Session 3: Additional Components

Smilei) Workshop

Advanced techniques

March 2022

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Motivation

Additional utilities to

- Reduce simulation time through physical approximations:
  Azimuthal Modes decomposition, **Laser Envelope model**,
  Macro-Particle Merging
- Advanced initialization:
  Laser Offset, **Relativistic Species Initialization**
- Reduce numerical artifacts of PIC codes:
  Current Filtering, **Perfectly Matched Layer**,
  Spectral Solvers

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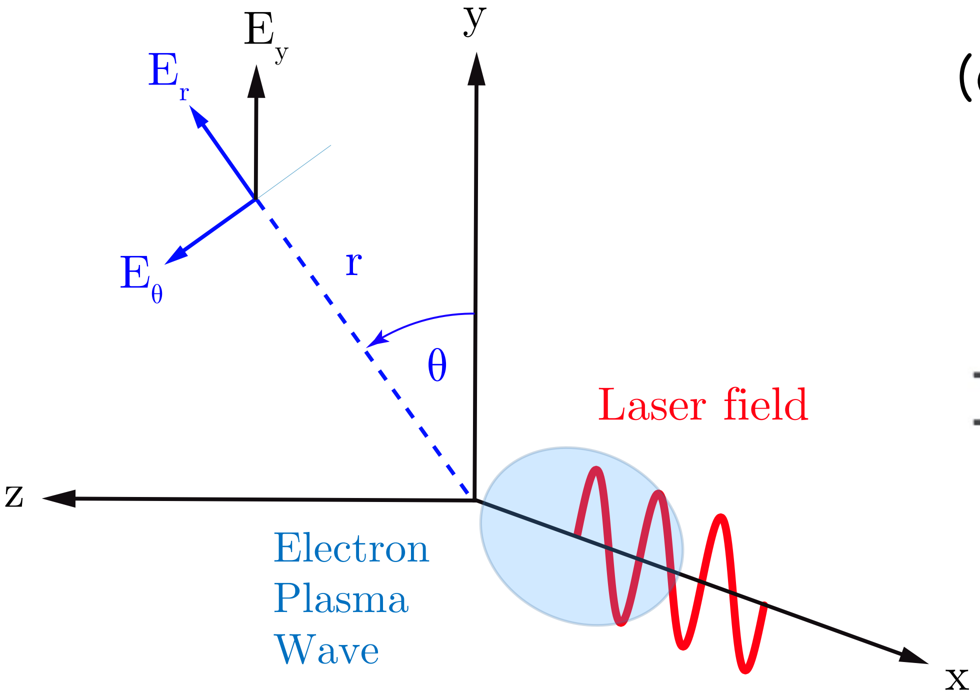
Azimuthal Modes decomposition ("AMcylindrical" geometry)

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 its wake are cylindrically symmetric:

(coefficient with **x,r** dependence) * [cos(**0*θ**)]

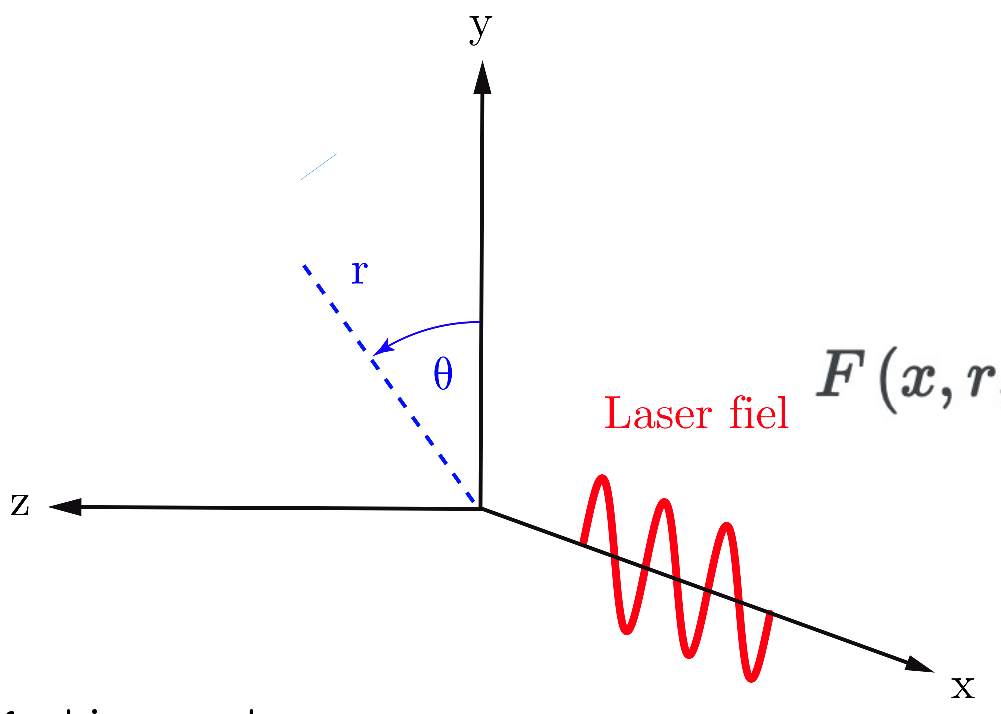
- Linearly polarized laser with cylindrically symmetric envelope:

$$\begin{aligned}\mathbf{E}_\perp(x,r,\theta,t) &= E_y(x,r,\theta,t)\mathbf{e_y}\\ &= E_r(x,r,\theta,t)\mathbf{e_r} + E_\theta(x,r,\theta,t)\mathbf{e}_\theta\\ &= E_y(x,r,t)[\cos(\theta)\mathbf{e_r} - \sin(\theta)\mathbf{e}_\theta].\end{aligned}$$

(coefficient with **x,r** dependence) * [cos(**1*θ**) or sin(**1*θ**)]

Azimuthal Modes decomposition: concept

Quasi-cylindrical set-up



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

Decomposition in Azimuthal modes for scalars and vector components components

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

2D grid instead of 3D grid!

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

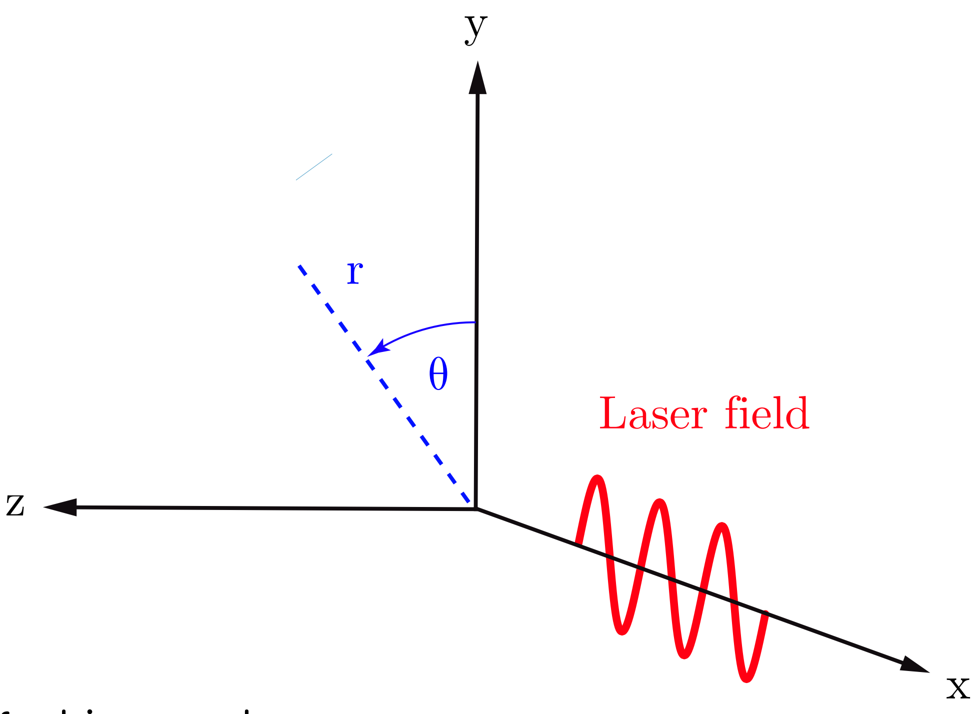
$$+ \tilde{F}^1_{real}\cos(\theta) + \tilde{F}^1_{imag}\sin(\theta)$$ m = 1

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

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

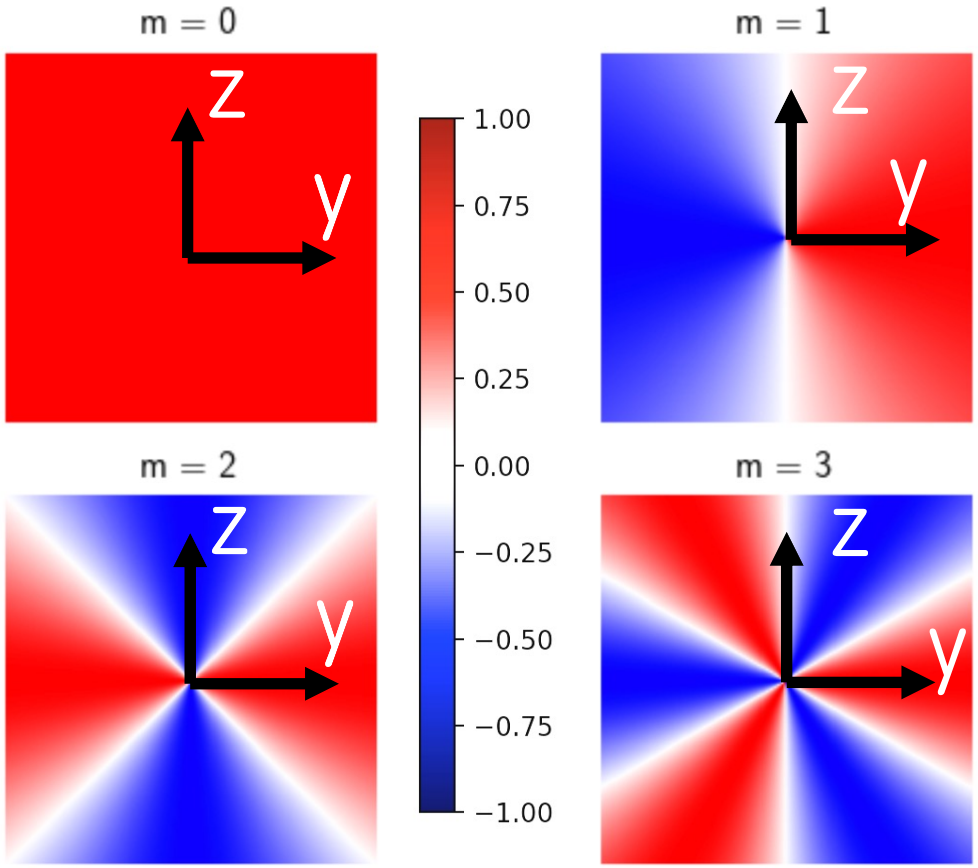
Azimuthal Modes decomposition: concept

Quasi-cylindrical set-up



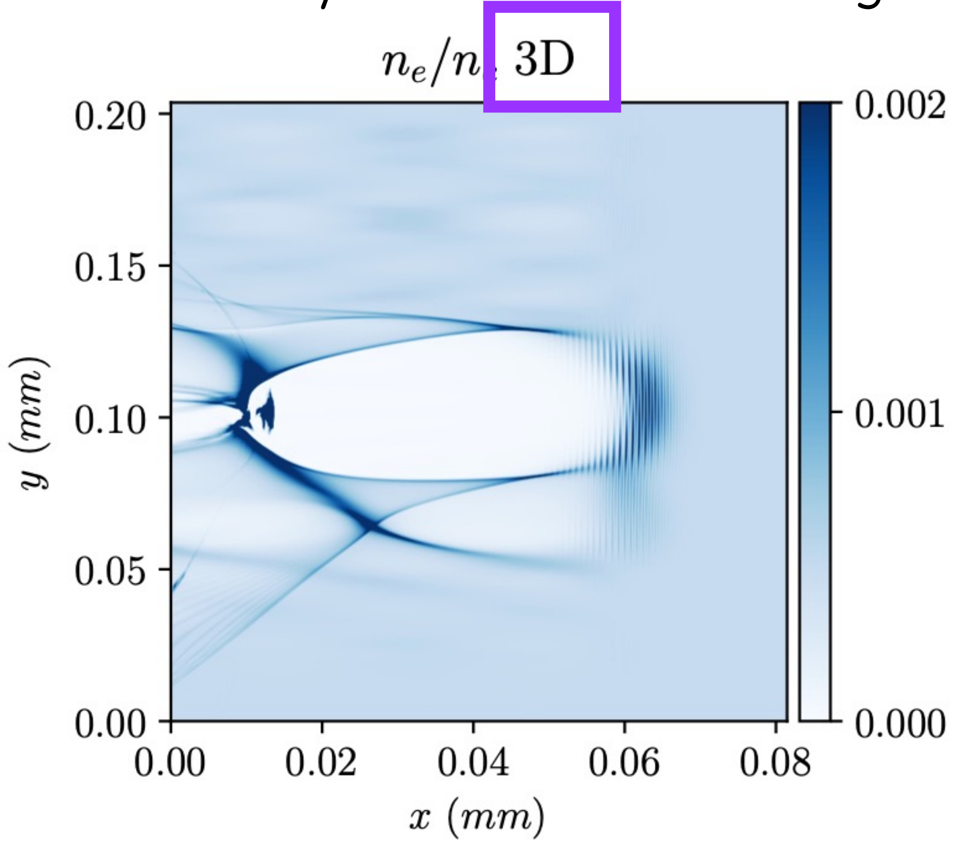
A. Lifschitz et al.,
J. Comp. Phys. (2008)

