Mesh Refinement in quasi-static codes

making plasma acceleration simulations in collider-relevant parameters feasible (and cheap)

Maxence Thévenet – DESY

MPA – plasma acceleration

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY.

Plasma acceleration is described by kinetic plasma dynamics

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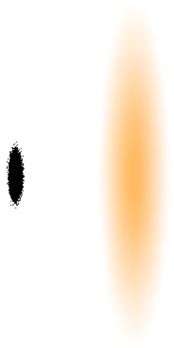

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E},$$

$$\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \mathbf{J},$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{v},$$

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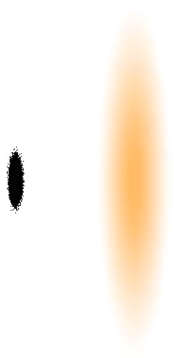

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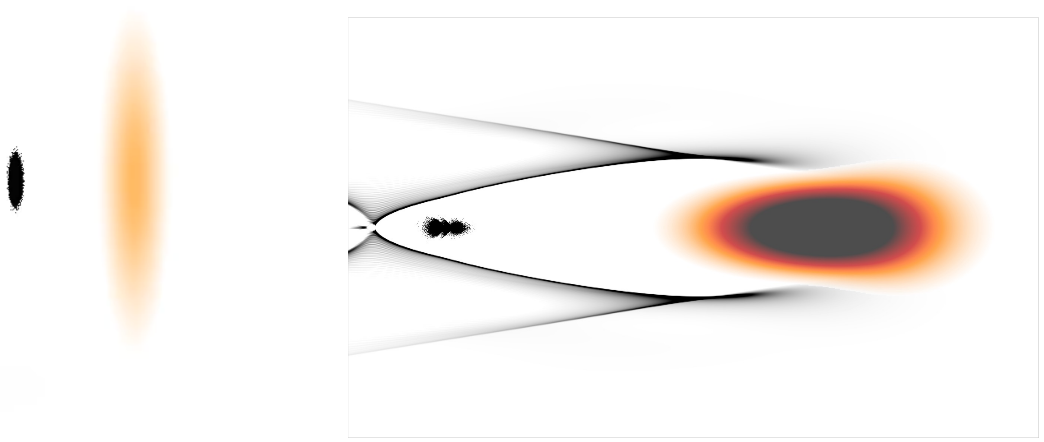

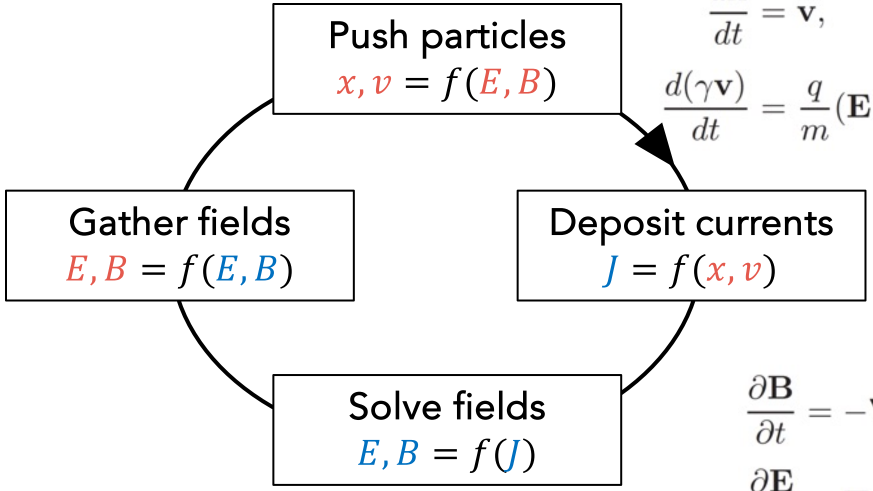

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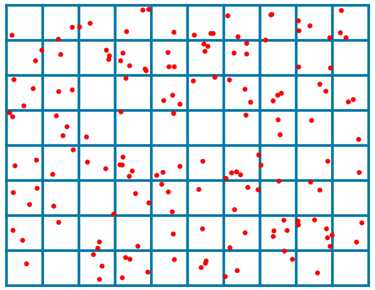
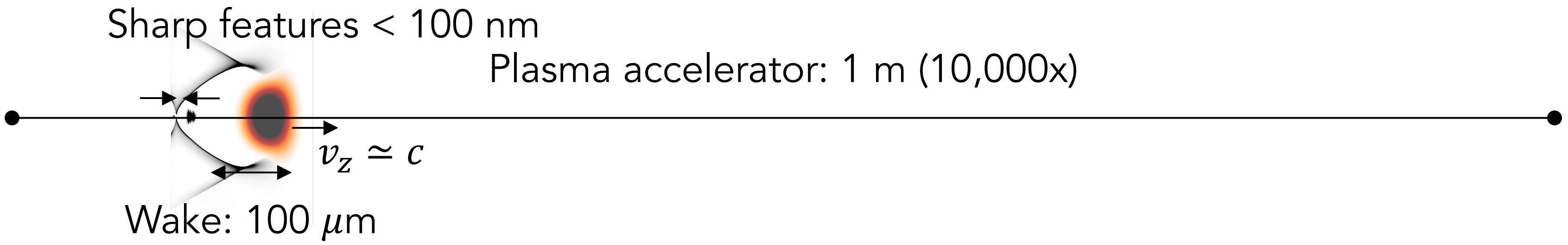


Regular mesh
Macroparticles

- *Lagrangian* description of plasma, *Eulerian* description of fields
- Physics can be added
- Time step limited by CFL condition: $\Delta t \simeq \frac{\Delta z}{c}$

→ 3D (EM) PIC simulations of plasma acceleration are very expensive

Quasi-static approximation helps simulations of plasma acceleration



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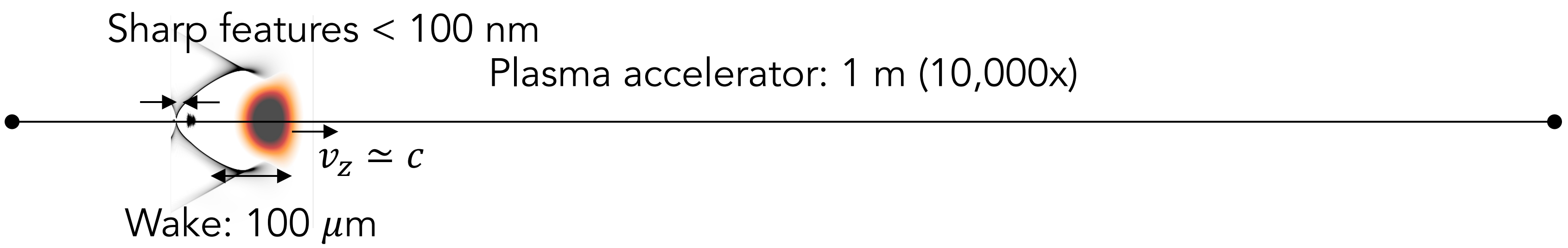

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Two main methods for larger time steps

- **Boosted frame method** [J.-L. Vay PRL **98**, 130405 (2007)]
  - Prone to Numerical Cherenkov Instability (NCI)
  - Mitigation methods exist [R. Lehe et al., PRE 94 (2016), M. Kirchen et al., Phys. Plasmas 23 (2016), A. Pukhov *JCP* 418 (2020)]

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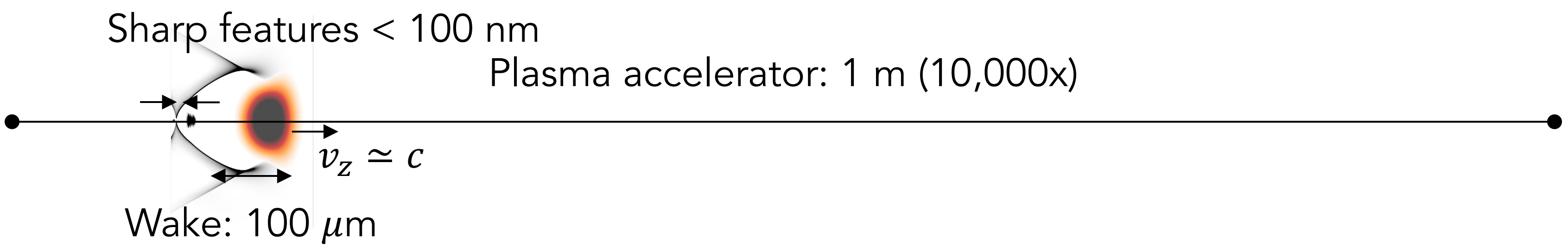

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  - Beam & wake: $\boldsymbol{v} \sim c\boldsymbol{e_z}$
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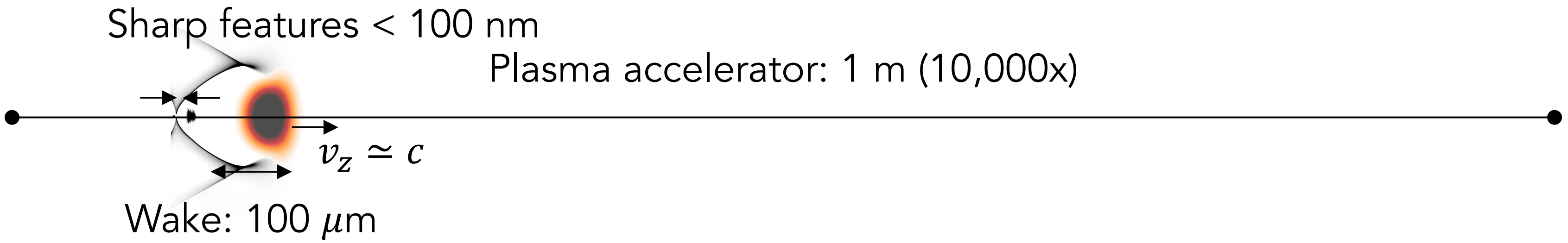

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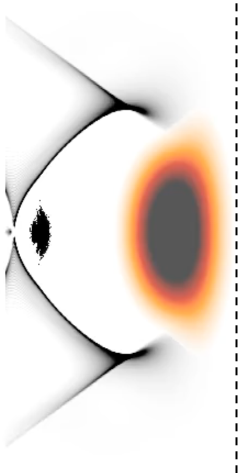

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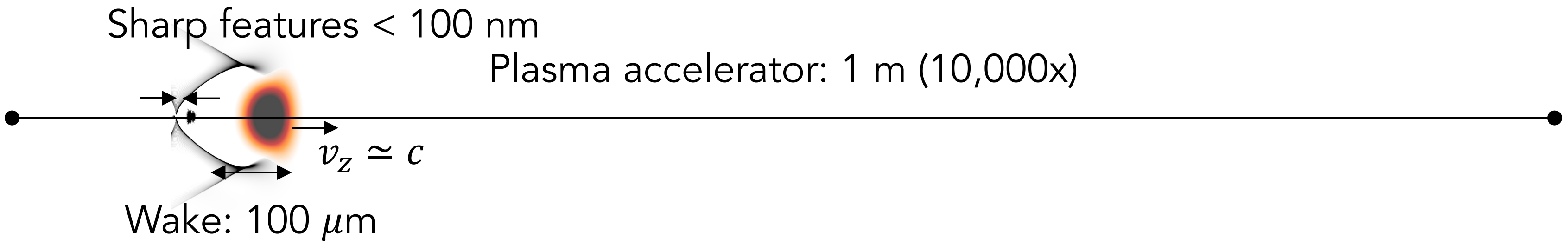

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$$\nabla_\perp^2 \psi = -\frac{1}{\epsilon_0}\left(\rho - \frac{1}{c} j_z\right)$$

$$E_x - c\,B_y = -\partial_x \psi$$

$$E_y + c\,B_x = -\partial_y \psi$$

$$\nabla_\perp^2 E_z = c\mu_0\left(\partial_x j_x + \partial_y j_y\right)$$

$$\nabla_\perp^2 B_x = \mu_0\left(-\partial_y j_z + \partial_\zeta j_y\right)$$

$$\nabla_\perp^2 B_y = \mu_0\left(\partial_x j_z - \partial_\zeta j_x\right)$$

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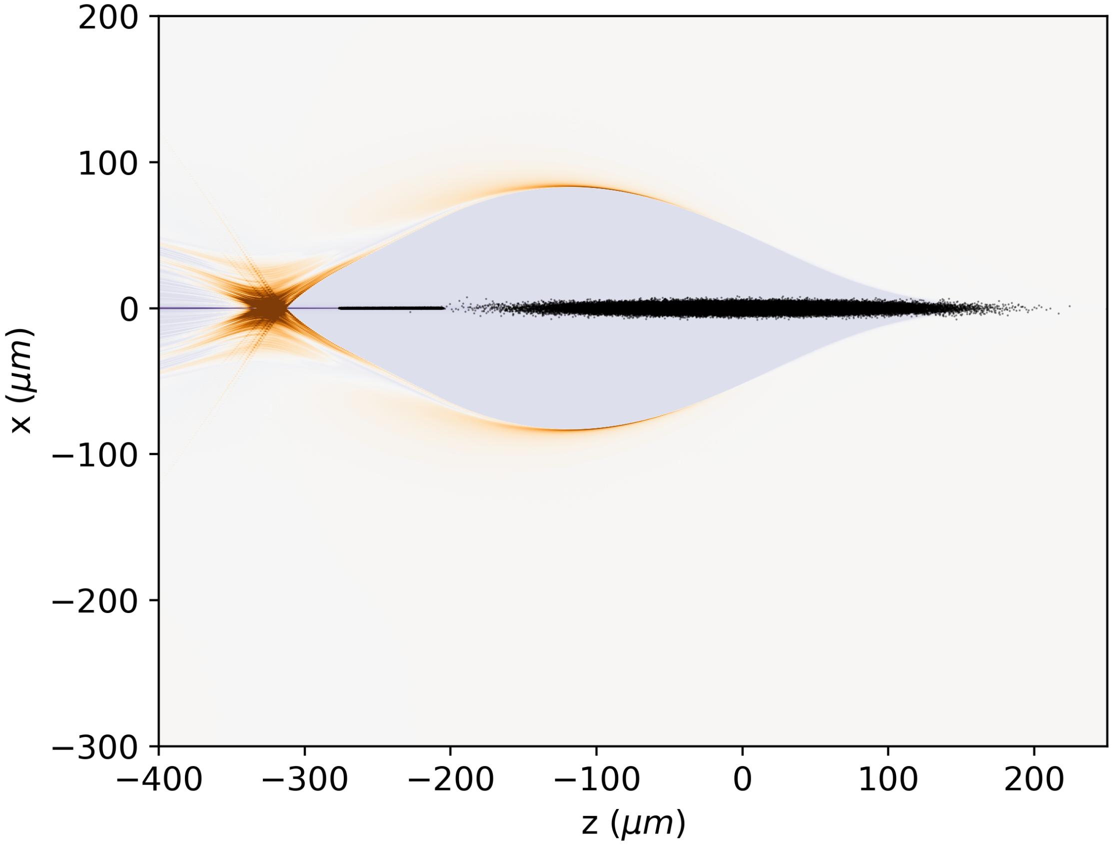
Scale discrepancies can make simulations impractical or unfeasible



Relevant for colliders, consistent with ESPP report

- <u>Driver</u>
  $Q = 2\ \mathrm{nC}$, $\epsilon_{x,y} = 10\ \mu\mathrm{m}$, $\mathcal{E} = 20\ \mathrm{GeV}$, $\Delta\mathcal{E} = 1\%$, $L = 53\ \mu\mathrm{m}$, matched

- <u>Witness</u>
  $Q = 833\ \mathrm{C}$, $\epsilon_{x,y} = 135\ \mathrm{nm}$, $\mathcal{E} = 175\ \mathrm{GeV}$, $\Delta\mathcal{E} = 0.35\%$, $L = 64\ \mu\mathrm{m}$ beam-loaded (SALAME), matched

- <u>Plasma</u> $n_0 = 10^{16}\mathrm{cm}^{-3}$, $r_b \simeq 100\ \mu\mathrm{m}$, ion spike $\simeq 10\ \mathrm{nm}$

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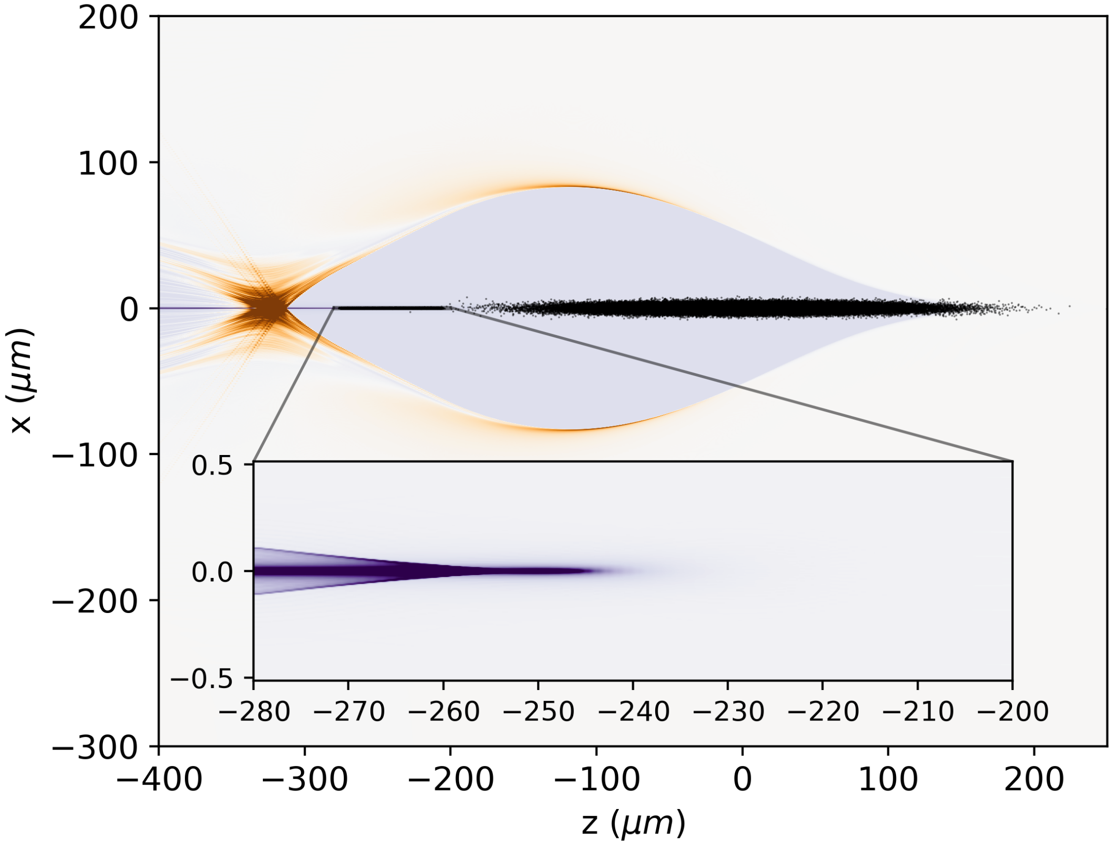

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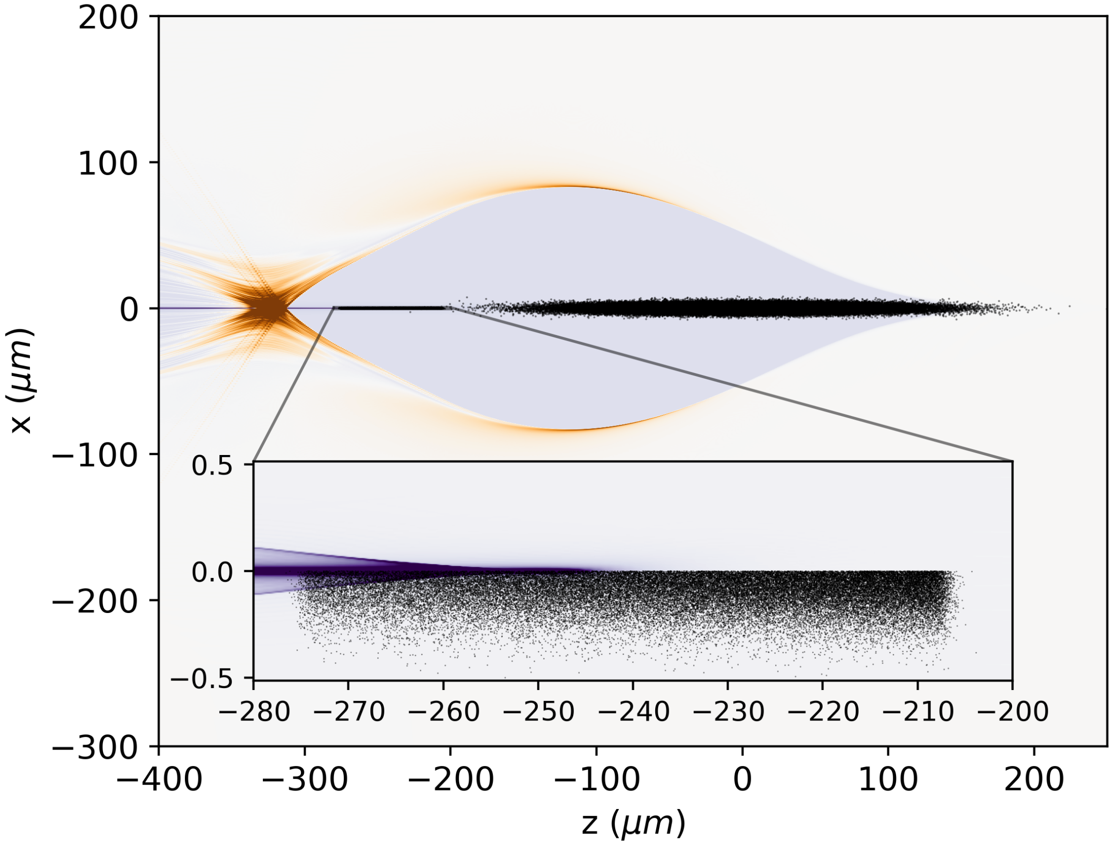

