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Advanced techniques

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Motivation

Additional utilities to

- Reduce simulation time through physical approximations and reduced model:
  Azimuthal Modes decomposition, Laser Envelope model, Macro-Particle Merging
- Reduce numerical artifacts of PIC codes via numerical techniques:
  Current Filtering, Non-standard Finite Difference Time Domain, Perfectly Matched Layer
- Handy tools for advanced initialization:
  Laser Offset, Relativistic Species Initialization

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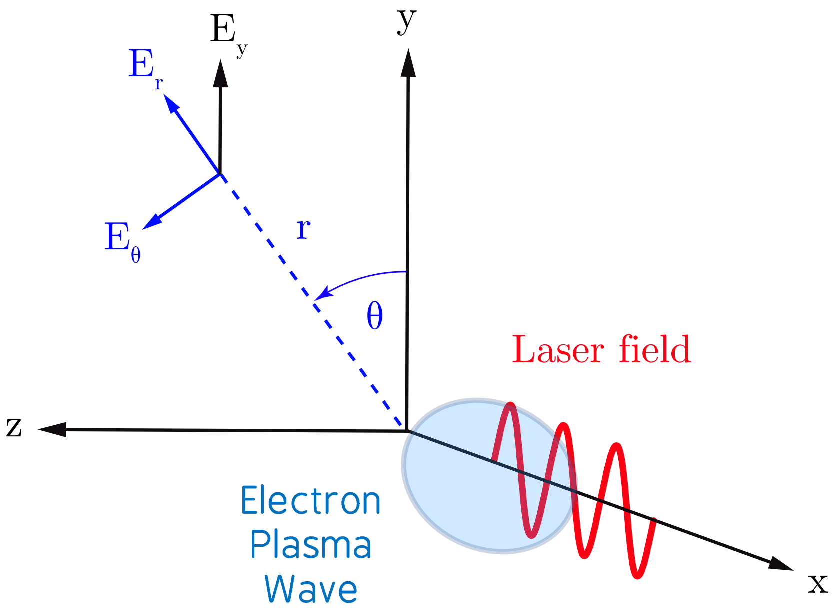
Azimuthal Modes decomposition (« AM-cylindrical » geometry)

Azimuthal Modes decomposition: concept

Example of quasi-cylindrical set-up:
Laser wakefield acceleration



A. Lifschitz et al., *J. Comp. Phys.* 228, 5 (2008)

Charge density, EM fields of laser wake are cylindrically symmetric:

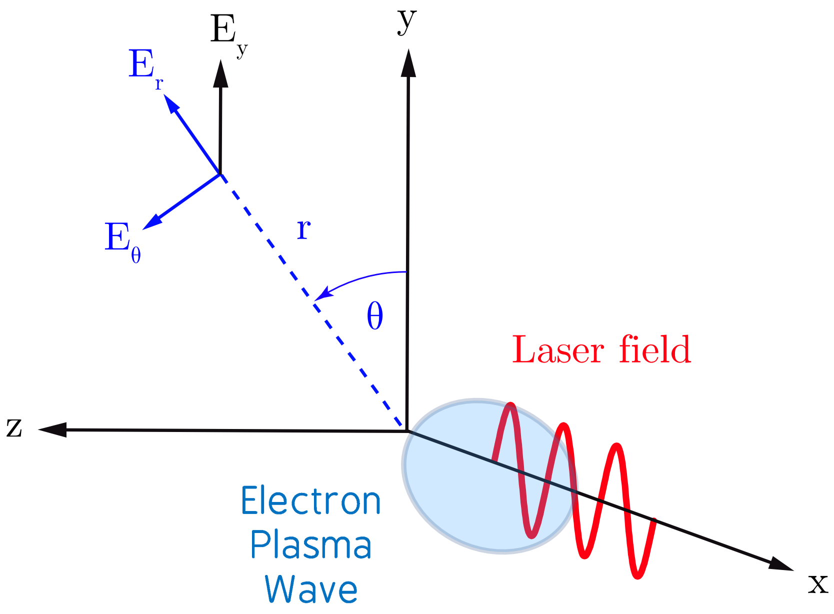
$$\rho(x,r,\theta,t) = \rho(x,r,t)[\cos(0\times\theta) + \sin(0\times\theta)]$$

Linearly polarized laser with cylindrically symmetric envelope:

$$\begin{aligned}\mathbf{E}_\perp(x,r,\theta,t) &= \mathbf{E}_y(x,r,\theta,t)\mathbf{e}_y \\ &= \mathbf{E}_y(x,r,\theta,t)\mathbf{e}_r + \mathbf{E}_y(x,r,\theta,t)\mathbf{e}_\theta \\ &= \mathbf{E}_y(x,r,t)[\cos(1\times\theta)\mathbf{e}_r - \sin(1\times\theta)\mathbf{e}_\theta]\end{aligned}$$

Azimuthal Modes decomposition: concept

Example of quasi-cylindrical set-up: Laser wakefield acceleration



A. Lifschitz et al., *J. Comp. Phys.* 228, 5 (2008)

Decomposition in *Azimuthal Modes* for scalars and vector components

$$F\left(x,r,\theta\right)=\tilde{F}^0_{real} \qquad m = 0$$

$$+\tilde{F}^1_{real}\cos(\theta)+\tilde{F}^1_{imag}\sin(\theta) \qquad m = 1$$

$$+\tilde{F}^2_{real}\cos(2\theta)+\tilde{F}^2_{imag}\sin(2\theta) \qquad m = 2$$

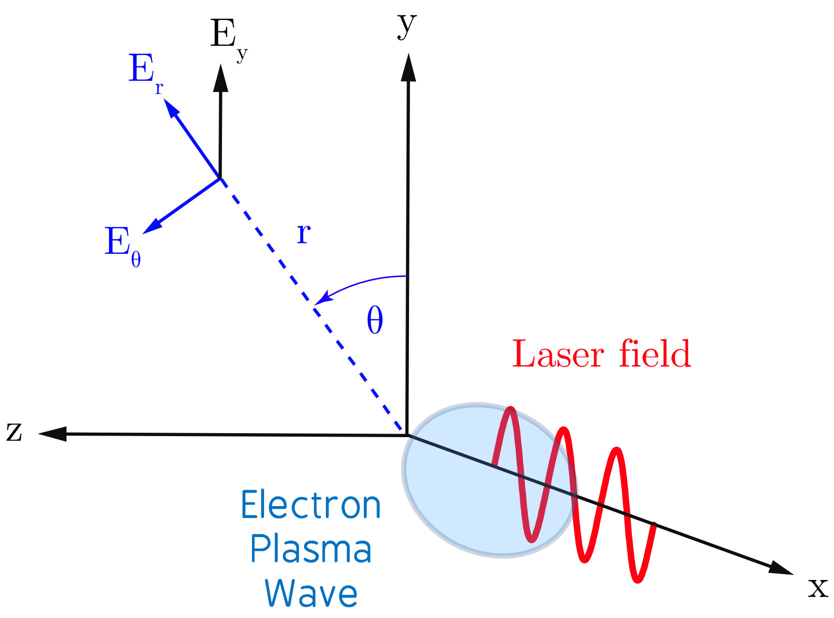
$+\ldots$ (the user chooses the highest m)

$$F\left(x,r,\theta\right)=\mathrm{Re}\left[\sum_{m=0}^{+\infty}\boxed{\tilde{F}^m\left(x,r\right)}\exp\left(-im\theta\right)\right]$$

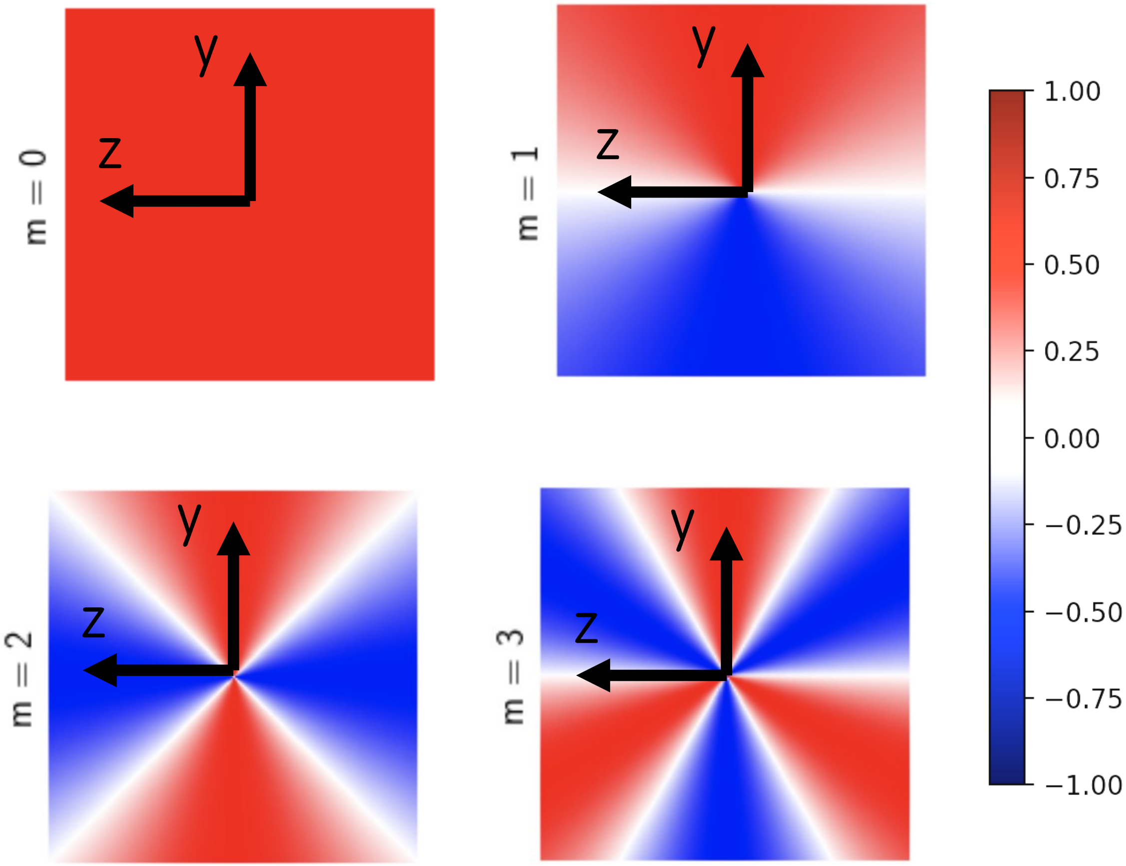
2D grid instead of 3D grid!

Azimuthal Modes decomposition: concept

Example of quasi-cylindrical set-up:
Laser wakefield acceleration

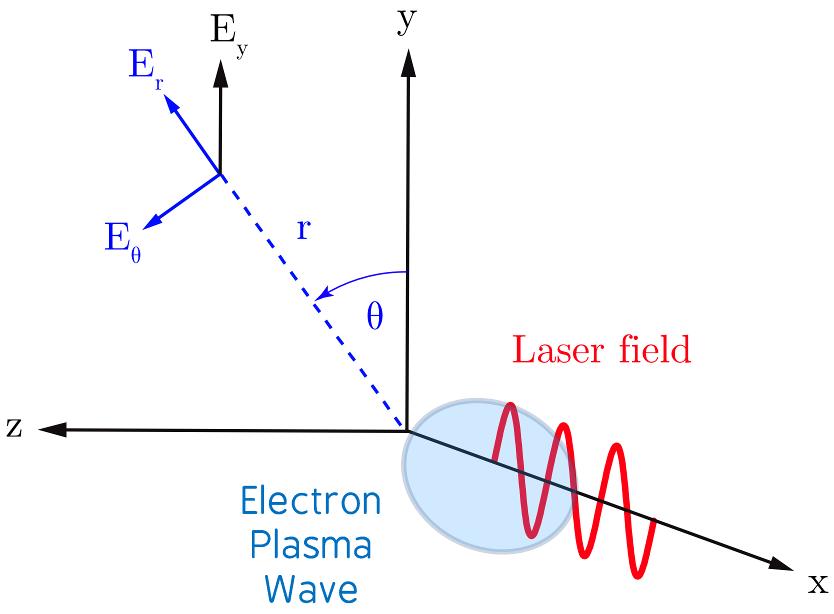


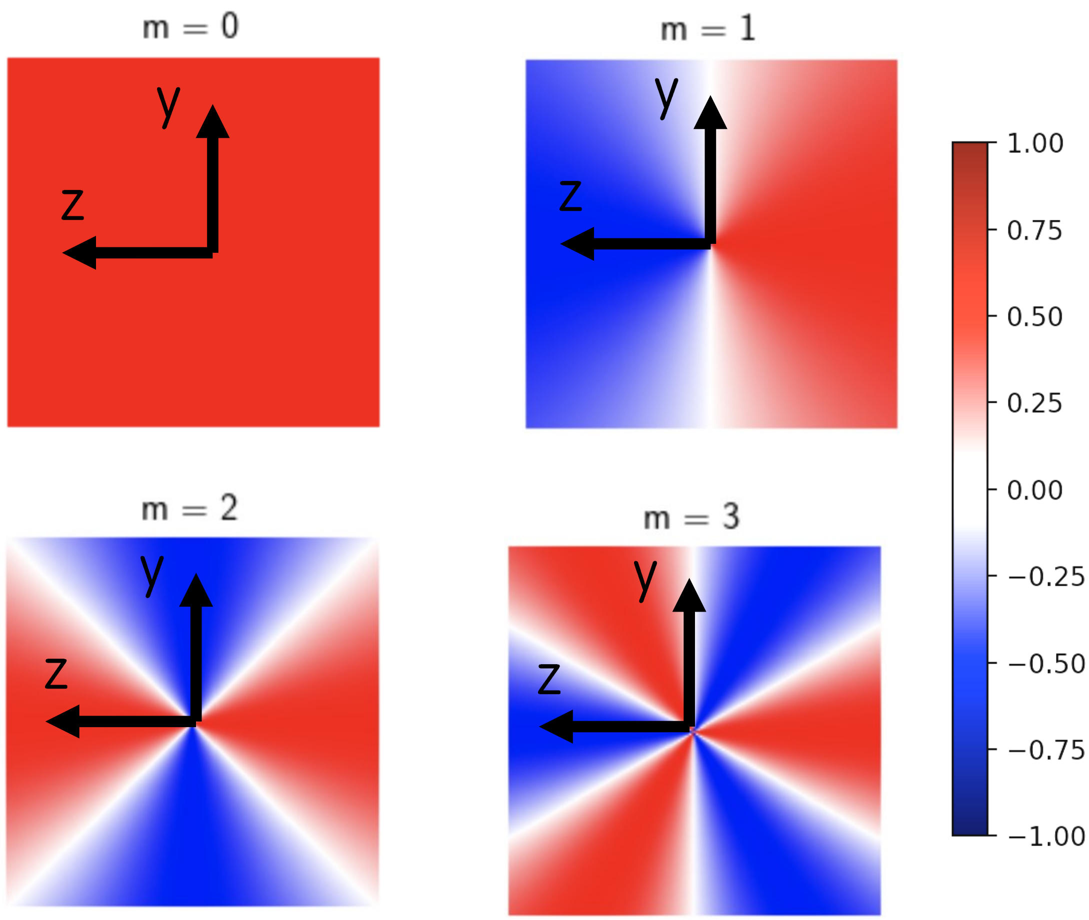
A. Lifschitz et al., *J. Comp. Phys.* 228, 5 (2008)



Azimuthal Modes decomposition: concept

Example of quasi-cylindrical set-up:
Laser wakefield acceleration

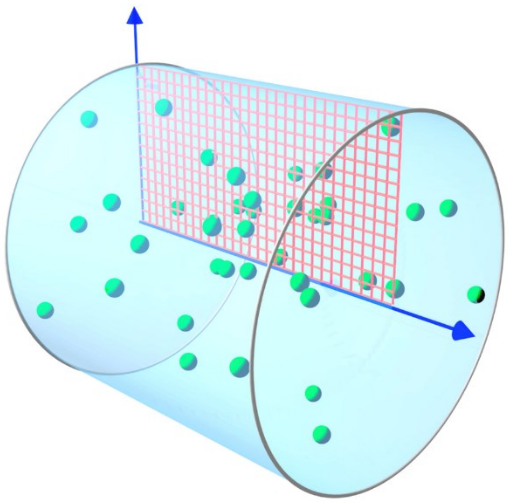




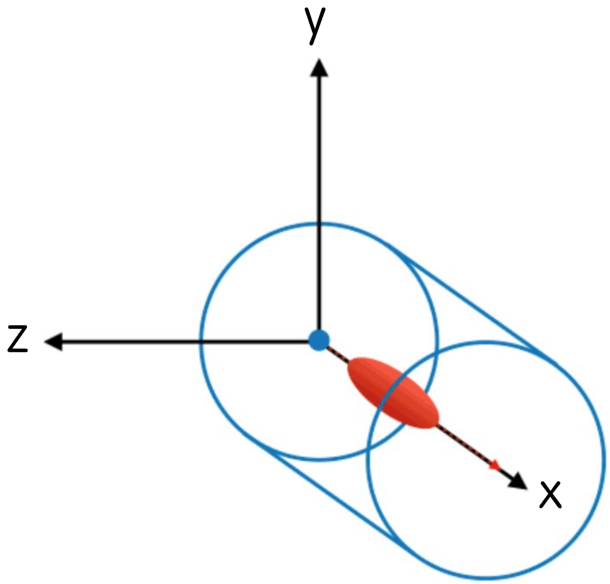
A. Lifschitz et al., *J. Comp. Phys.* 228, 5 (2008)

Grids are 2D, particles are 3D !