Azimuthal modes Re [$e^{-im\theta}$]
(scalar field or vector component)



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

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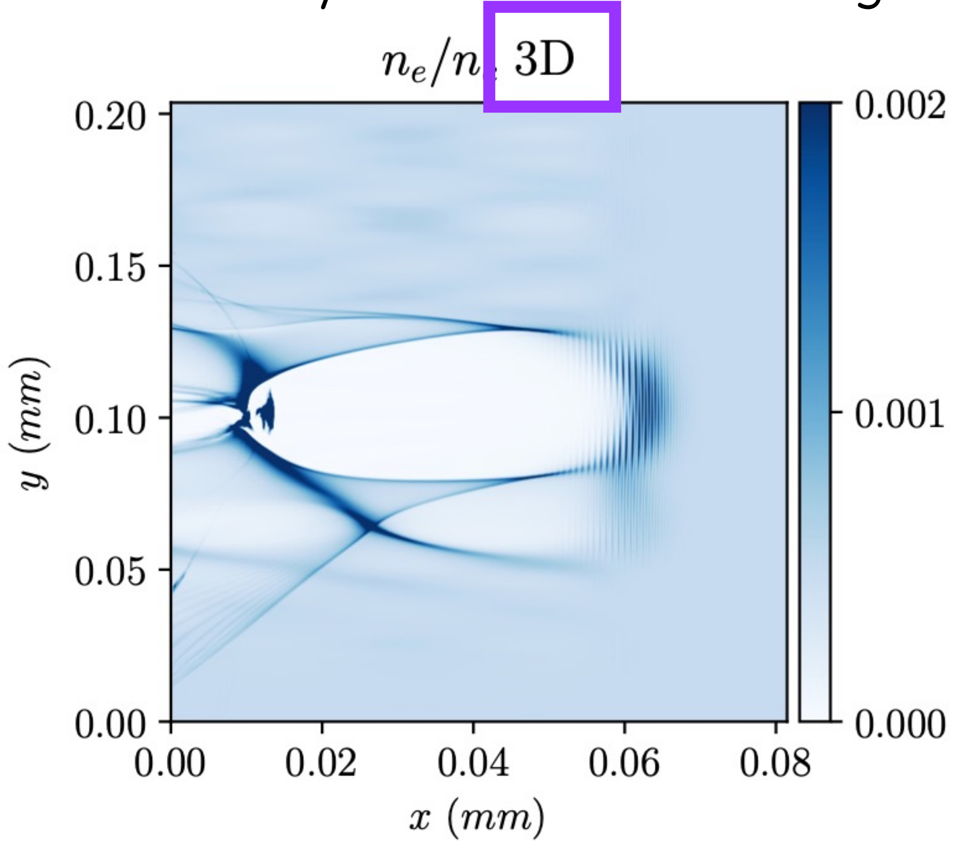

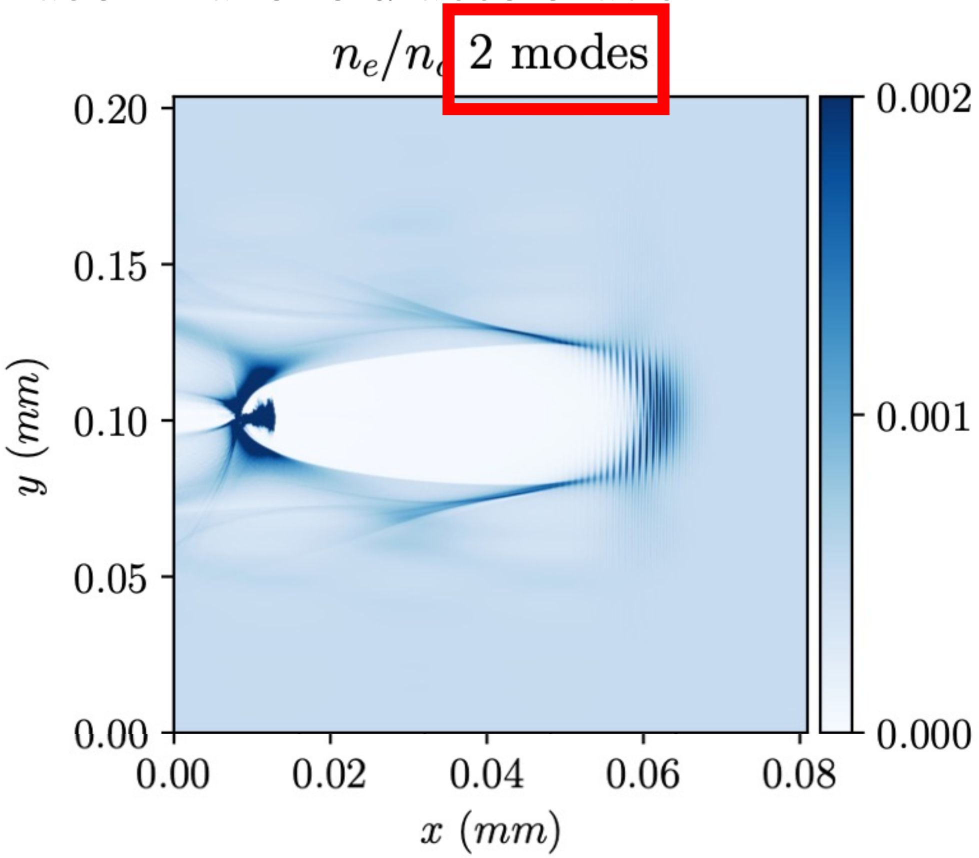

I. Zemzemi, PhD thesis http://llr.in2p3.fr/IMG/pdf/thesis_postfinal_zemzemi.pdf

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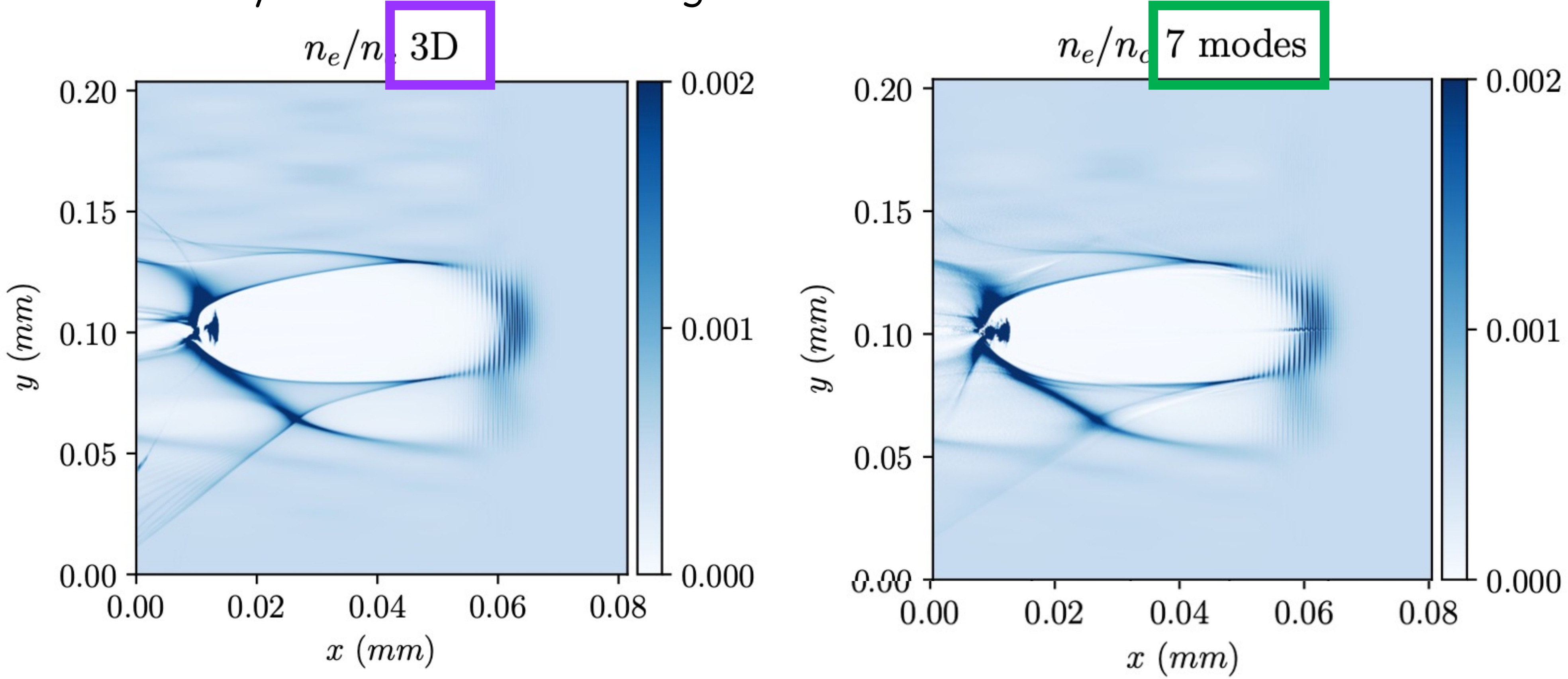


I. Zemzemi, PhD thesis http://llr.in2p3.fr/IMG/pdf/thesis_postfinal_zemzemi.pdf

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	Adaptative vectorization

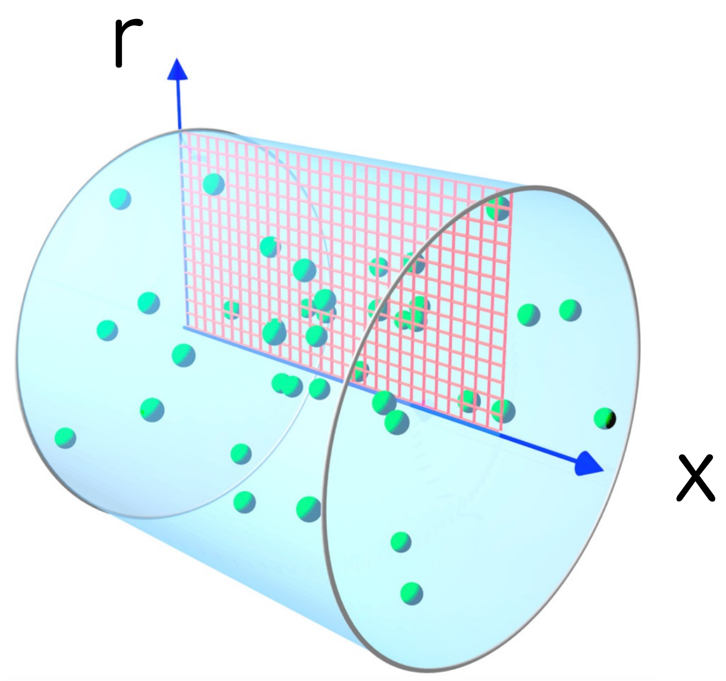
Warning: very asymmetric case,
normally 2-3 modes are enough for laser wakefield acceleration