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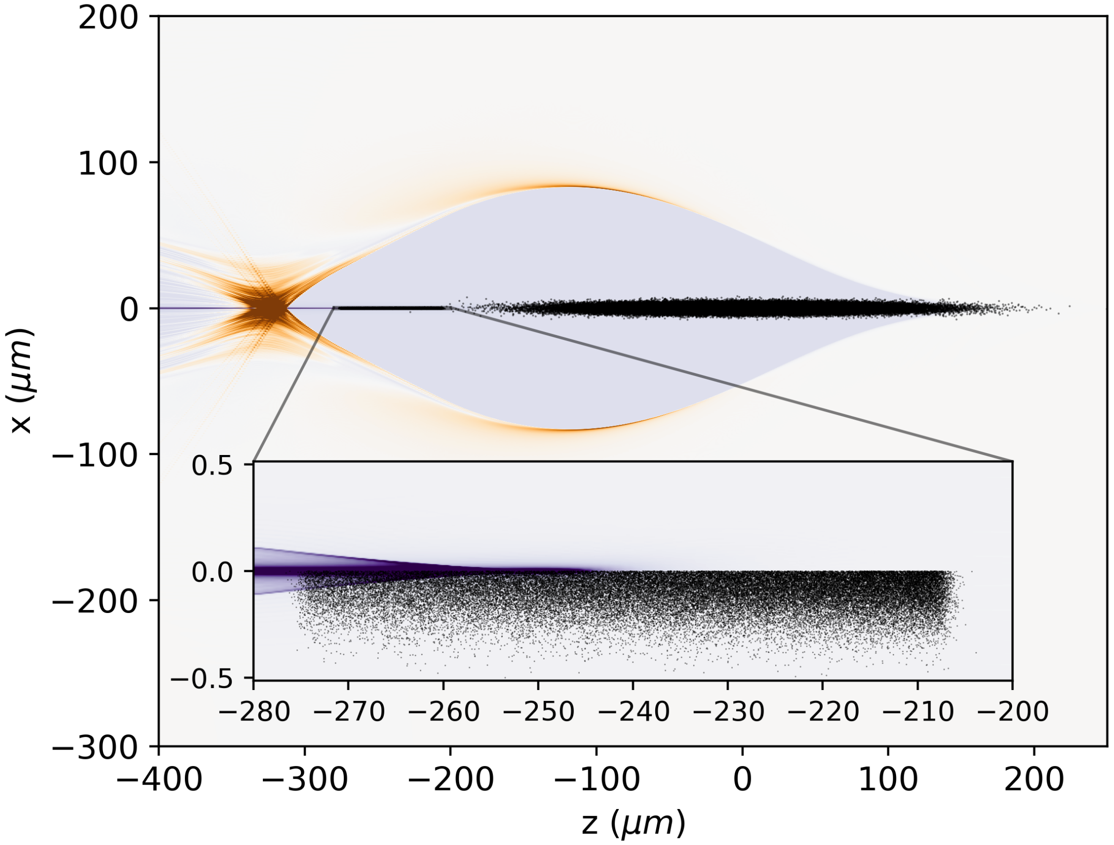

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Solutions exist (*see presentation by J.-L. Vay*)

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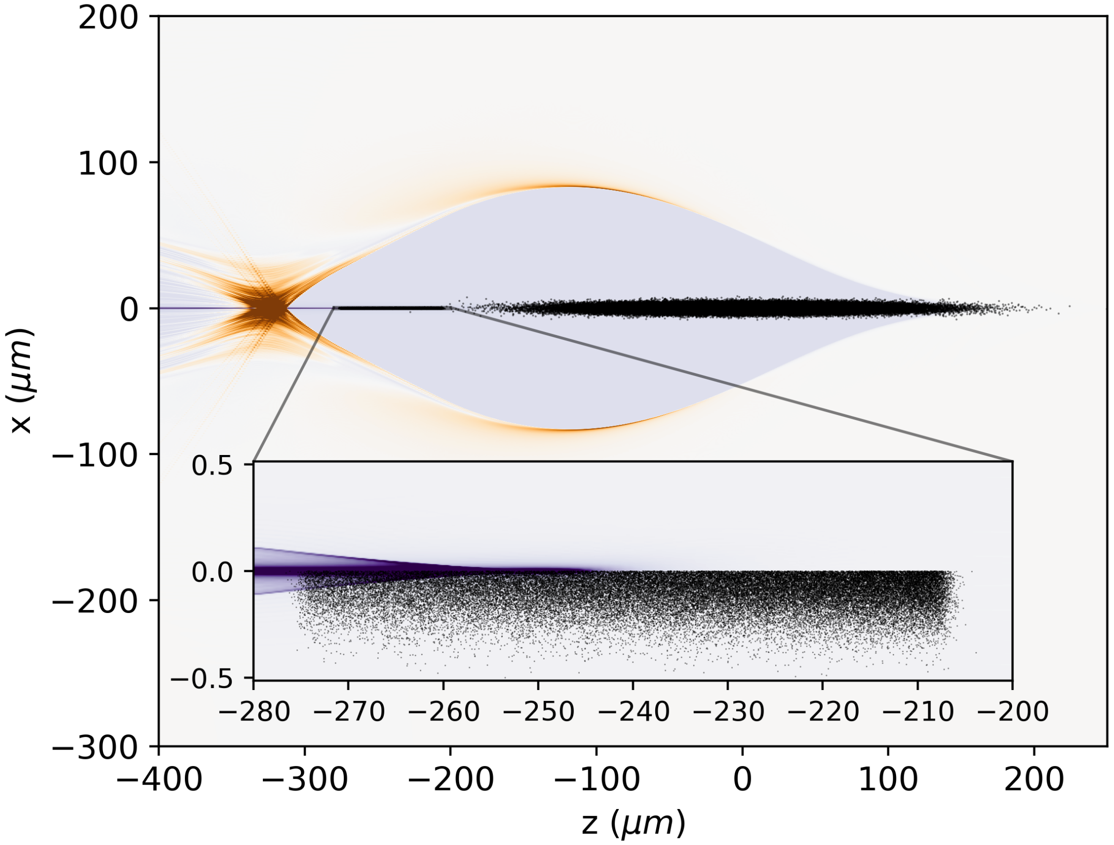

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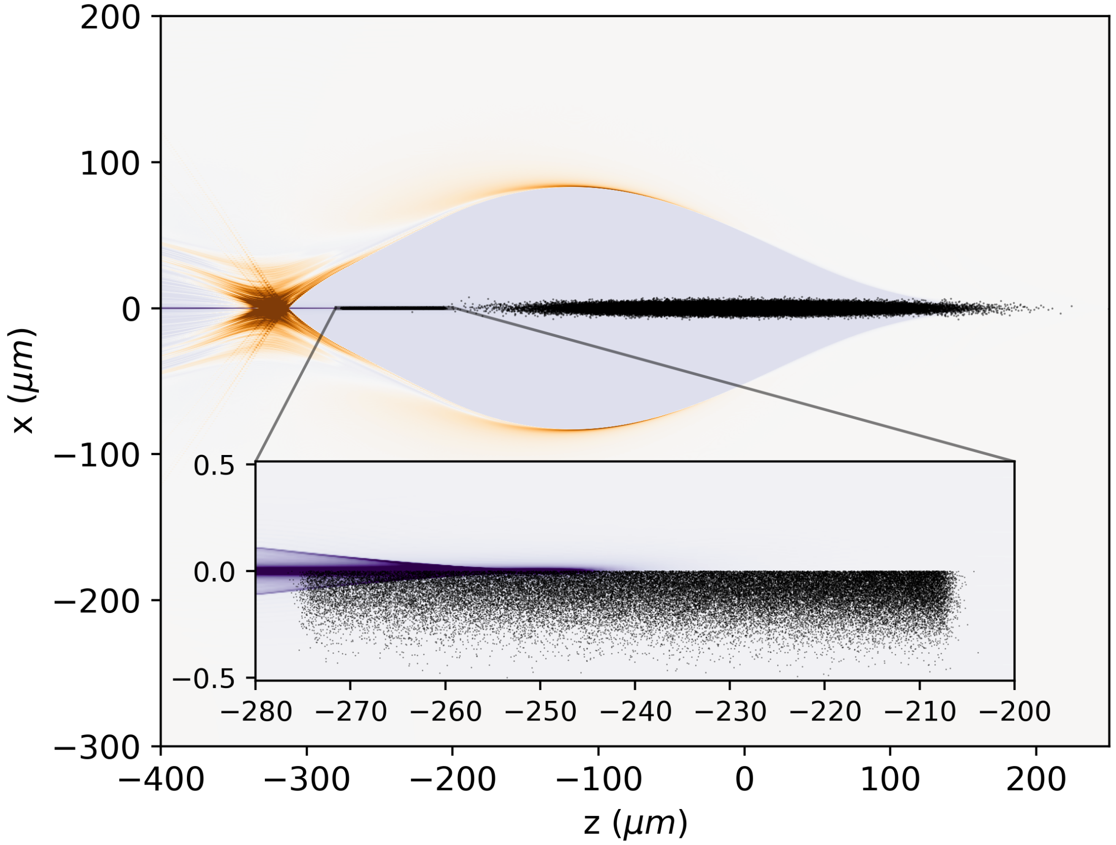

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➢ We will discuss mesh refinement in **two (open-source) codes**

HiPACE++ WakeT

HiPACE++: 3D advanced quasi-static PIC on GPU

Beam-driven or laser-driven plasma acceleration

Combine performance and usability

- **Laptop to supercomputer** - CPUs/GPUs (powered by AMReX)
- **Open-source** - documented, openPMD, CI
- **Multi-physics** - lasers & beams, collisions, ionization, RR
- **Advanced methods** - explicit solver, in-situ diagnostics, two unit systems, SALAME, adaptive time step, etc.

BLAST
BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

https://github.com/Hi-PACE/hipace

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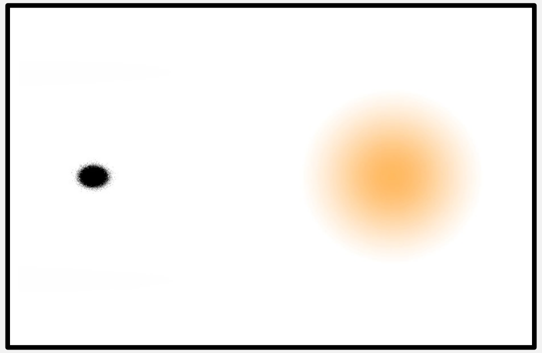

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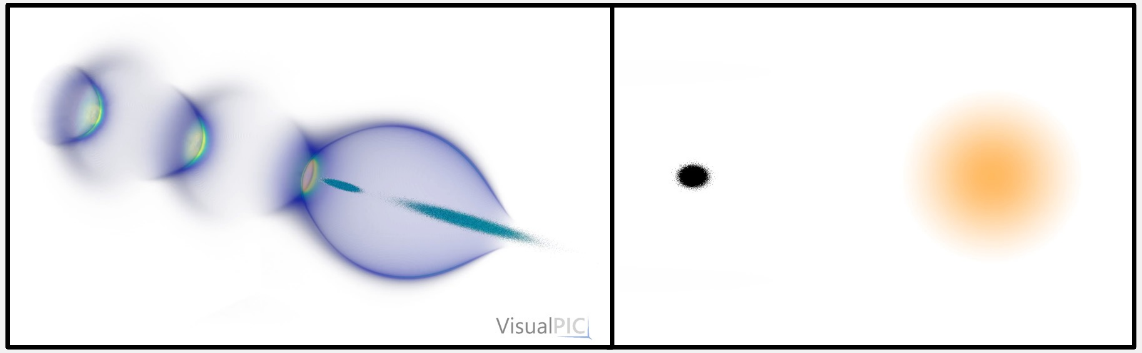

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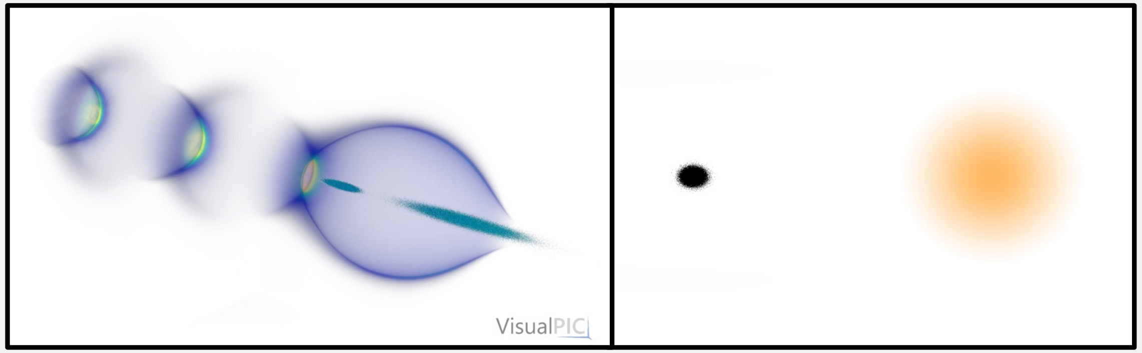

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Runtime (seconds)	6	556
Cost (node-hours)	6	11900

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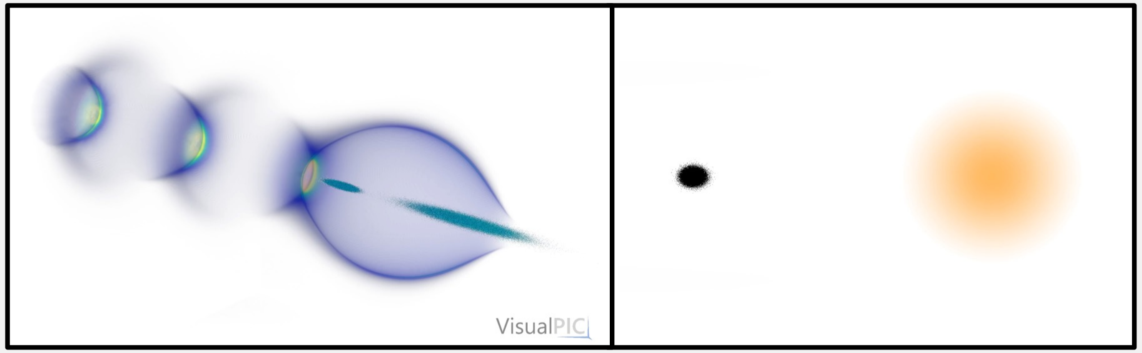

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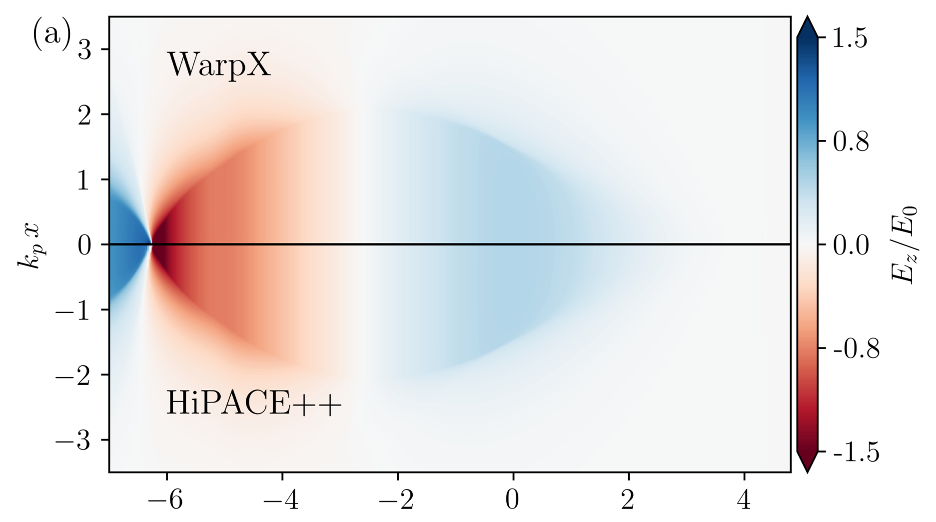

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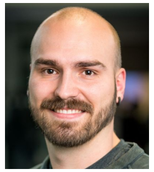
HiPACE++ – The Team

Advanced algorithms and high-performance computing for fast and energy-efficient 3D simulations of plasma acceleration – for everyone

Maxence Thévenet (lead)

Severin Diederichs

Alexander Sinn



Axel Huebl

Rémi Lehe

Jean-Luc Vay

Andrew Myers

Weiqun Zhang

Carlo Benedetti

DESY – MPA

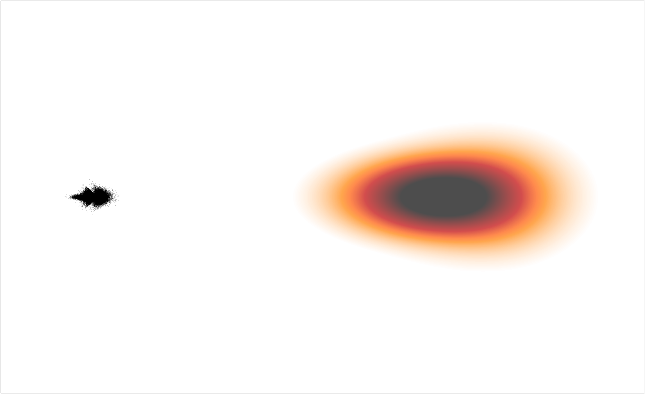
LBNL – AMP
ECP *project WarpX*

LBNL – AMCR
AMReX developers

LBNL – BELLA

- ➢ Started mid-2020
- ➢ International project, open-source
- ➢ New contributors most welcome!

In QS PIC, plasma and laser/particle beams are treated differently



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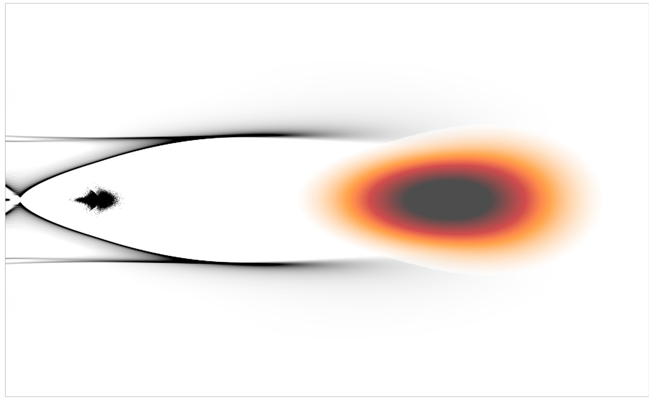

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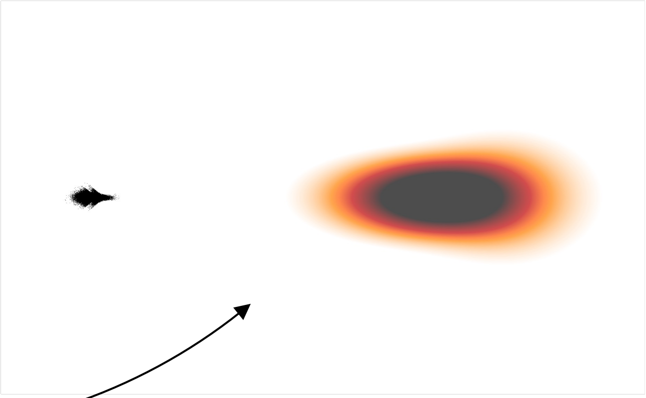

Large $\Delta t \gg \Delta z/c$

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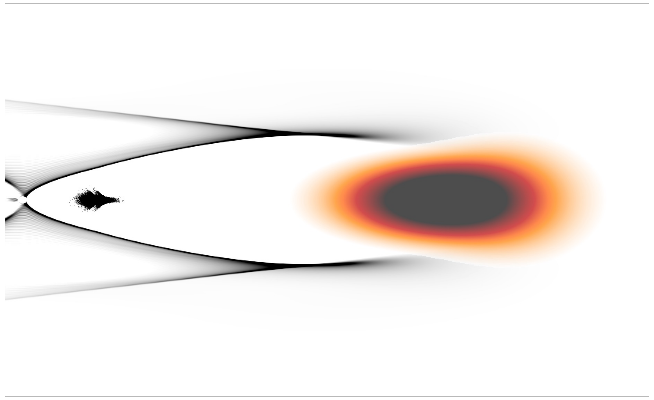

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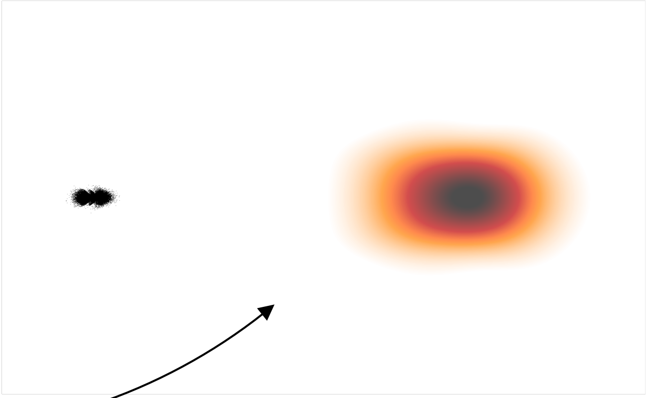

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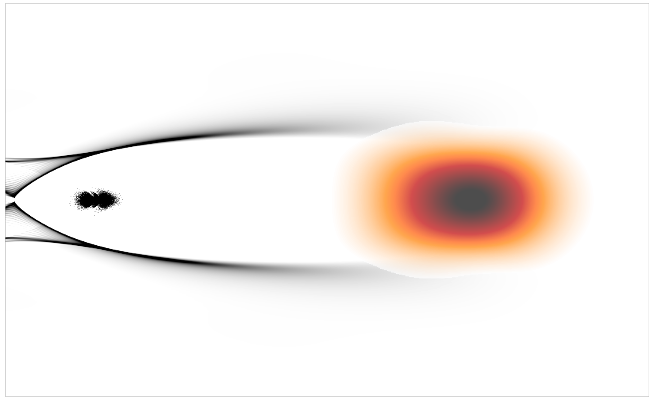

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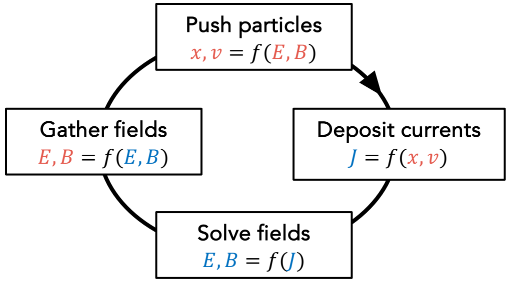