EM Fields, density:
Defined on RZ grid

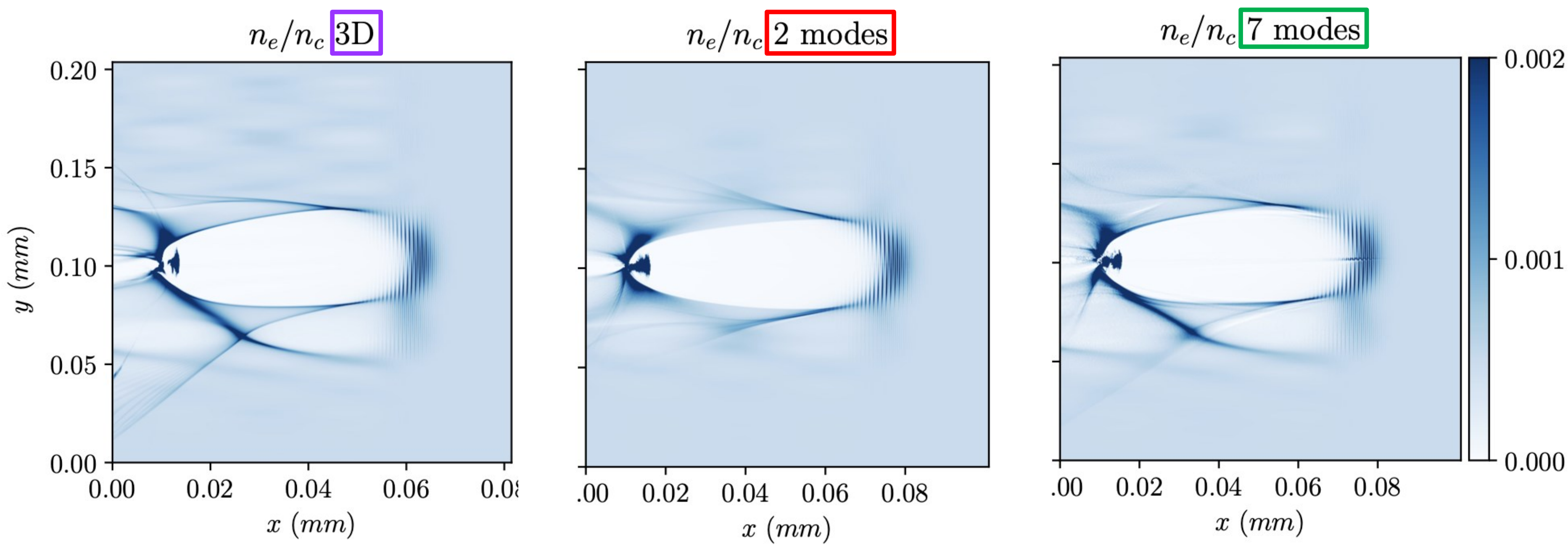


Particle coordinates, Probe coordinates:
3D space (remember the reference axes)



Azimuthal Modes decomposition: comparison with 3D

Warning: very asymmetric case,
normally 2-3 modes are enough for laser wakefield acceleration



I. Zemzemi, PhD thesis http://llr.in2p3.fr/IMG/pdf/thesis_postfinal_zemzemi.pdf

Azimuthal Modes decomposition: comparison with 3D

Speed-up compared with 3D:

	~50	~30	~20	
Simulation	2 modes	5 modes	7 modes	3D
Particles per cell	56	56	56	4
CPU-hours	16496	27483	37413	800000
Number of cores	1536	1536	1536	16000
Vectorization	None	None	None	Adaptive vectorization

Warning: very asymmetric case,
normally 2-3 modes are enough for laser wakefield acceleration

I. Zemzemi, PhD thesis http://llr.in2p3.fr/IMG/pdf/thesis_postfinal_zemzemi.pdf

Azimuthal Modes decomposition: how to use it

```
Main.geometry       = "AMcylindrical"
Main.number_of_AM = N_modes

Species.position_initialization = "regular"
Species.regular_number = [Nx,Nr,Ntheta]
```

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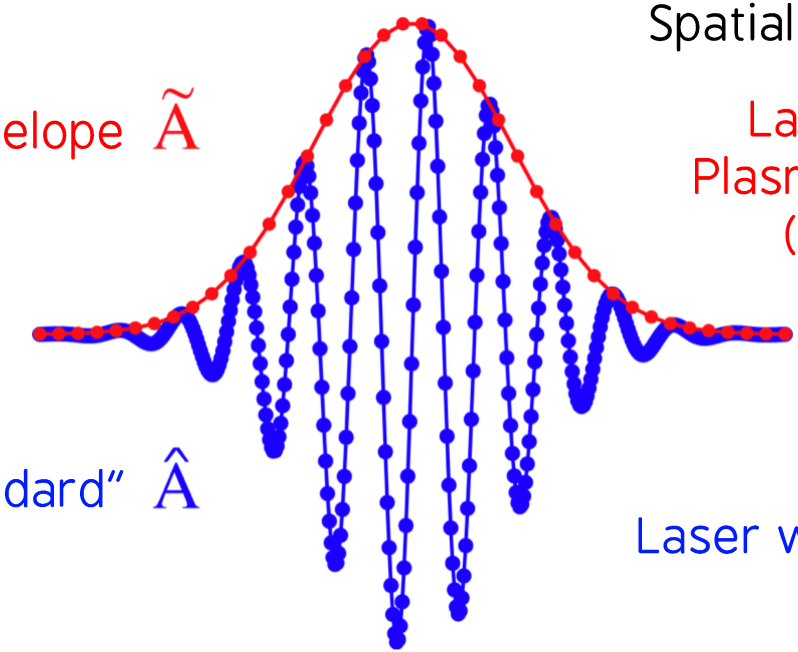
Laser Envelope Model

Laser Envelope Model: concept

Laser Envelope $\tilde{A}$

Laser "Standard" $\hat{A}$



Spatial variation scales:

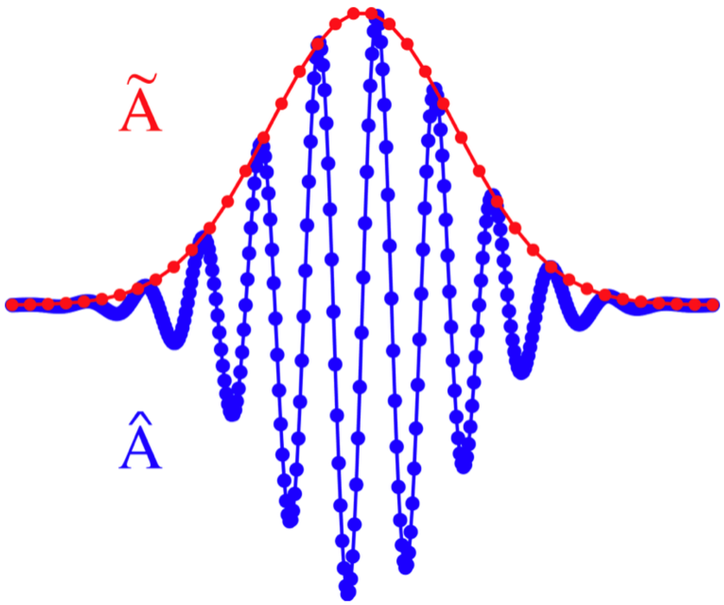
Laser length ~ Plasma wavelength (10-100 μm)

Laser wavelength ~1 μm

In this figure: $$\frac{\text{Points sampling Laser "Standard"}}{\text{Points sampling Laser Envelope}} = 10$$

With a Laser Envelope, larger Δx and Δt can be used!

Envelope Equations: Propagation and plasma coupling



Laser Envelope

$$\hat{A}(\mathbf{x},t) = Re\left[\tilde{A}(\mathbf{x},t)e^{ik_0(x-ct)}\right]$$

D'Alembert's Equation

$$\nabla^2\hat{A} - \partial_t^2\hat{A} = -\hat{J}$$

Envelope Equation: $\nabla^2\tilde{A} + 2i\left(\partial_x\tilde{A} + \partial_t\tilde{A}\right) - \partial_t^2\tilde{A} = \chi\tilde{A}$ Plasma Susceptibility

D. Terzani and P. Londrillo, Comput. Phys. Comm. 242, 49 (2019)

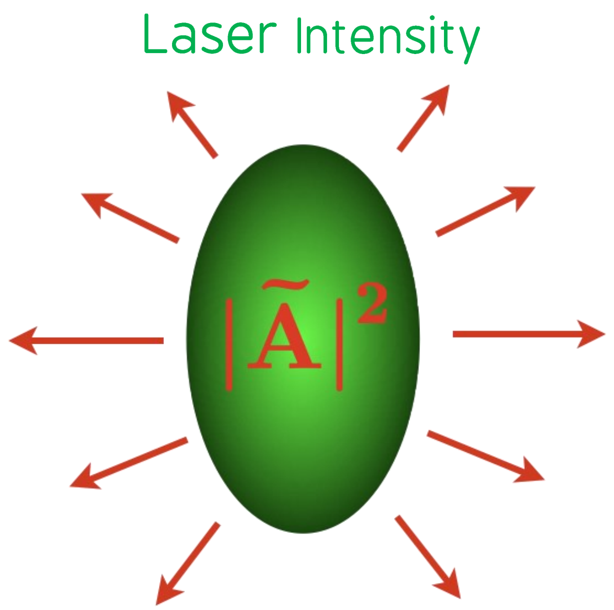
Ponderomotive equation of motion for macroparticles

Equations of motion for the macro-particles
(here electrons):

$$\frac{d\bar{\mathbf{x}}_p}{dt} = \frac{\bar{\mathbf{u}}_\mathbf{p}}{\bar{\gamma}_p}$$

$$\frac{d\bar{\mathbf{u}}_p}{dt} = r_s \left(\bar{\mathbf{E}}_p + \frac{\bar{\mathbf{u}}_p}{\bar{\gamma}_p} \times \bar{\mathbf{B}}_p \right) - r_s^2 \frac{1}{4\bar{\gamma}_p} \nabla \left(|\tilde{A}_p|^2 \right)$$

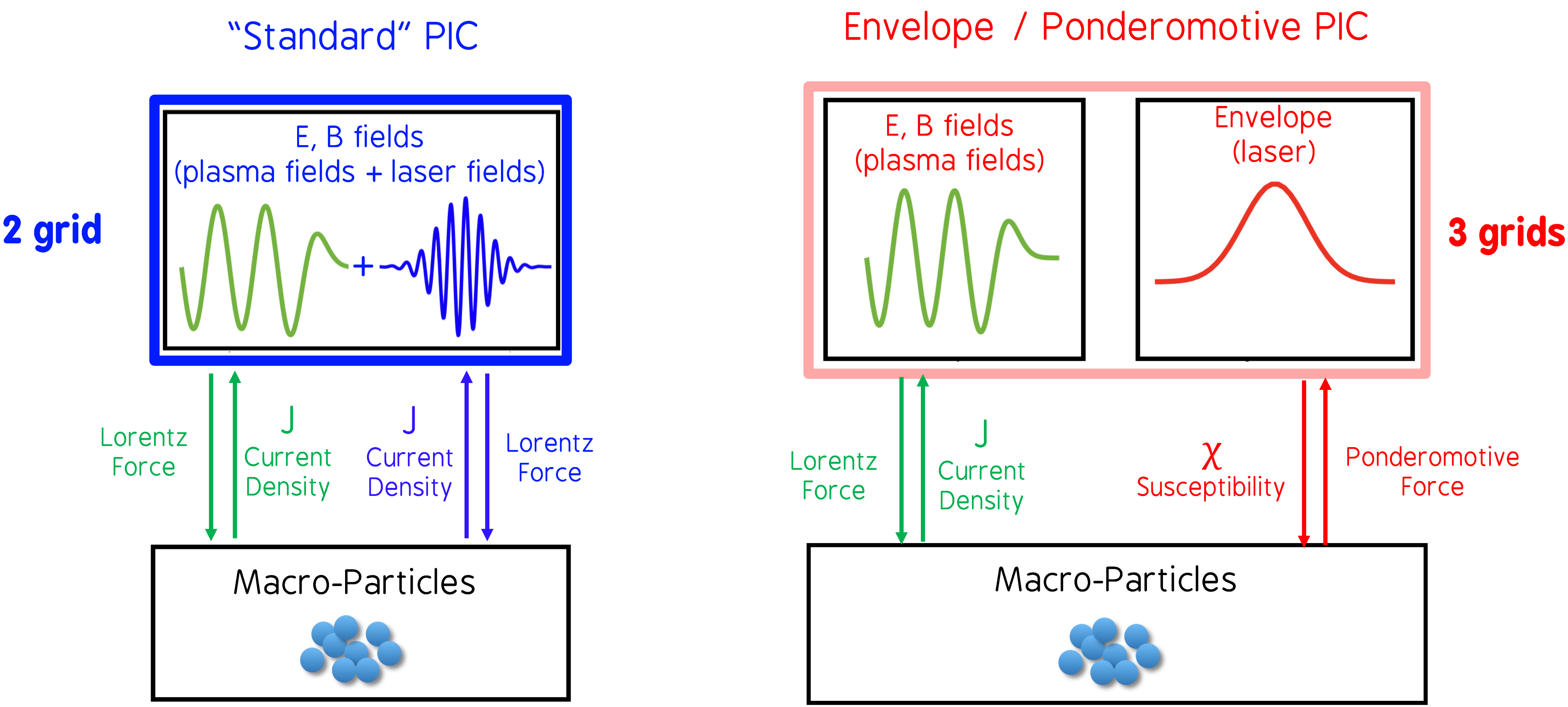
Lorentz Force — Ponderomotive Force



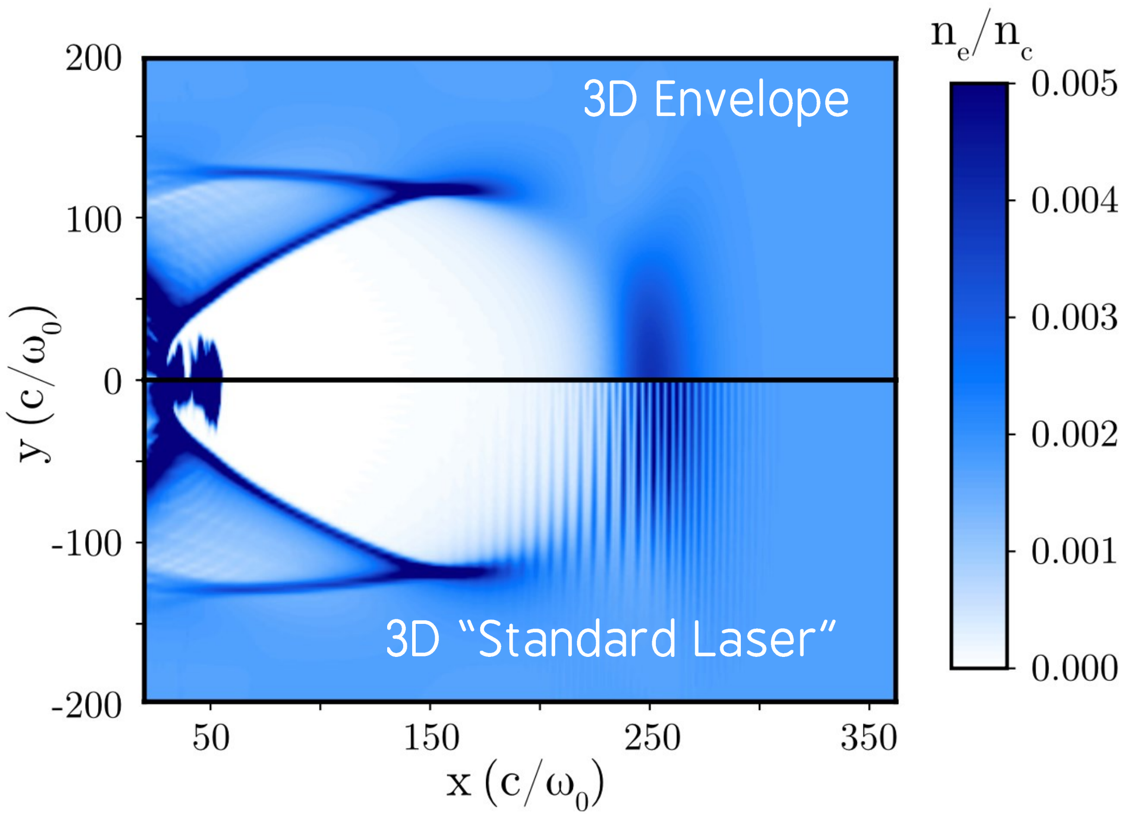
Ponderomotive force acts as a radiation pressure