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

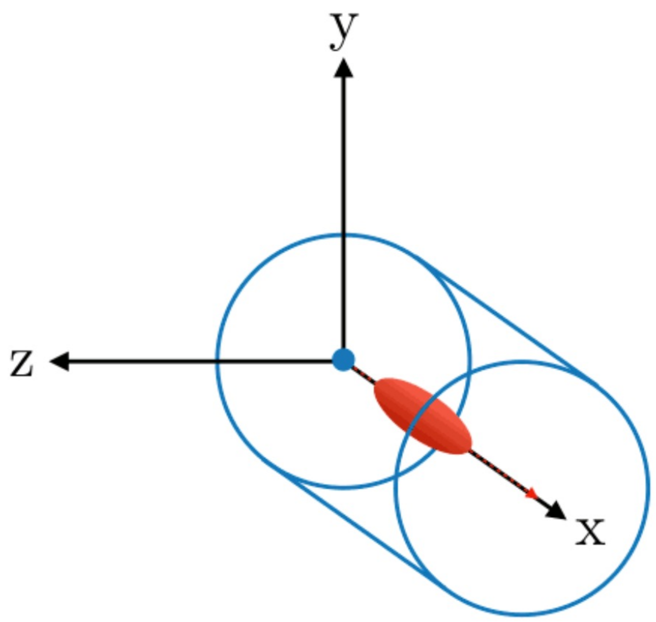
Azimuthal Modes decomposition: how to use it

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

EM Fields, density:
Defined on RZ grid



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



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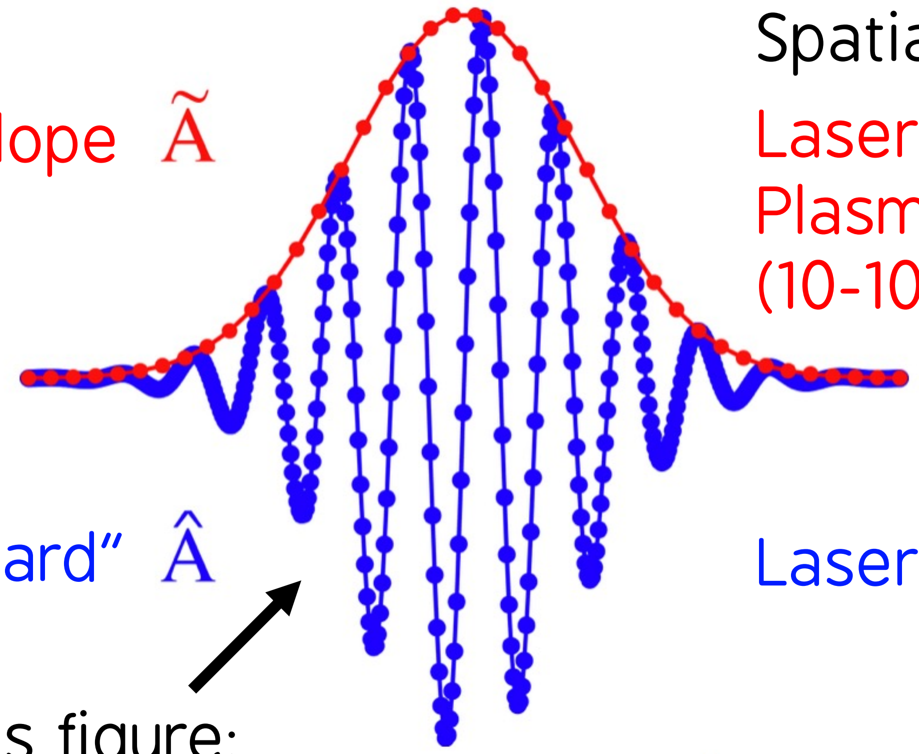
Laser Envelope Model

Laser Envelope Model: concept

Laser Envelope $\tilde{A}$



Laser "Standard" $\hat{A}$

Spatial variation scales:

Laser length ~ Plasma wavelength (10-100 µm)

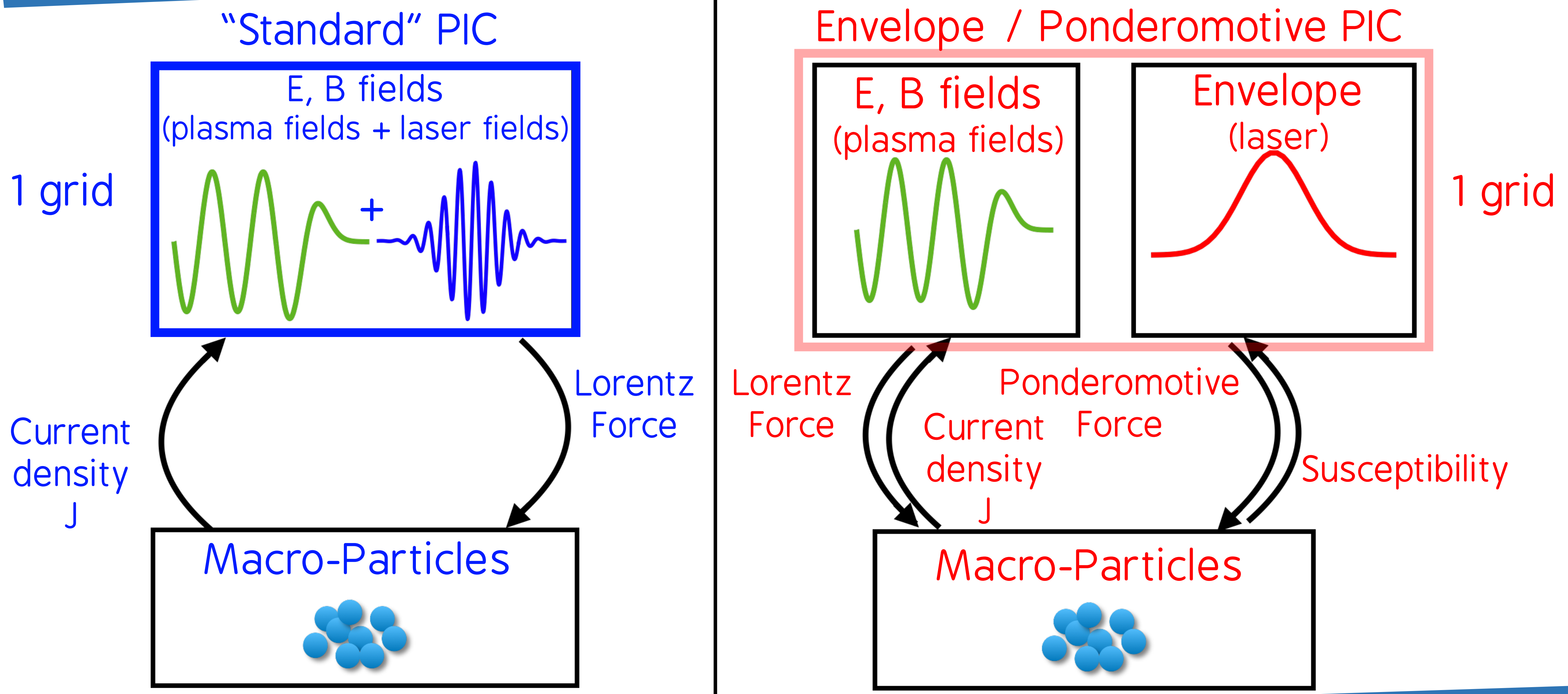
Laser wavelength ~1 µm

In this figure:

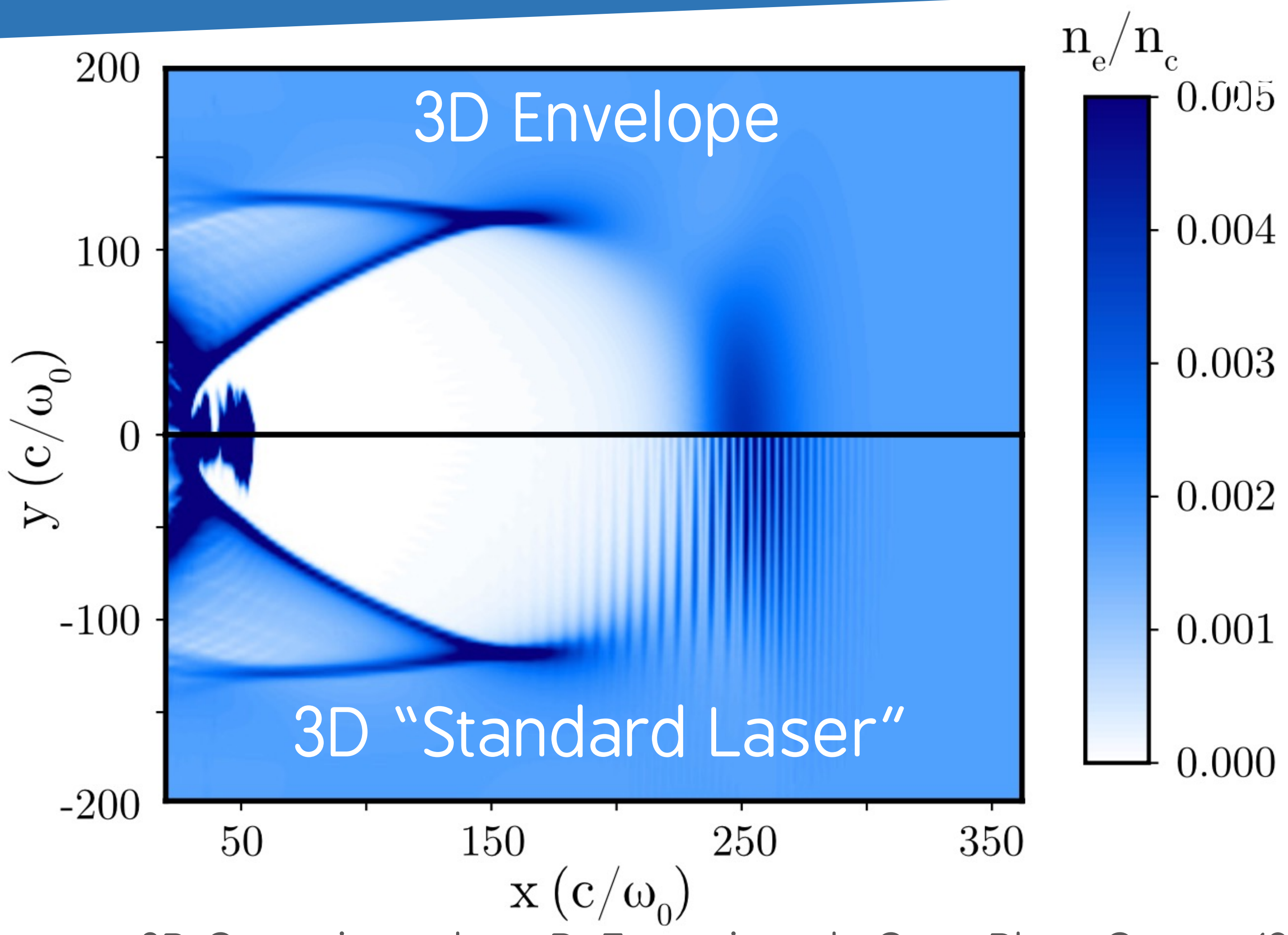
$$\frac{\text{Points sampling Laser "Standard"}}{\text{Points sampling Laser Envelope}} = 10$$

