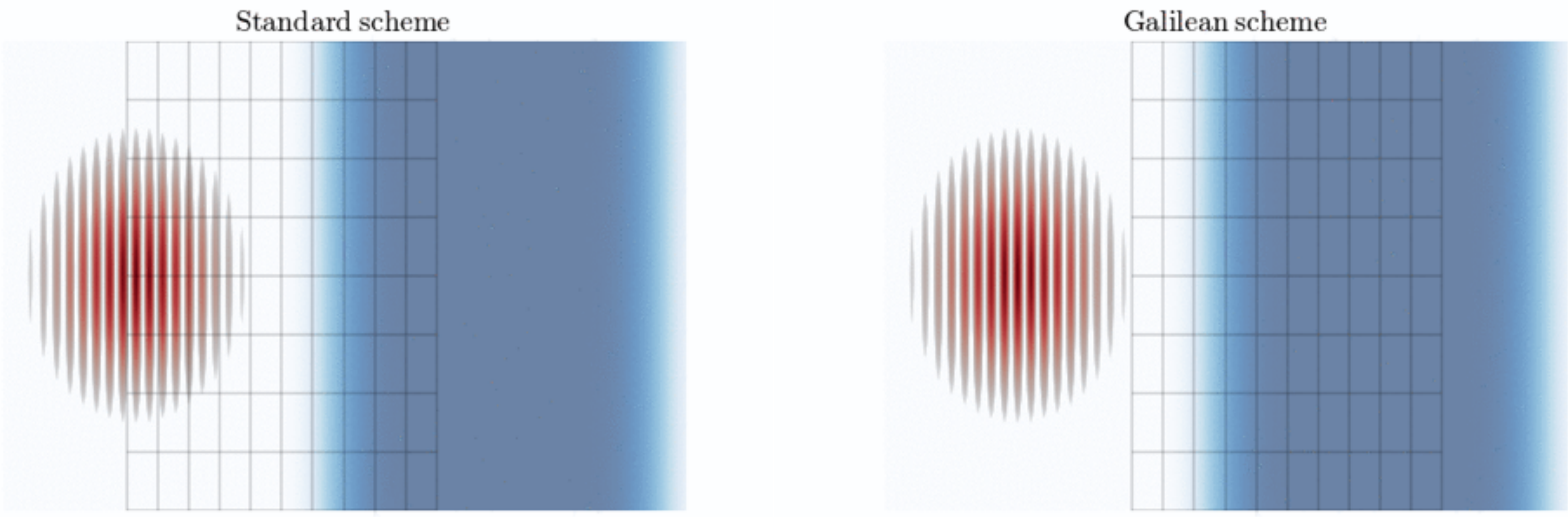
- Use small dt to decouple instability from physics
- Tweak the dispersion relation of the Maxwell solver at the main unstable frequency

P. Yu et al, CPC, **197**, 144-152 (2015)

Galilean transformation

- Simulates physics in a grid that moves with the plasma.
- Requires PSATD solver.
  M. Kirchen et al., PoP (2016)
  R. Lehe et al., PRE (2016)

The Galilean scheme: concept



Proposed by
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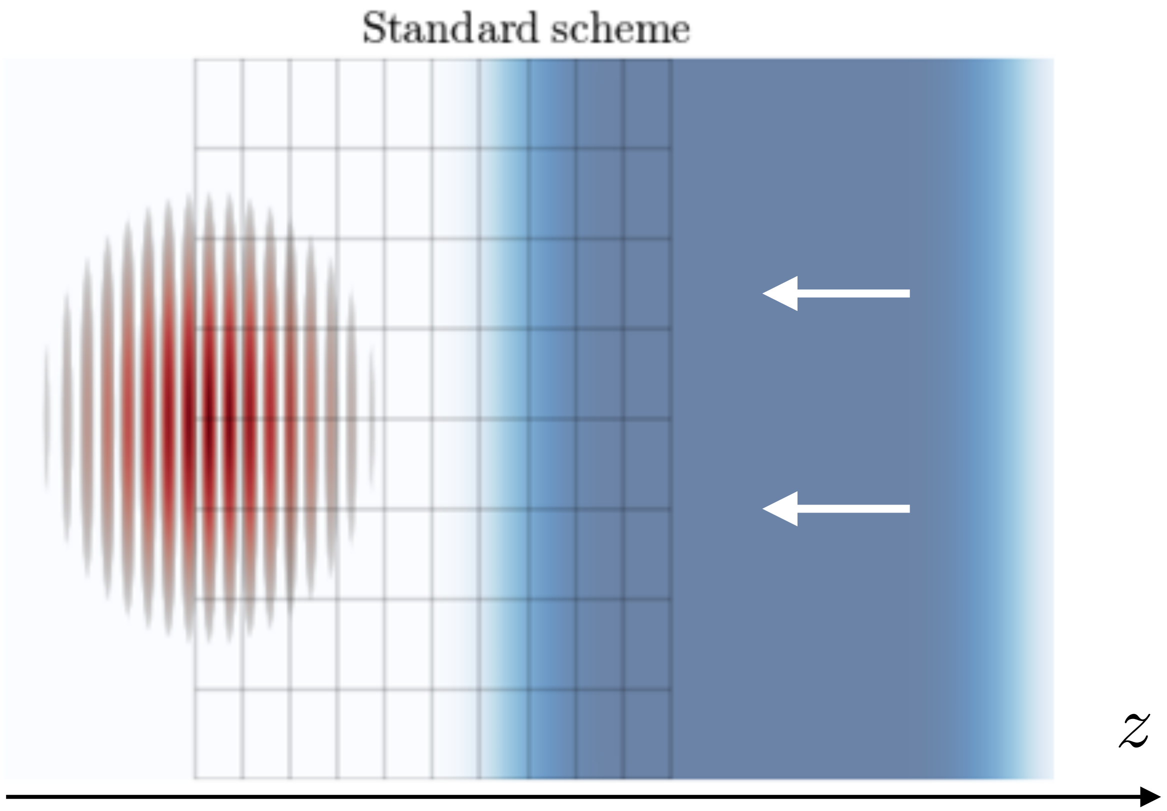
Intuition: The numerical instability arises because the bulk of the plasma **flows** through a **fixed grid**.