B. Quesnel and P. Mora, Phys. Rev. E 58, 3719 (1998)

Laser Envelope Model: Resume



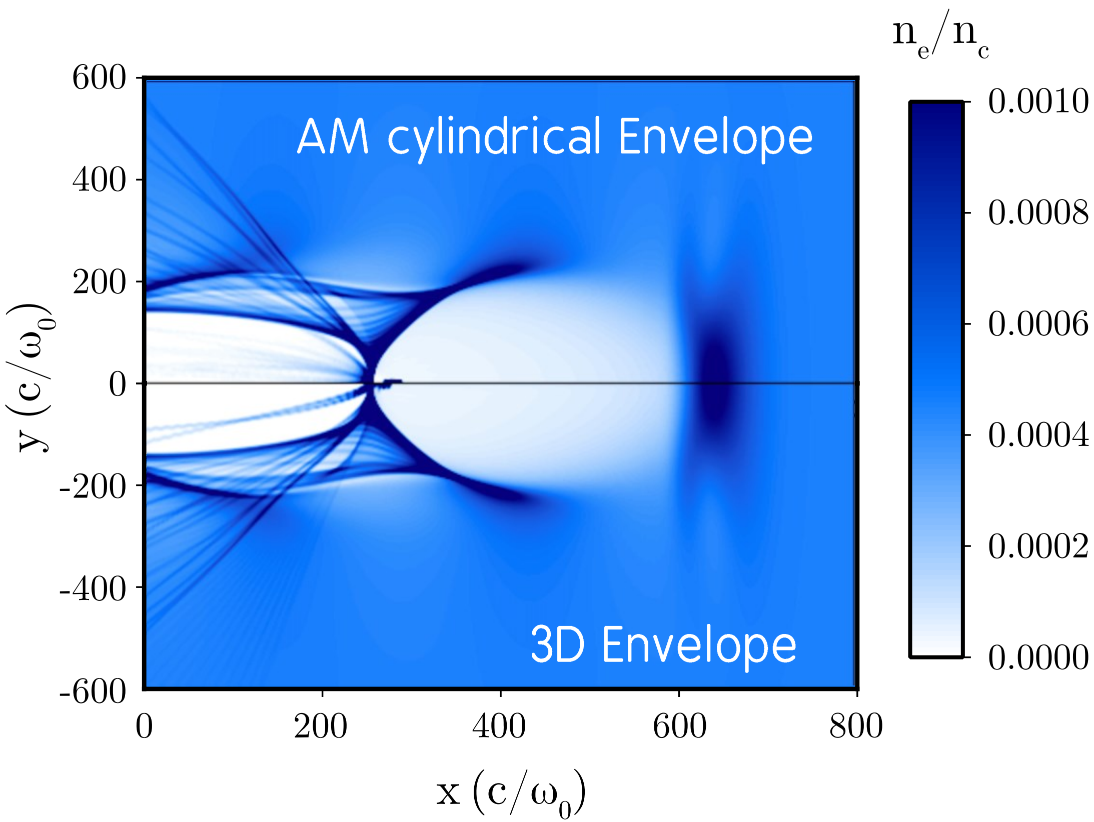
Laser Envelope Model vs full 3D (Standard)



$$\frac{T_{\text{Standard PIC 3D}}}{T_{\text{Envelope PIC 3D}}} > 20$$

3D Cartesian solver: D. Terzani et al., Com .Phys. Comm. (2019), F. Massimo et al., PPCF. (2019)

The envelope exists also in AM !



$$\frac{T_{\text{Envelope PIC 3D}}}{T_{\text{Envelope PIC cylindrical}}} > 100$$

2D cylindrical solver: F. Massimo et al., J. Phys.: Conf. Ser. (2020)

Envelope: how to use it

```
LaserEnvelopeGaussian3D(
    a0              = 1.,
    focus           = [150., 40., 40.],
    waist           = 30.,
    time_envelope   = tgaussian(center=150., fwhm=40.),
    envelope_solver = 'explicit',
    Envelope_boundary_conditions = [ ["reflective"] ],
    polarization_phi = 0.,
    ellipticity      = 0.
)
```

Envelope: how to use it

```
Main.geometry      = “AMcylindrical”
Main.number_of_AM = 1


LaserEnvelopeGaussianAM(
    a0              = 1.,
    focus           = [150., 0.],
    waist           = 30.,
    time_envelope   = tgaussian(center=150., fwhm=40.),
    envelope_solver = 'explicit_reduced_dispersion',
    Envelope_boundary_conditions = [ ["PML"] ],
    polarization_phi = 0.,
    ellipticity      = 0.
)
```

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Tunnel Ionization with Laser Envelope Model

Laser Envelope Model: Tunnel ionization module

Challenge: Simulate from laser tunneling ionization **without field peaks**

```
Species.ionization_model = "tunnel_envelope_averaged"
```

- Averaged ionization rate

M. Chen et al., J. Comput. Phys. 236, 220 (2013)

- Statistical reconstruction of electron transverse momenta

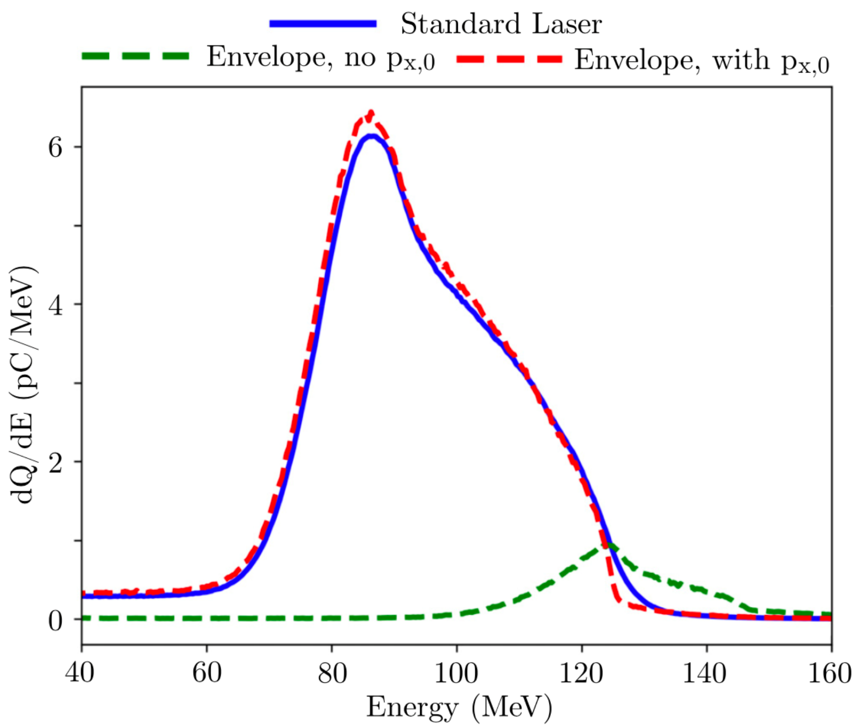
P. Tomassini et al., Phys. Plasmas 24, 103120 (2017)

- Statistical reconstruction of electron longitudinal momenta (important for relativistic regimes)

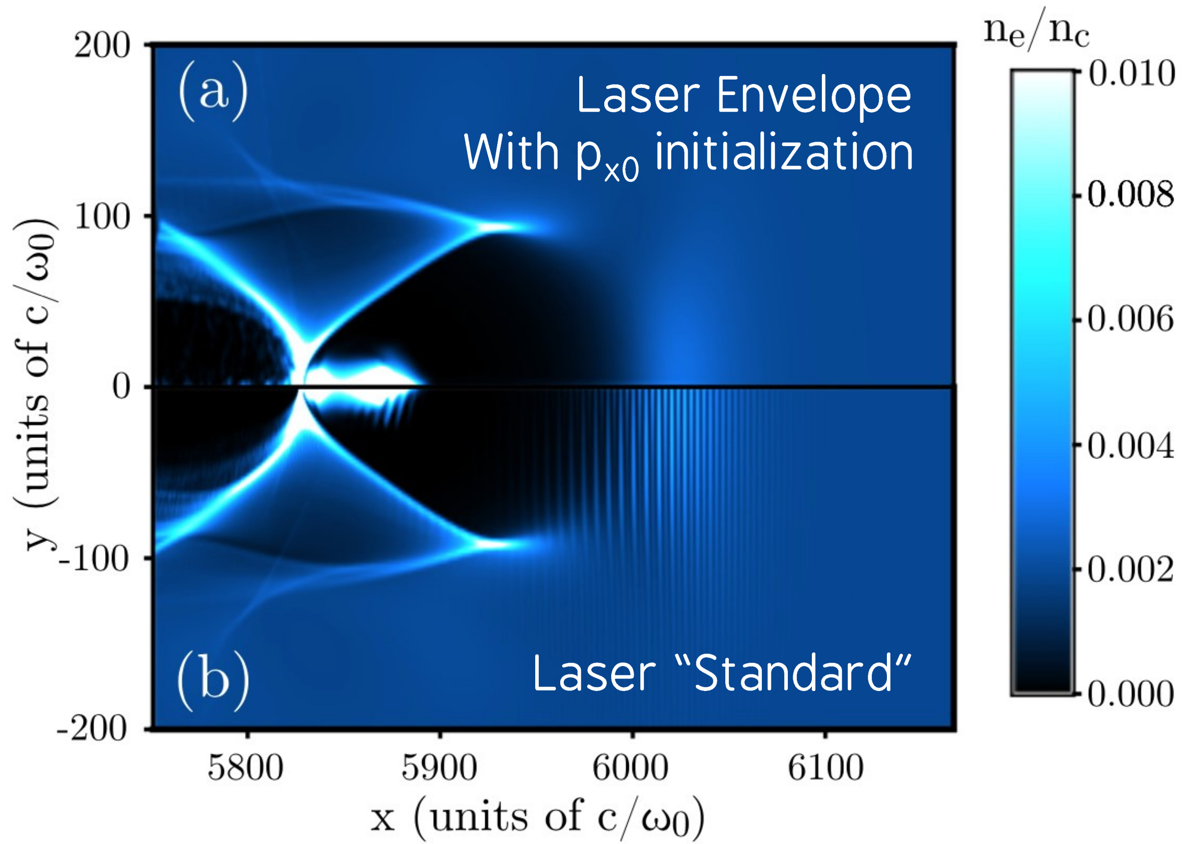
F. Massimo et al., Phys. Rev. E 102, 033204 (2020)

Introduced with **Smilei)**
for all geometries

Laser Envelope Model: LWFA with ionization injection



AM Cylindrical LWFA simulation at 800 um



F. Massimo et al., Phys. Rev. E (2020)

Laser Envelope Model: LWFA with ionization injection

F. Massimo et al., Phys. Rev. E (2020)	AM cylindrical (2 modes) Simulation time: 9.3 kcpu-hours	AM cylindrical (1 mode) Simulation time: 30 minutes, 1 cpu-core
L = 800 µm	Standard laser	Envelope, 1 particle per cell
Q [pC]	175	179
$2\sigma_x$ [μm]	3.4	3.5
$2\sigma_y$ [μm]	2.3	2.4
$2\sigma_z$ [μm]	1.1	1.2
$\varepsilon_{n,y}$ [mm-mrad]	3.9	4.0
$\varepsilon_{n,z}$ [mm-mrad]	1.2	1.2
E_{avg} [MeV]	90.2	89.6
σ_E/E [rms, %]	11.91	11.52
	Tunnel ionization	Envelope tunnel ionization

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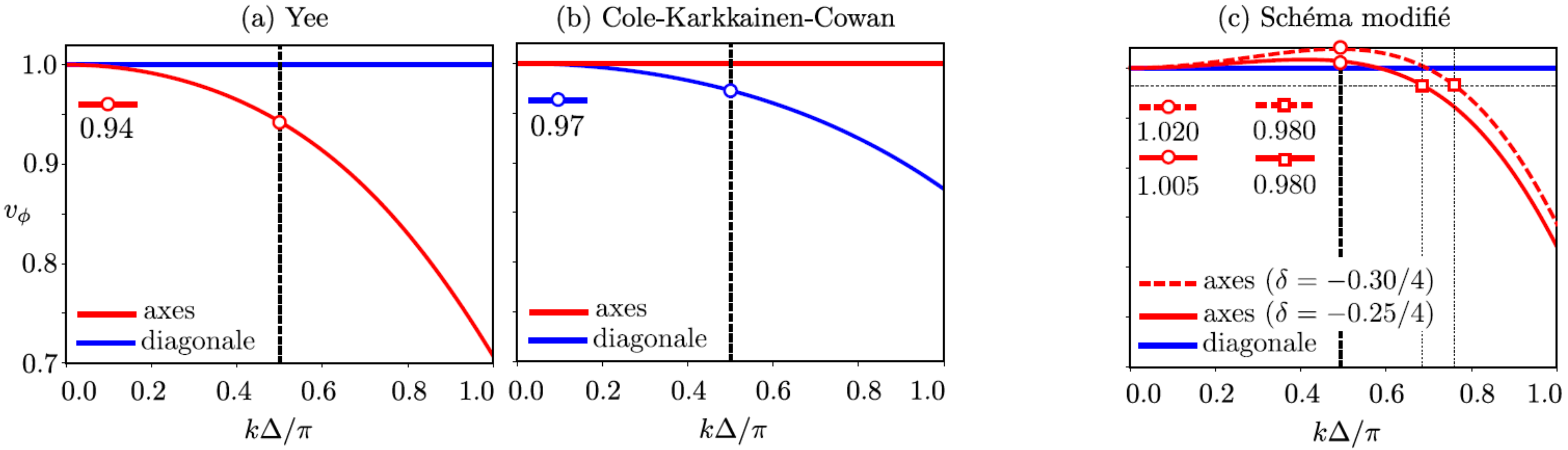
Advanced Fields Solvers

Why having advanced fields solvers ?

One example : Numerical dispersion in 2D

Standard
Finite Difference Time Domain (FDTD)

Non Standard
(FDTD)

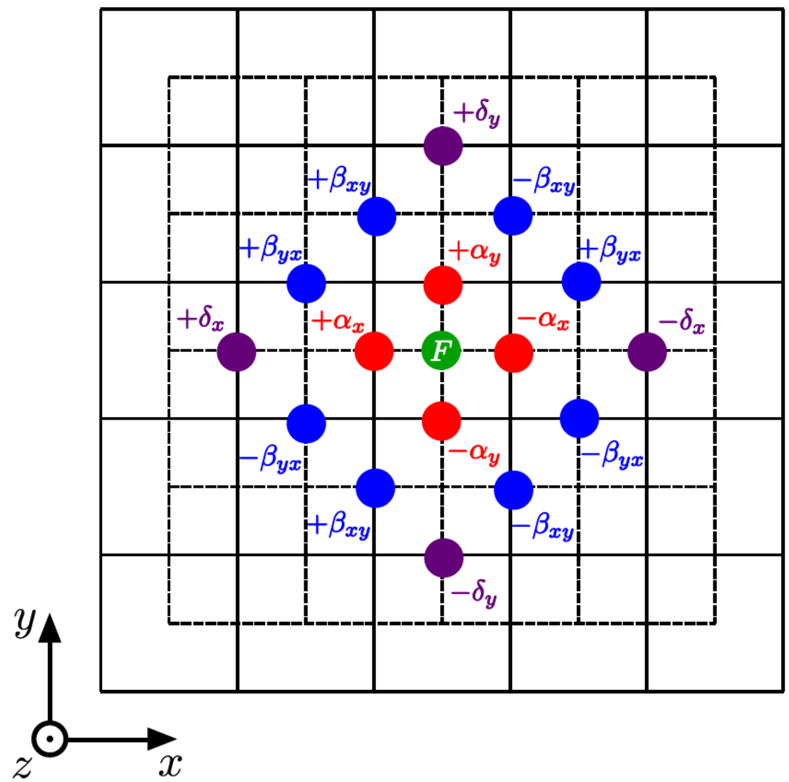


Pro : Computationally efficient
Con : Dispersive and anisotropic

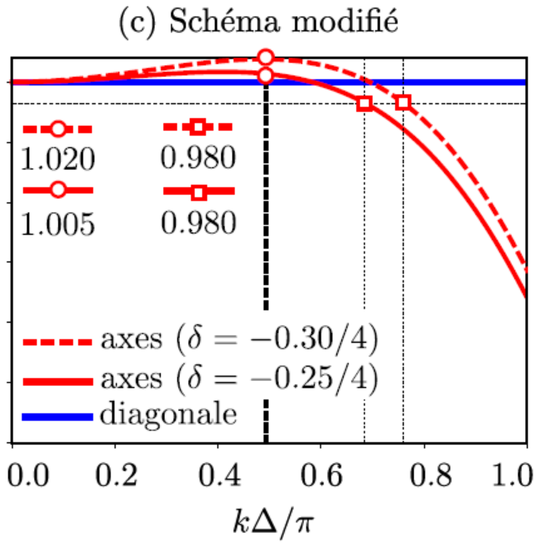
Pro : Less Dispersive and more isotropic
Con : Less local and more operations

Why having advanced fields solvers ?