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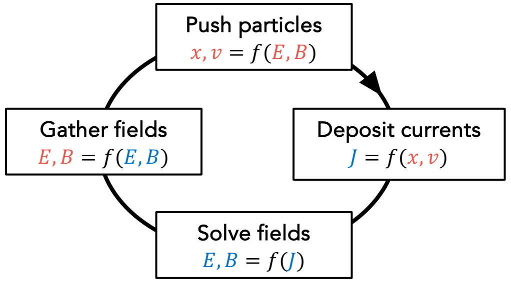
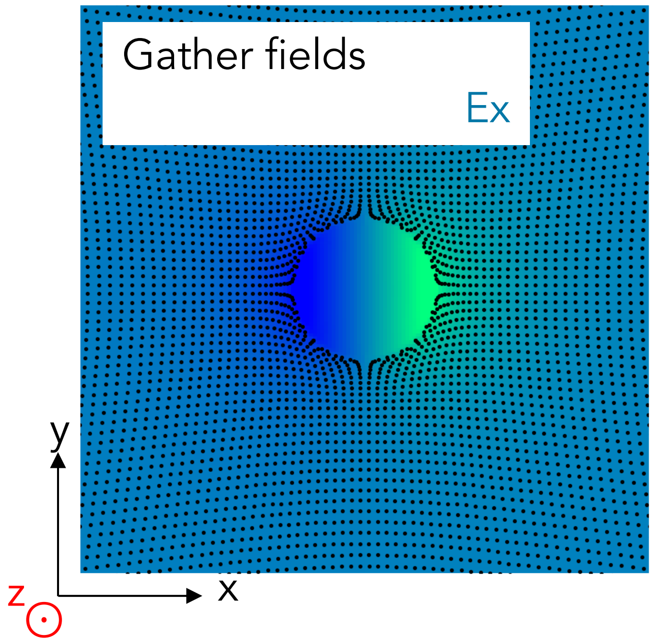


2D slice
Field & particles



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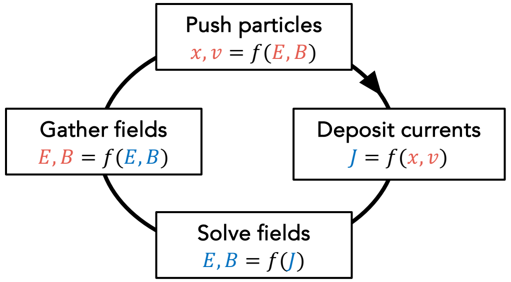

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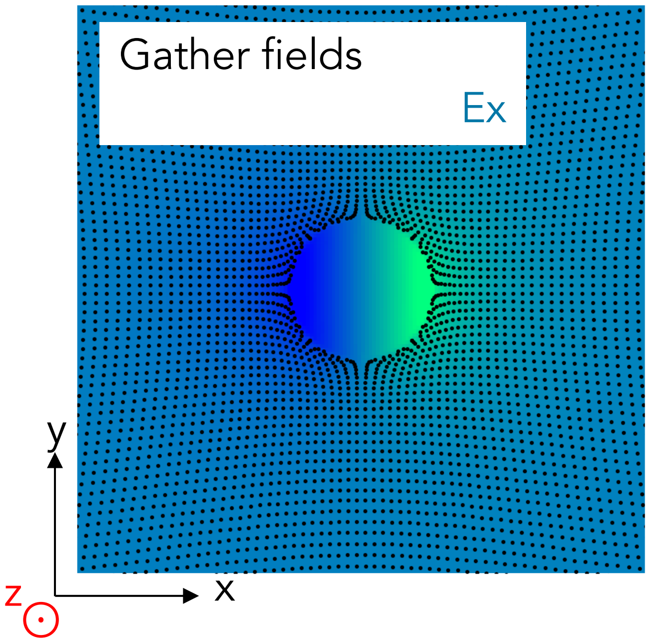
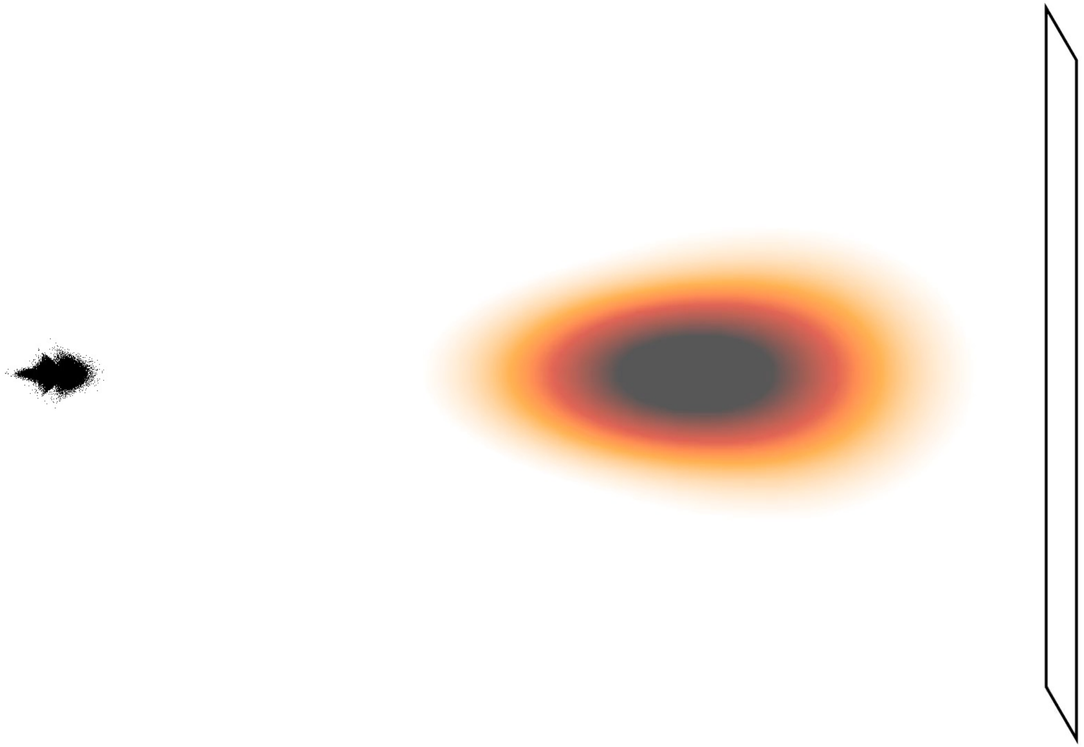
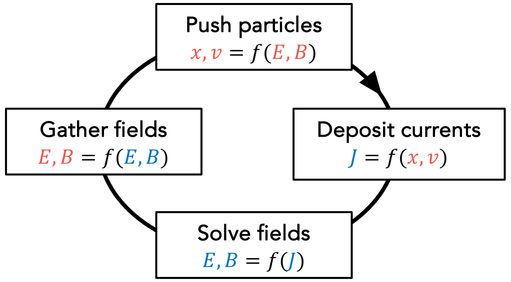


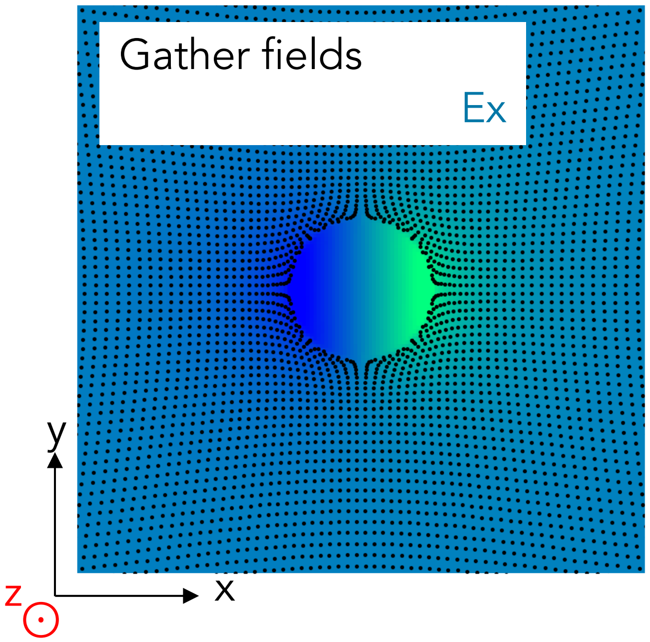
- All PIC operations occur on the 2D transverse domain
- Plasma particles are advanced in ζ (z), <u>not in time</u>
- (specific to HiPACE++: beams and lasers also advanced in the swipe)
- A simulation does $\boldsymbol{n_t}\times\boldsymbol{n_z}$ **PIC iterations on domain** $\boldsymbol{n_x}\times\boldsymbol{n_y}$
- (EM PIC: does $\boldsymbol{n_t}$ **PIC iterations on domain** $\boldsymbol{n_x}\times\boldsymbol{n_y}\times\boldsymbol{n_z}$)

The plasma response is computed with a swipe from head to tile





2D slice
Field & particles



- All PIC operations occur on the 2D transverse domain
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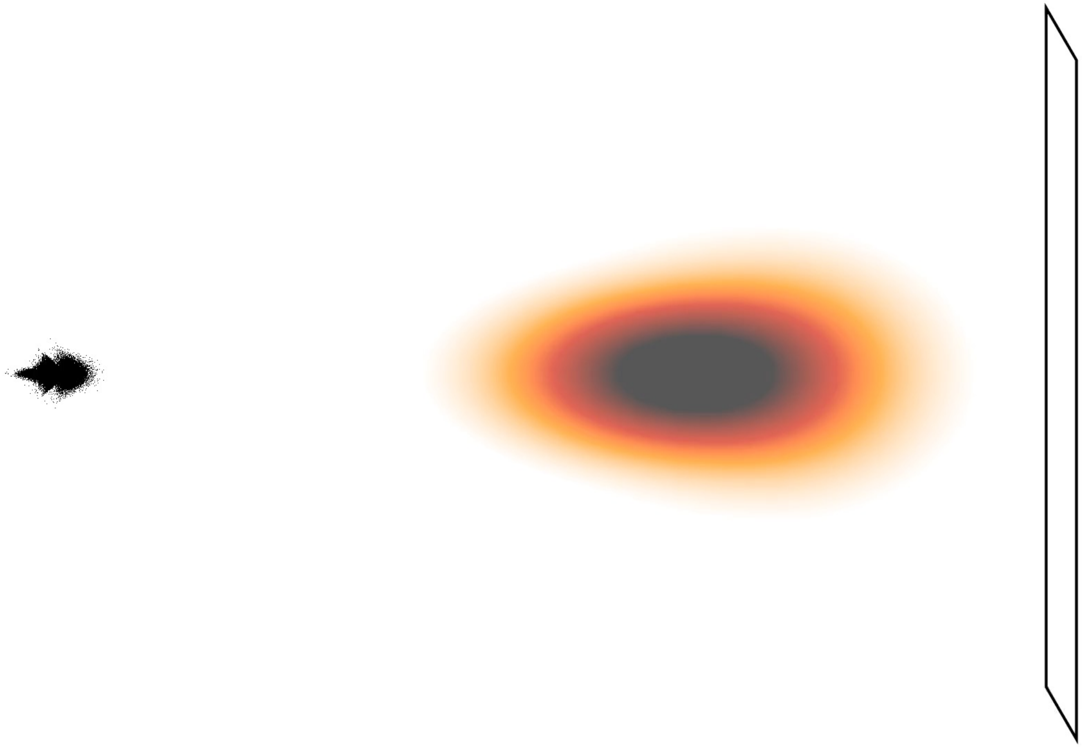

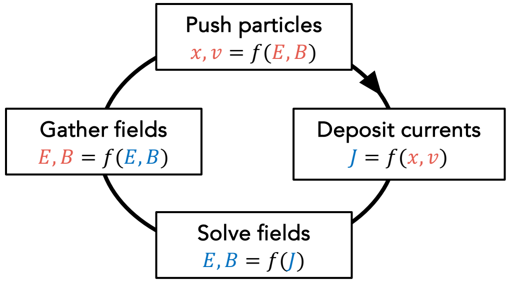

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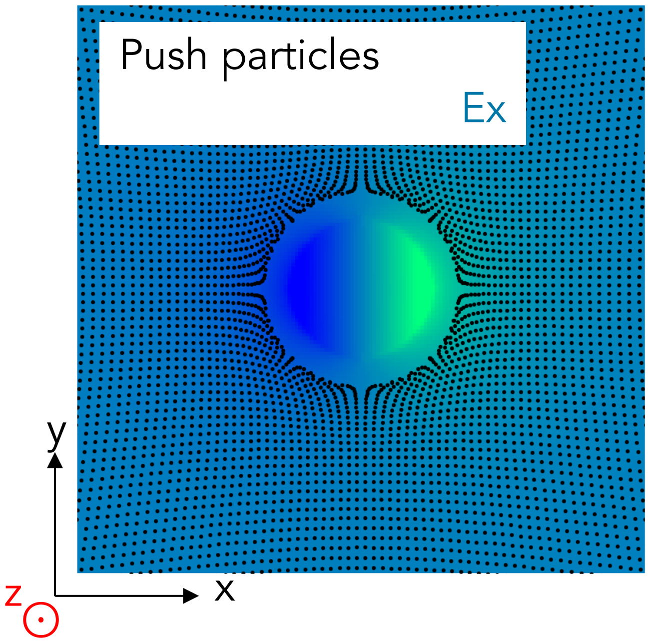

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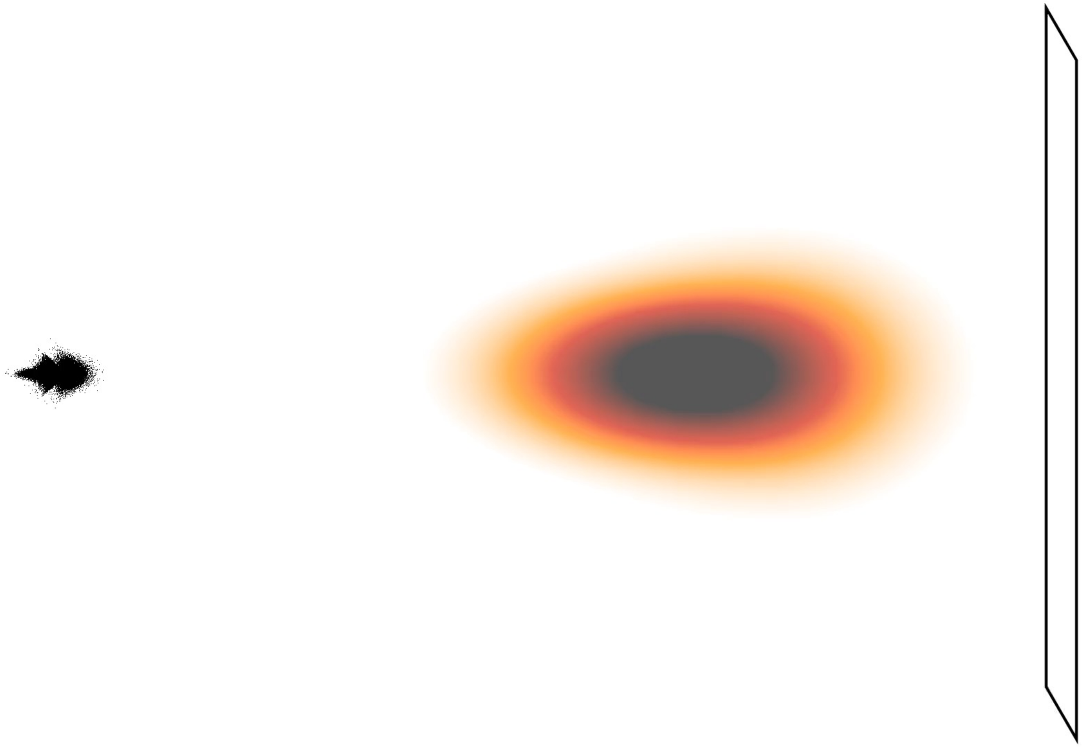

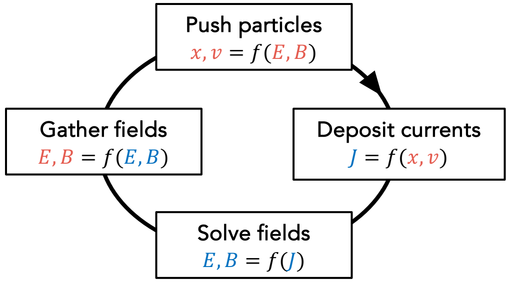

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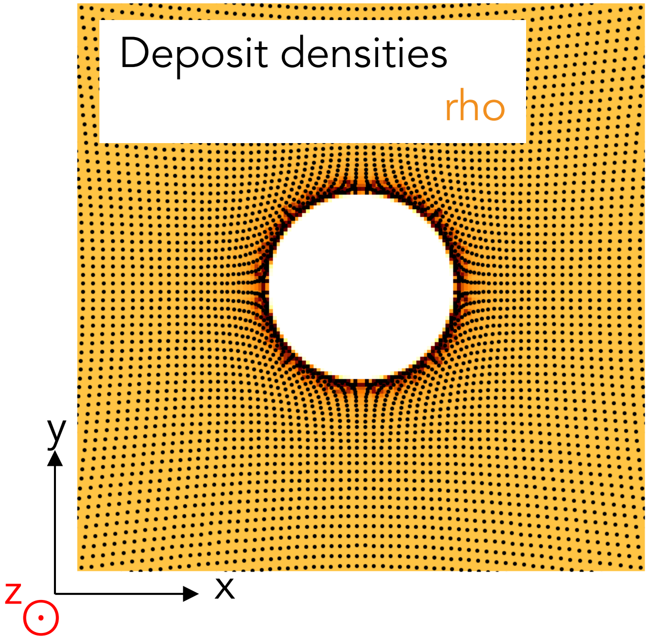

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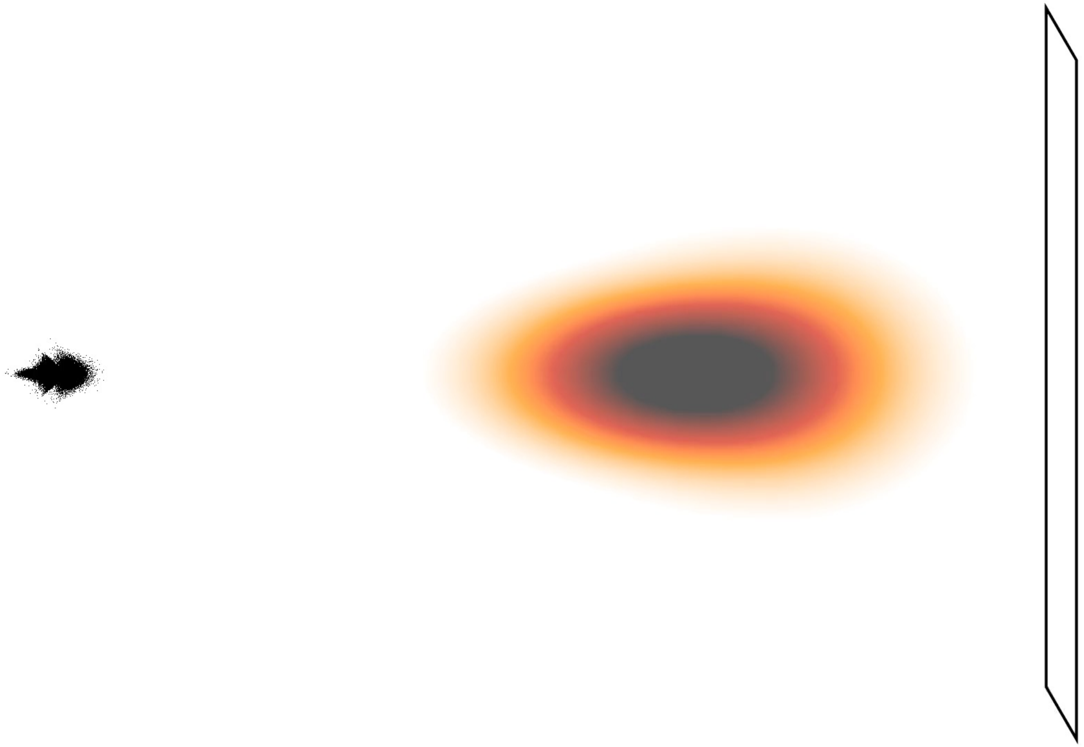

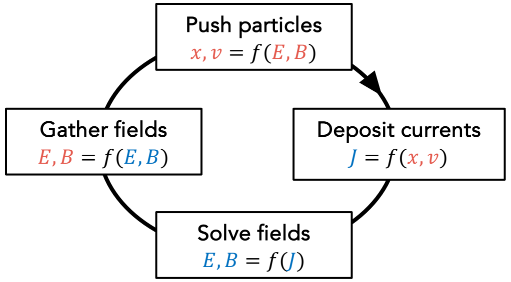

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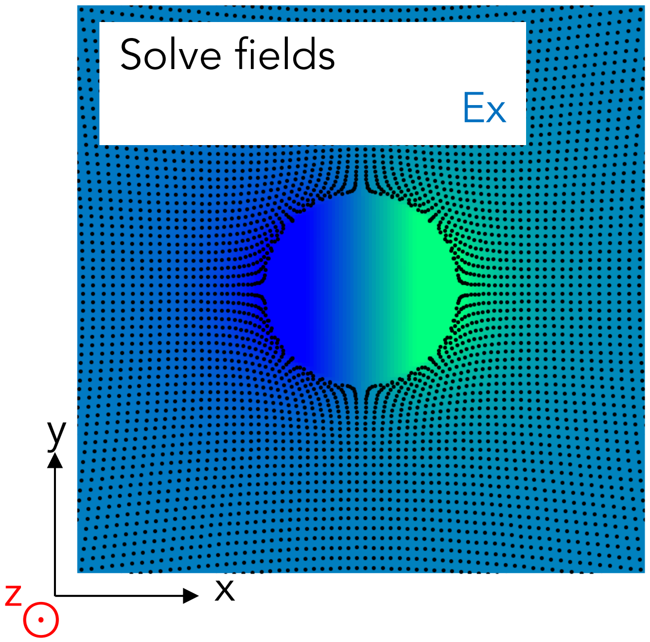