Solution: The grid should **move along** with the plasma.

The Galilean scheme: mathematical formulation



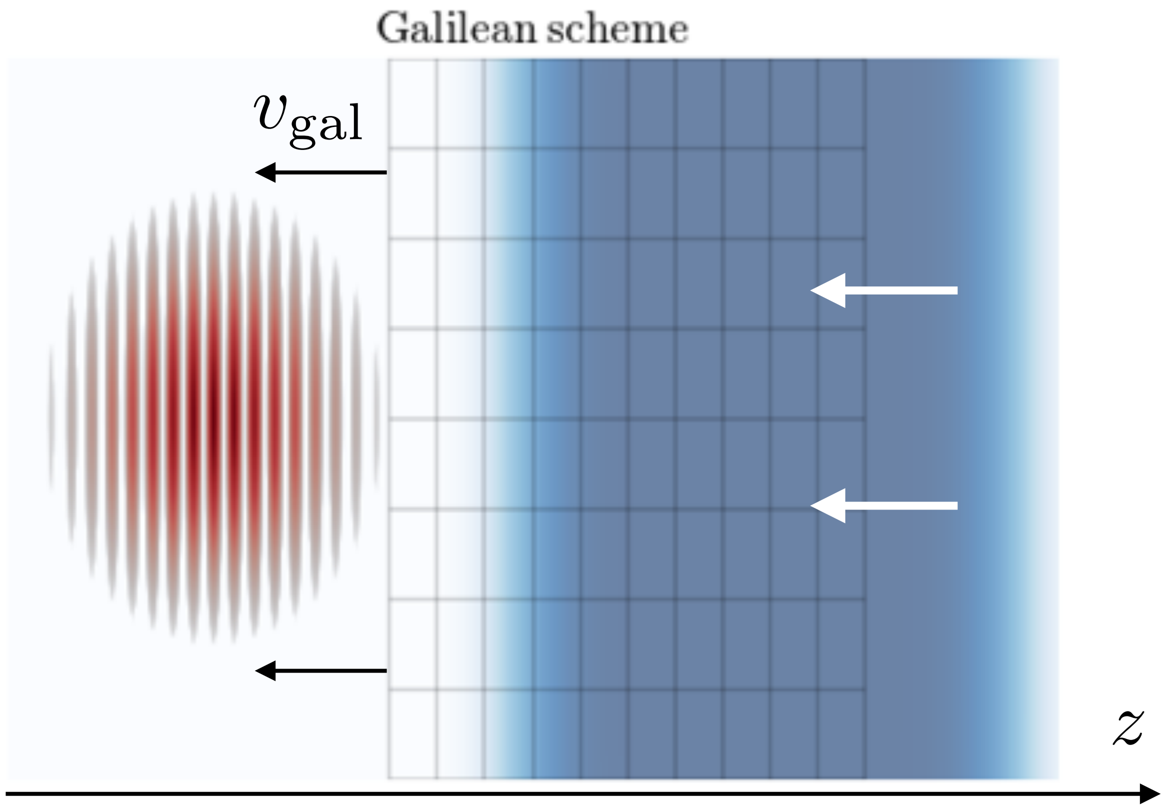
Grid = **fixed values of** z

Integrate on the grid

$$\frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E}$$

$$\frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} = \nabla \times \boldsymbol{B} - \mu_0 \boldsymbol{j}$$