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

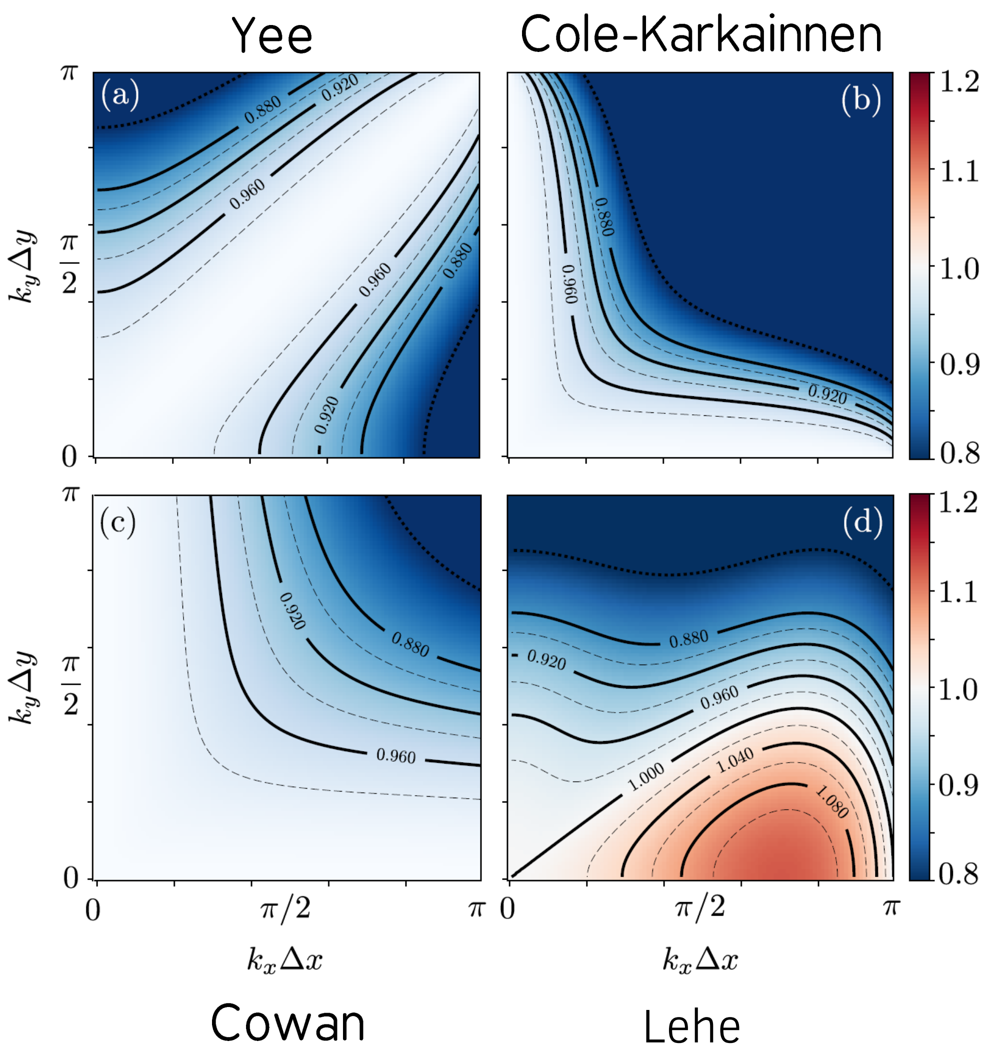


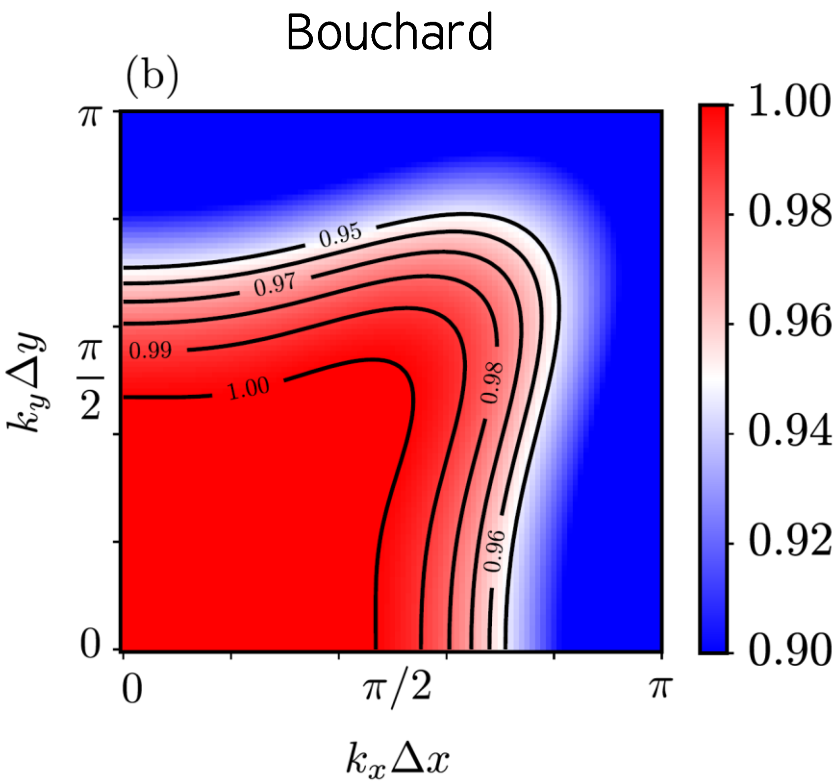
Non Standard
(FDTD)



Pro : Less Dispersive and more isotropic
Con : Less local and more operations

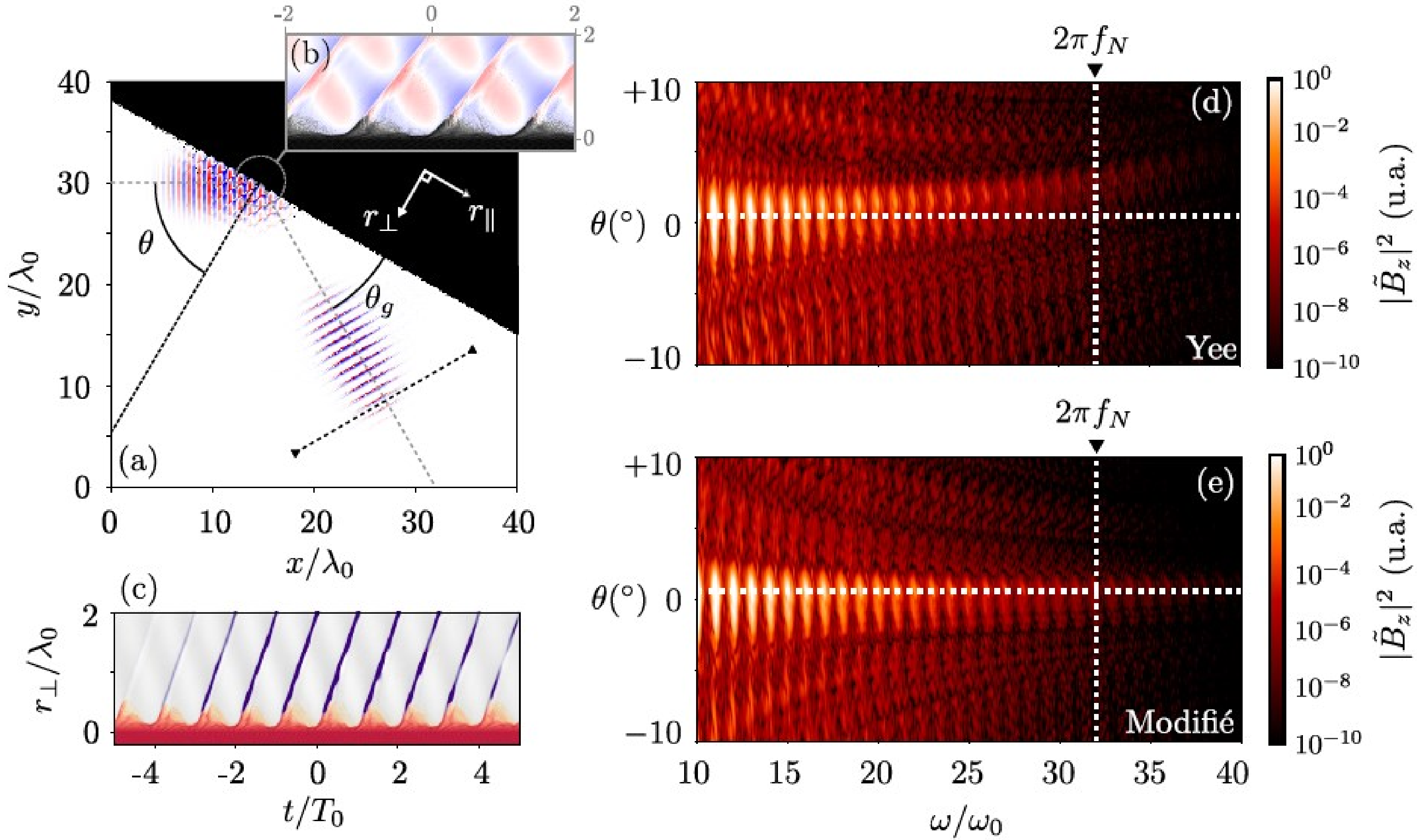
Why having advanced fields solvers ?





Pro : Less Dispersive and more isotropic
Con : Less local and more operations
Sacrifice high-frequency

X-UV Generation when a laser impinge a solid target at a given angle



G. Bouchard, PhD thesis https://theses.hal.science/tel-02967252

How to use it

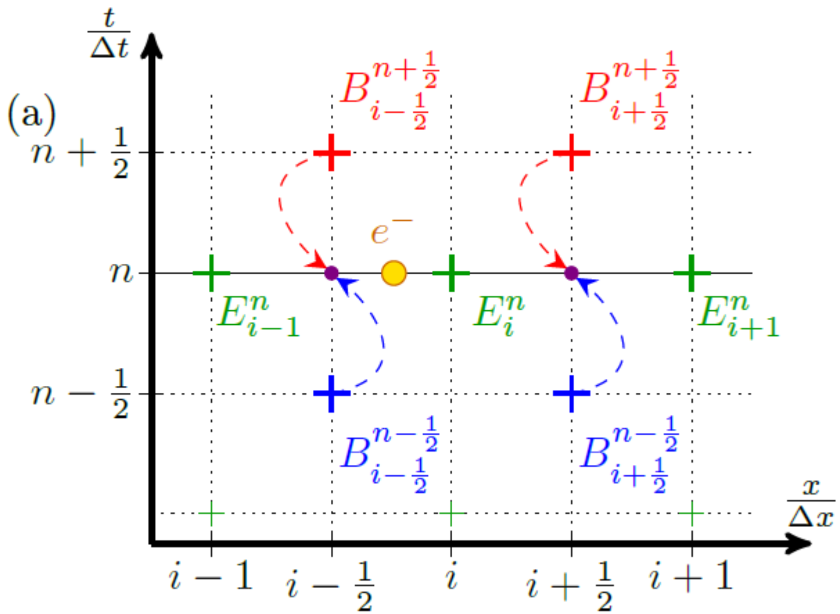
```
#Laser wavelength
L0 = 2.*numpy.pi
dx = L0/10.

Main(
    …
    geometry = "2Dcartesian", #3Dcartesian as well
    cell_length = [dx,dx],
    timestep = dx/2,
    maxwell_solver = "Bouchard",
    …
)
```

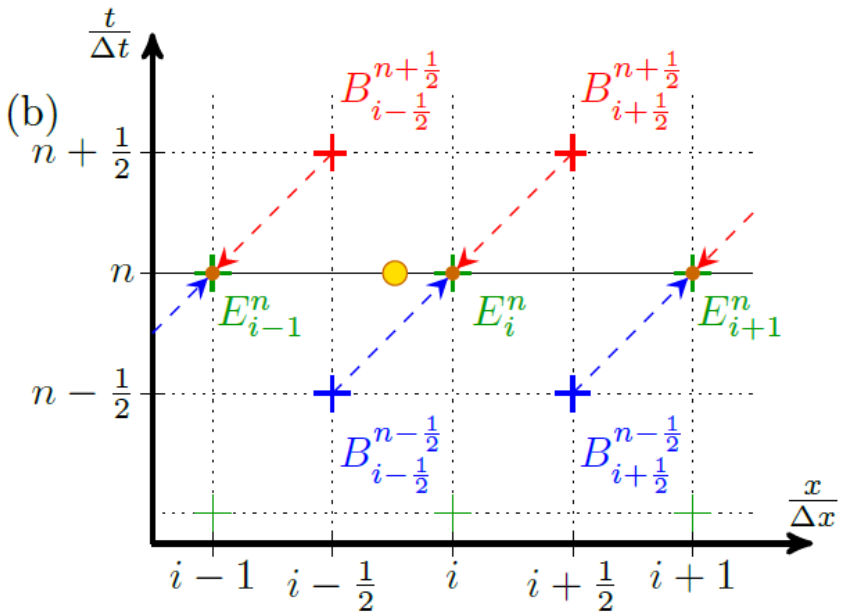
B-translated interpolation scheme (B-TIS3)

A new interpolation scheme

Standard Field gathering/interpolation



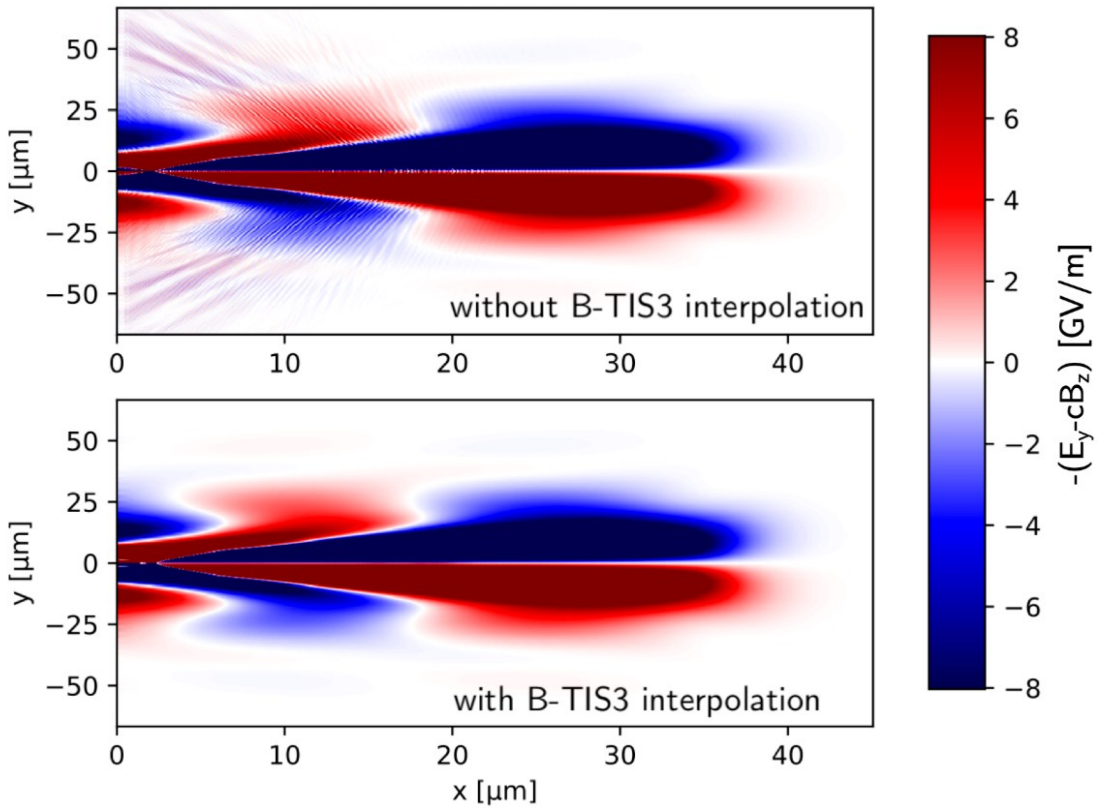
Non Standard Field gathering/interpolation



Bourgeois & Davoine, *J. Comput. Phys.*, vol. 413, 2020, 109426.
Bourgeois & Davoine, *J. of Plasma Physics*, 2023, 89 (2).