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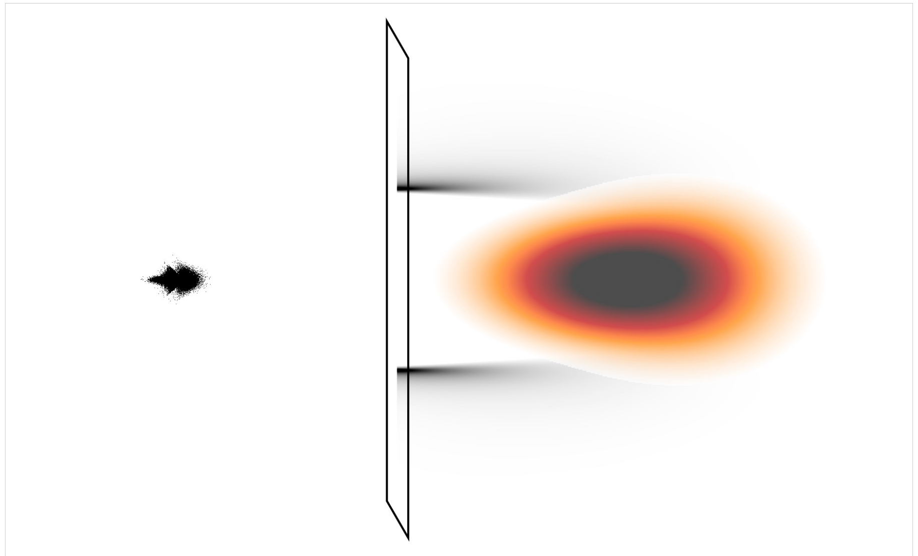
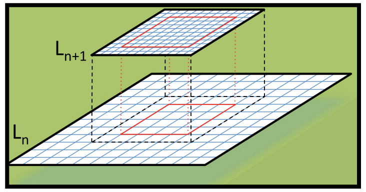
Mesh Refinement in HiPACE++



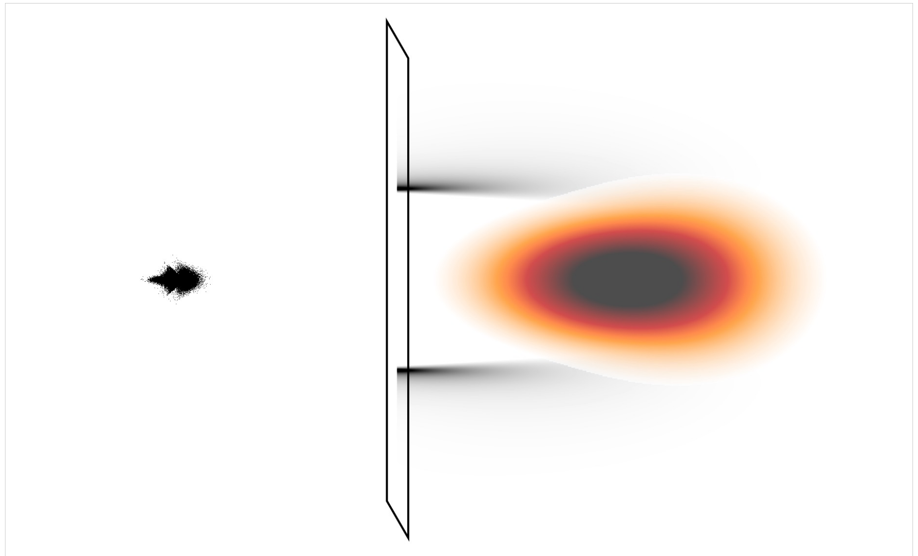
- <u>Deposit densities</u> (beam and plasma) $\rho, \vec{J}, S_x, S_y$
- <u>Solve fields</u> ($E_x - cB_y, E_y + cB_x, E_z. B_z$) and ($B_x. B_y$)
- <u>Advance</u> plasma <u>particles</u> by 1 slice ($-\Delta\zeta$)
- <u>Advance</u> beam <u>particles</u> by 1 time step ($+\Delta t$)

Mesh Refinement in HiPACE++

- MR in electrostatic PIC



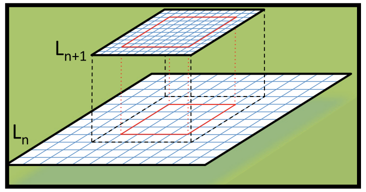
J.-L. Vay et al., Comput. Sci. & Disc. 5, 014019 (2012)

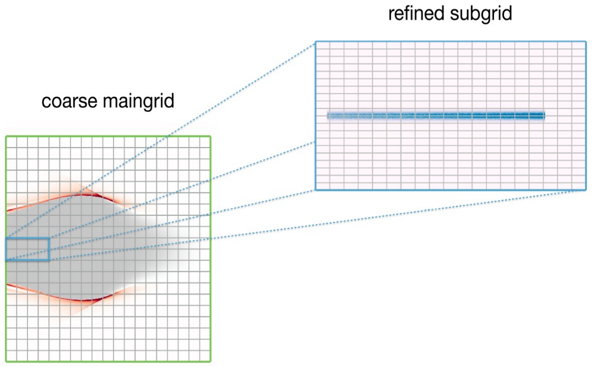


- Deposit densities (beam and plasma) $\rho, \vec{J}, S_x, S_y$
- Solve fields $(E_x - cB_y, E_y + cB_x, E_z . B_z)$ and $(B_x . B_y)$
- Advance plasma particles by 1 slice ($-\Delta\zeta$)
- Advance beam particles by 1 time step ($+\Delta t$)

Mesh Refinement in HiPACE++

- ➢ MR in electrostatic PIC
- ➢ MR with quasi-static PIC, no crossing





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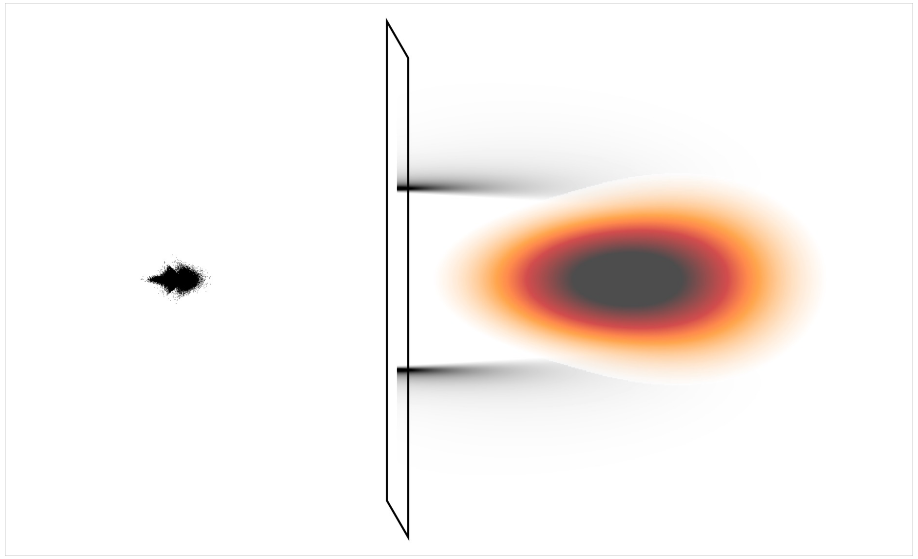
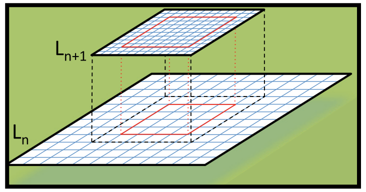
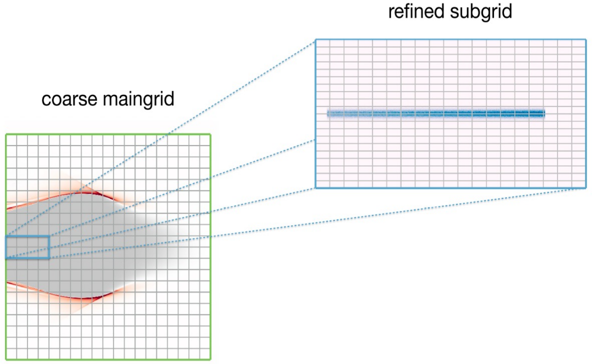


- Deposit densities (beam and plasma) $\rho, \vec{J}, S_x, S_y$
- Solve fields $(E_x - cB_y, E_y + cB_x, E_z. B_z)$ and $(B_x. B_y)$
- Advance plasma particles by 1 slice $(-\Delta\zeta)$
- Advance beam particles by 1 time step $(+\Delta t)$

Mesh Refinement in HiPACE++

- MR in electrostatic PIC
- MR with quasi-static PIC, no crossing

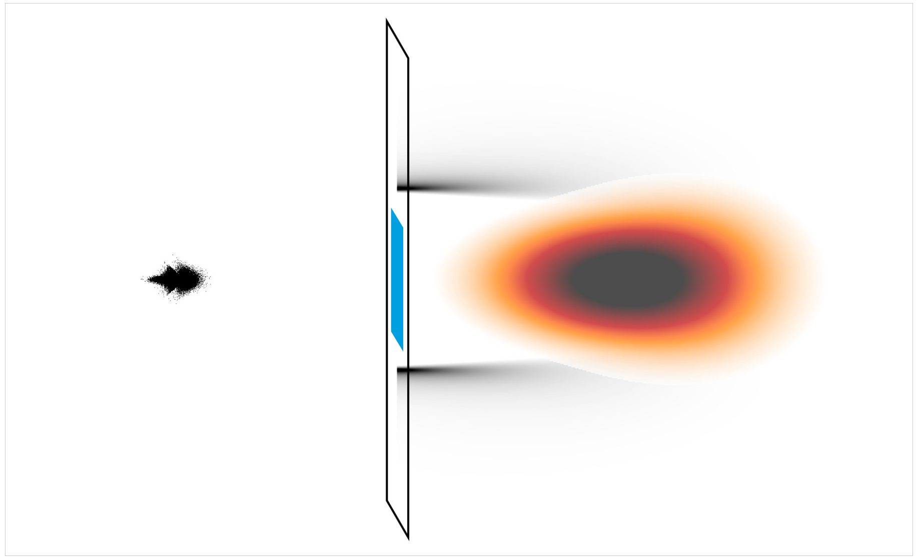




Severin Diederichs

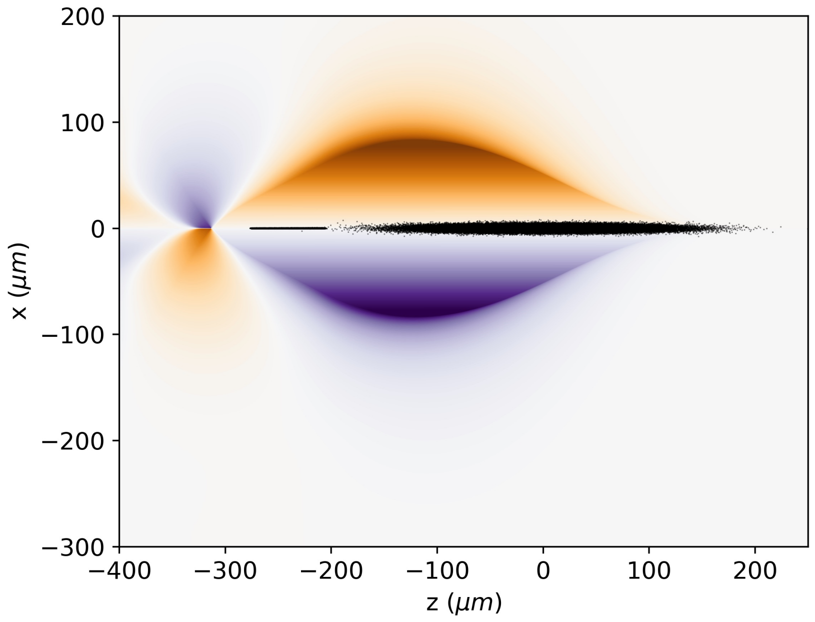
Alexander Sinn

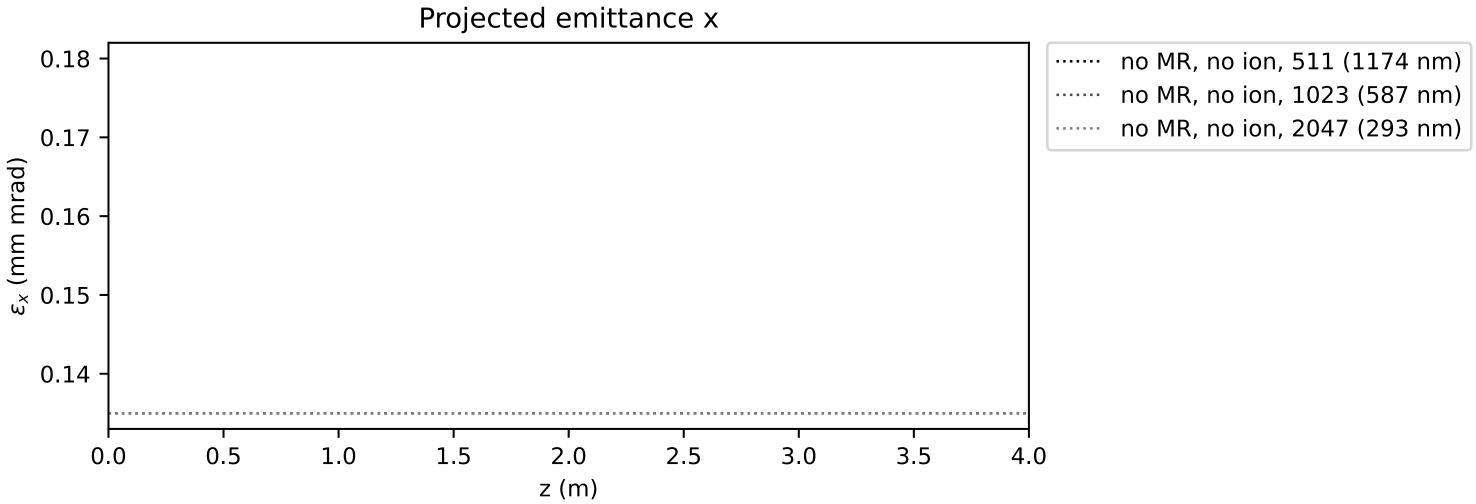
J.-L. Vay et al., Comput. Sci. & Disc. 5, 014019 (2012)	T. J. Mehrling et al., IEEE, AAC (2018)



- Deposit densities (beam and plasma) $\rho, \vec{J}, S_x, S_y$
  on all levels
- Solve fields $(E_x - cB_y, E_y + cB_x, E_z. B_z)$ and $(B_x. B_y)$
  BC on fine patch, solve, Interpolate in ghost cells
- Tag by level
- Advance plasma particles by 1 slice $(-\Delta\zeta)$
- Advance beam particles by 1 time step $(+\Delta t)$

Converged simulations in collider-relevant range are ~~feasible~~ cheap





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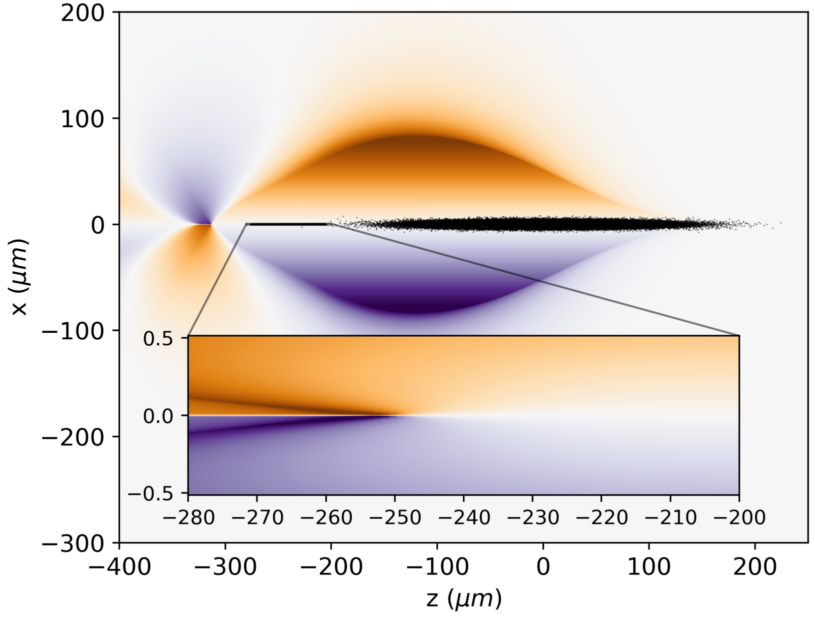

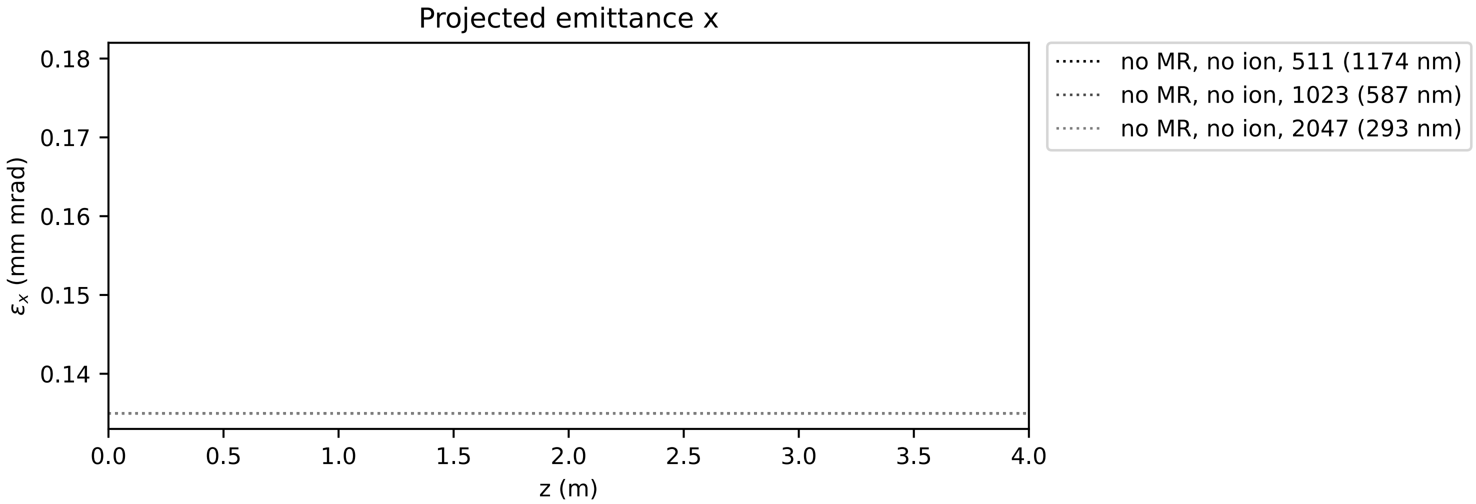

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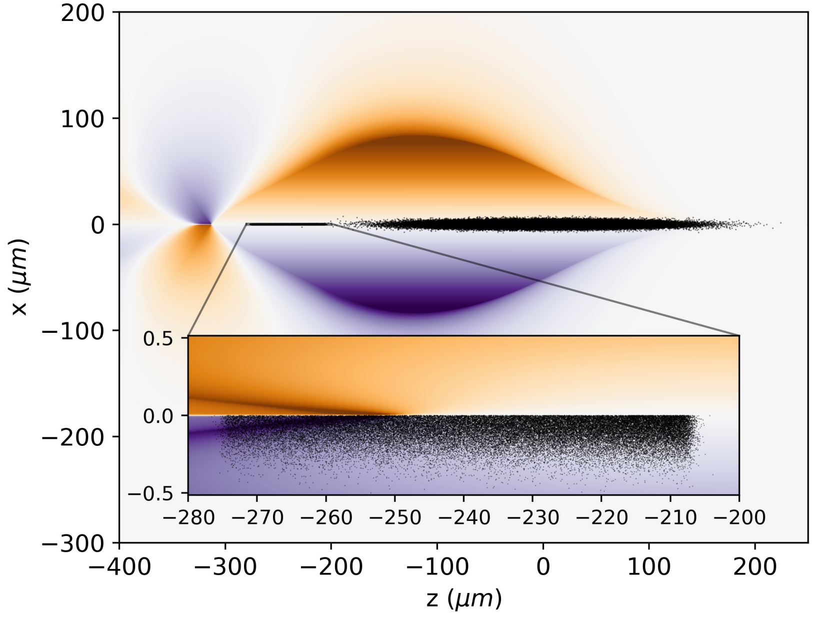

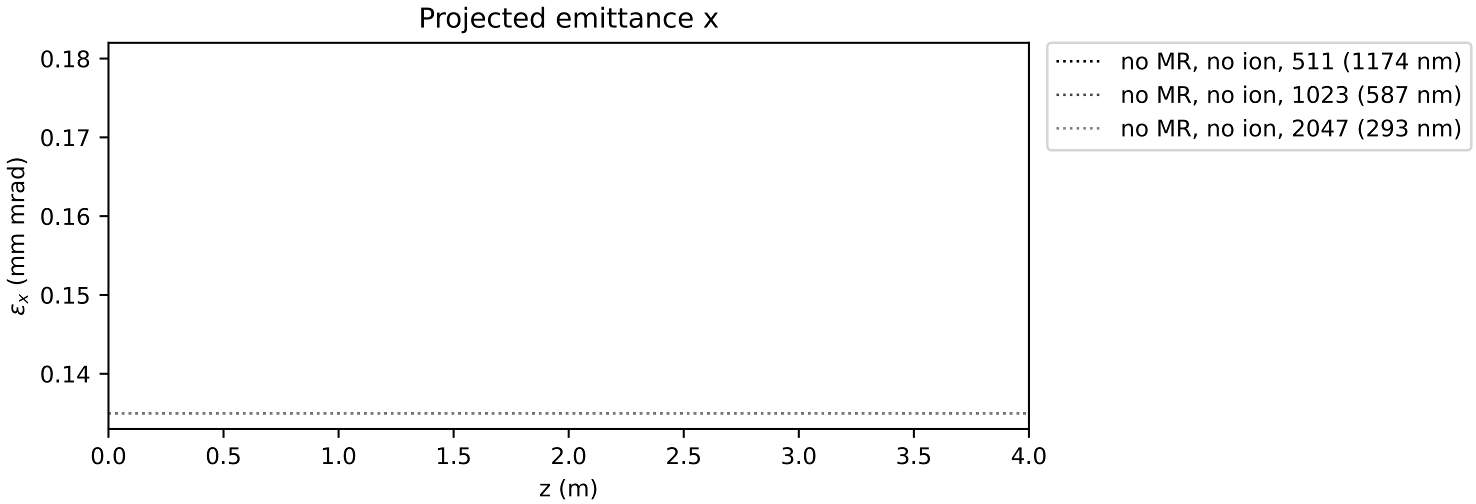

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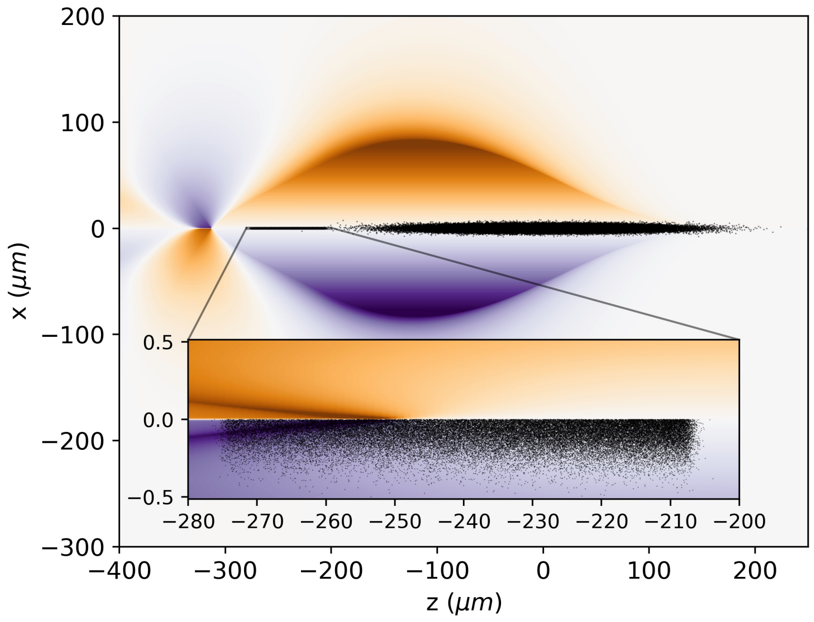