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

Laser Envelope Model: concept



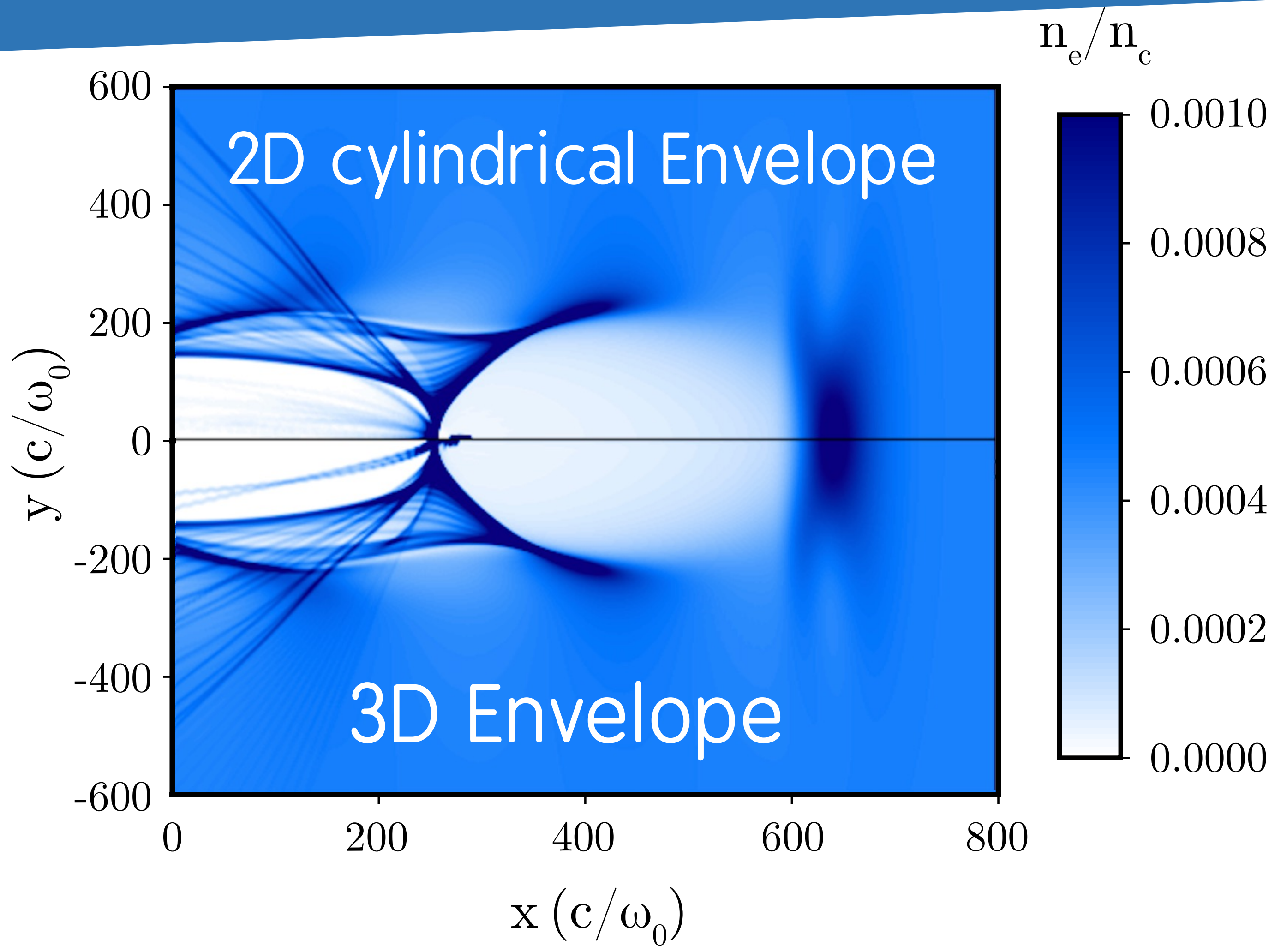
Laser Envelope Model, 3D Cartesian



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

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

Laser Envelope Model, cylindrical geometry (N_AM_modes= 1)



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

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

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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)

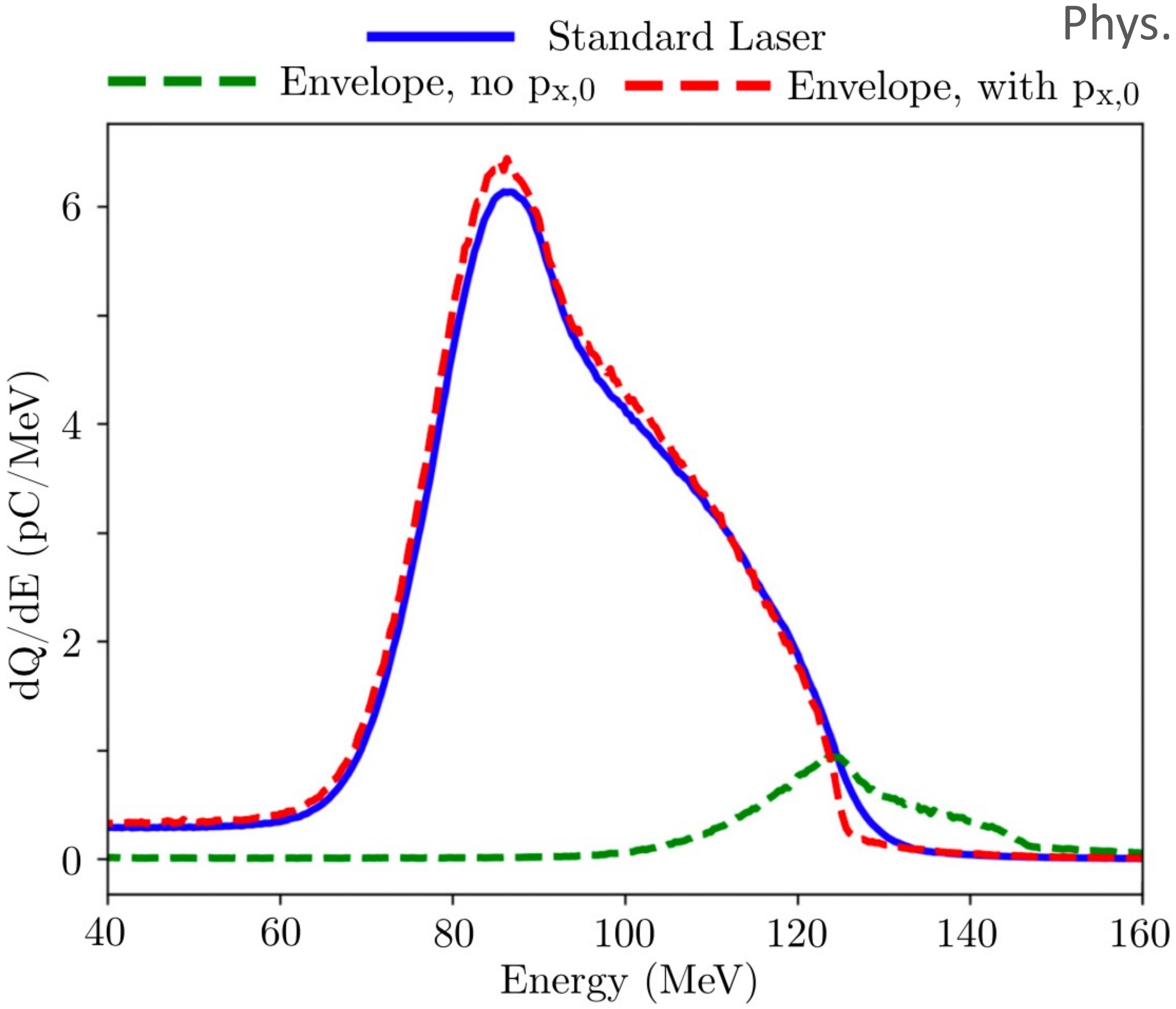
  F. Massimo et al., Phys. Rev. E 102, 033204 (2020)

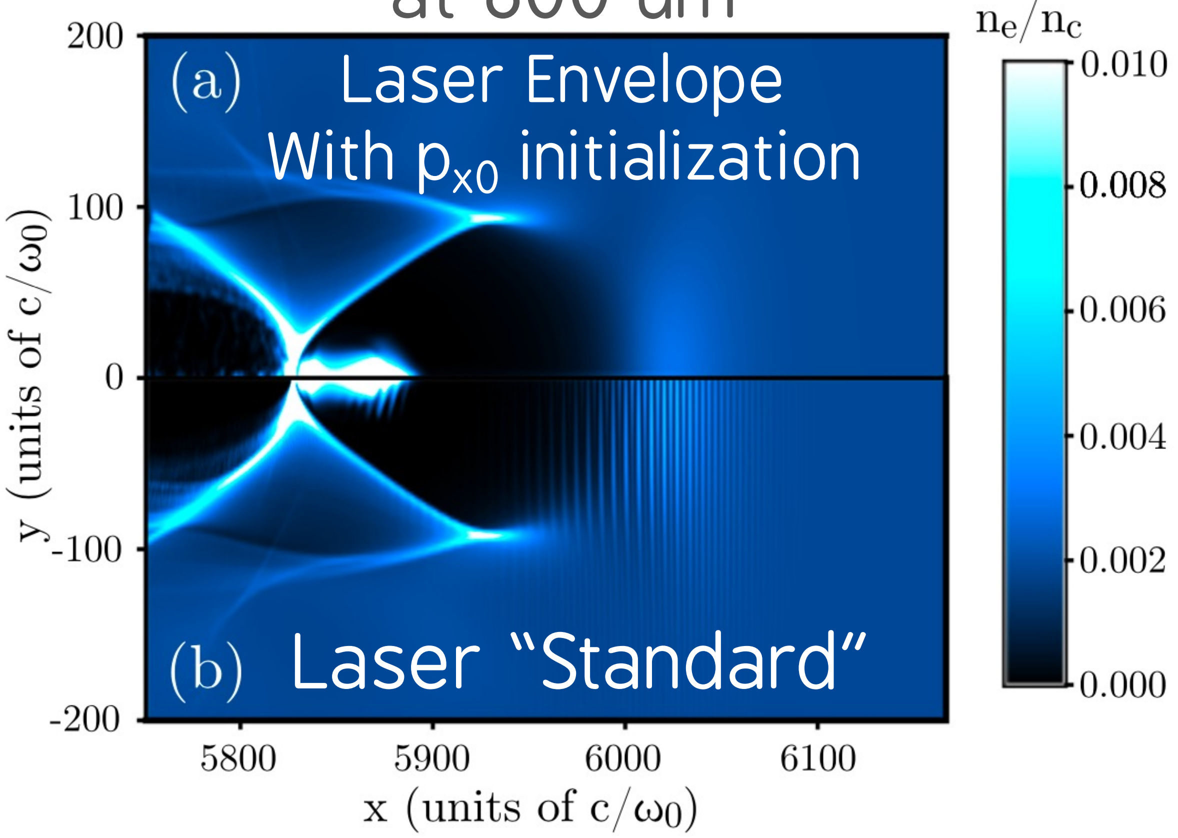
Introduced with Smilei) for all geometries

Laser Envelope Model: LWFA with ionization injection

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

AM Cylindrical LWFA simulation at 800 um





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
$E_{\rm avg}$ [MeV]	90.2	89.6
σ_E/E [rms, %]	11.91	11.52
	Tunnel ionization	Envelope tunnel ionization

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Macro-Particle Merging

Particle Merging: when should we use it?

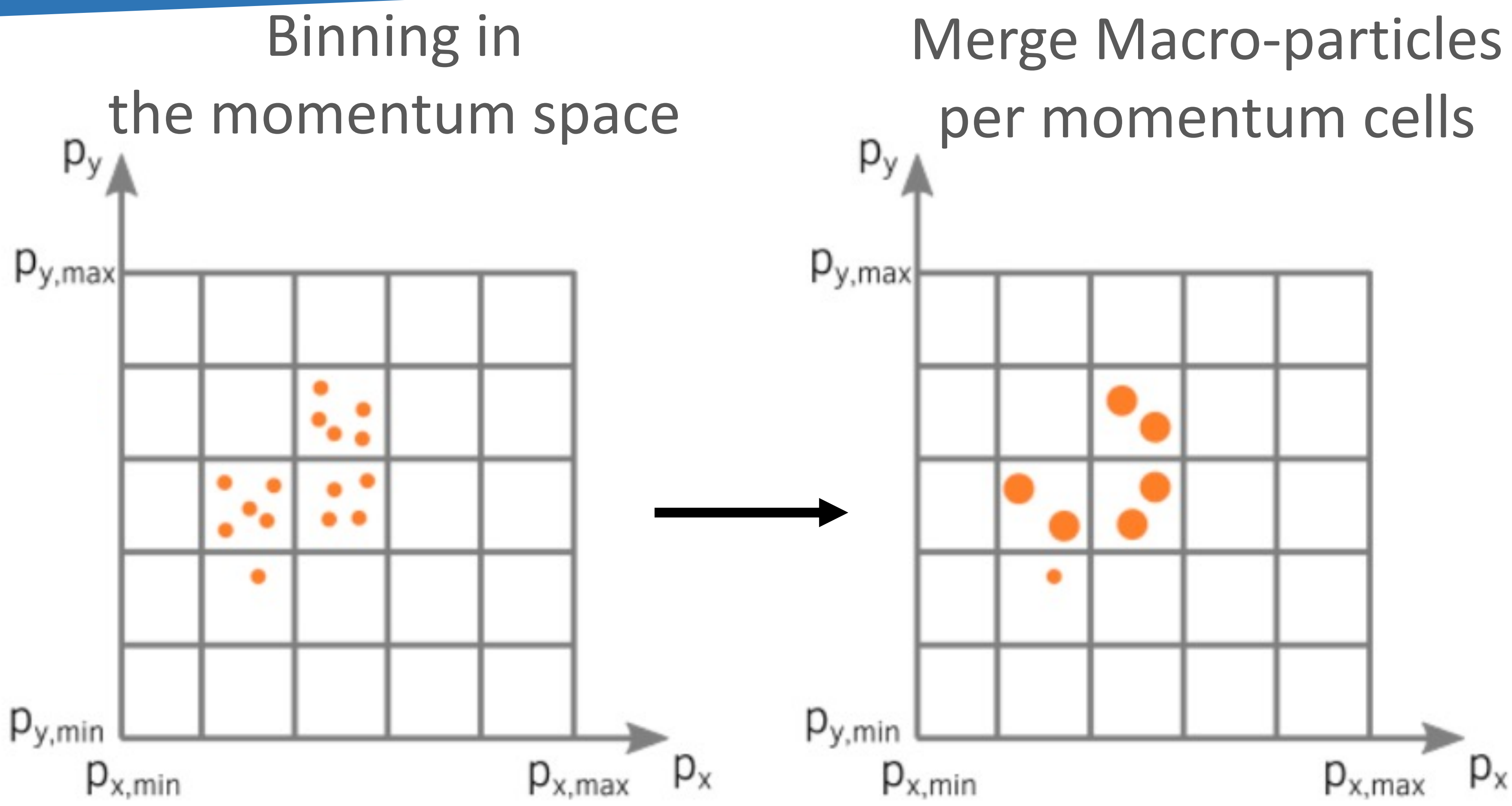
- Macro-particles accumulate in a fraction of the simulation
  (e.g. Weibel collision shocks, laser wakefield acceleration)