A Laser Wake Field Acceleration scenario

Force acting on particles in presence of fields that move at speed close to the speed of light in the x direction



How to use it

```
Main(
    …
    use_BTIS3_interpolation = True,
    …
)

DiagProbe(
    …
    fields    = ["By", Bz", "ByBTIS3", "BzBTIS3"
    …
)
```

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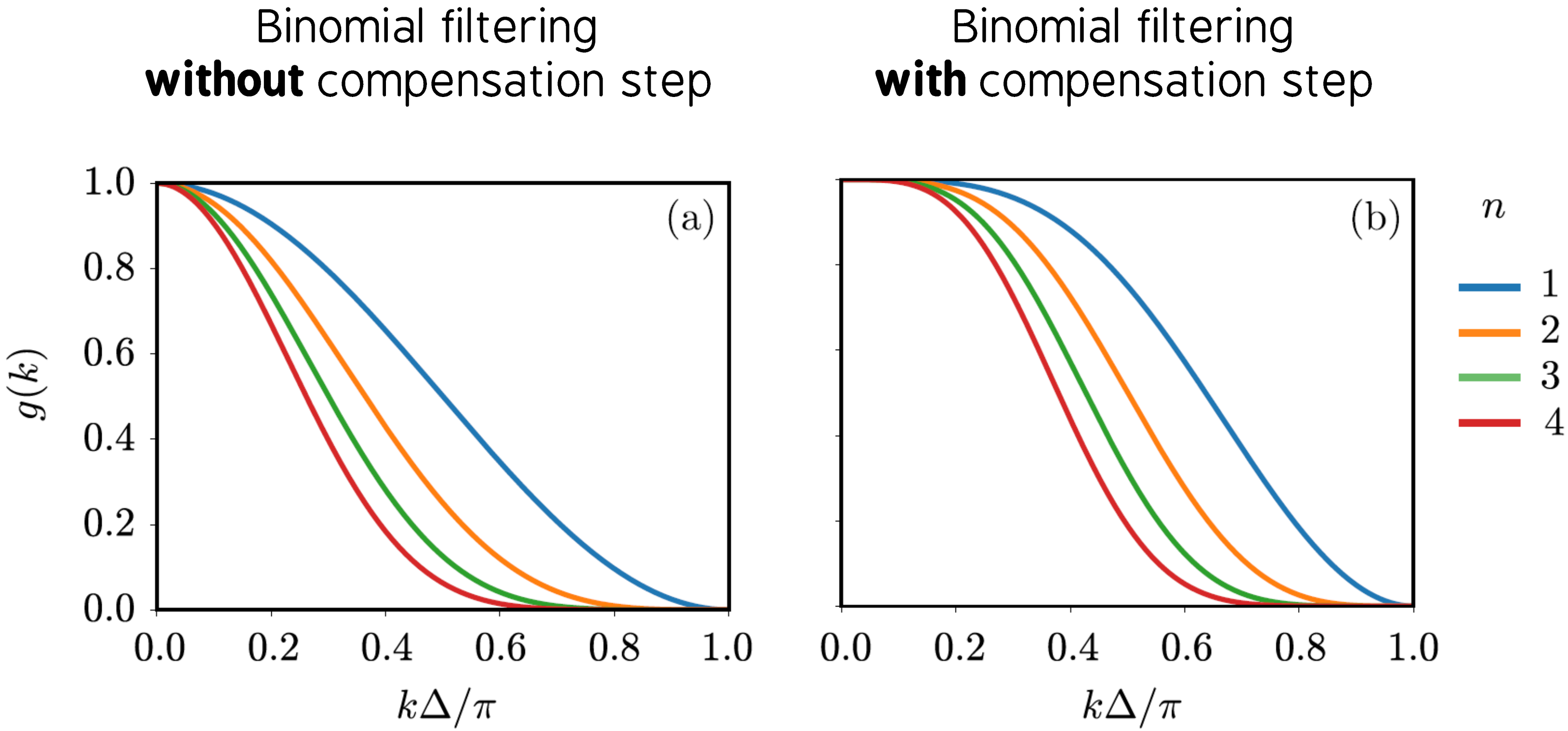
Current Spatial Filtering

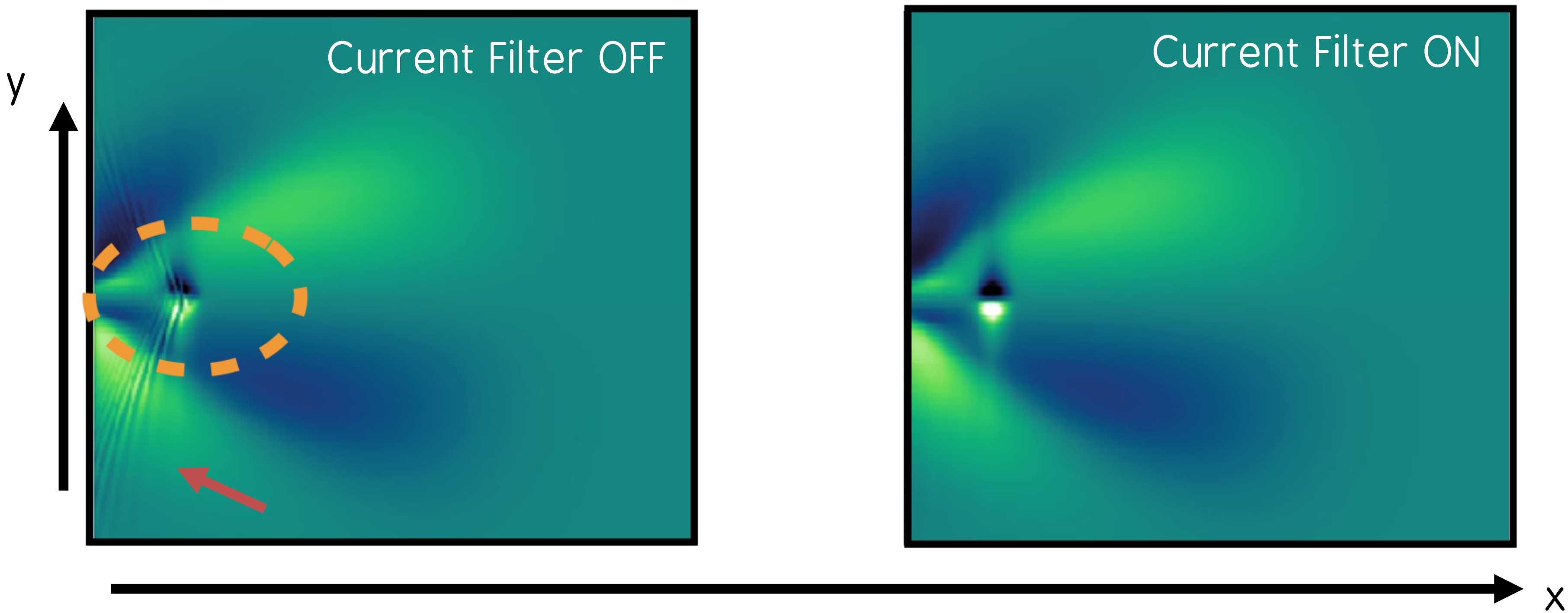
Current Filtering on current density (space filtering)



Reduce (supress) high frequency contribution of the current density without altering low frequency physics

Current Filtering: reduction of numerical Cherenkov radiation

Ey from LWFA simulation with Laser Envelope

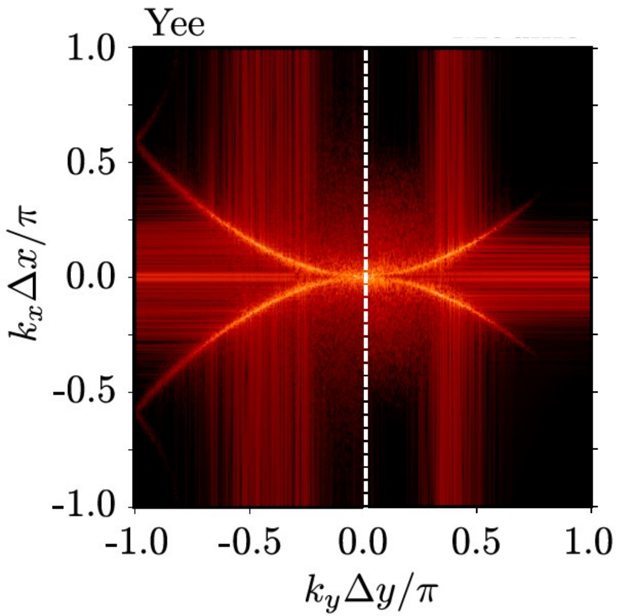


Filtering can reduce Numerical Cherenkov Radiation

J.-L.Vay, Journ. Comput. Phys. 230 (2011)

Consider an advanced field solver

3 passes of binomial filtering
with Yee solver

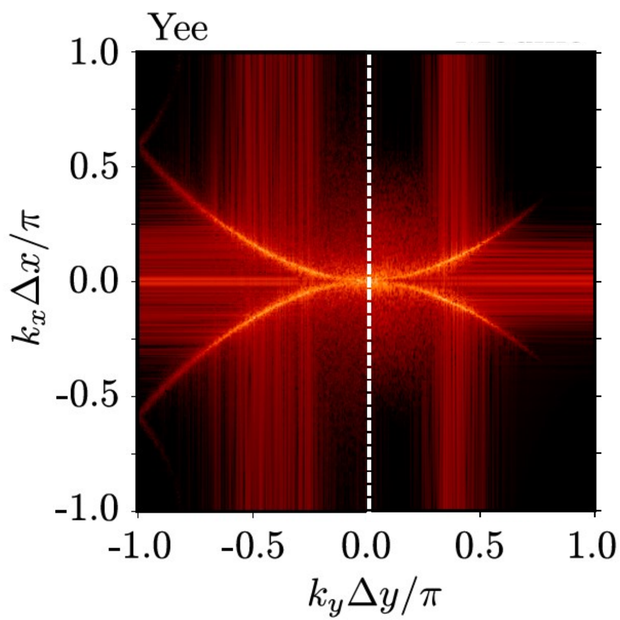


Cherenkov at low frequency
can not be filtered

G. Bouchard, PhD thesis https://theses.hal.science/tel-02967252

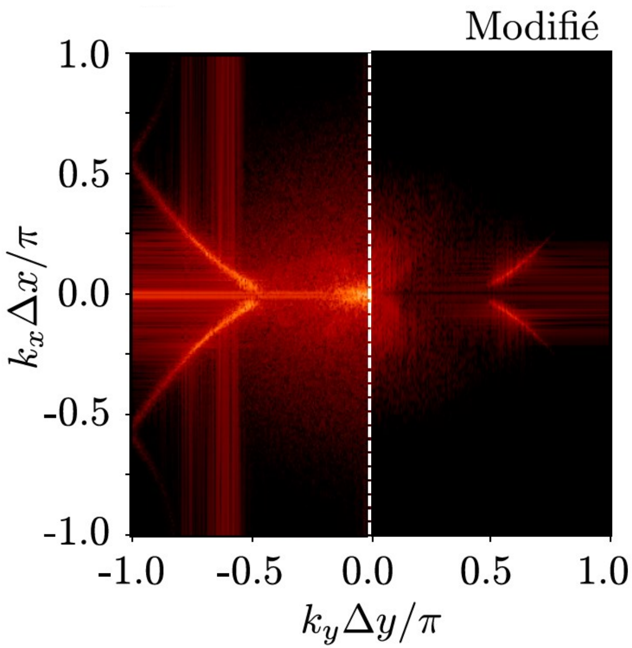
Consider an advanced field solver

3 passes of binomial filtering
with Yee solver



Cherenkov at low frequency
can not be filtered

3 passes of binomial filtering
with advanced solvers



Only band-frequency
Cherenkov

G. Bouchard, PhD thesis https://theses.hal.science/tel-02967252

Current Filtering: how to use it

Available
in all geometries

```
CurrentFilter(
        model     = “binomial",
        passes    = [1]
)
```

Current Filtering: how to use it

Available
in all geometries

```
CurrentFilter(
        model      = "customFIR",
        passes     = [1],
        kernelFIR = [0.25,0.5,0.25]
)
```

Warning: filtering increases the time spent on communications consider adding also Single Domain Multiple Decomposition

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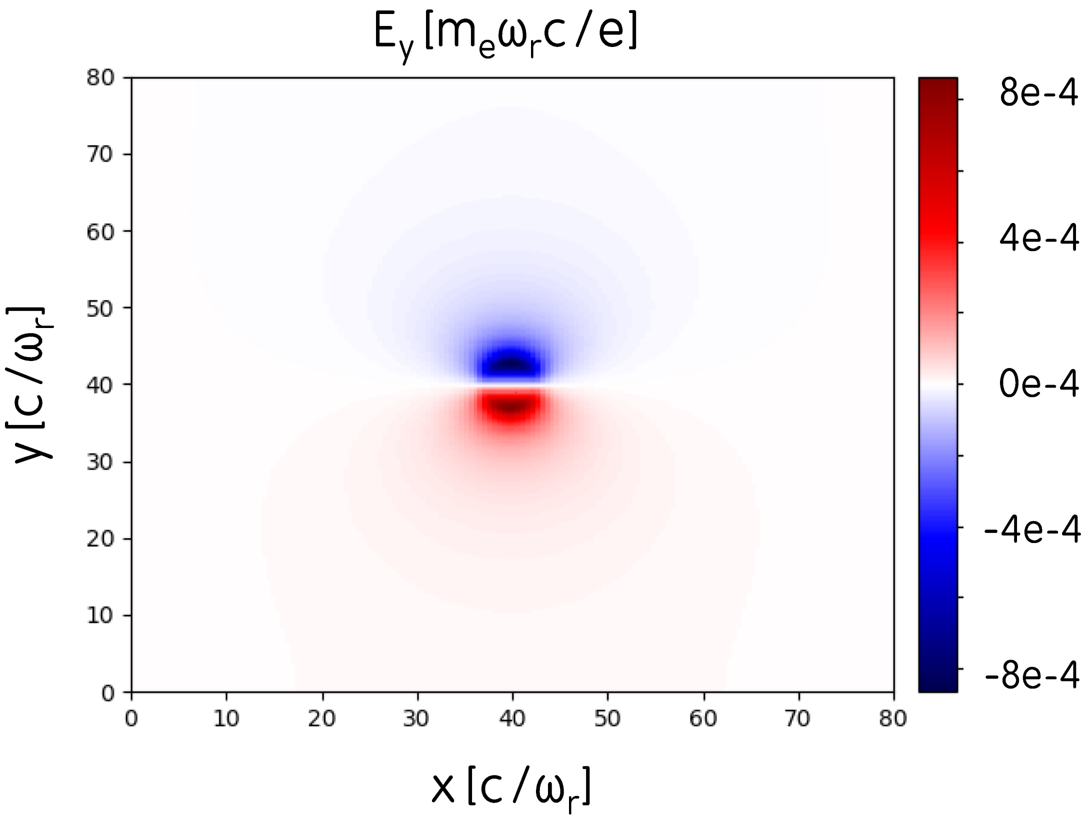
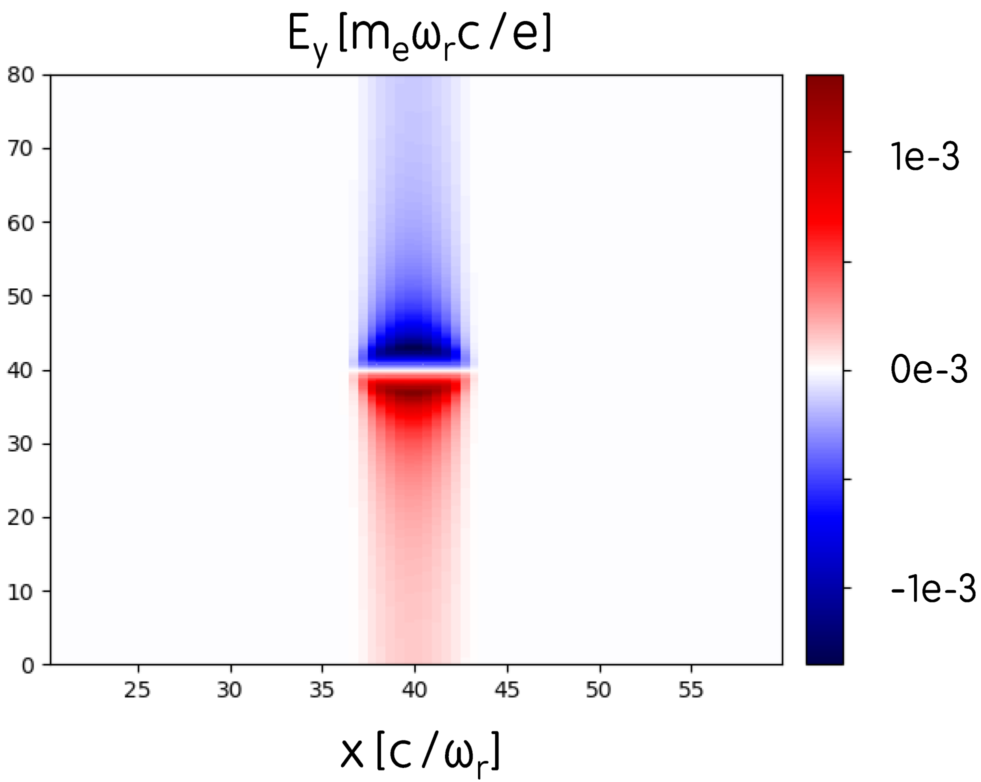
Field initialization of relativistic Species

Relativistic Species Initialization example: electron sphere

$\gamma_0 \sim 1$ ($v_x << c$)



$\gamma_0 = 200$ (relativistic, $v_x \sim c$, E~100 MeV)



Relativistic Species Initialization: how to use it

```
Main(
        …
        solve_poisson = False,
        solve_relativistic_poisson = True,
        …
        )
```

Warning:
if relativistic solver is used, do not use also the classical one!

```
Species(
        …
        # Relativistic field initialization:
        relativistic_field_initialization = "True",
        …
        )
```