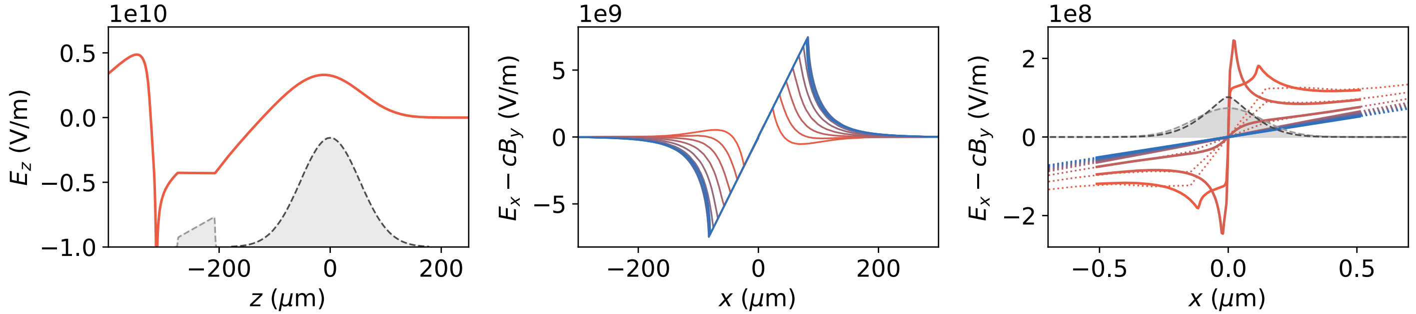

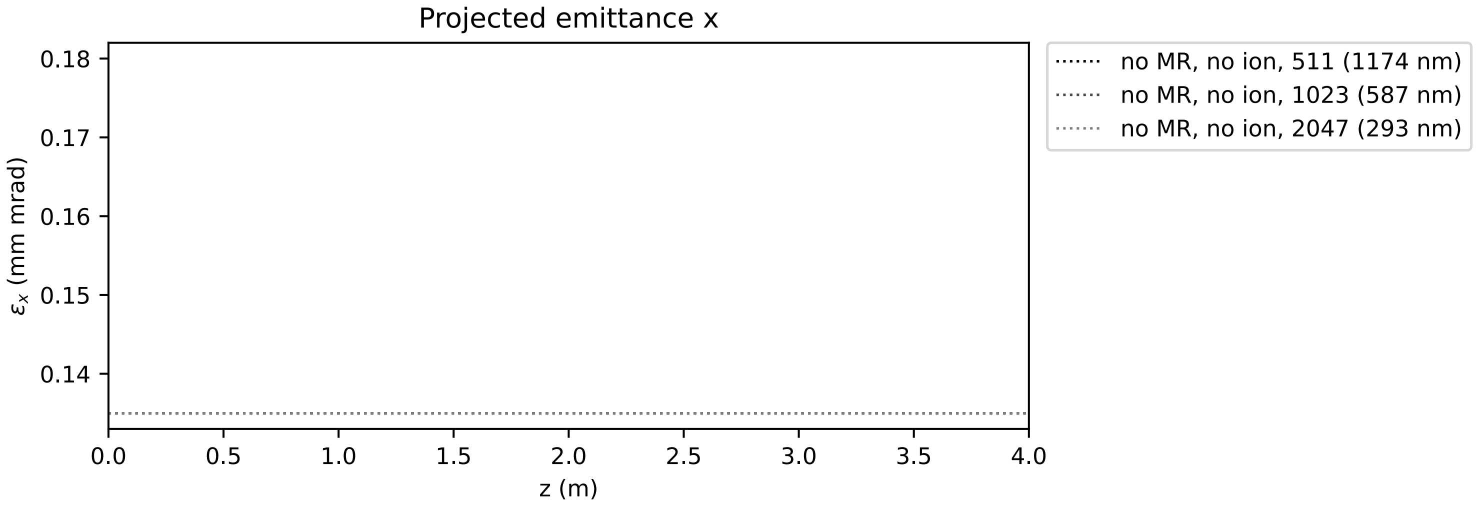

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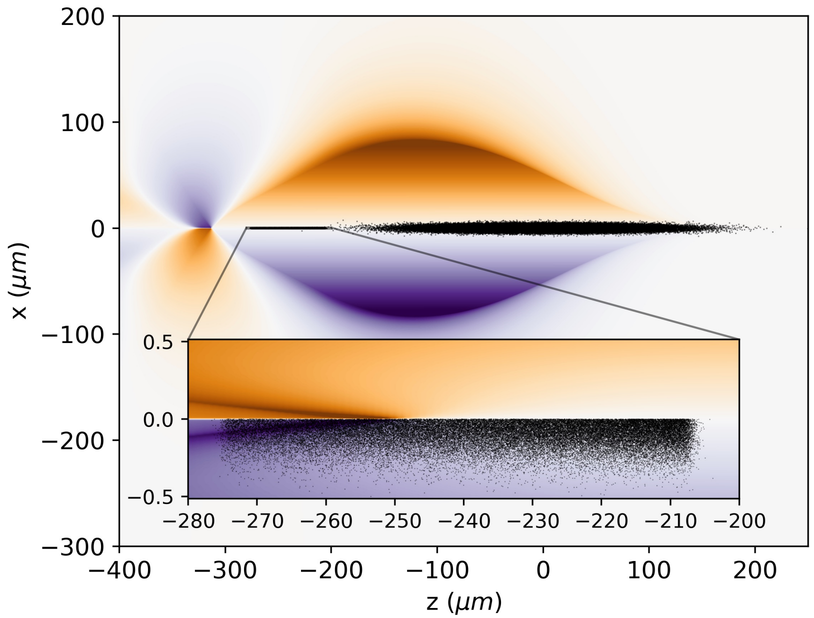

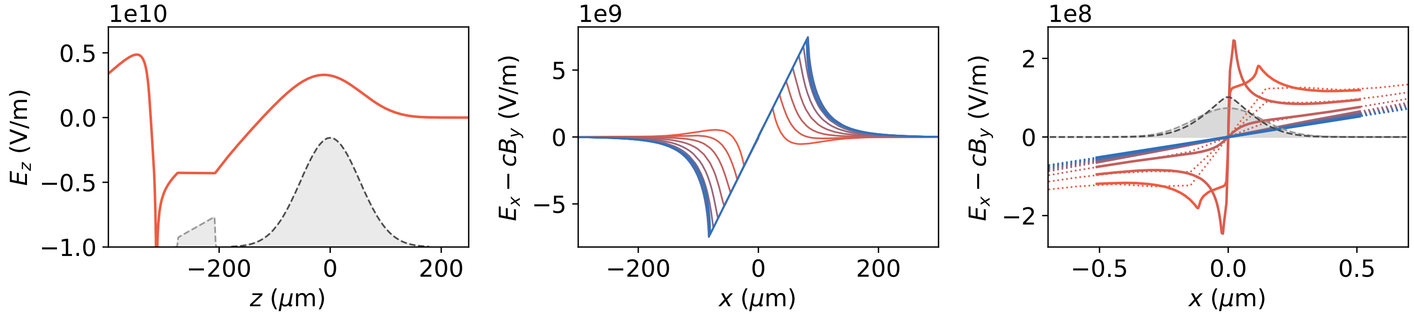

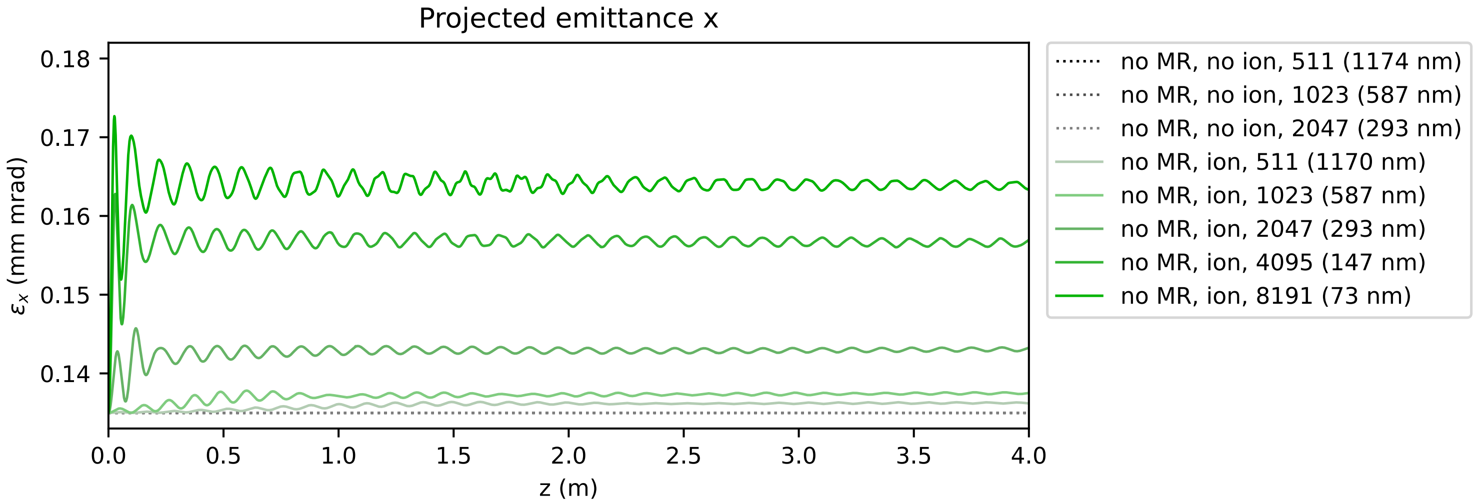

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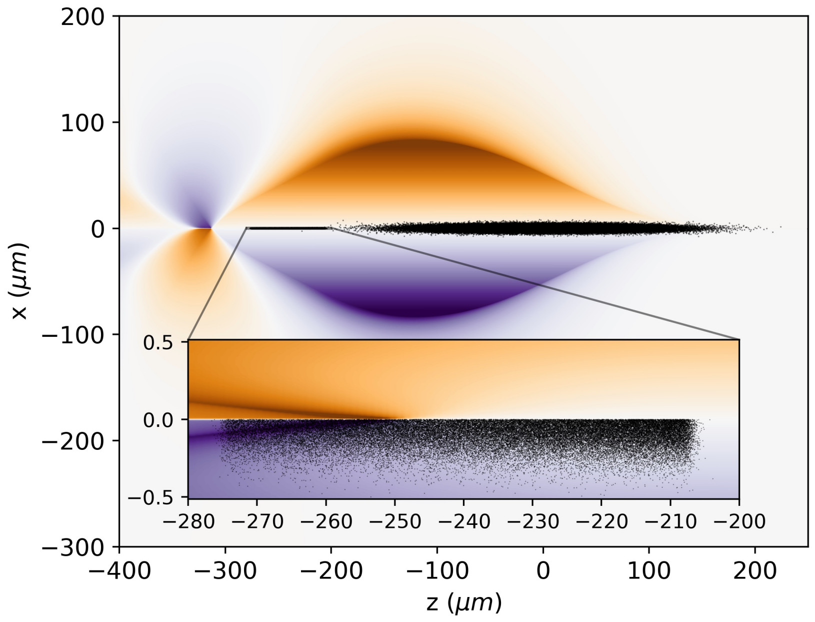

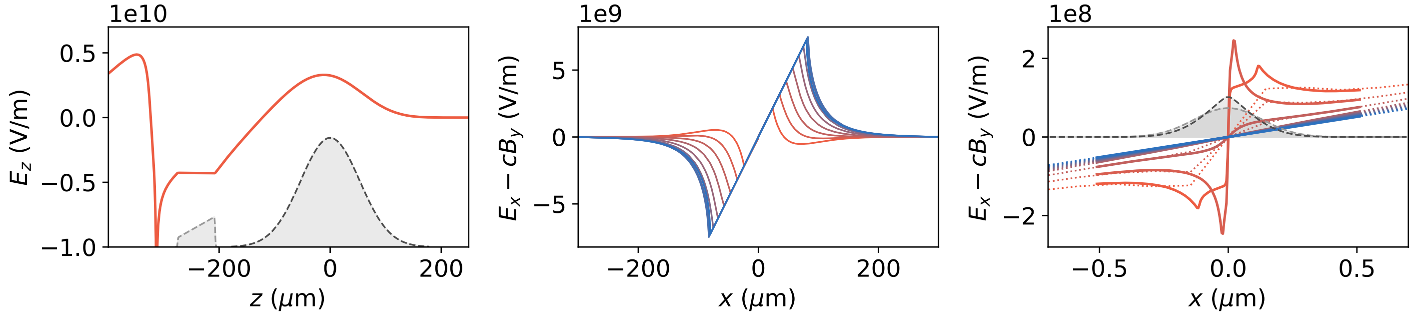

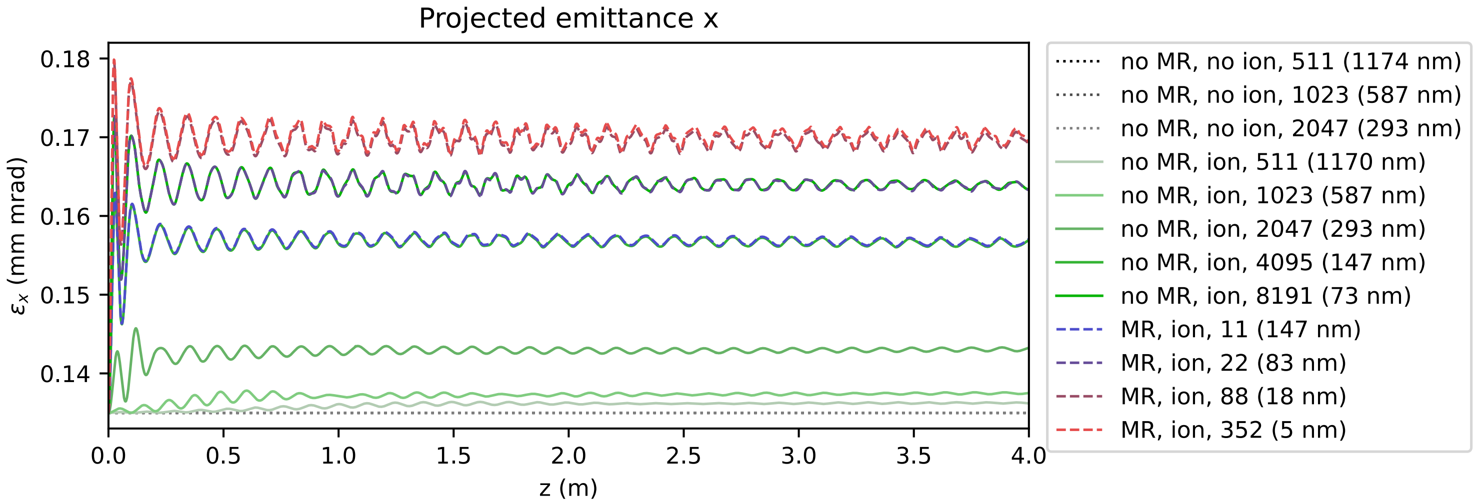

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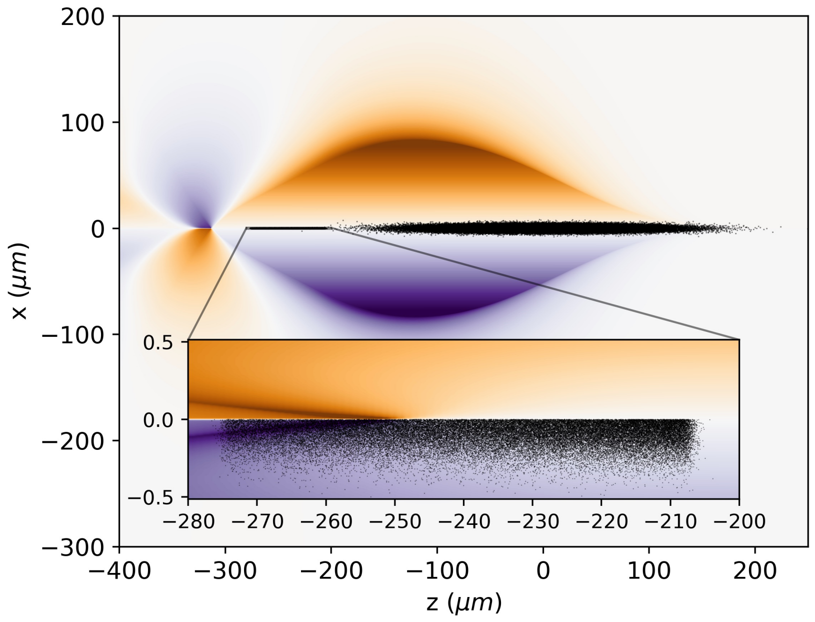

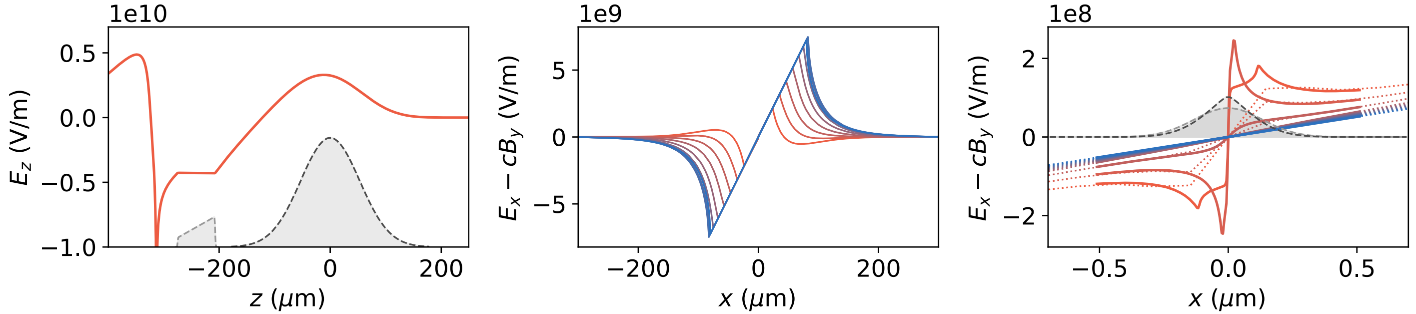

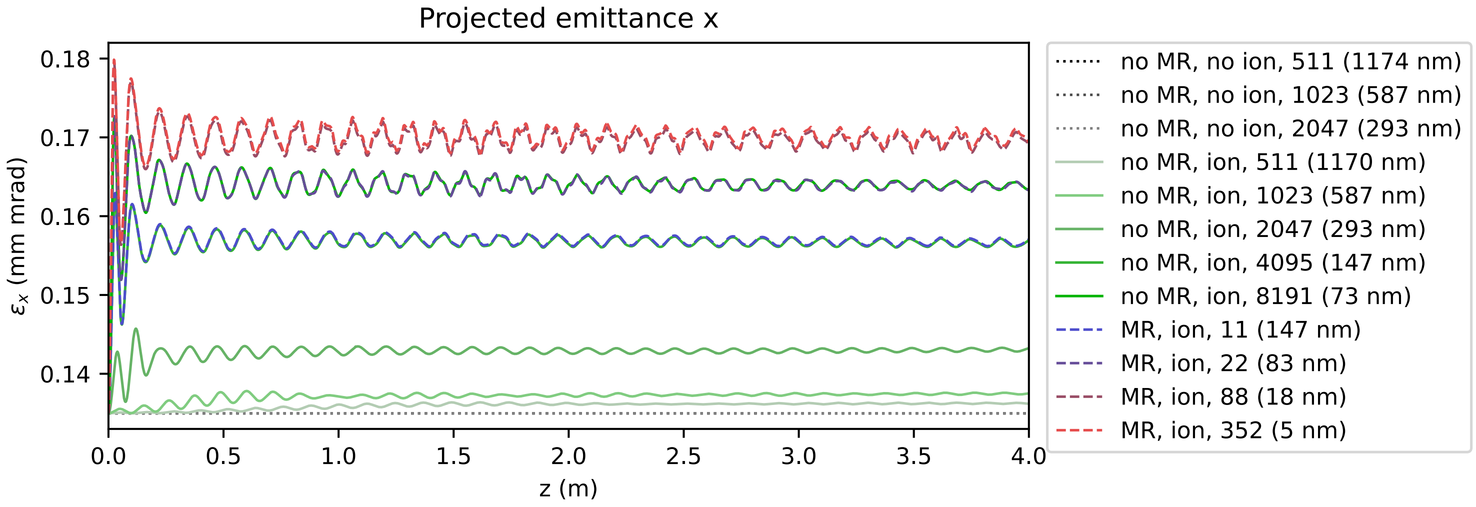

- Fine everywhere = Coarse + MR
- MR allows for convergence at modest cost

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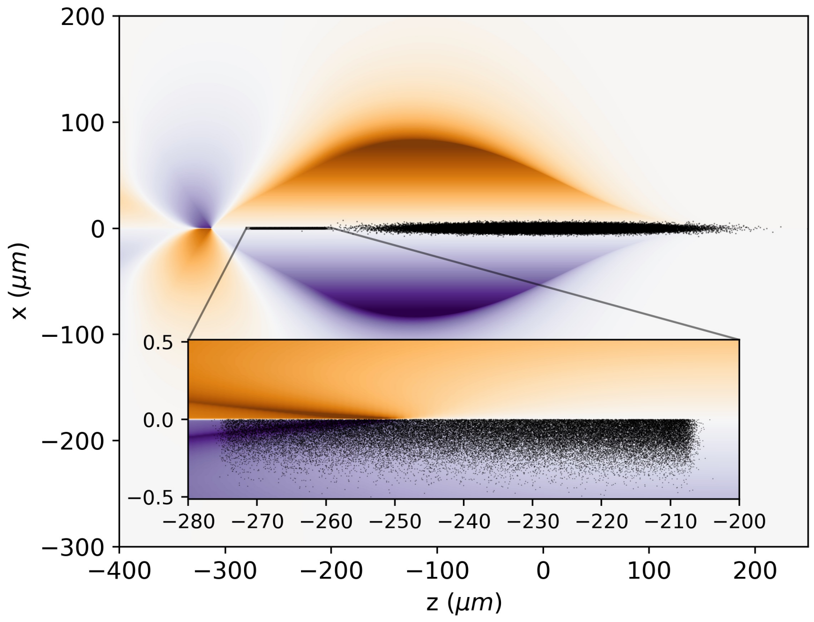