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

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

Particle Merging: Smilei implementation

For each cell:



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

Particle Merging: concept

Conserved macro-particle quantities:

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

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

$$\mathbf{p}_t = \sum_{k \in M} w_k \mathbf{p}_k$$ 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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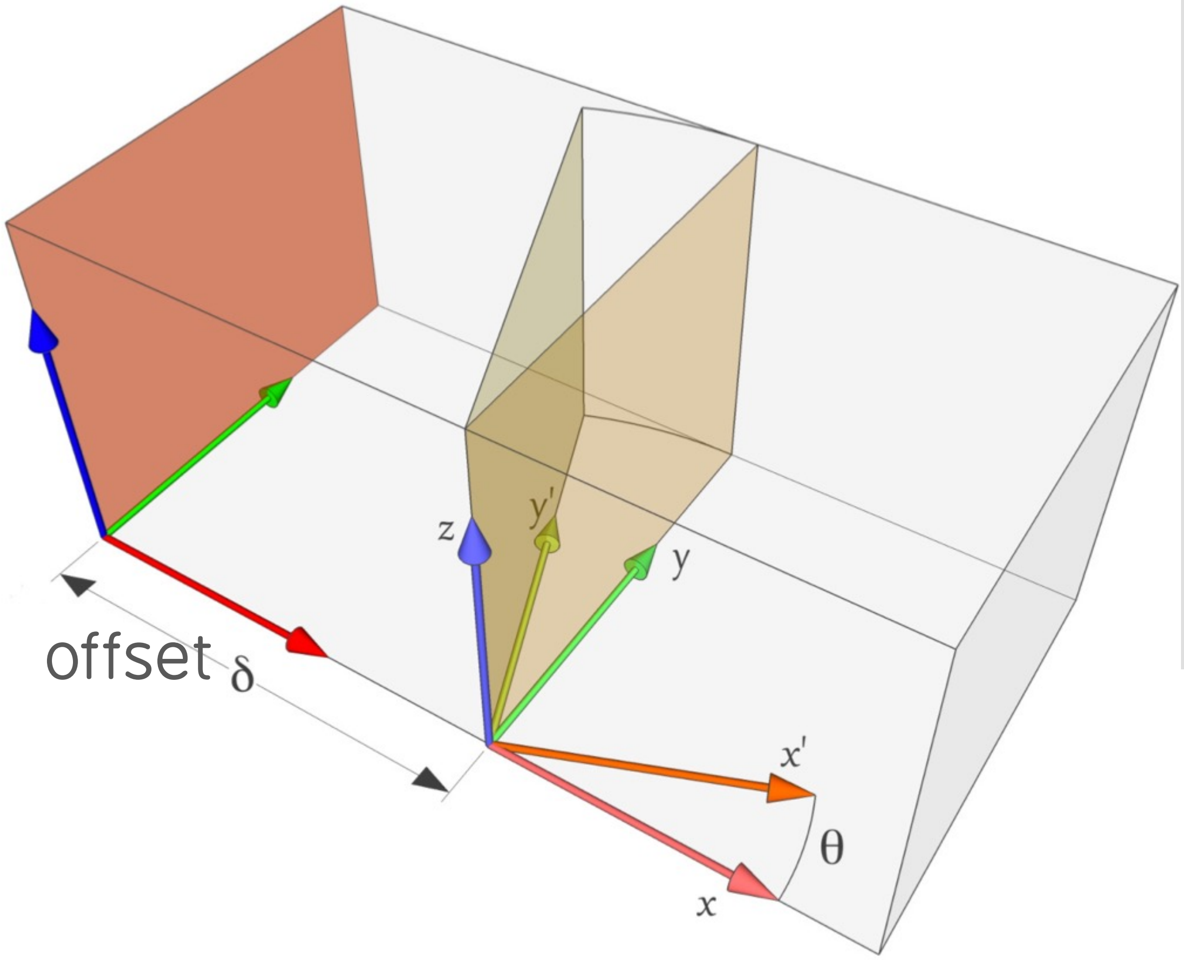
Laser Offset

Laser Offset: Laser profile known on tilted plane

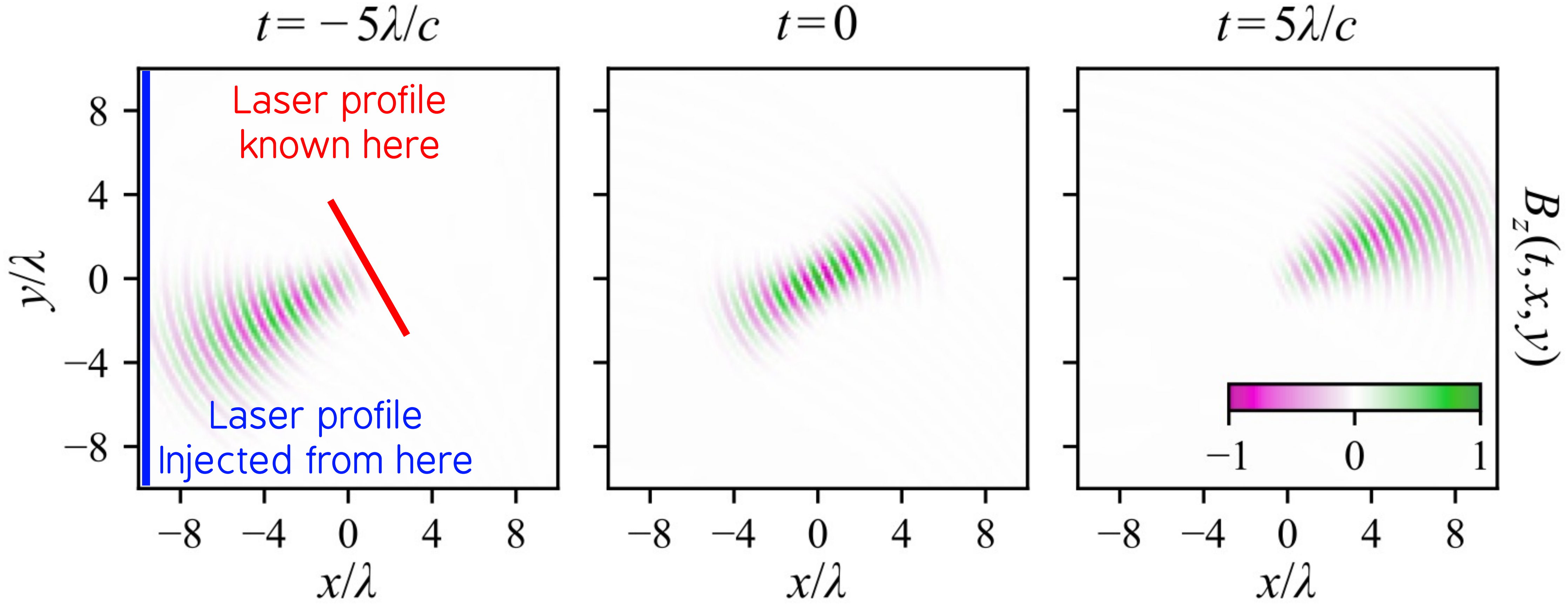



```
LaserOffset(
      box_side = "xmin",
      space_time_profile =
      [ By_profile, Bz_profile ],
      offset = 10.,
      extra_envelope = tconstant(),
      angle = 10./180.*3.14159
      …
      )
```

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

Laser Offset: tilted plane injection

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



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Field initialization of relativistic Species