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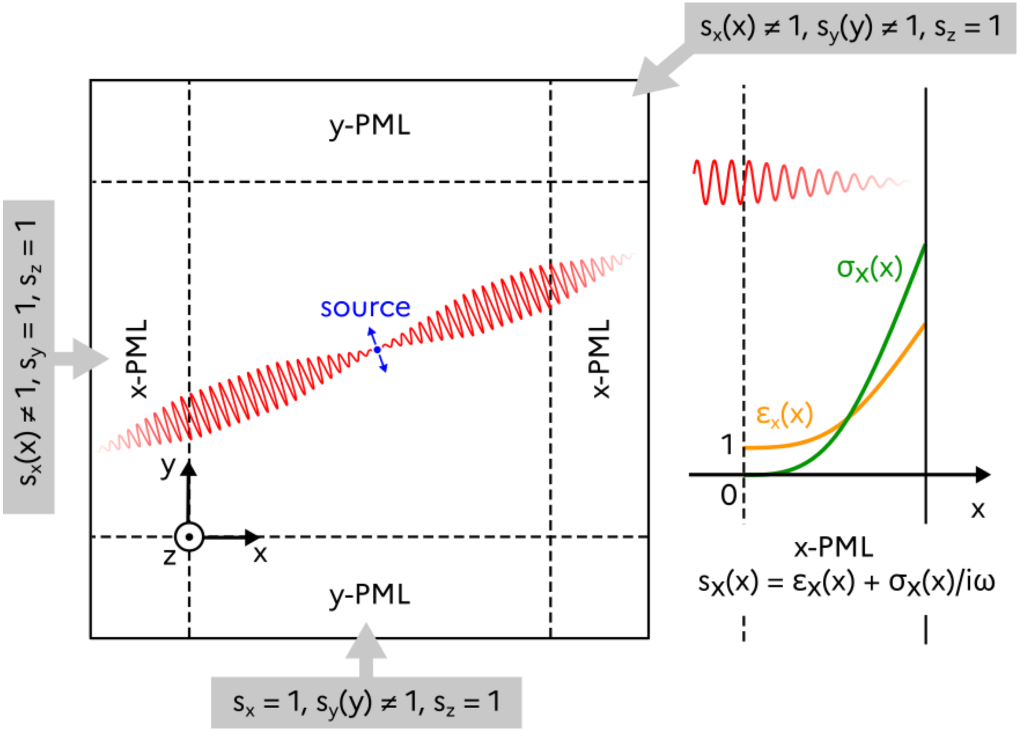
Perfectly Matched Layer

Perfectly Matched Layer (PML): Concept



In Smilei)

- For all geometries
- For standard fields and envelope

Maxwell Faraday

$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = -i\omega\mu_0 \boxed{\frac{s_y s_z}{s_x}} H_x$$

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = -i\omega\mu_0 \boxed{\frac{s_x s_z}{s_y}} H_y$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -i\omega\mu_0 \boxed{\frac{s_x s_y}{s_z}} H_z$$

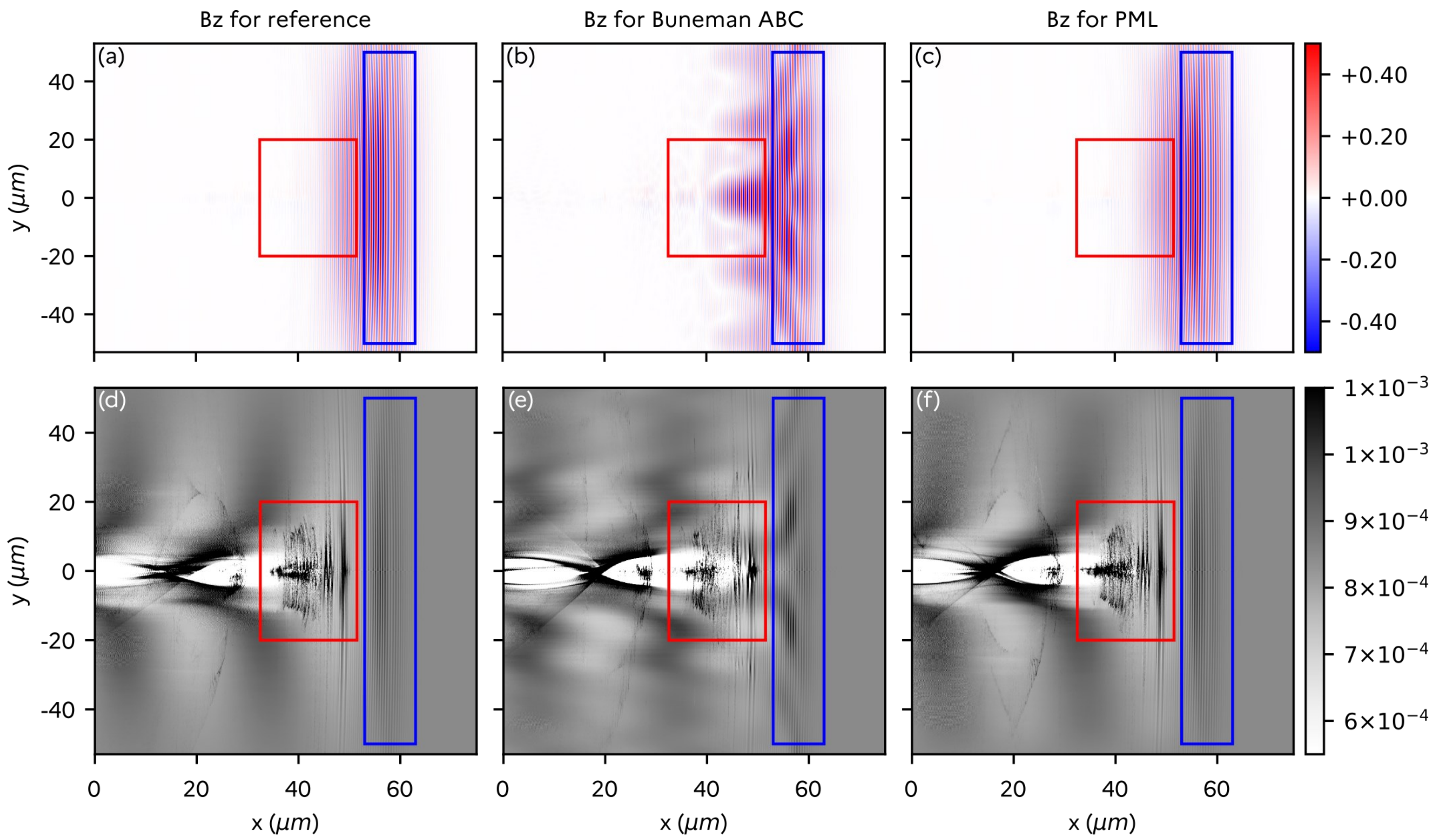
Maxwell Ampere

$$\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} = i\omega\varepsilon_0 \boxed{\frac{s_y s_z}{s_x}} E_x$$

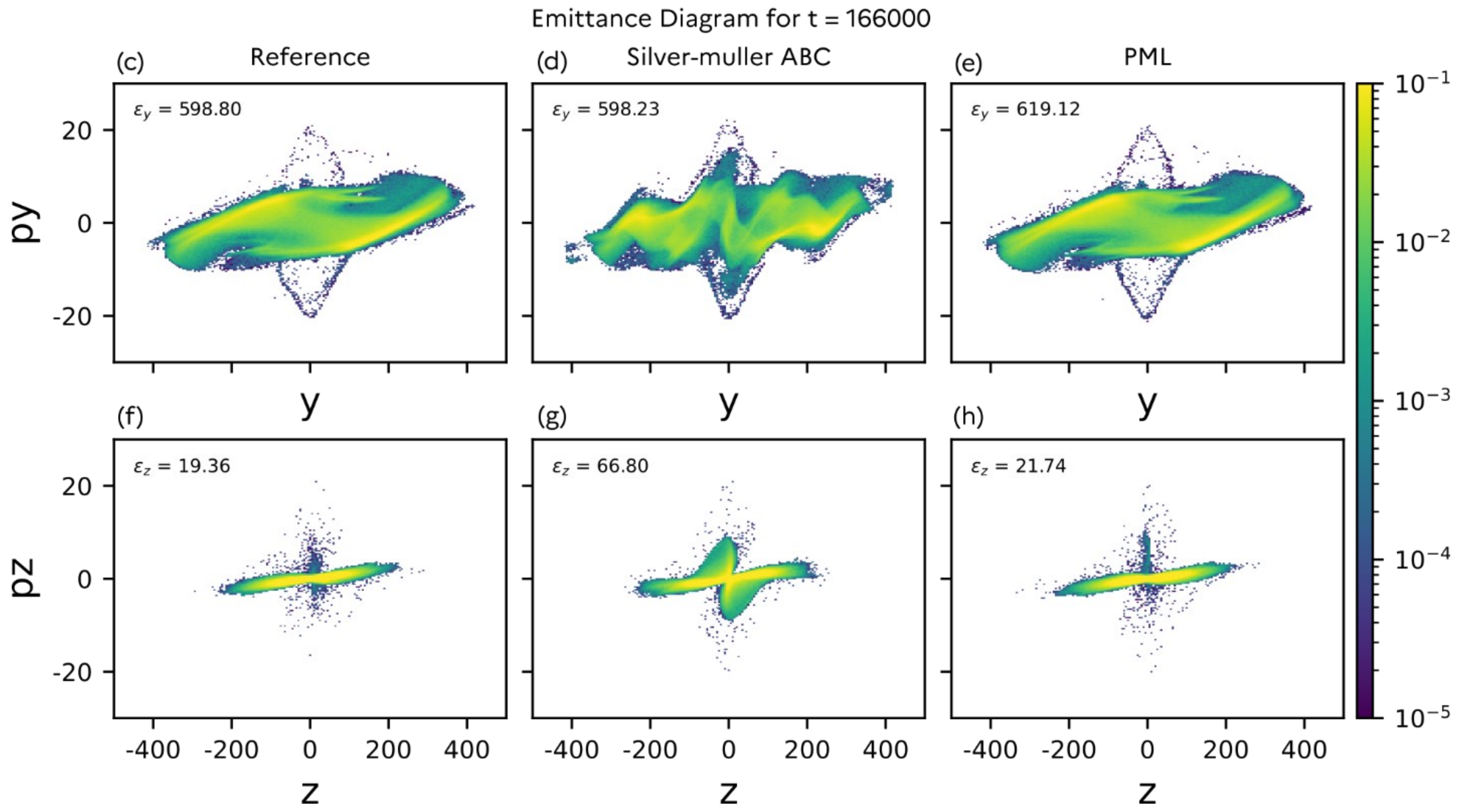
$$\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = i\omega\varepsilon_0 \boxed{\frac{s_x s_z}{s_y}} E_y$$

$$\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} = i\omega\varepsilon_0 \boxed{\frac{s_x s_y}{s_z}} E_z$$

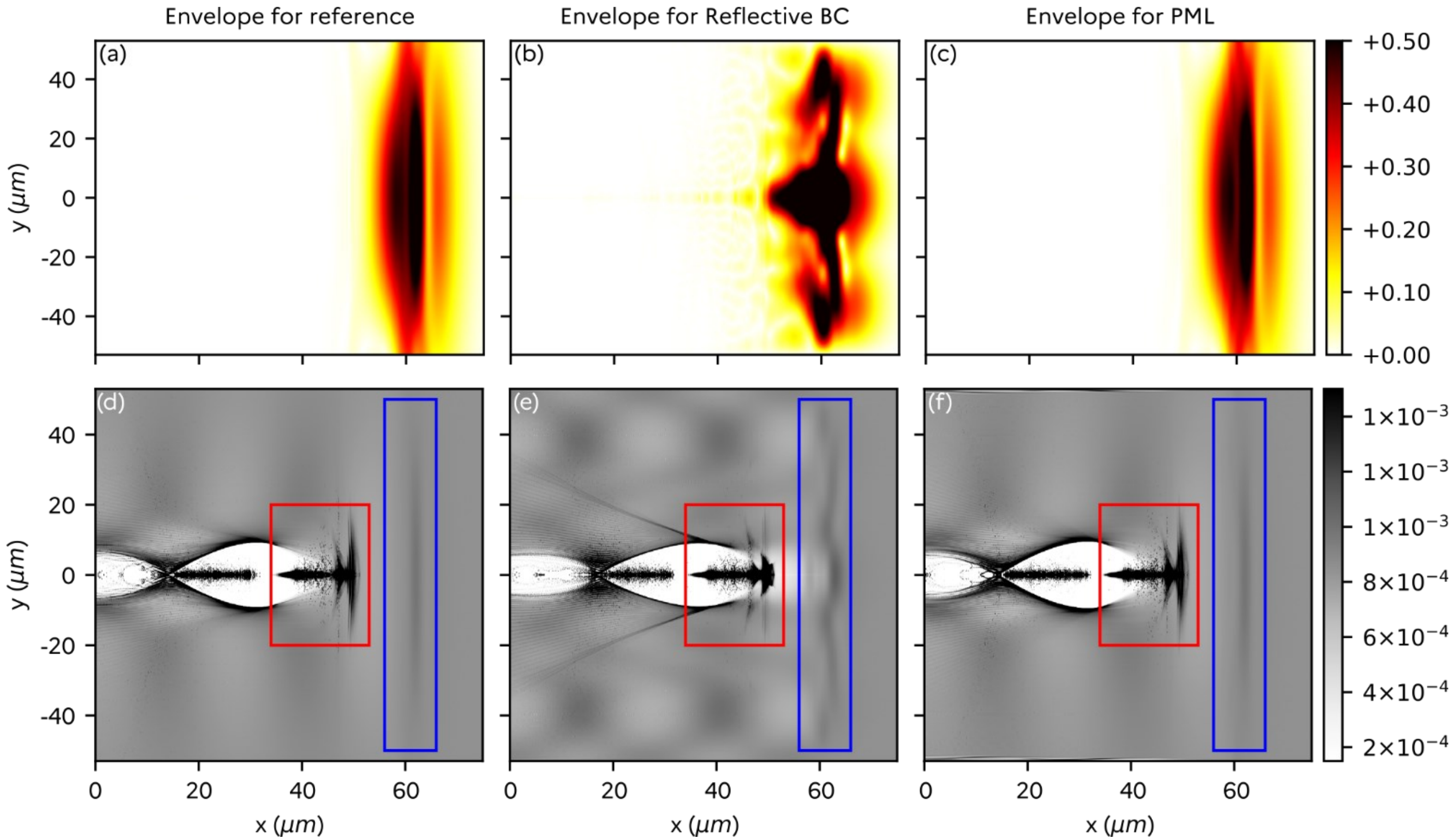
LWFA in Cylindrical geometry



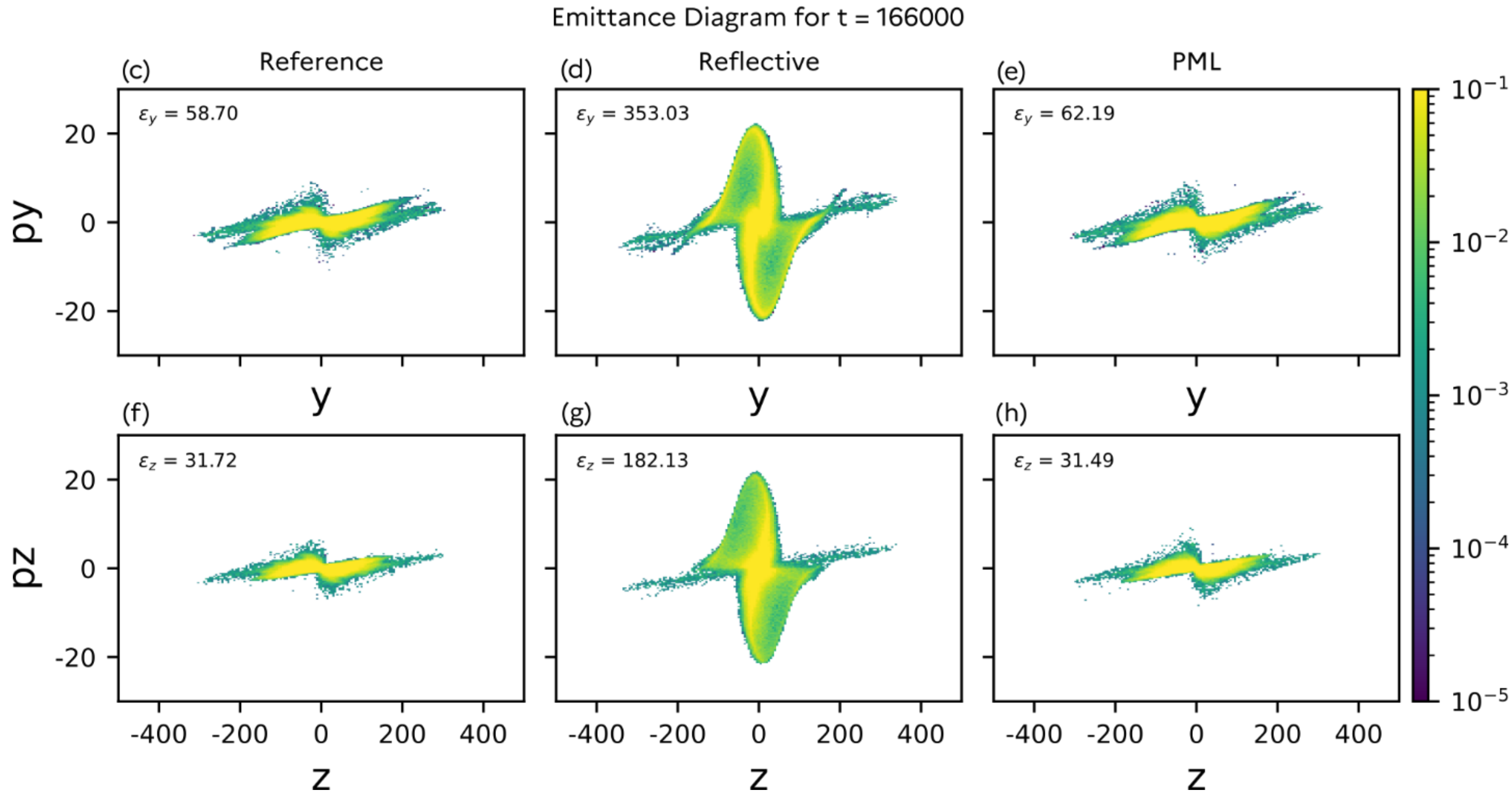
LWFA in Cylindrical geometry



LWFA in Cylindrical geometry (envelope)



LWFA in Cylindrical geometry (envelope)



How to use it… in 2D or 3D cartesian geometry

```
Main(
    …
    number_of_pml_cells = [ [20] ],
    pml_sigma = [lambda x : 20 * x**2],
    pml_kappa = [lambda x : 1 + 79 * x**4],
    …
)
```

How to use it… in AM geometry

```
def sigma(u):
    return 20. * u**2
def integrate_sigma(u):
    return 20./3. * u**3
def kappa(u):
    return 1 + 79. * u**4
def integrate_kappa(u):
    return u + 79./5. * u**5

Main(
    …
    number_of_pml_cells = [ [20] ],
    pml_sigma = [sigma_x, sigma_r, integrate_sigma_r],
    pml_kappa = [kappa_x, kappa_r, integrate_kappa_r],
    …
)
```

How to use it... with envelope (experimental)

```
Main(
     …
     number_of_pml_cells = [ [20] ],
     pml_sigma = [lambda x : 20 * x**2],
     pml_kappa = [lambda x : 1 + 79 * x**4],
     …
)
```

```
LaserEnvelopeGaussianAM(
     …
     envelope_solver = 'explicit’,
     Envelope_boundary_conditions = [["PML","PML"],["PML","PML"]],
     Env_pml_sigma_parameters = [[0.9,2],[80.0,2],[80.0,2]],
     Env_pml_kappa_parameters = [[1.00,1.00,2],[1.00,1.00,2],[1.00,1.00,2]],
     Env_pml_alpha_parameters = [[0.90,0.90,1],[0.65,0.65,1],[0.65,0.65,1]]
     …
)
```

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Conclusion and Perspectives

Conclusions and Perspectives

Recent Advanced techniques review:

- Azimuthal modes decomposition ("AMcylindrical" geometry);
- Laser Envelope model with envelope ionization module;
- Non-Standard Finite Difference Time Domain;
- BTIS3;
- Customized FIR filter;
- Initialization of relativistic Species' fields;
- Perfectly Matched Layer Standard/Envelope;

Recent Advanced techniques not review in this presentation (but could be useful):

- Macro-Particle Merging;
- Tilted plane injection for Laser.