assuming $\boldsymbol{j}(x, y, z, t)$ is constant over one timestep



Grid = **fixed values of** $z' = z - v_{\mathrm{gal}} t$

Integrate on the grid

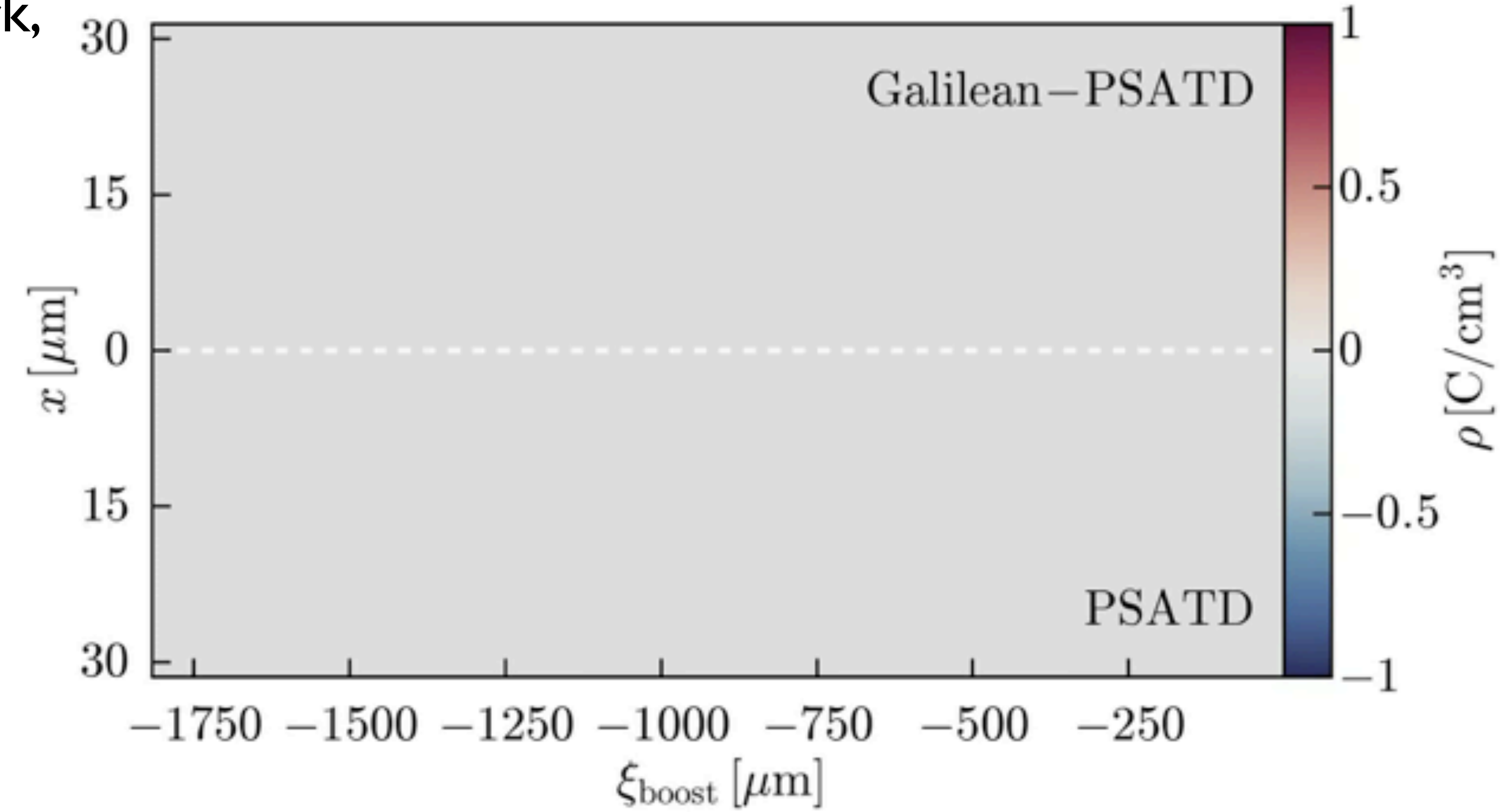
$$\left(\frac{\partial}{\partial t} - \boldsymbol{v}_{gal} \cdot \boldsymbol{\nabla}'\right) \boldsymbol{B} = -\boldsymbol{\nabla}' \times \boldsymbol{E}$$

$$\frac{1}{c^2}\left(\frac{\partial}{\partial t} - \boldsymbol{v}_{gal} \cdot \boldsymbol{\nabla}'\right) \boldsymbol{E} = \boldsymbol{\nabla}' \times \boldsymbol{B} - \mu_0 \boldsymbol{j}$$

assuming $\boldsymbol{j}(x, y, z', t)$ is constant over one timestep

Implementation in the code FBPIC

When the Galilean equations are implemented in a PSATD framework, the instability is suppressed!



Concept & applications:
M. Kirchen et al., PoP (2016)
Algorithm & math:
R. Lehe et al., PRE (2016)

Conclusion

- **EM PIC face many challenges for accurate simulations**
- **In many cases, spectral (PSATD) solver can mitigate those challenges, at the cost of a more intricate MPI pattern.**
- **But PSATD is not a universal solution, and other solutions exist.**

Thank you for your attention