Relativistic Species Initialization: field computation

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

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

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

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

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

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

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

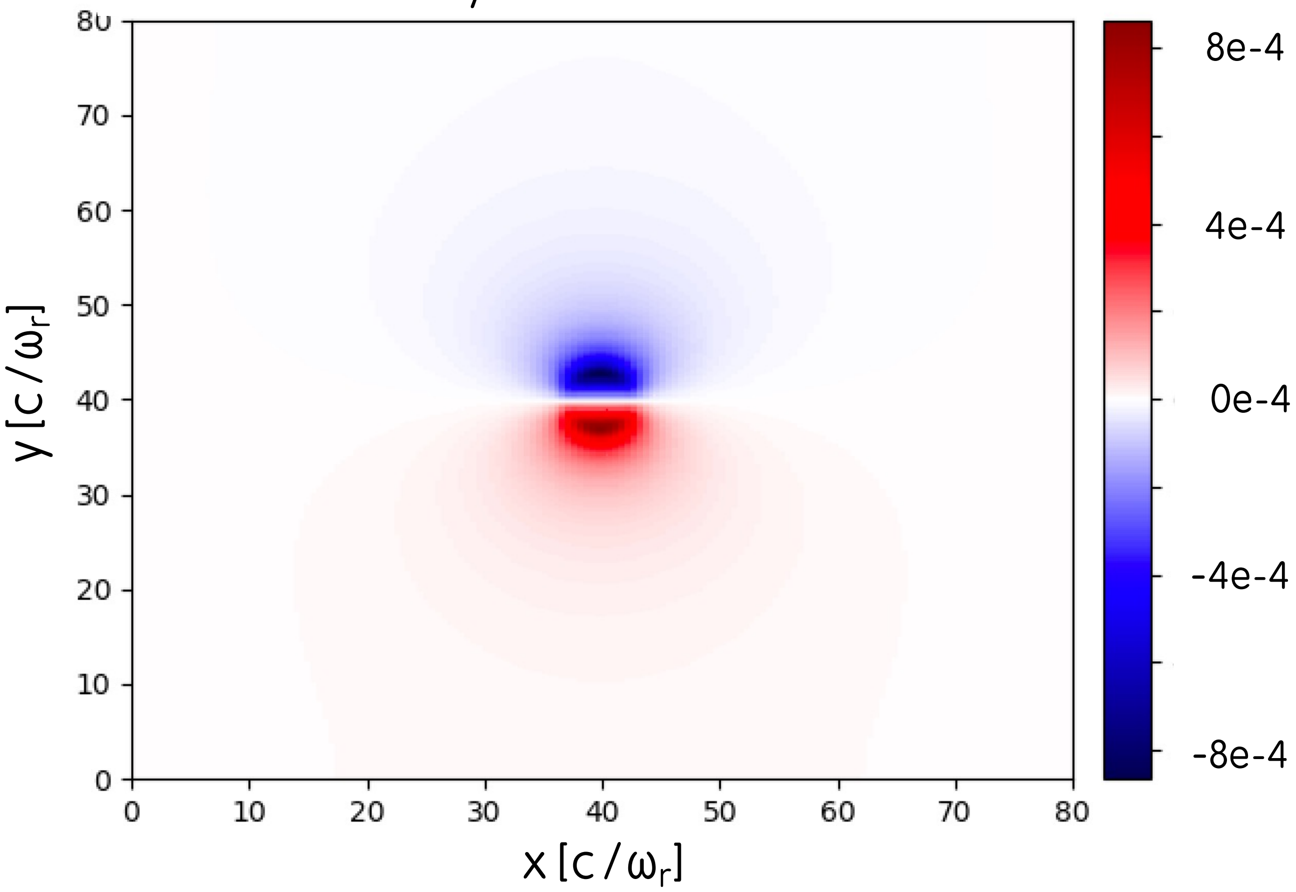
Hypothesis: negligible energy spread

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

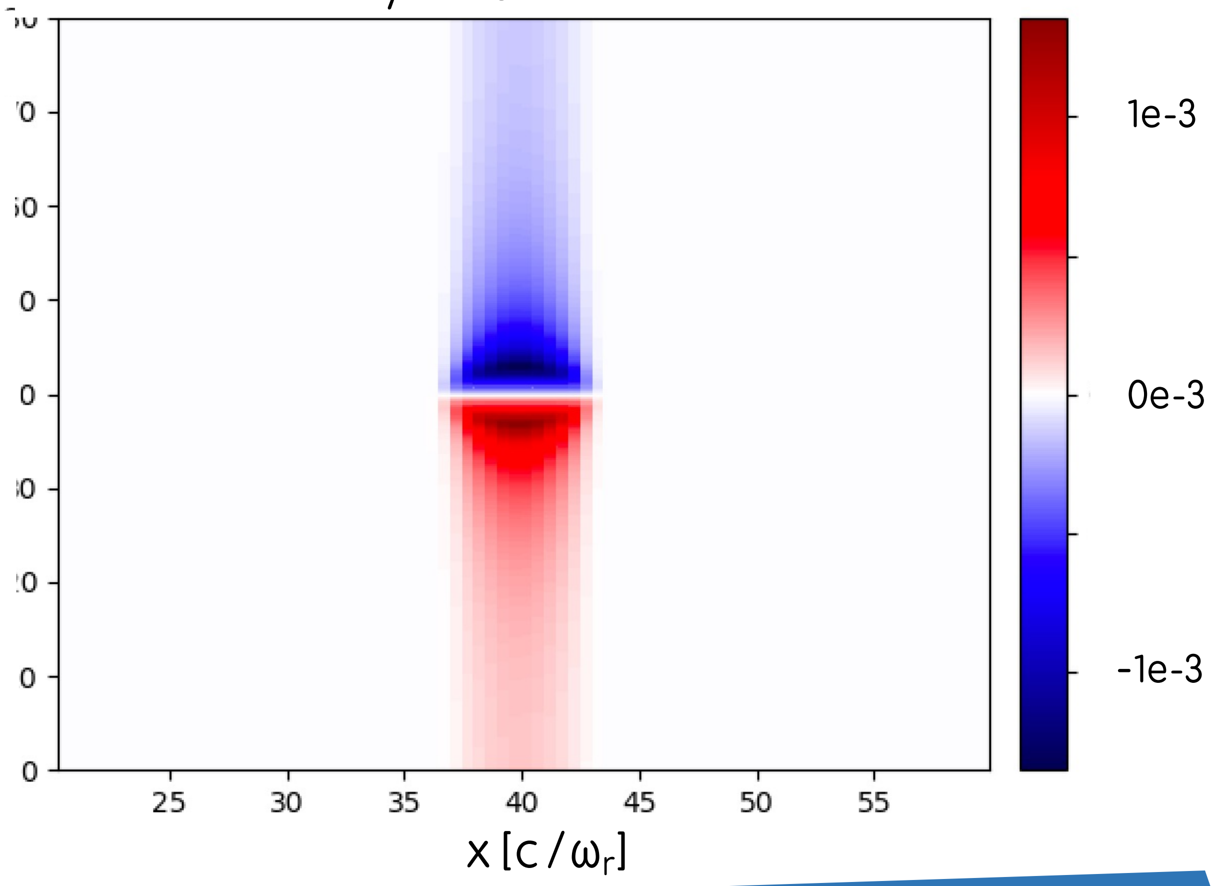
F. Massimo, et al, NIMA (2016)

Relativistic Species Initialization example: electron sphere

$\gamma_0 = 1$ (immobile, $v_x = 0$)



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



Relativistic Species Initialization: how to use it

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


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

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

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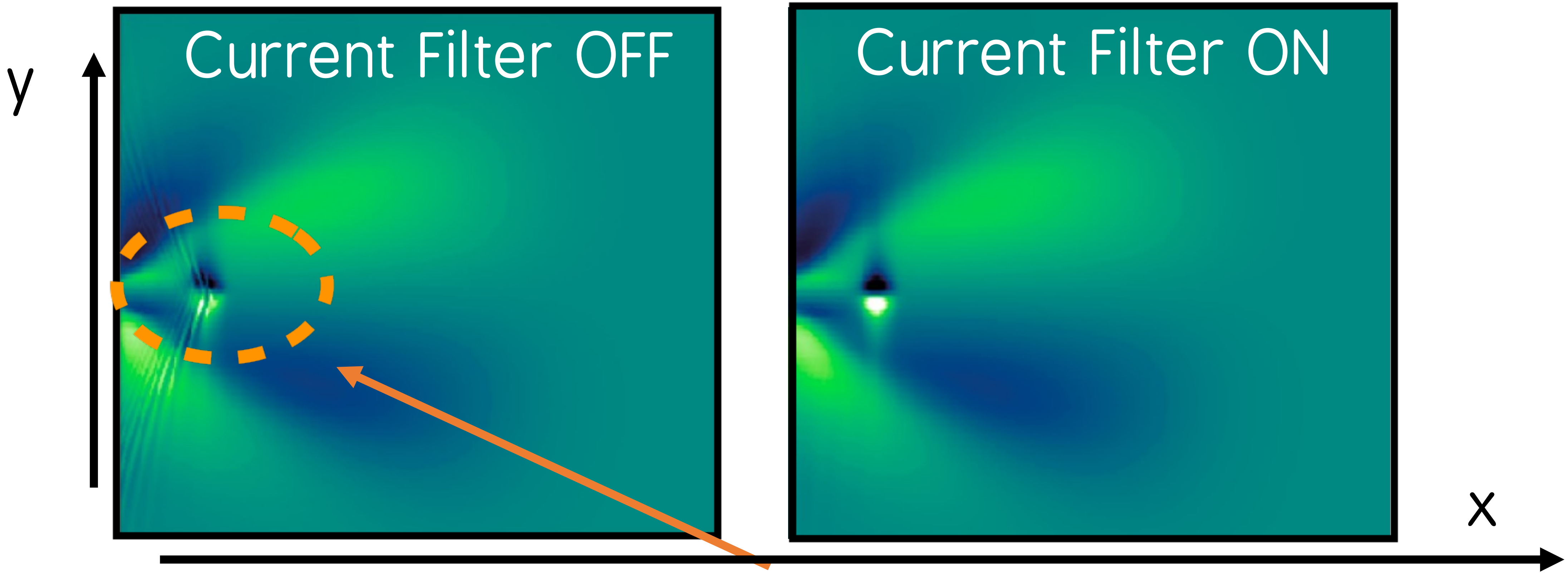
Current Filtering

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)

Current Filtering: how to use it

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

Available
in all geometries

Warning: filtering increases the time spent on communications: consider adding also Single Domain Multiple Decomposition (cf. Arnaud's talk)

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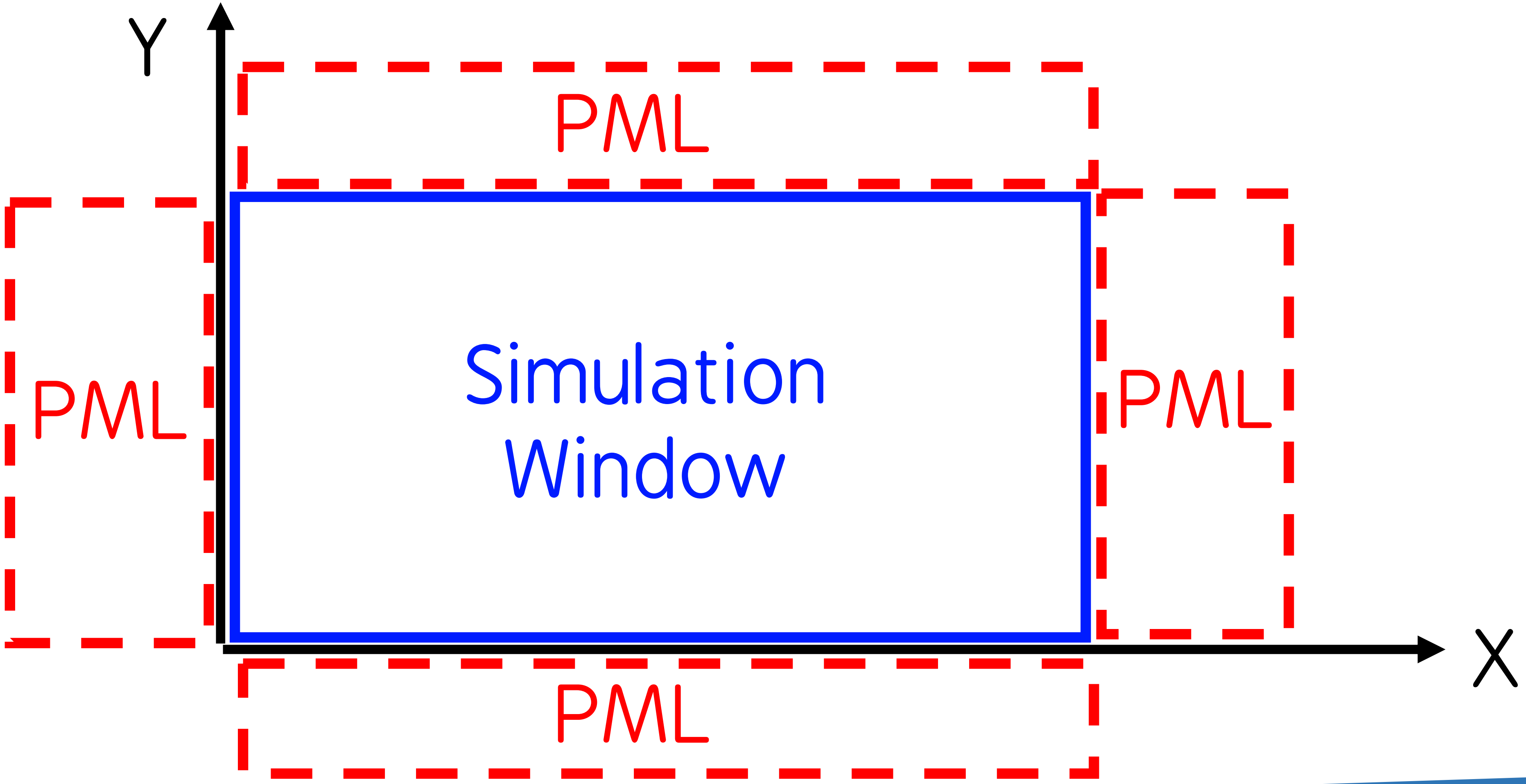
Perspectives: Perfectly Matched Layer