Work in progress and perspectives:

Multi-grid Multi-domain decomposition.

Acknowledgements

Thanks and keep Smileing ;)

Thanks for supporting this event

Contributing labs, institutions & funding agencies

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Back-up slide for questions

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Field initialization of relativistic Species

Relativistic Species Initialization: field computation

Immobile Species ($\gamma_0 = 1$):
Poisson's Equation

$$\nabla^2 \Phi = -\rho$$

$$\mathbf{E} = \Big(-\, \partial_x \Phi, -\partial_y \Phi, -\partial_z \Phi \Big)$$

Moving Species ($\gamma_0 > 1$) :
"Relativistic" Poisson's Equation

$$\left(\frac{1}{\gamma_0^2} \partial_x^2 + \nabla_\perp^2 \right) \Phi = -\rho$$

$$\mathbf{E} = \Big(-\frac{1}{\gamma_0^2} \partial_x \Phi, -\partial_y \Phi, -\partial_z \Phi \Big)$$

$$\mathbf{B} = \frac{\beta_0}{c} \hat{\mathbf{x}} \times \mathbf{E}$$

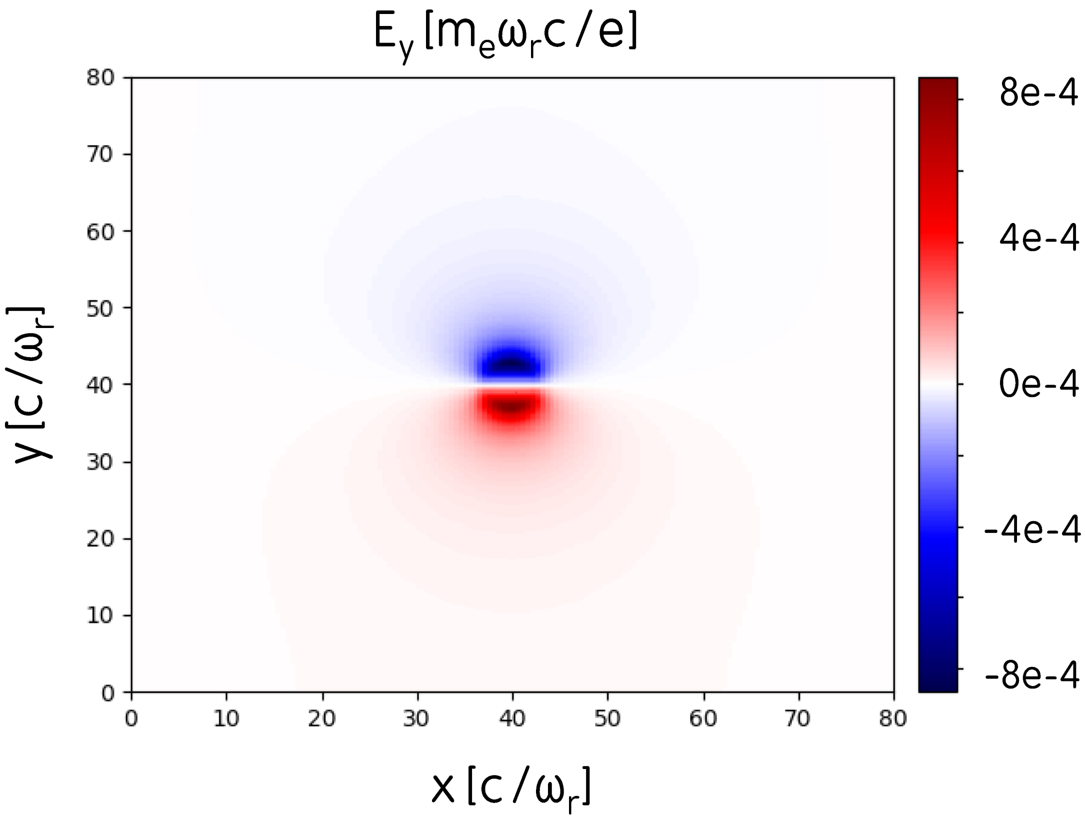
Hypothesis: negligible energy spread

J.-L. Vay, Phys. Plas. (2008)

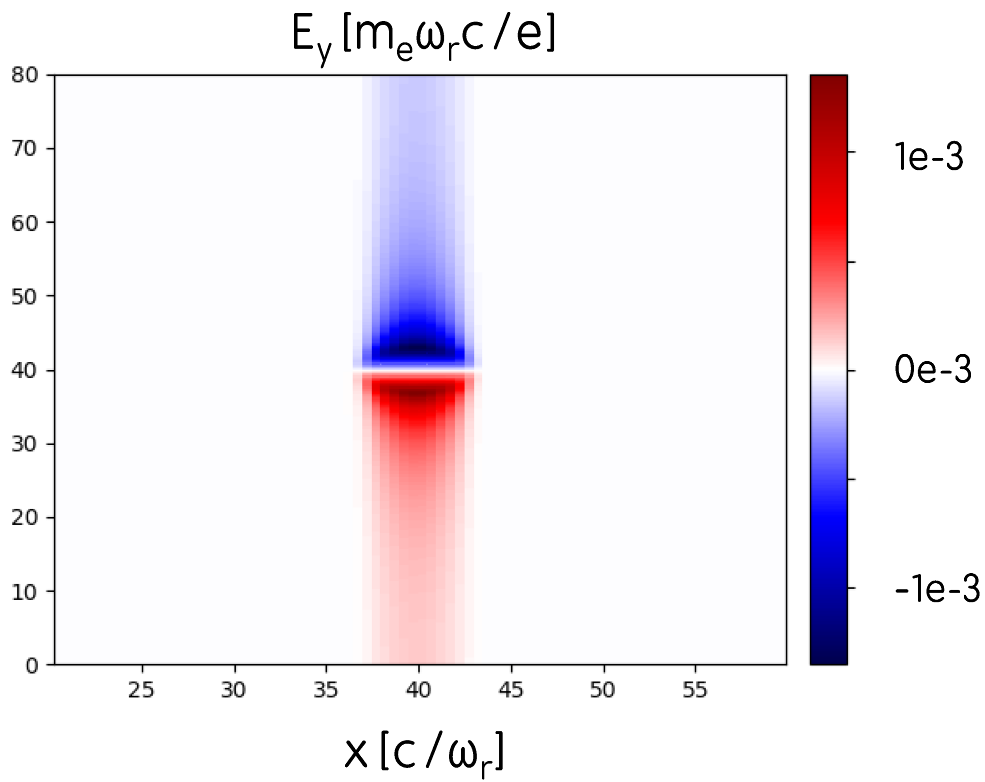
F. Massimo, et al, NIMA (2016)

Relativistic Species Initialization example: electron sphere

$\gamma_0 \sim 1$ ($v_x << c$)

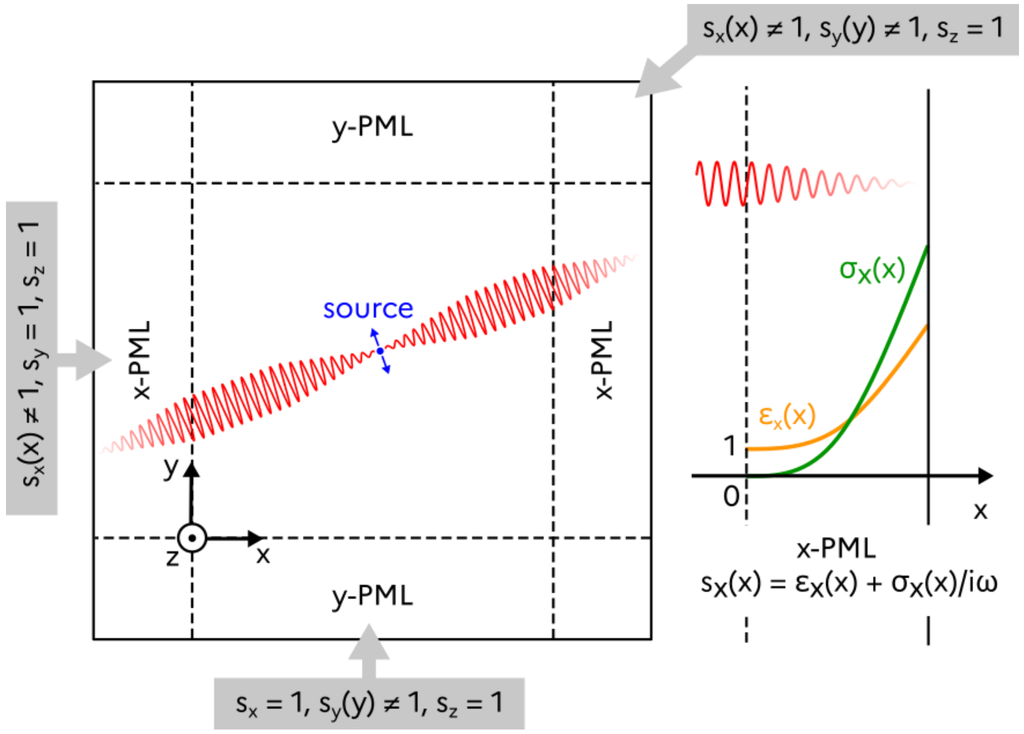


$\gamma_0 = 200$ (relativistic, $v_x \sim c$, E~100 MeV)



Perfectly Matched Layer

Perfectly Matched Layer (PML): Concept



In Smilei)

- For all geometries
- For standard fields and envelope

Maxwell Faraday

$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = -i\omega\mu_0 \boxed{\frac{s_y s_z}{s_x}} H_x$$

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = -i\omega\mu_0 \boxed{\frac{s_x s_z}{s_y}} H_y$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -i\omega\mu_0 \boxed{\frac{s_x s_y}{s_z}} H_z$$

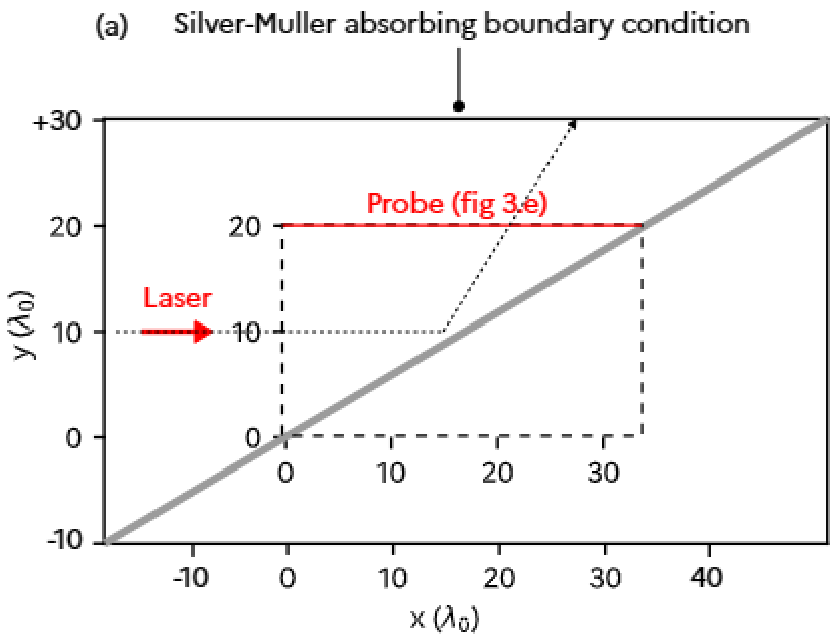
Maxwell Ampere

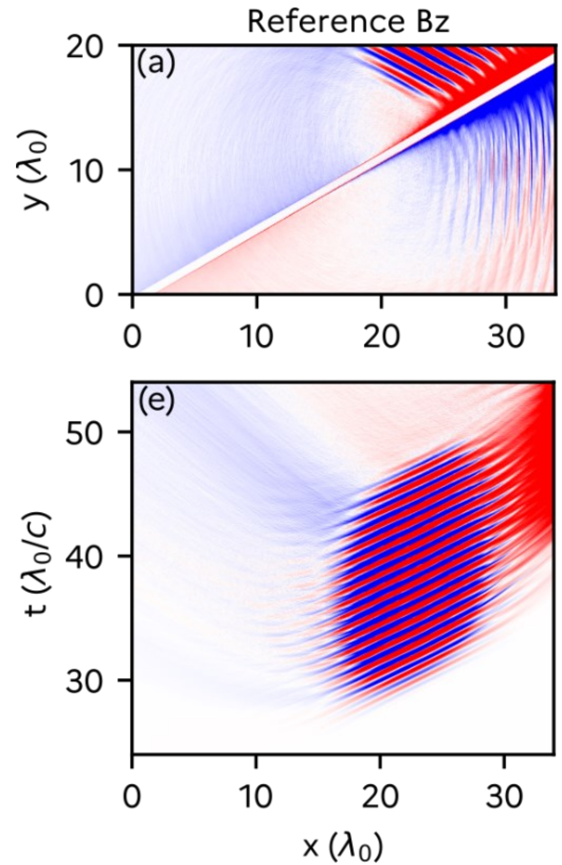
$$\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} = i\omega\varepsilon_0 \boxed{\frac{s_y s_z}{s_x}} E_x$$

$$\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = i\omega\varepsilon_0 \boxed{\frac{s_x s_z}{s_y}} E_y$$

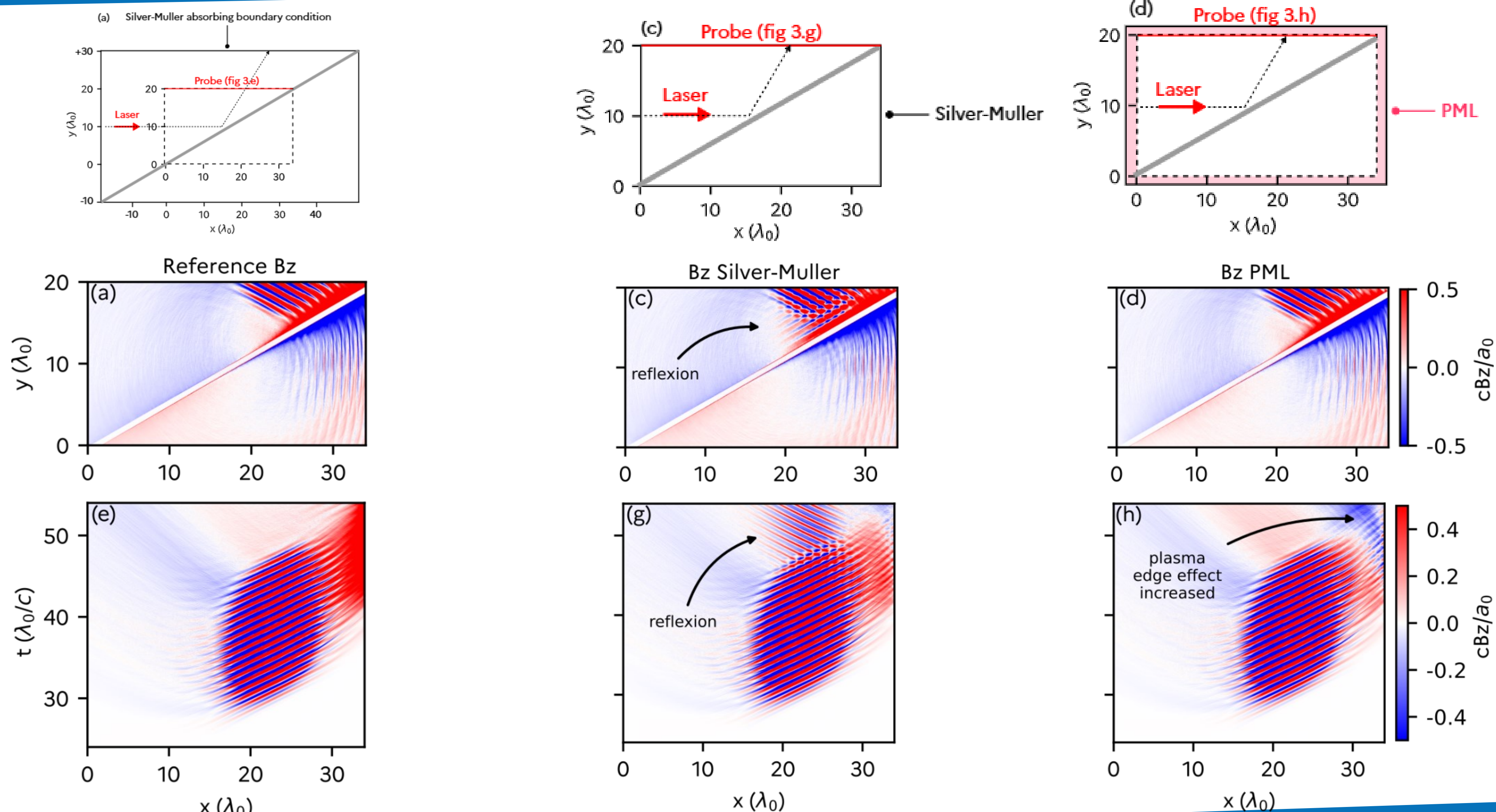
$$\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} = i\omega\varepsilon_0 \boxed{\frac{s_x s_y}{s_z}} E_z$$

X-UV emission from laser and overdense plasma foil interaction





X-UV emission from laser and overdense plasma foil interaction



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Macro-Particle Merging

Particle Merging: when should we use it?