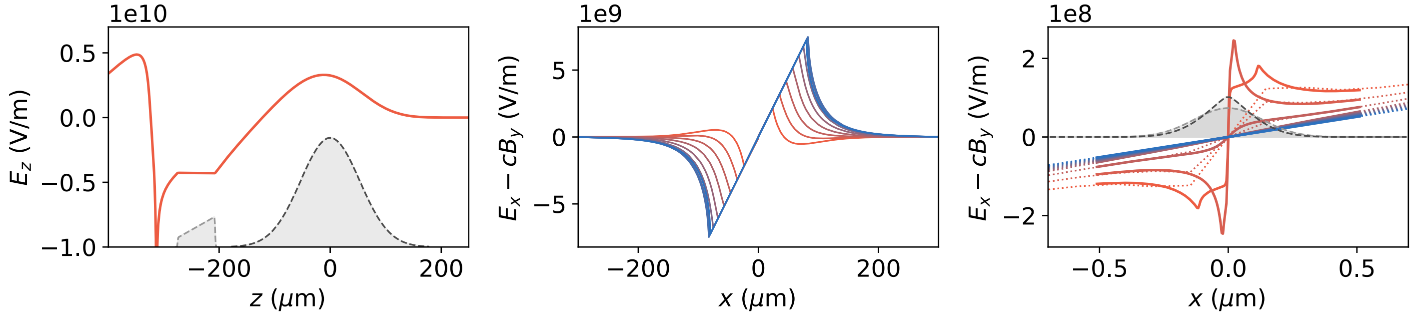

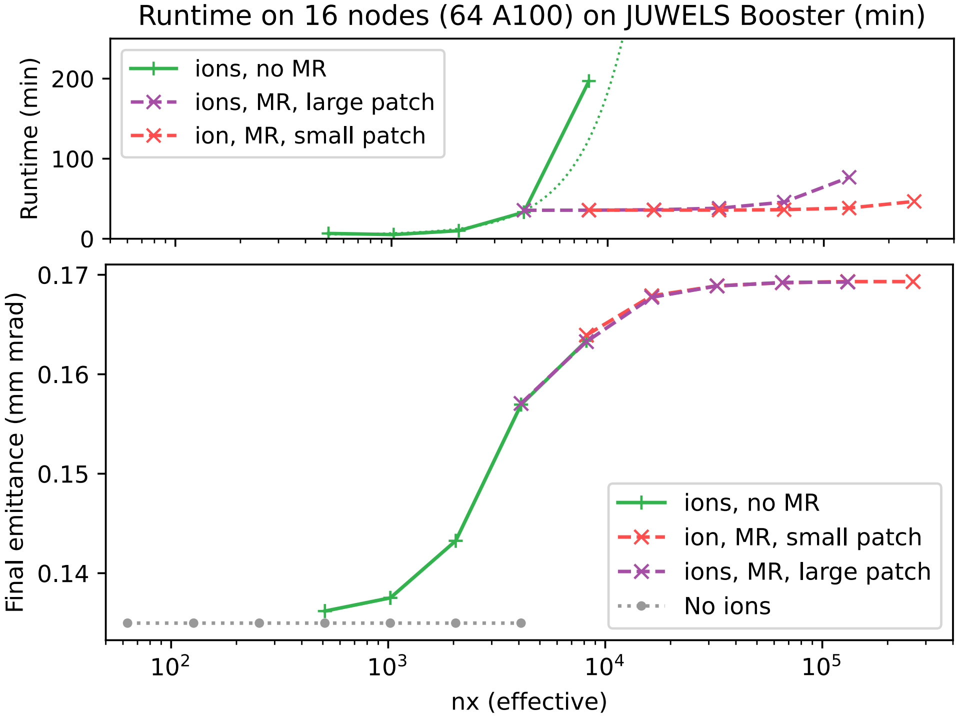

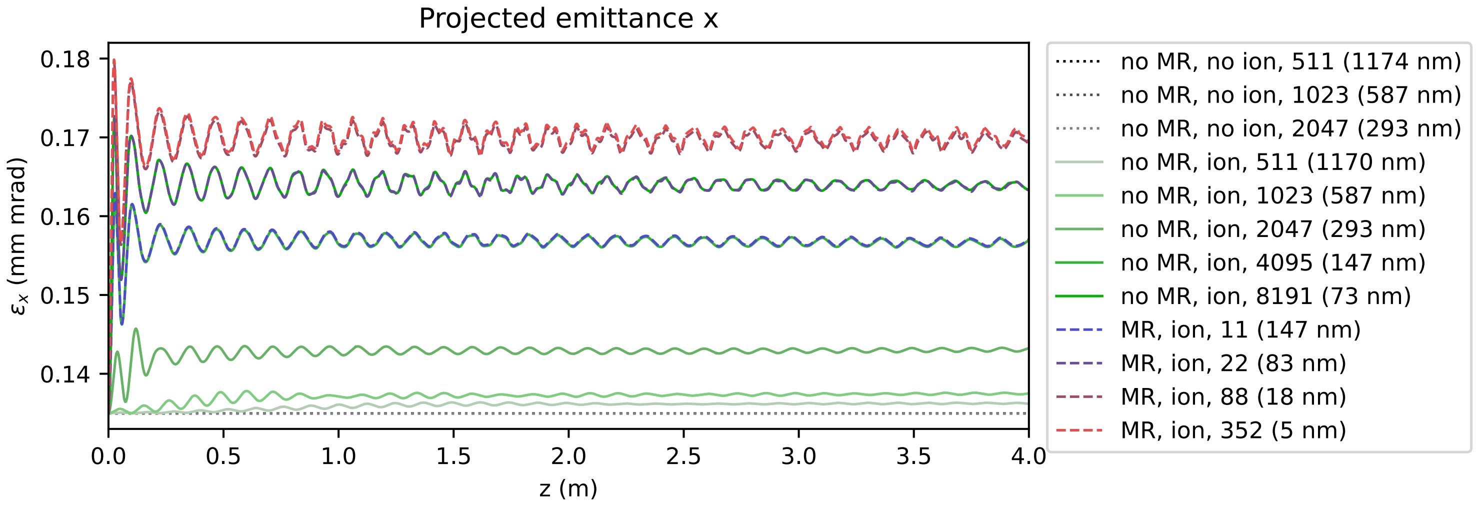

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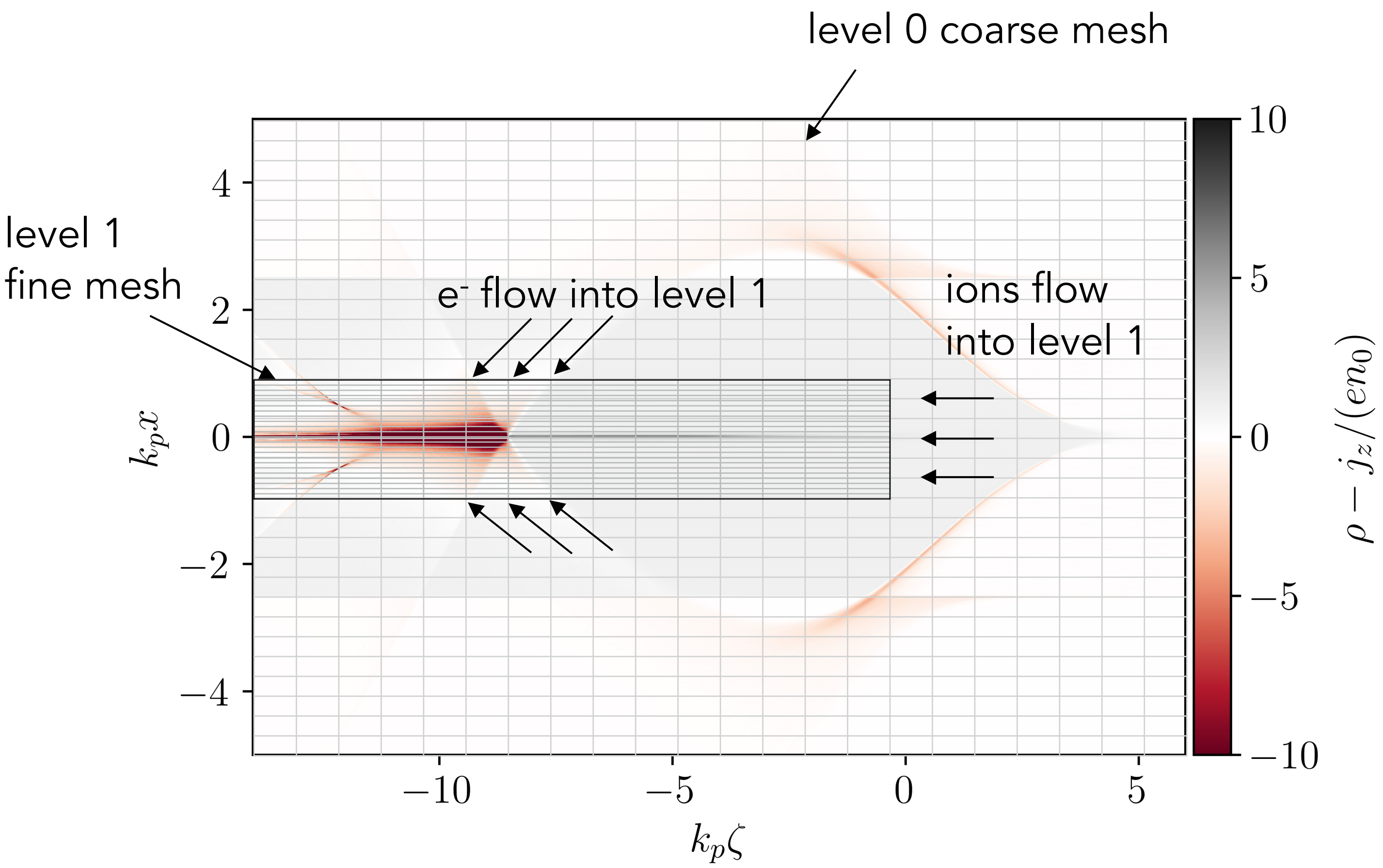
Challenging positron acceleration simulations benefit from MR



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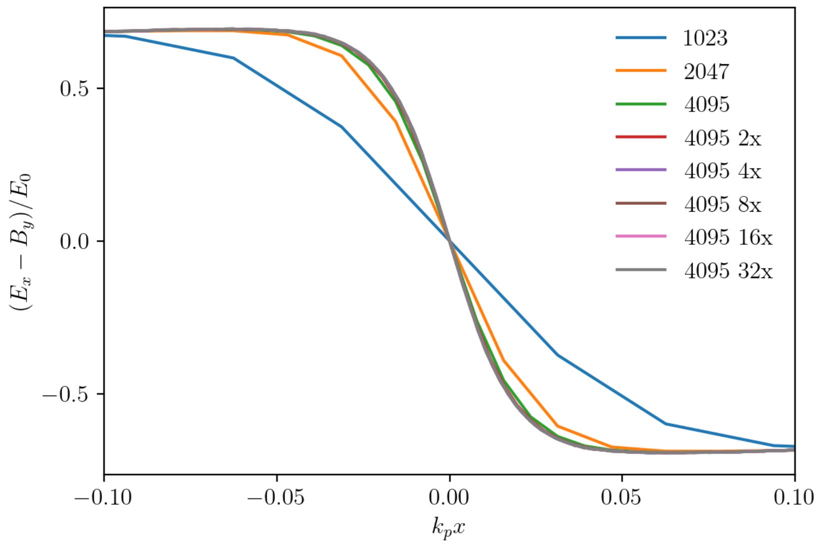

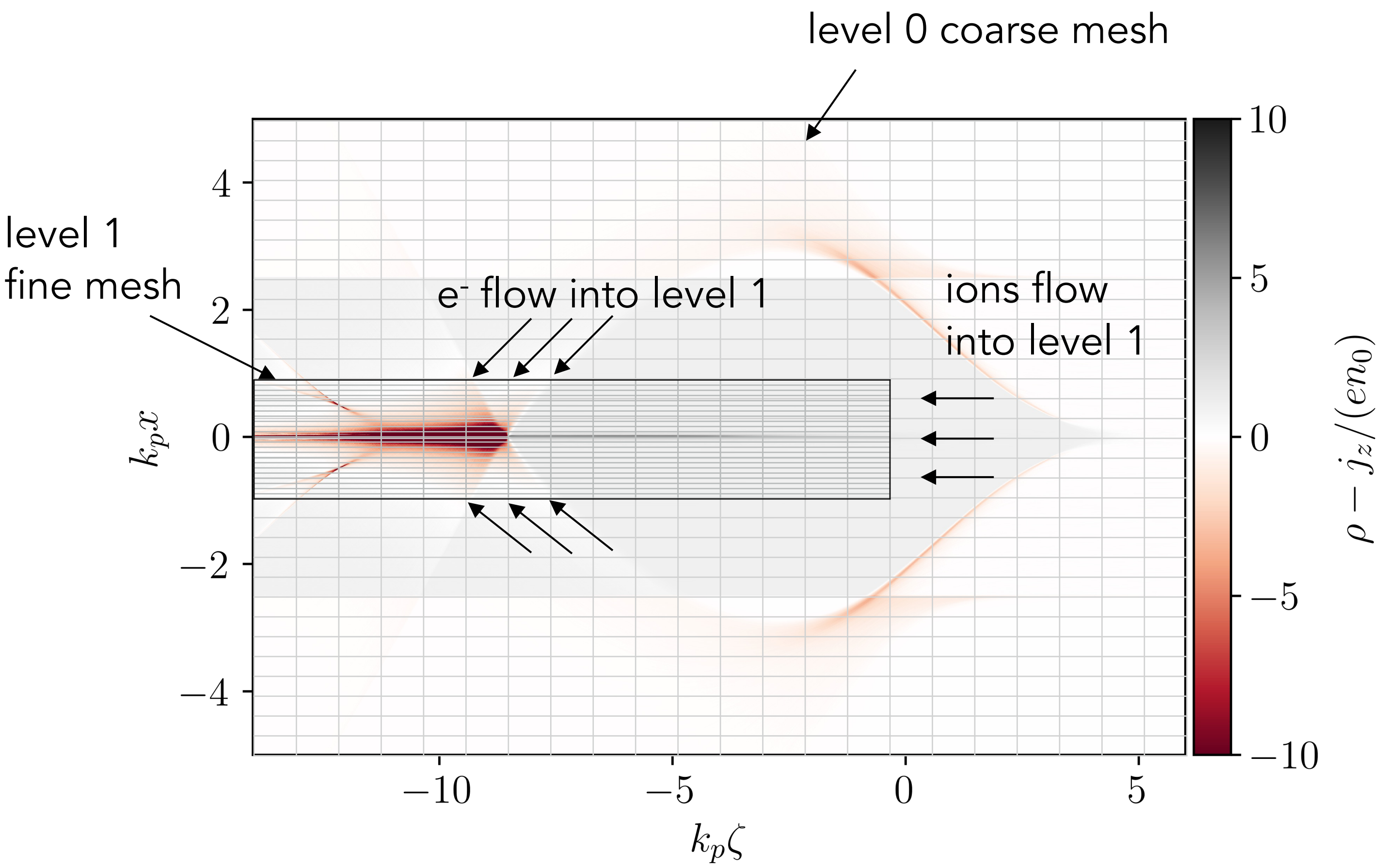

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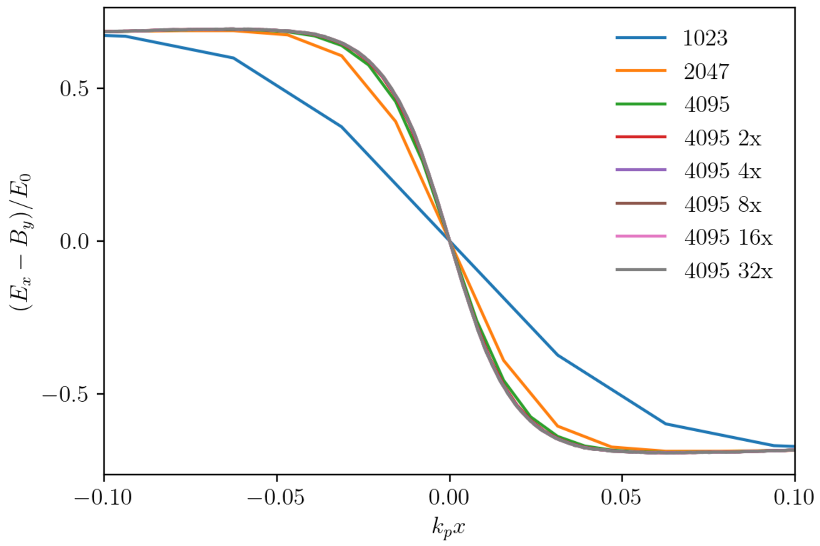