Perfectly Matched Layer (PML): Concept

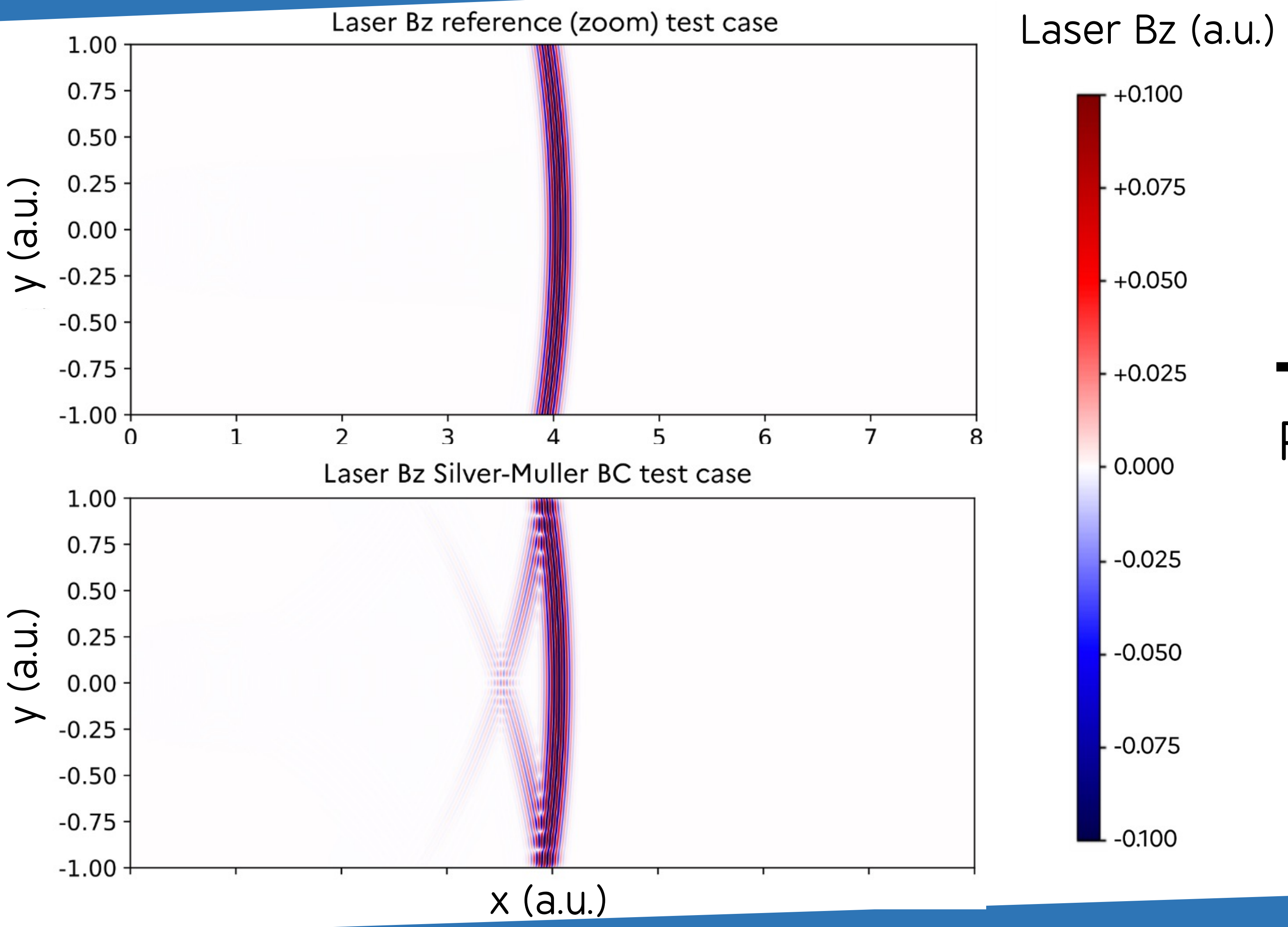
PML: layer of fictious absorbing medium



Perfectly Matched Layer: Standard Laser

Reference (Very large window, zoomed)

Silver-Müller Boundary Conditions

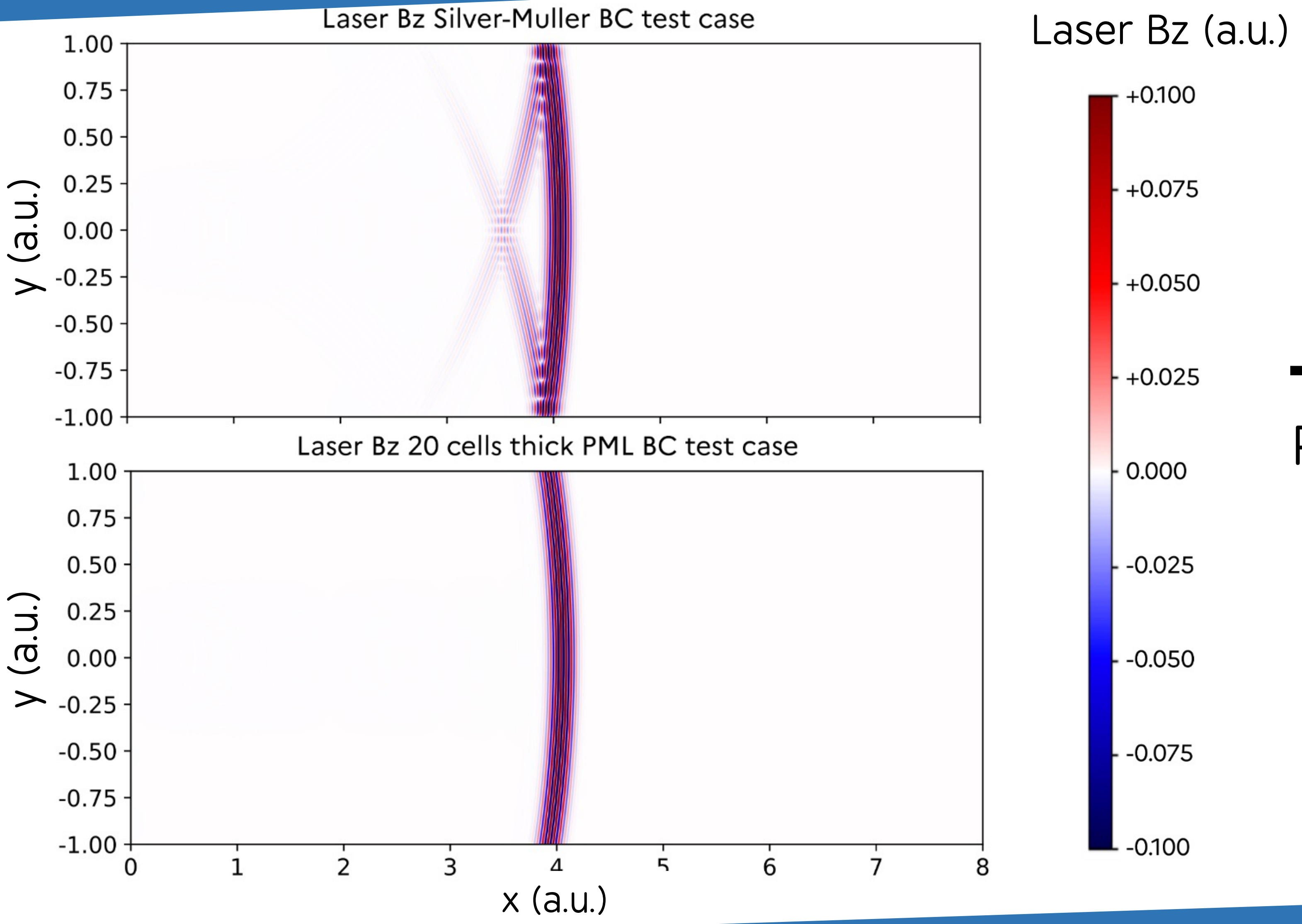


Propagation direction

Perfectly Matched Layer: Standard Laser

Silver-Müller Boundary Conditions

Perfecly Matched Layer



Propagation direction

Perfectly Matched Layer: Standard Laser

Silver-Müller Boundary Conditions

Perfecly Matched Layer

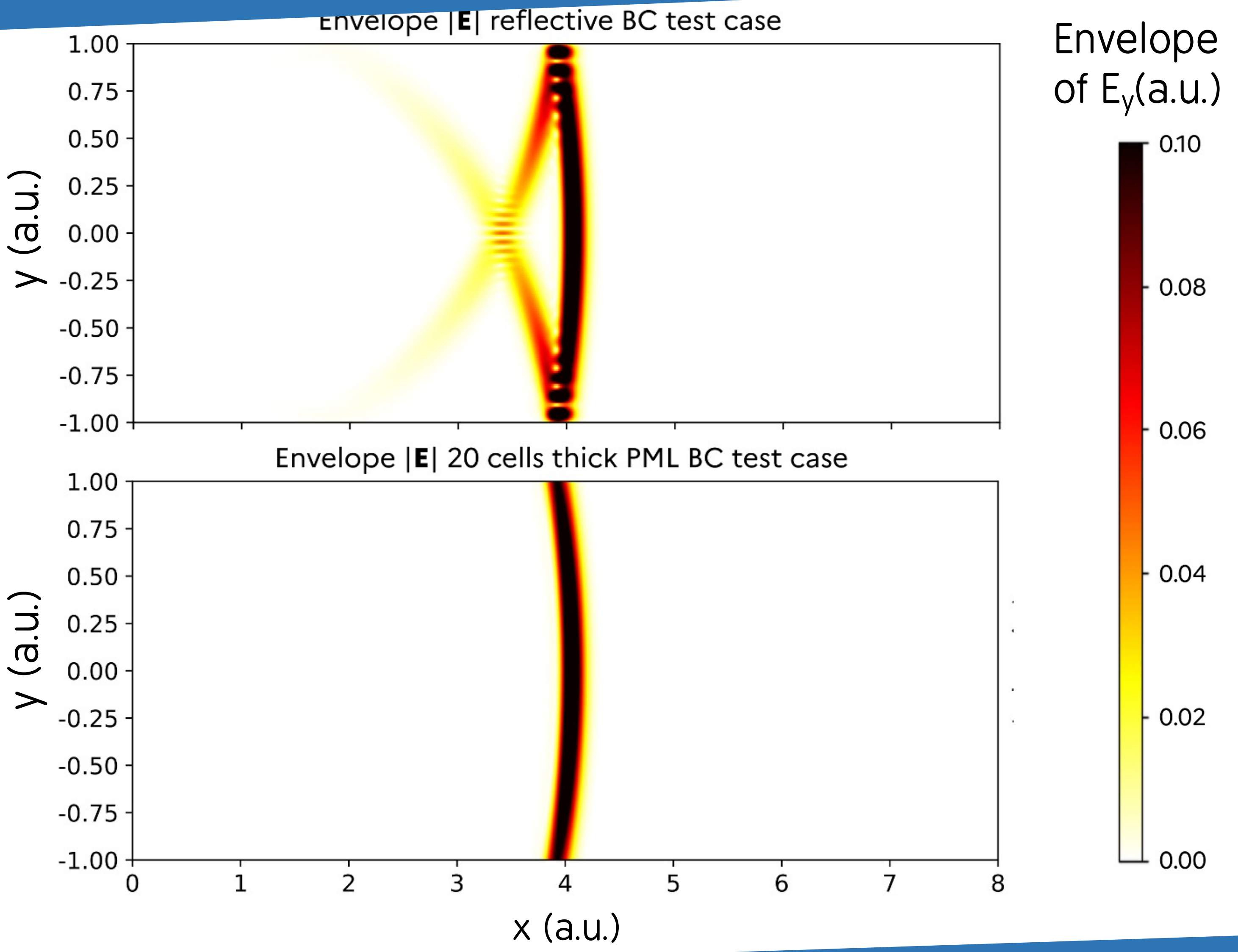
Already Released!

Propagation direction

Perfectly Matched Layer: Laser Envelope

Present Envelope Boundary Conditions

Perfecly Matched Layer for Envelope



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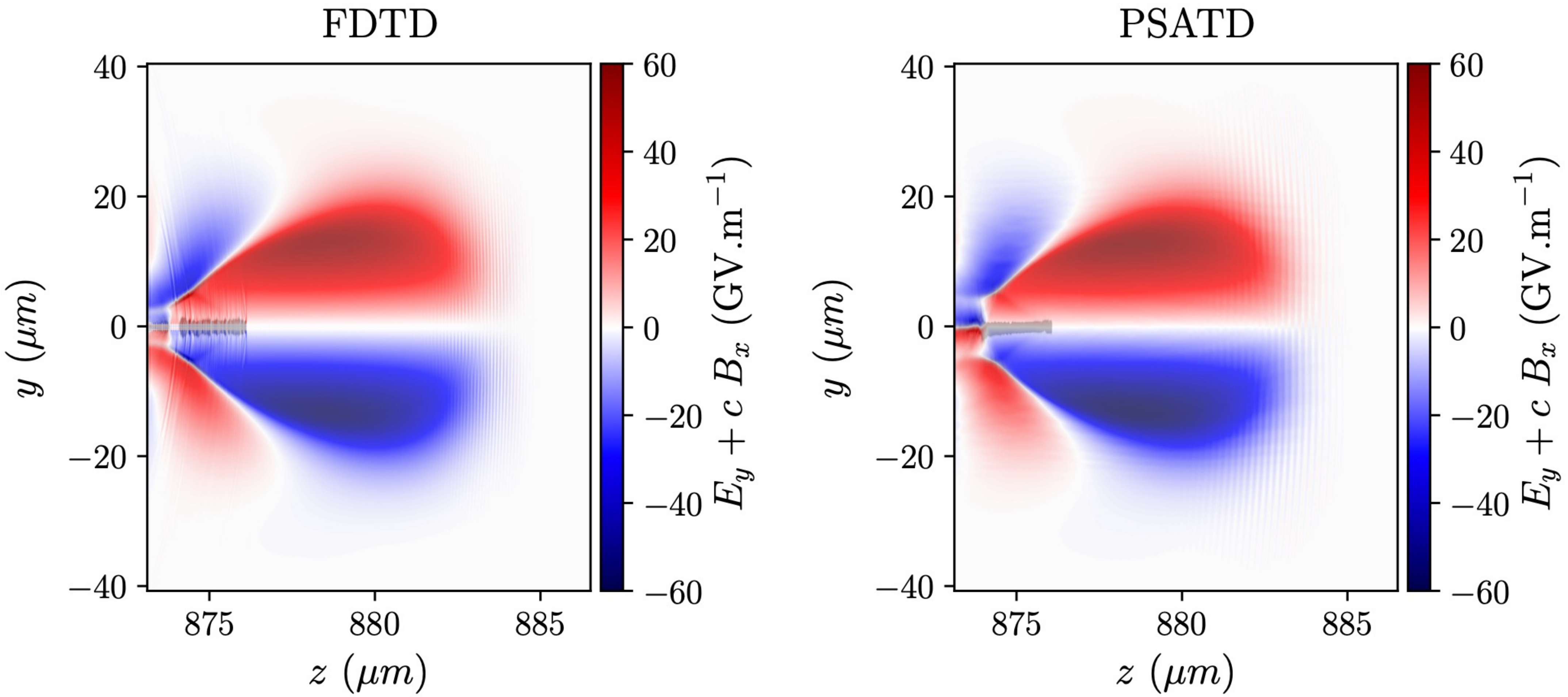
Perspectives: Spectral Solvers