- Macro-particles accumulate in a fraction of the simulation
  (e.g. Weibel collision shocks, laser wakefield acceleration)

- Macro-particles are generated in a large quantity due to some additional physical phenomenon
  (e.g. ionization, macro-photon emission, QED cascades…)

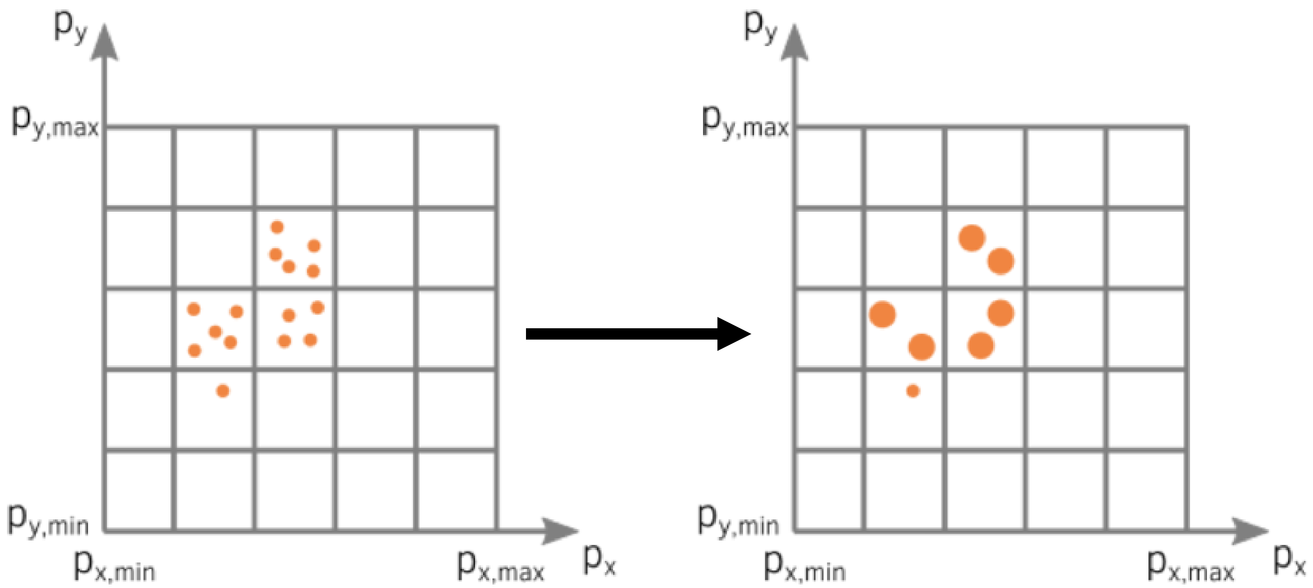
- Macro-particles travel in large quantities outside interesting physical regions

Particle Merging: Smilei implementation

For each cell:

Binning in the momentum space

Merge Macro-particles per momentum cells



M. Vranic et al., Comp. Phys. Comm. (2015)

Particle Merging: concept

Conserved macro-particle quantities:

$$w_t = \sum_{k \in \mathrm{M}} w_k$$ Total weight

$$\varepsilon_t = \sum_{k \in \mathrm{M}} w_k \varepsilon_k$$ Total energy

$$\mathbf{p}_t = \sum_{k \in \mathrm{M}} w_k \mathbf{p}_k$$ Total momentum

Merging M macro-particles into macro-particles a and b:

$$w_t = w_a + w_b$$
$$\mathbf{p}_t = w_a \mathbf{p}_a + w_b \mathbf{p}_b$$
$$\varepsilon_t = w_a \varepsilon_a + w_b \varepsilon_b$$

$$\varepsilon_a^2 = p_a^2 + 1$$
$$\varepsilon_b^2 = p_b^2 + 1$$

M. Vranic et al., Comp. Phys. Comm. (2015)

Particle Merging: how to use it

In the namelist, Particle Merging is part of the Species block:

```
Species(
        …
        # Merging
        merging_method  = "vranic_spherical",
        merge_every     = 5,
        # other merging parameters
        …
)
```

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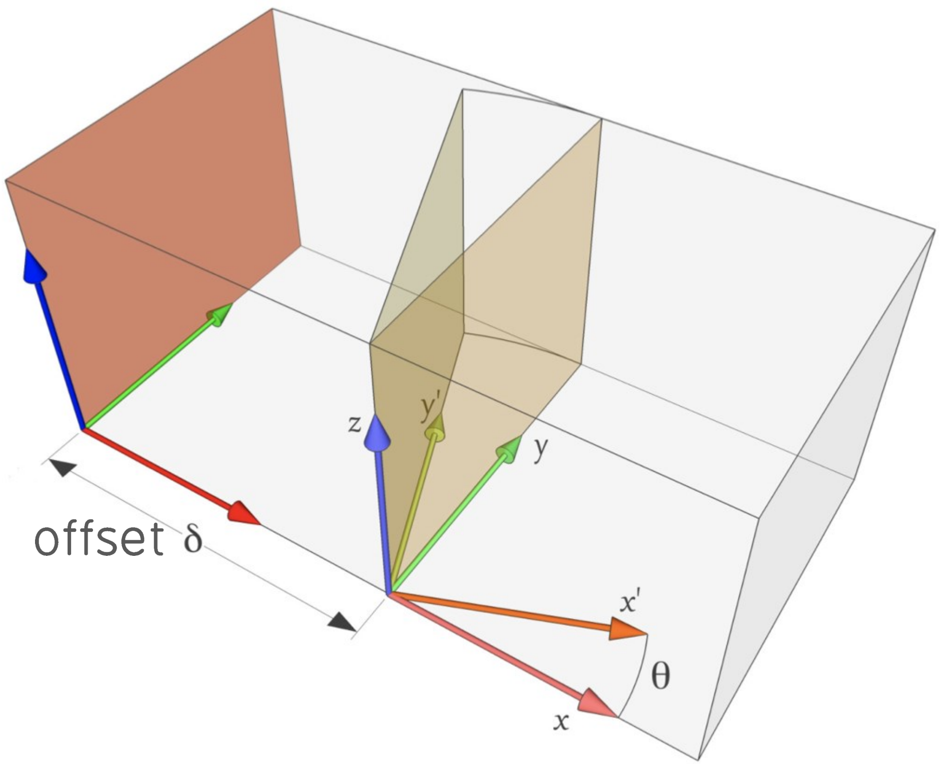
Laser Offset

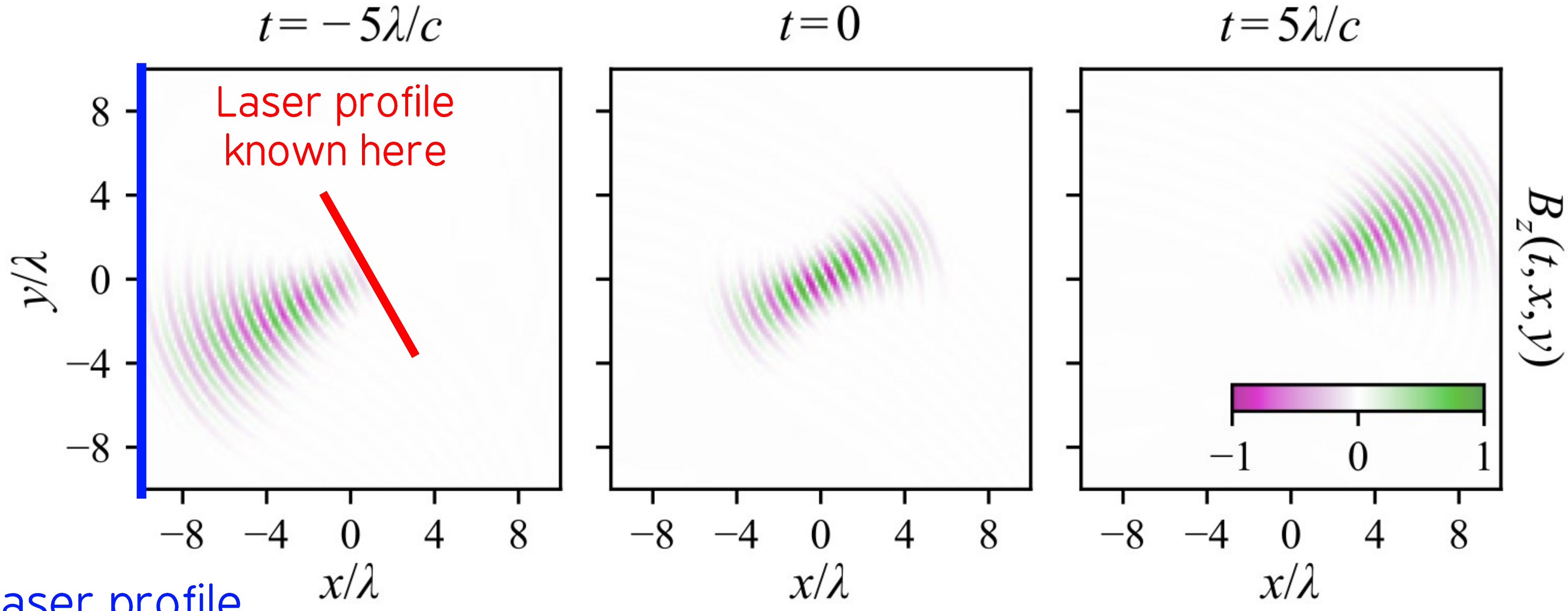
Laser Offset: Laser profile known on tilted plane



F. Perez and M. Grech, Phys. Rev. E (2019)

Title

Sometimes the laser profile is known on a plane other than a window border



Laser profile
Injected from here

How to use it

```
LaserOffset(
        …
        box_side = "xmin",
        space_time_profile = [ By_profile, Bz_profile ],
        offset = 10.,
        extra_envelope = tconstant(),
        angle = 10./180.*3.14159
        …
)
```

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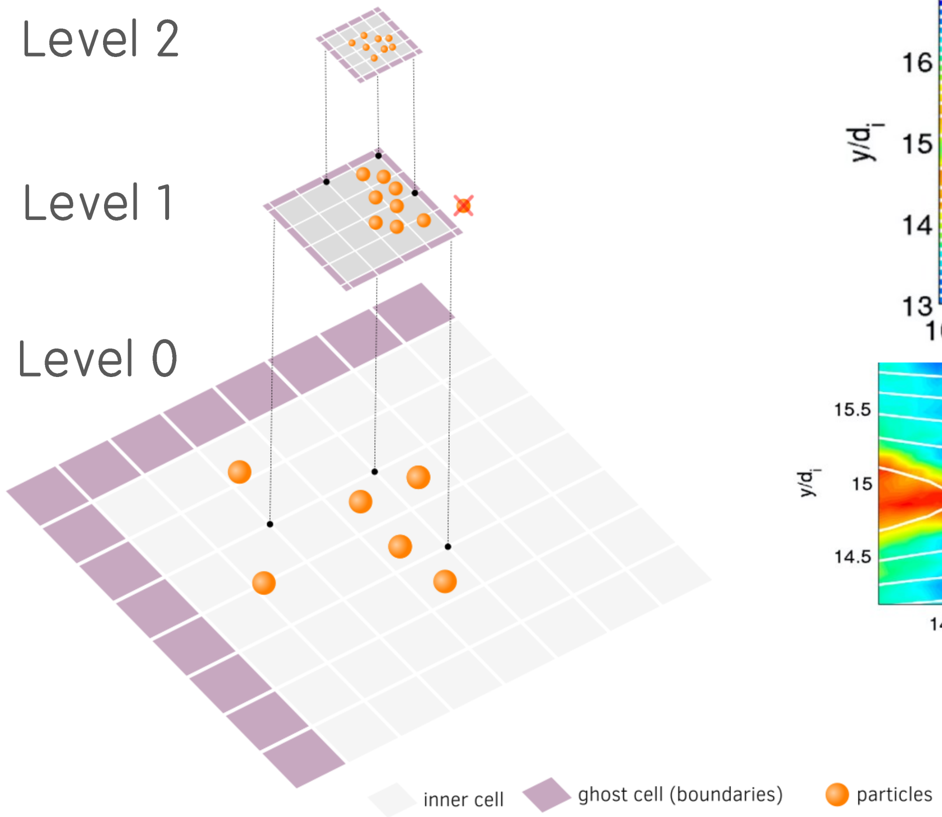
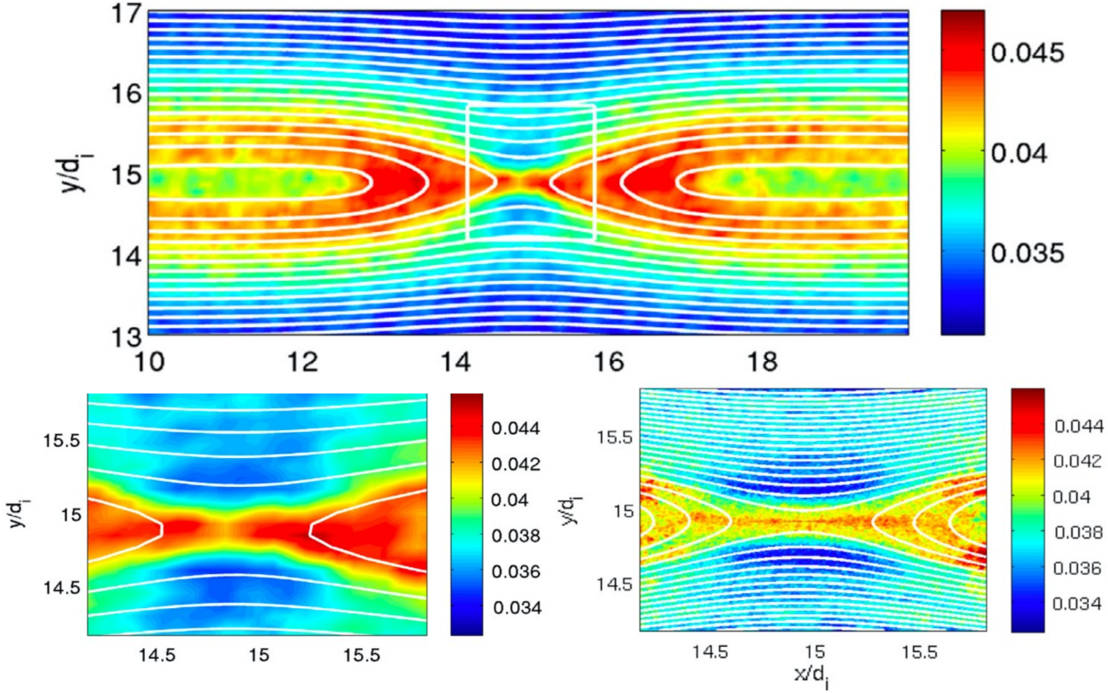
Perspectives: Multi-Level-Multi-Domain PIC

Multi-Level Multi-Domain Particle in Cell



Magnetic Reconnection Simulation



A. Beck et al., J. Comp. Phys. (2014)