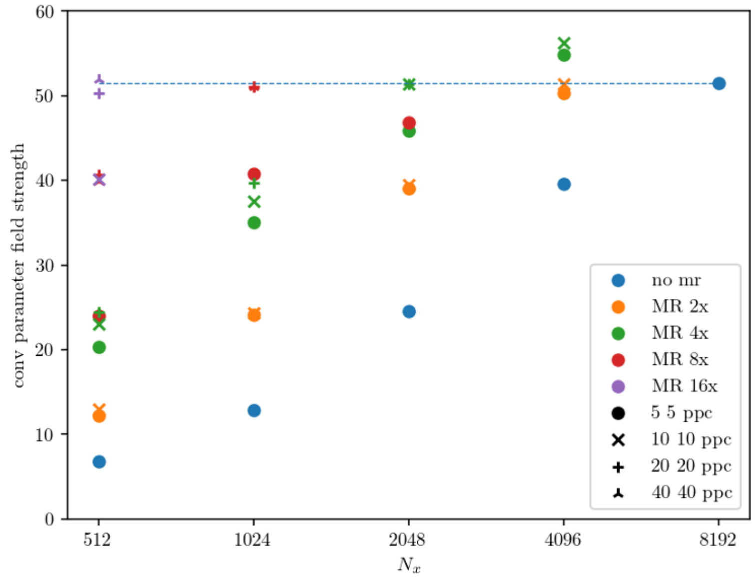

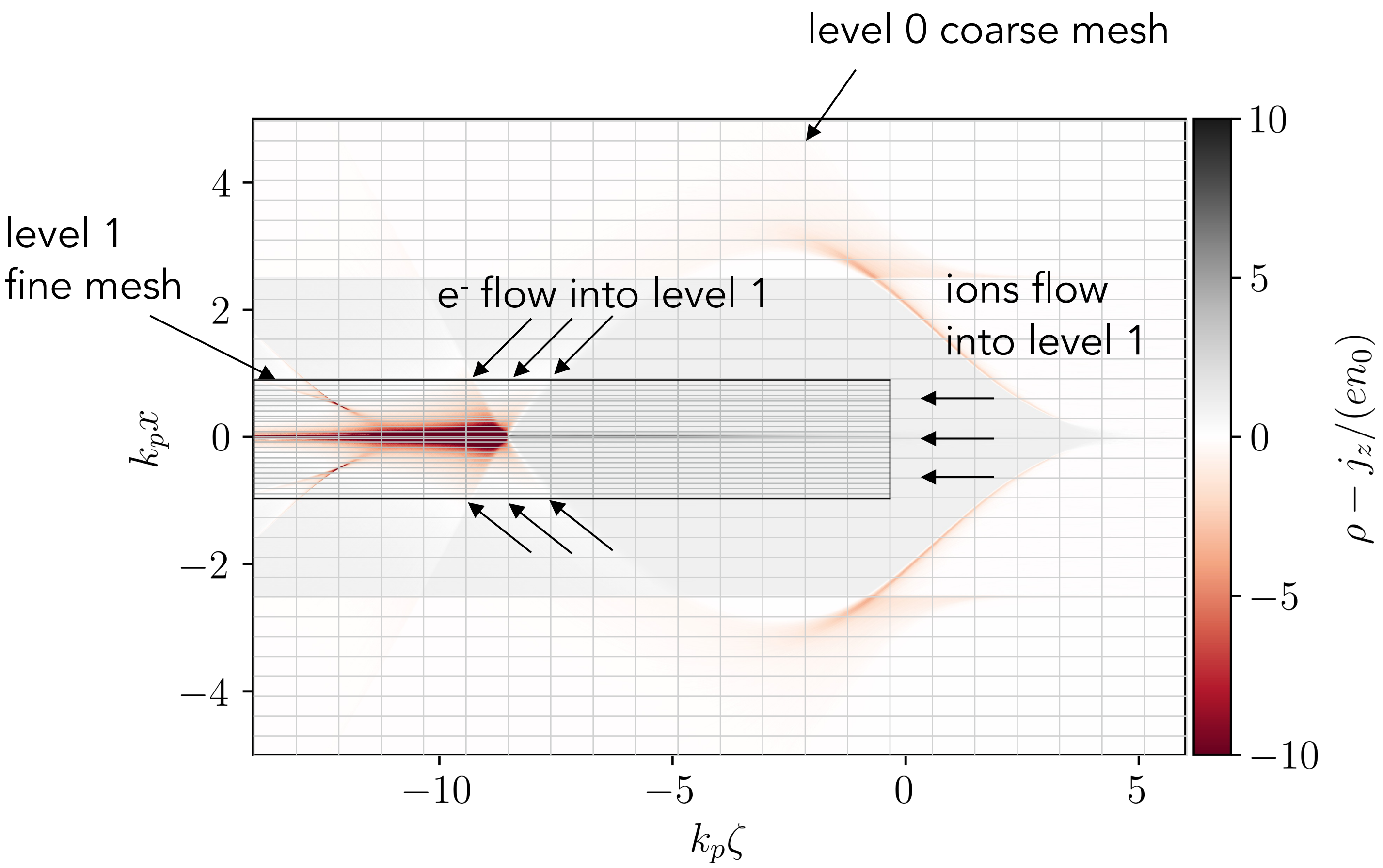

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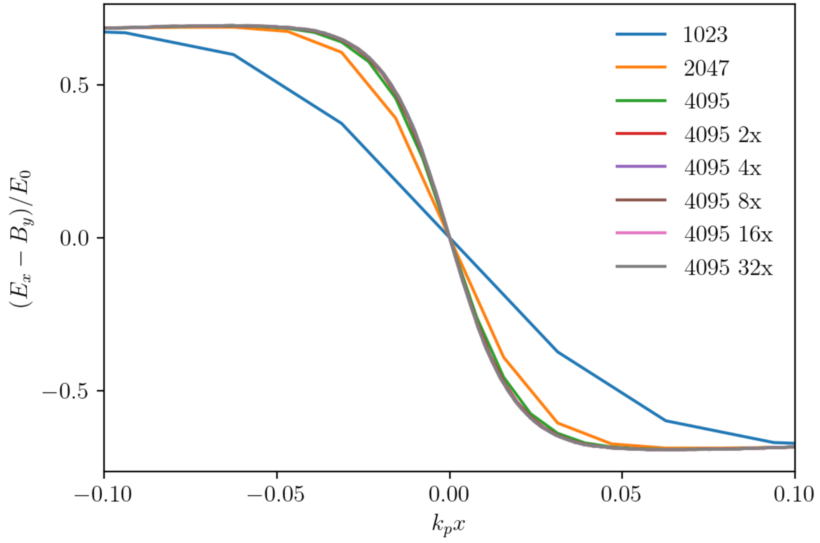
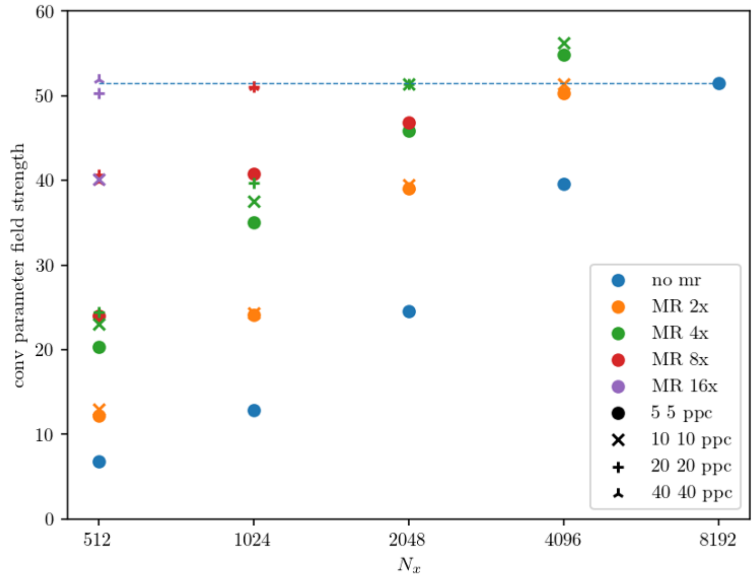
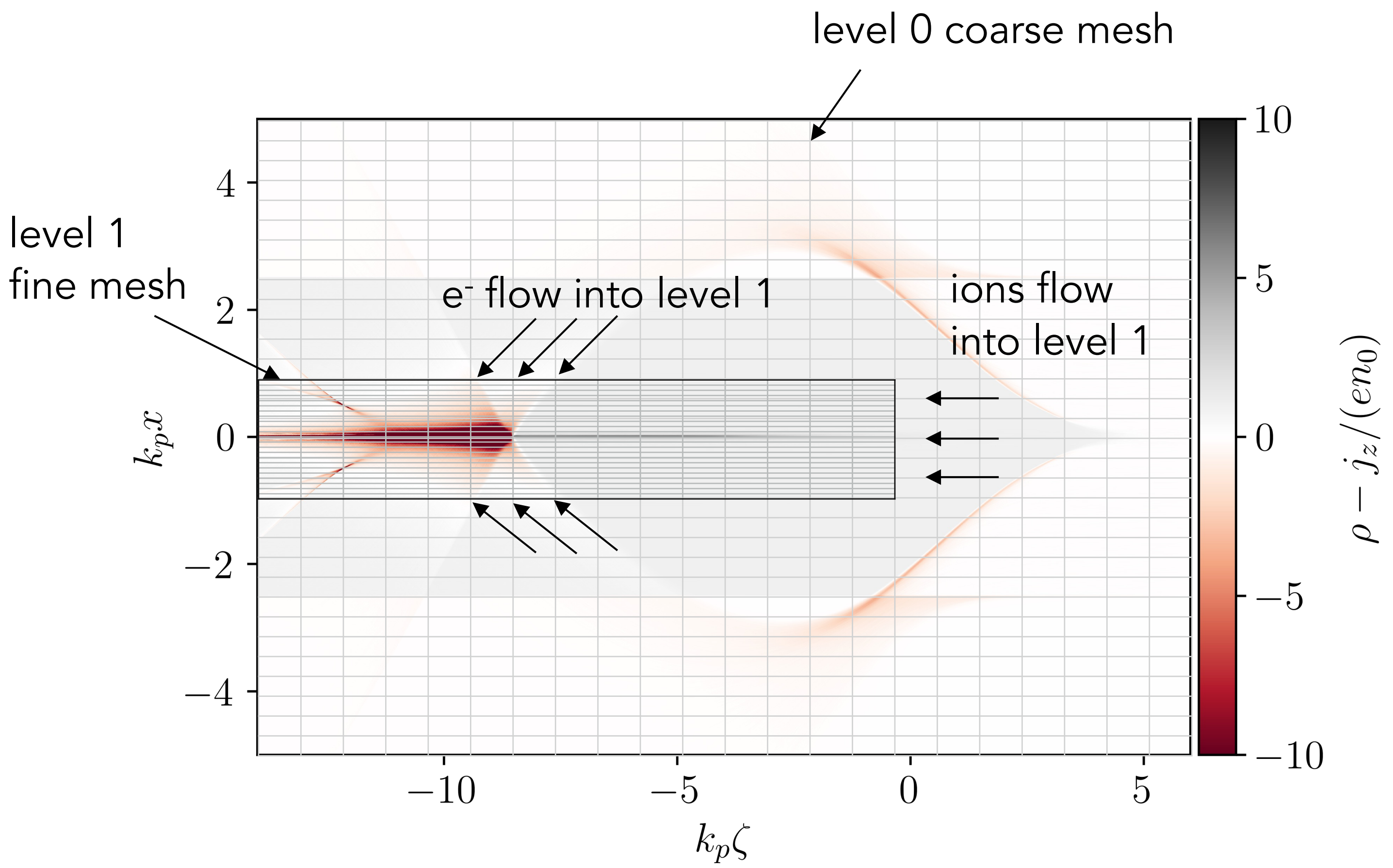






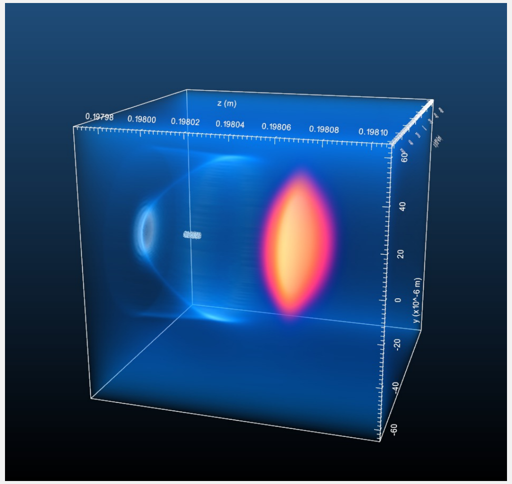
- ➢ Coarse resolution + MR = fine resolution everywhere
- ➢ MR allows for convergence at modest cost

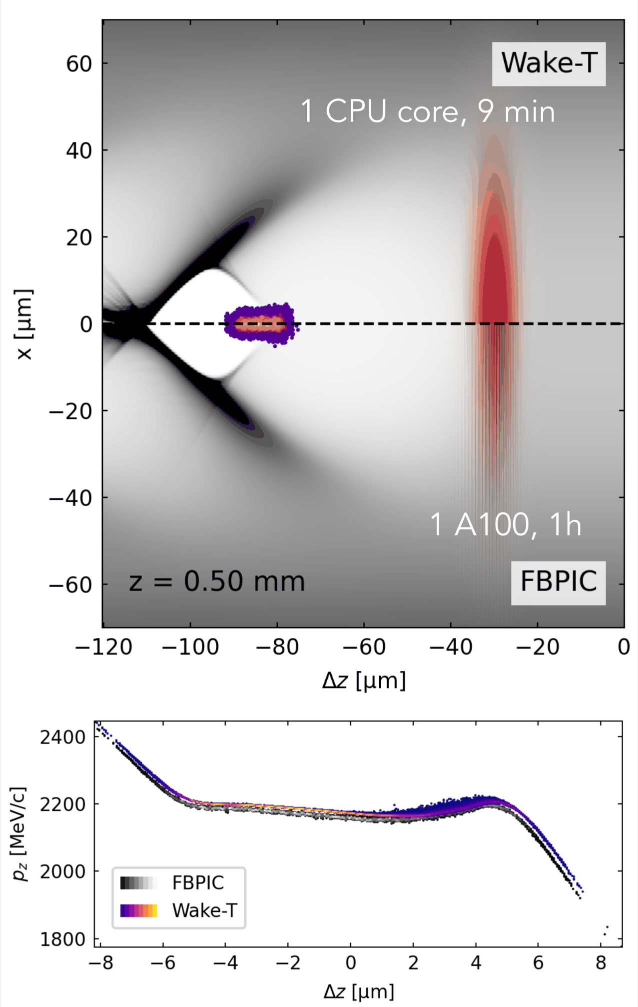
Wake-T: multi-stage axisymmetric simulations on a laptop

Ángel Ferran Pousa

<u>Wake</u>field particle <u>T</u>racker [1]

- 2D (RZ) axisymmetric, quasi-static
- Particle beam or laser pulse drivers [2]
- Gridless model based on explicit solver [3]
- Python, open-source, openPMD
- Beam optics





→ Multi-stage simulations within second/minutes on a laptop

https://github.com/AngelFP/Wake-T
https://wake-t.readthedocs.io

[1] A. Ferran Pousa et al., J. Phys.: Conf. Ser. (2019)
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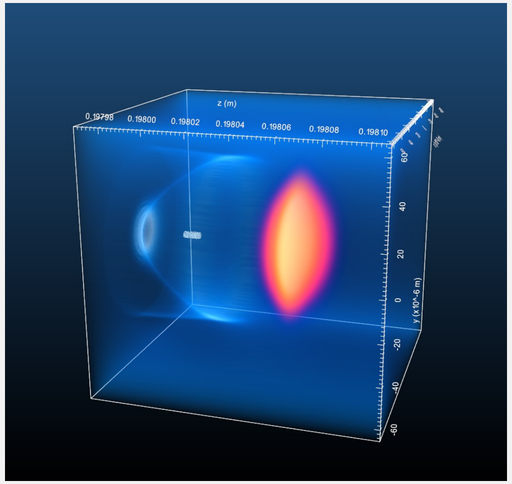

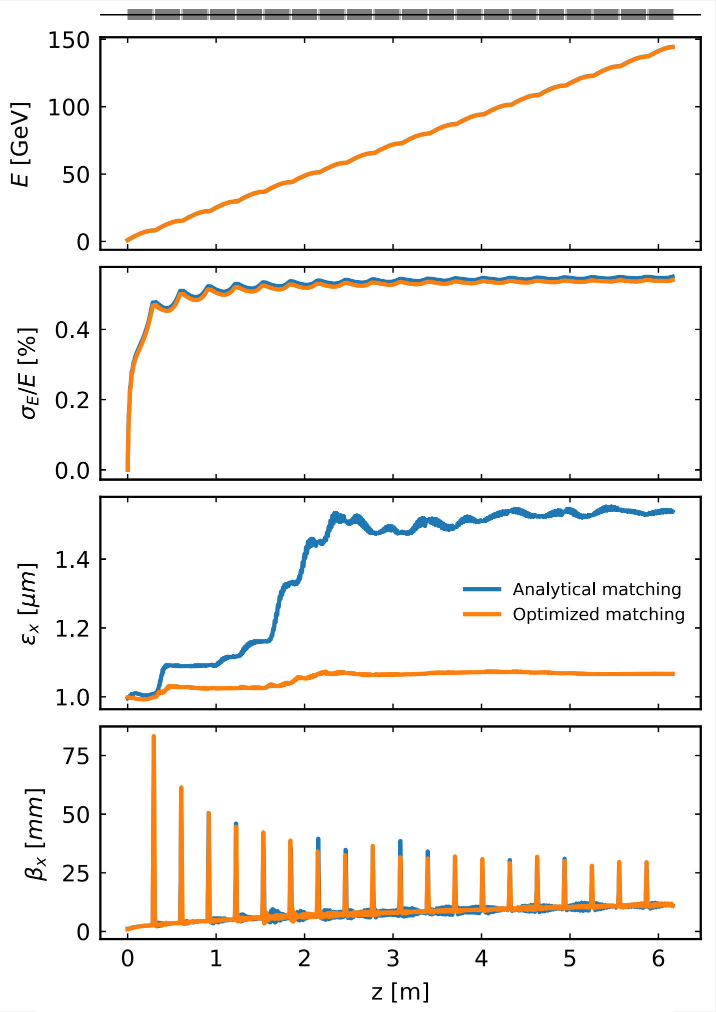

A. Ferran Pousa, IPAC 2023

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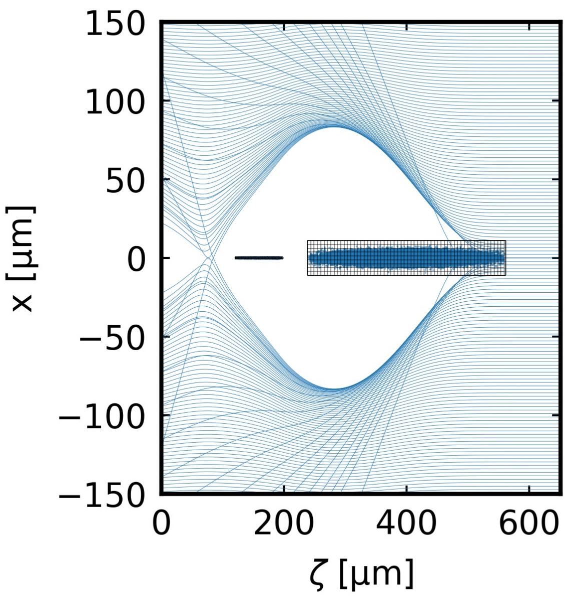
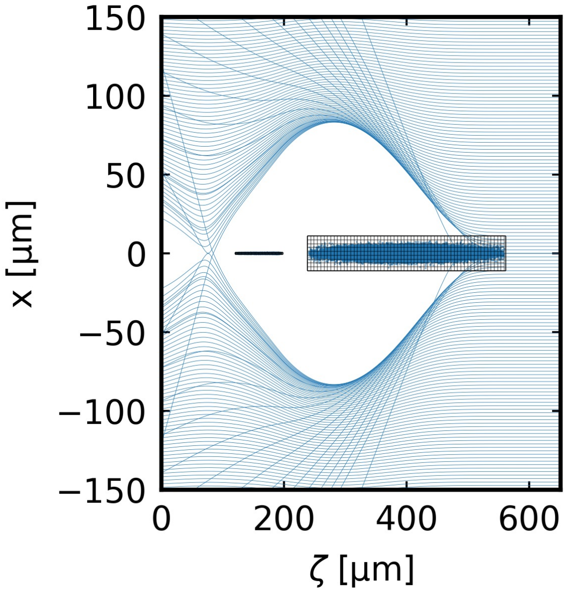
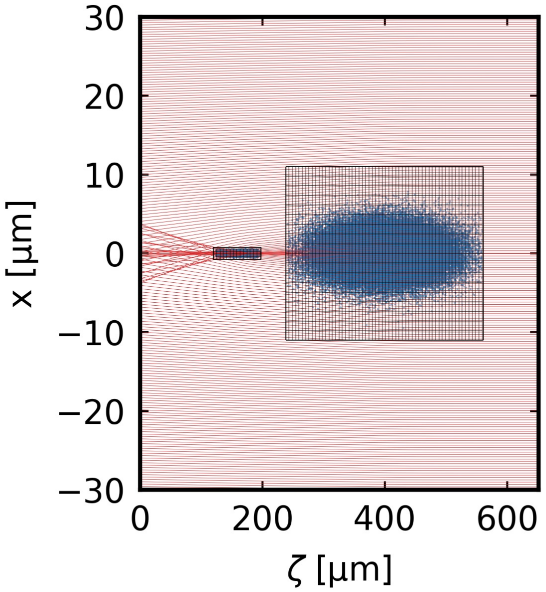
Wake-T: an adaptive grid in a gridless method



Wake-T: an adaptive grid in a gridless method





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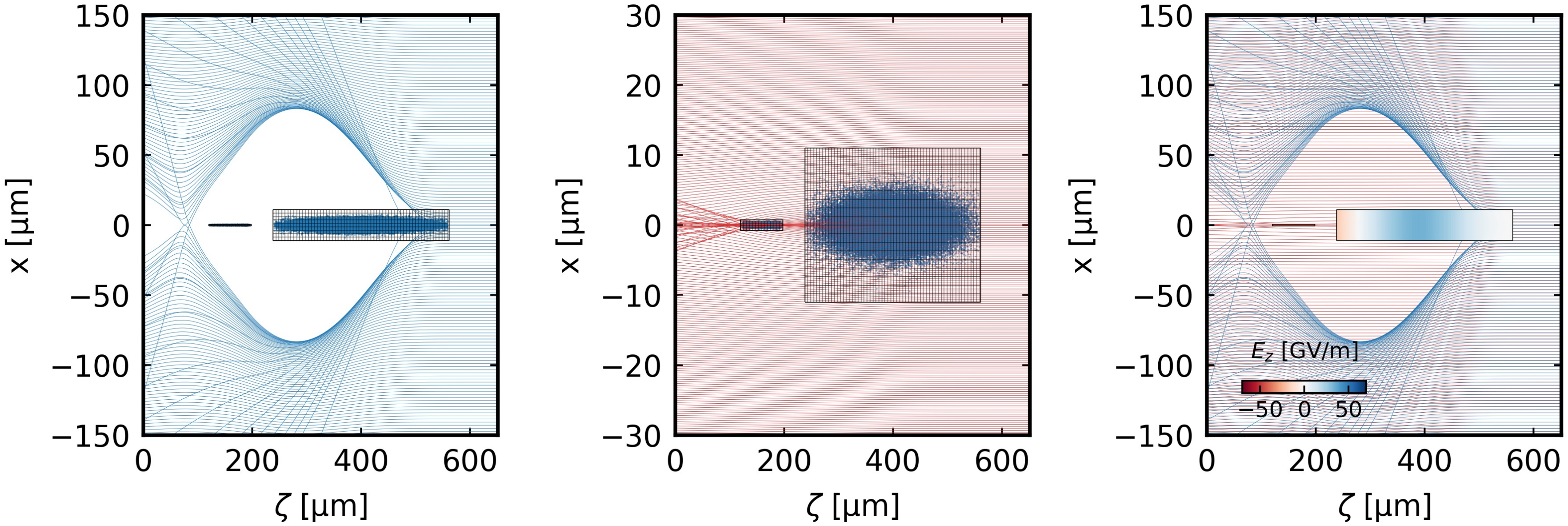
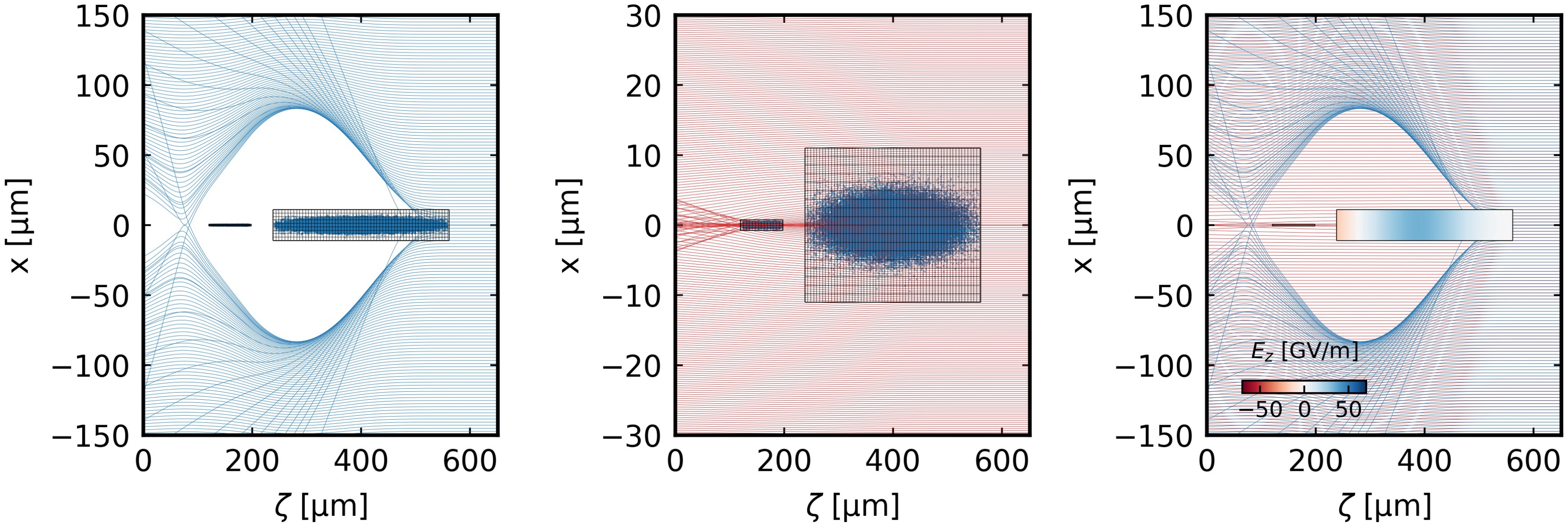
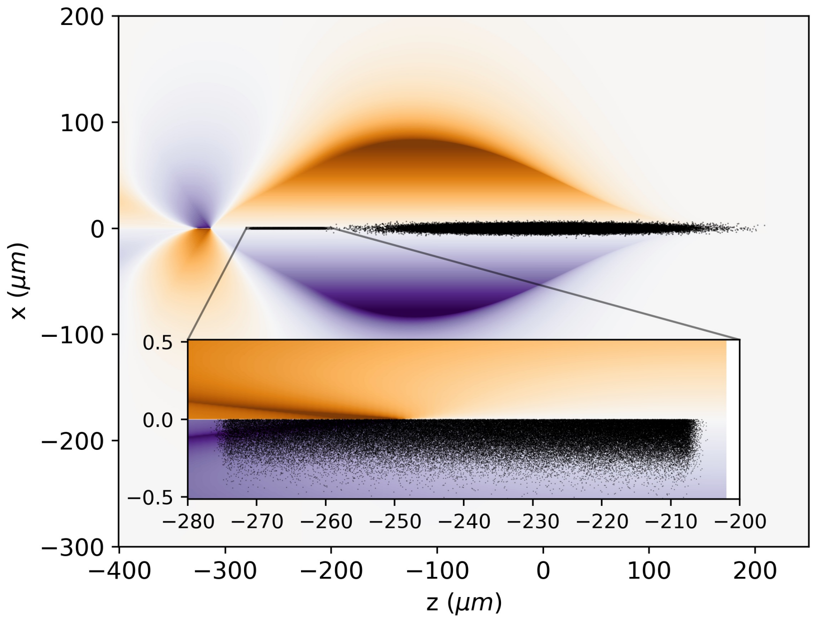