Pseudo Spectral Analytical Time Domain solver



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

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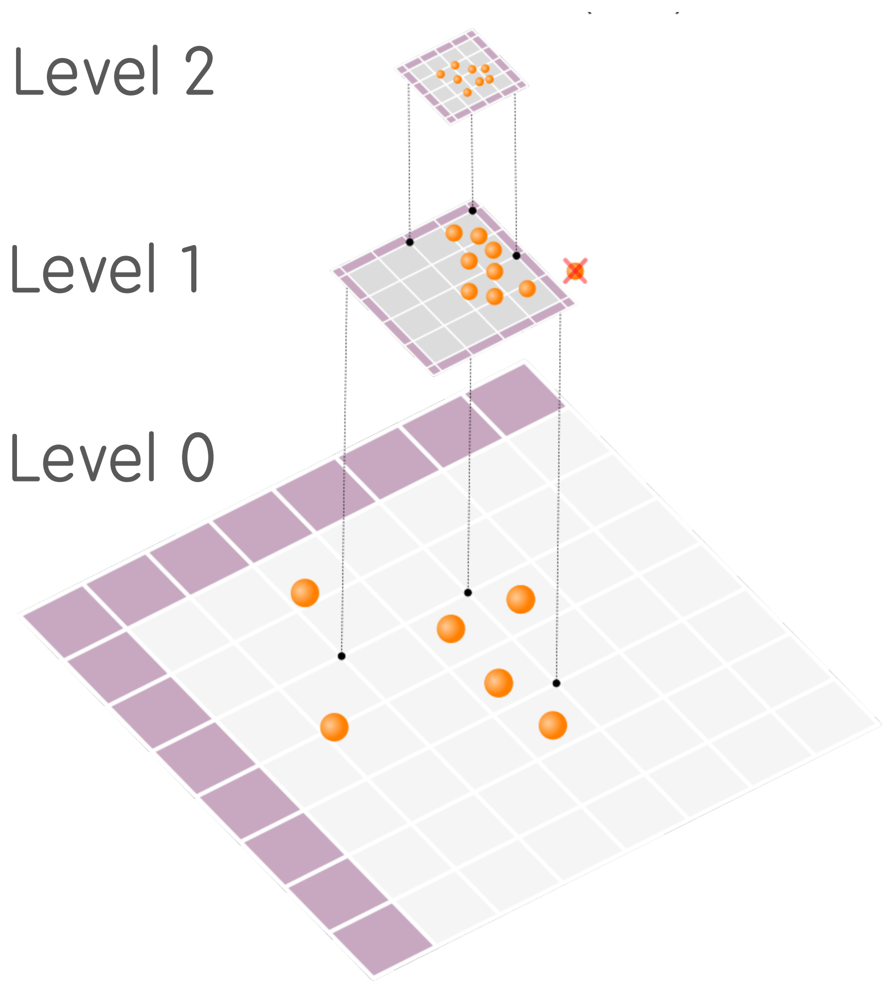
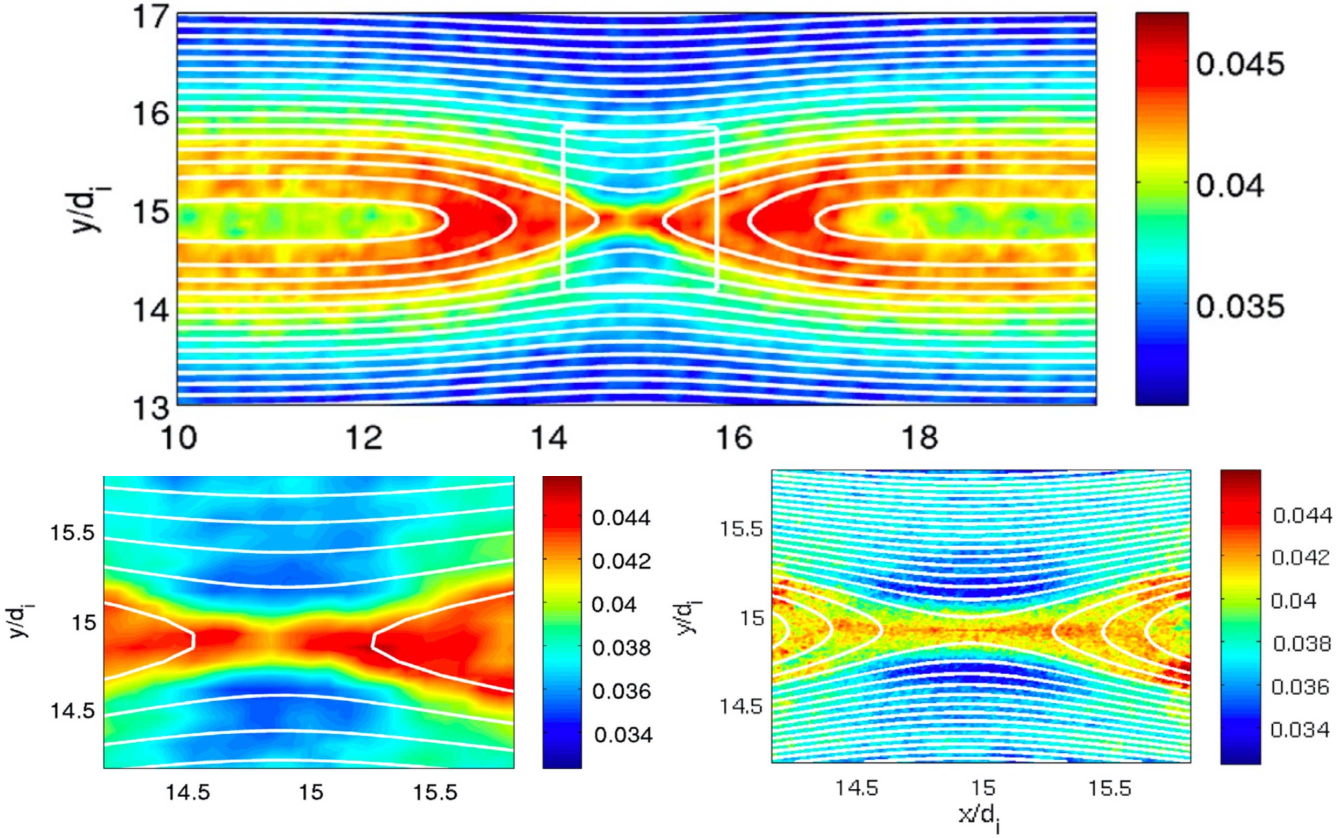
Perspectives: Multi-Level-Multi-Domain PIC

Multi-Level Multi-Domain Particle in Cell



Magnetic Reconnection Simulation



M. E. Innocenti et al., J. Comp. Phys. (2013)

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

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Conclusions and perspectives

Conclusions and Perspectives

Recent Advanced techniques:

- Azimuthal modes decomposition ("AMcylindrical" geometry)
- Laser Envelope model with envelope ionization module
- Macro-Particle Merging
- Initialization of relativistic Species' fields
- Tilted plane injection for Laser
- Customized FIR filter,
- Perfectly Matched Layer

Work in progress and perspectives:

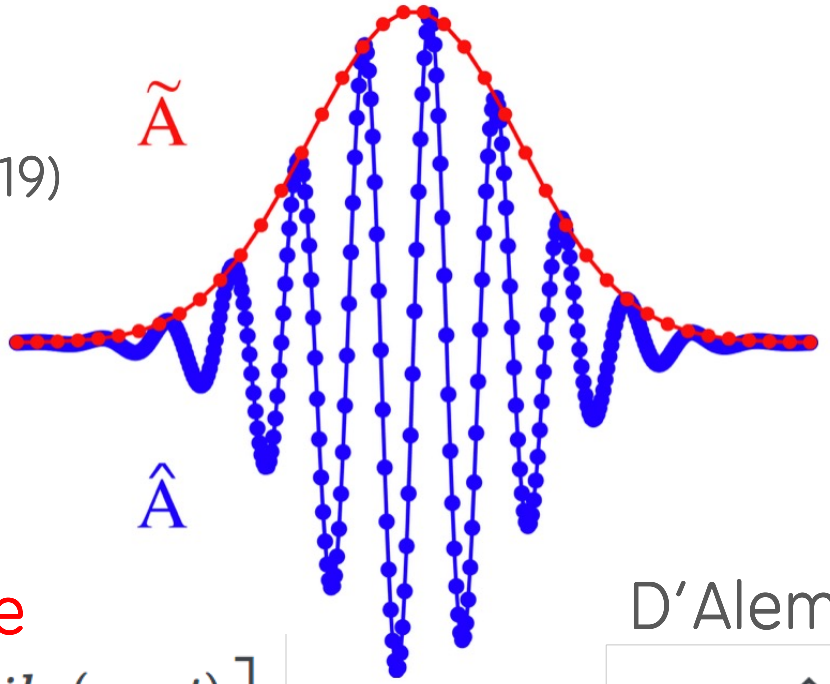
- Perfectly Matched Layer for Laser Envelope
- Multi-grid Multi-domain decomposition
- Spectral Solvers

What advanced features would you need?

Additional Slides

Envelope Equation

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



Laser Envelope

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

D'Alembert's Equation

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

Envelope Equation:

$$\nabla^2\tilde{A} + 2i\left(\partial_x\tilde{A} + \partial_t\tilde{A}\right) - \partial_t^2\tilde{A} = \boxed{\chi}\tilde{A}$$

Plasma Susceptibility

Ponderomotive equations of motion

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

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

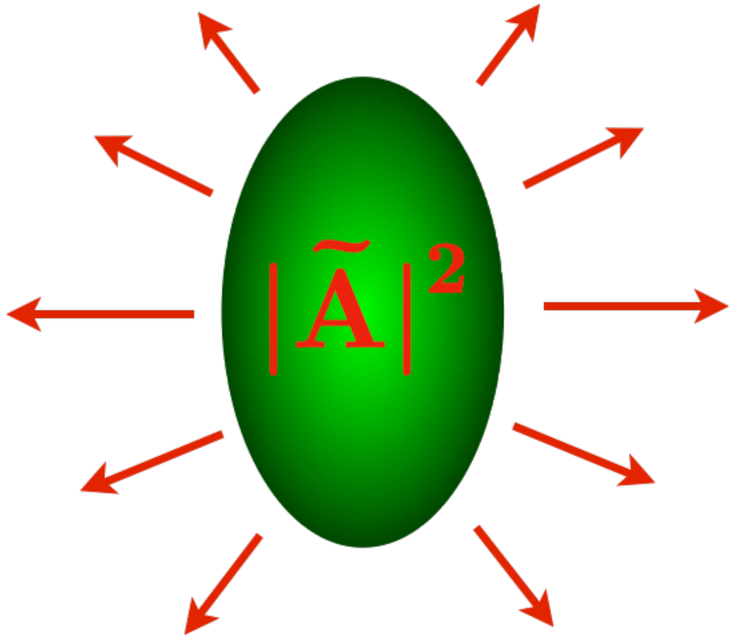
$$\frac{d\bar{\mathbf{x}}_p}{dt} = \frac{\bar{\mathbf{u}}_p}{\bar{\gamma}_p}$$

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

Lorentz Force

Ponderomotive Force

Laser Intensity



Ponderomotive force acts as a radiation pressure