Wake-T: an adaptive grid in a gridless method



- ➢ Plasma advance does not need a grid
- ➢ Beam advance uses an adaptive grid

Realistic simulations of collider parameters on a laptop w/ Wake-T



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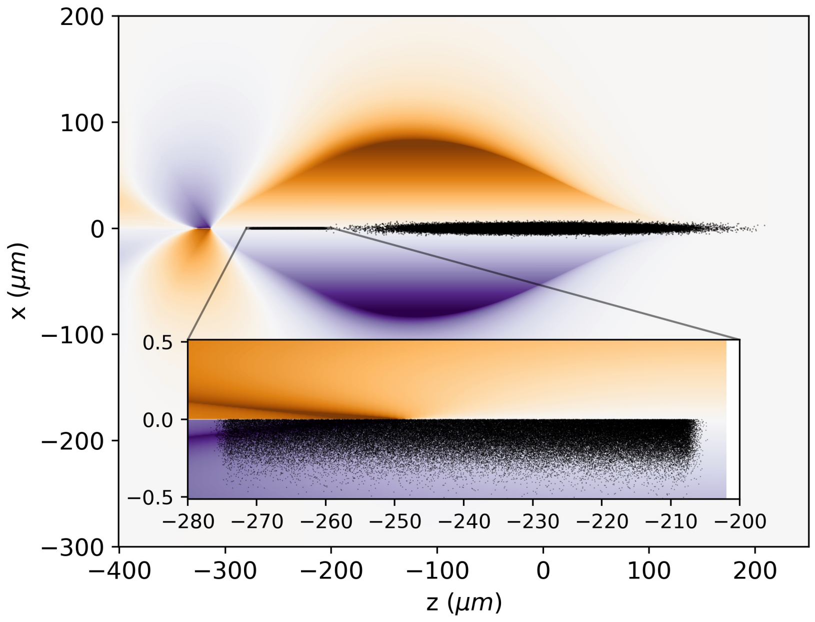

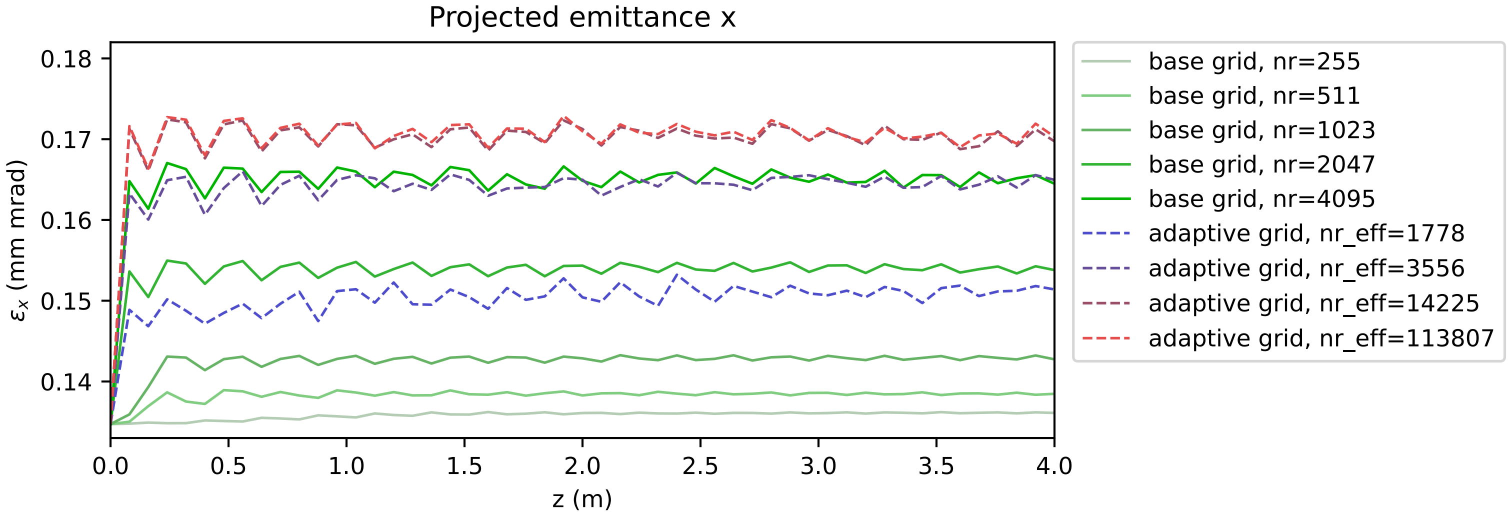

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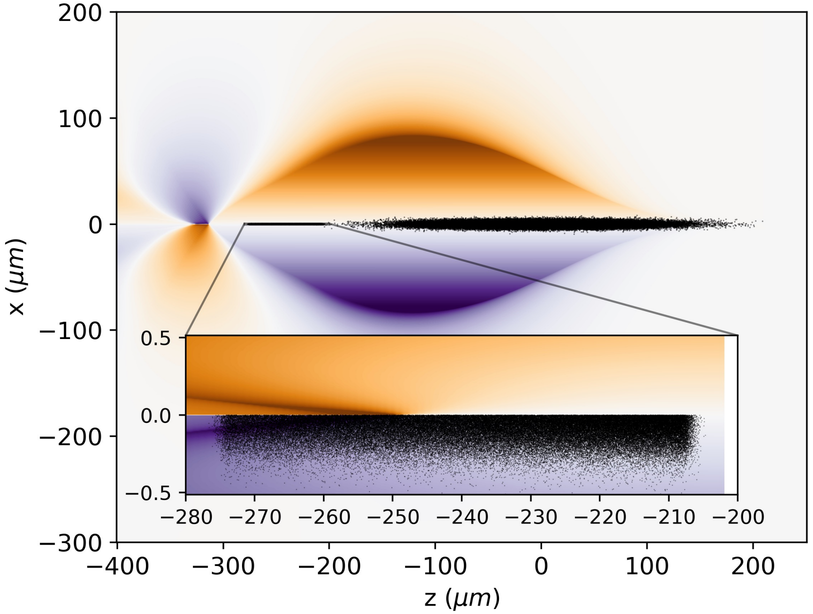
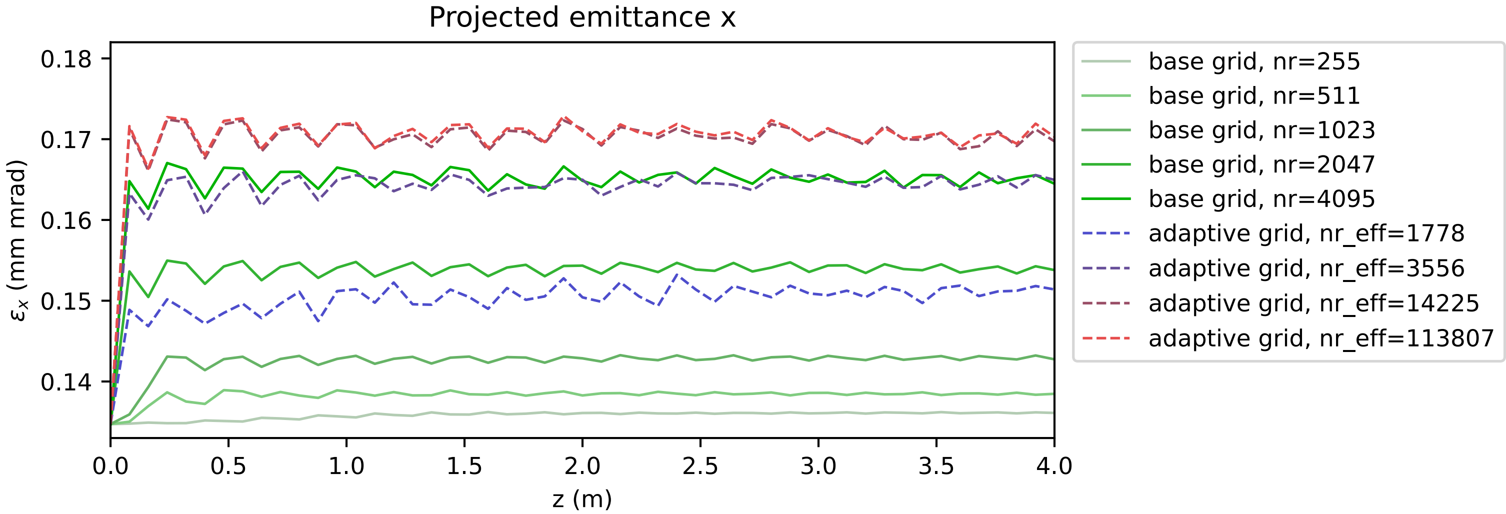
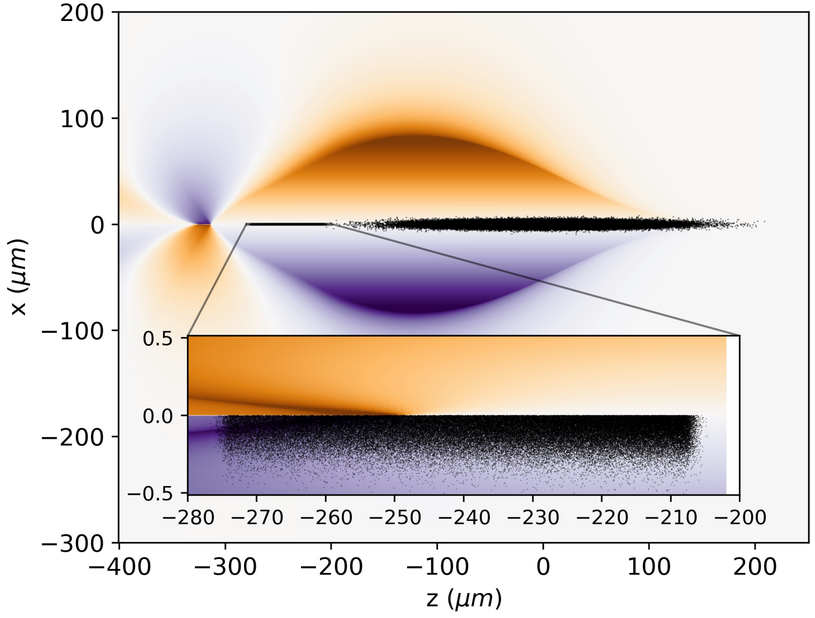
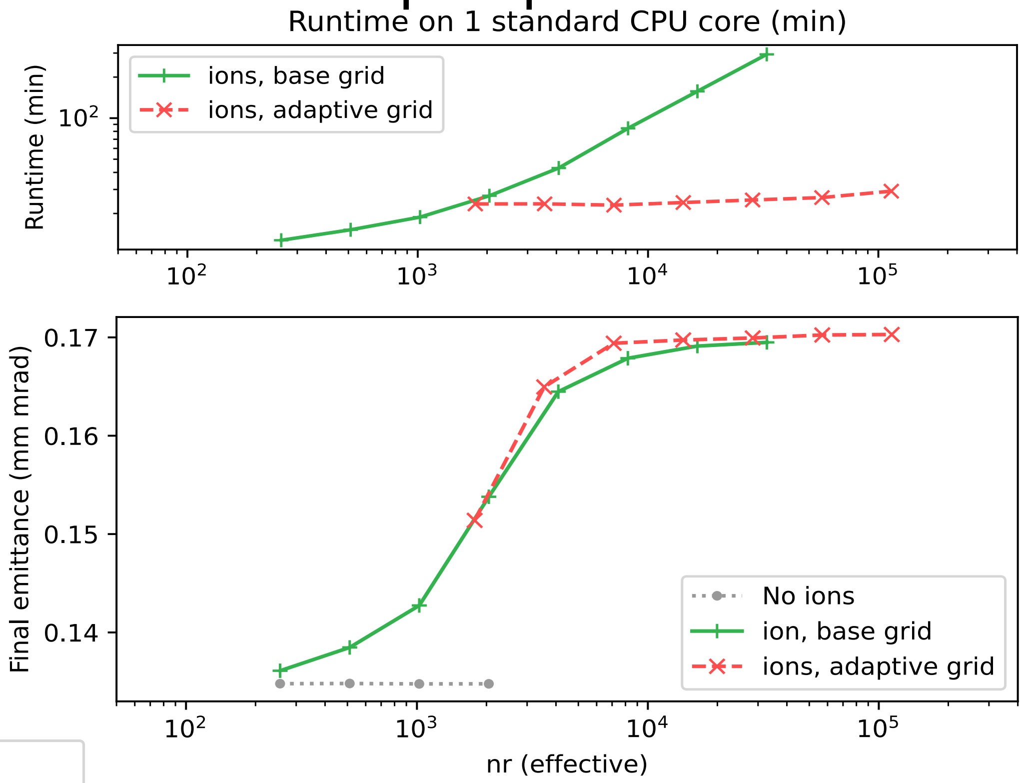


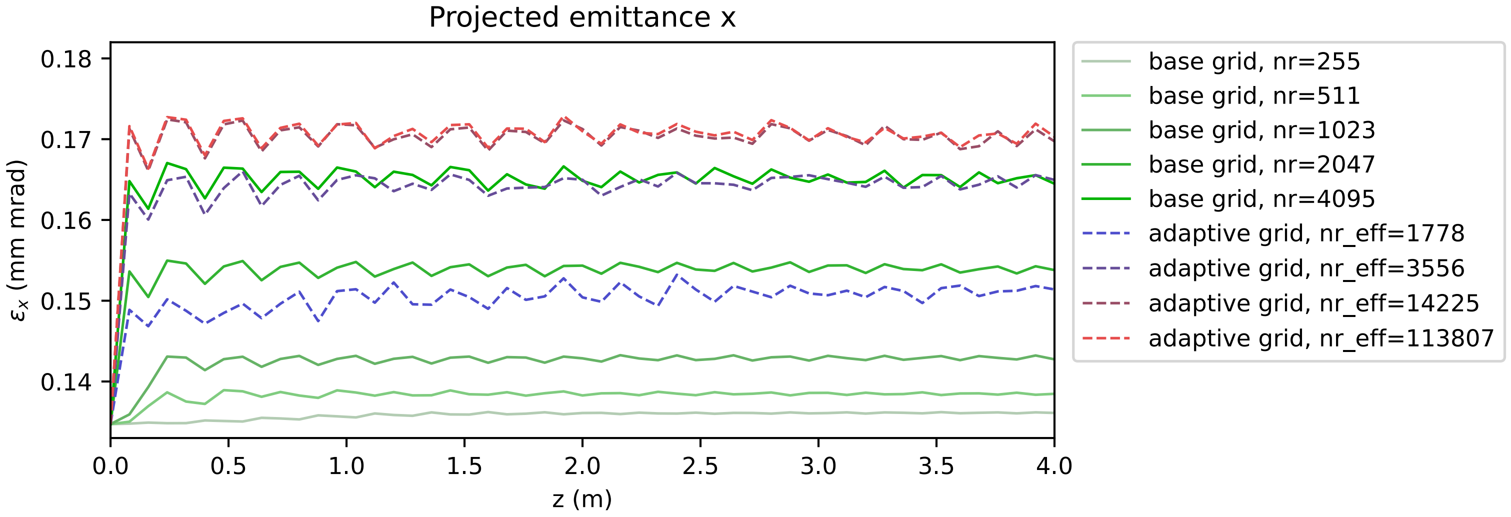


- Adaptive grid = fine resolution everywhere
- MR allows for convergence at modest cost

Realistic simulations of collider parameters on a laptop w/ Wake-T

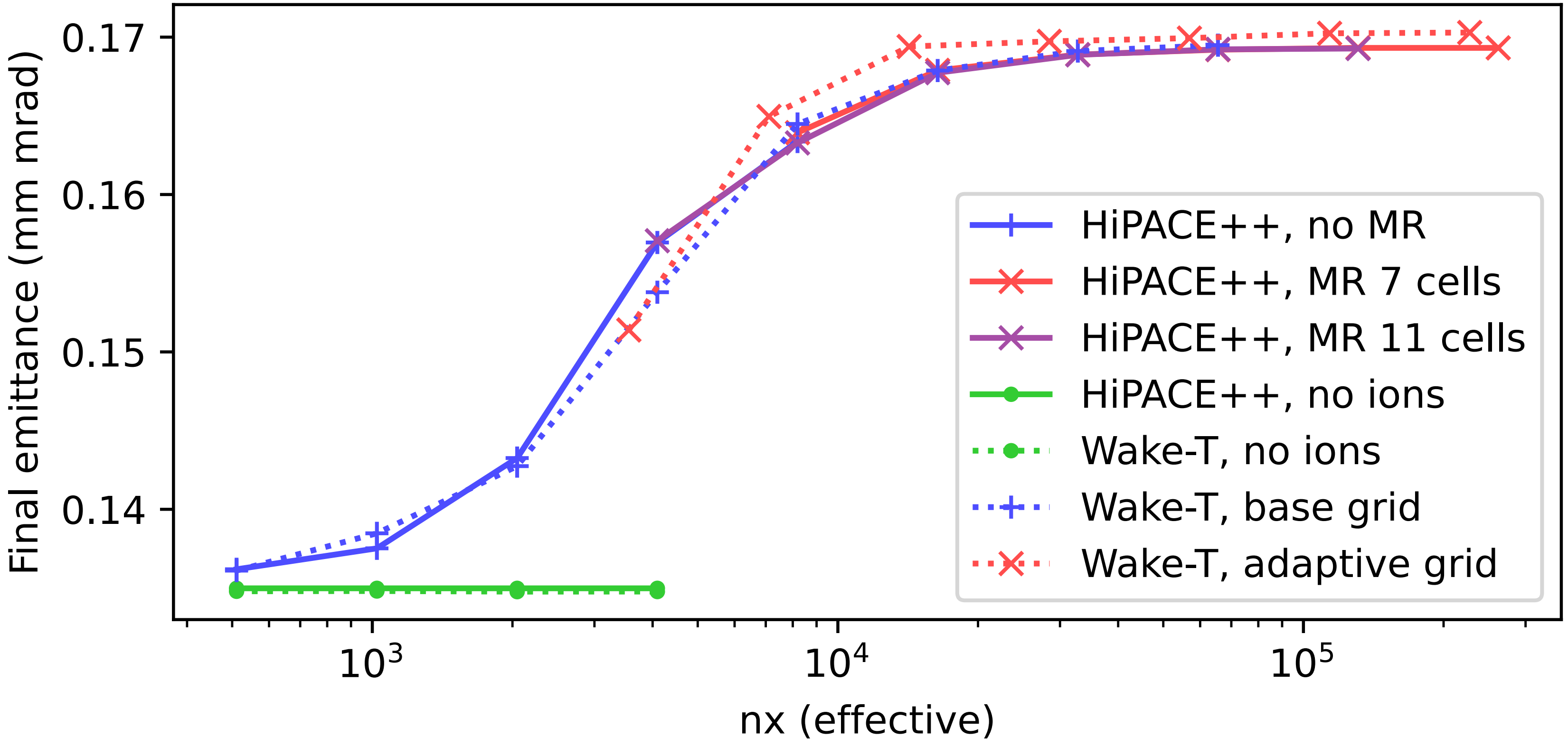






- ➢ Adaptive grid = fine resolution everywhere
- ➢ MR allows for convergence at modest cost

HiPACE++ and Wake-T converge to the same (?) result



Conclusion

- We implemented mesh refinement in HiPACE++ and adaptive grid in Wake-T.
- This allows for converged simulations in collider-relevant parameters.
- Full-physics realistic simulations are *very* affordable.

Perspective

- Simplify usage of mesh refinement.
- Adress low-hanging fruits for performance optimization.
- Interact with the community towards realistic simulations of collider design.

Wait, wait, two more slides!

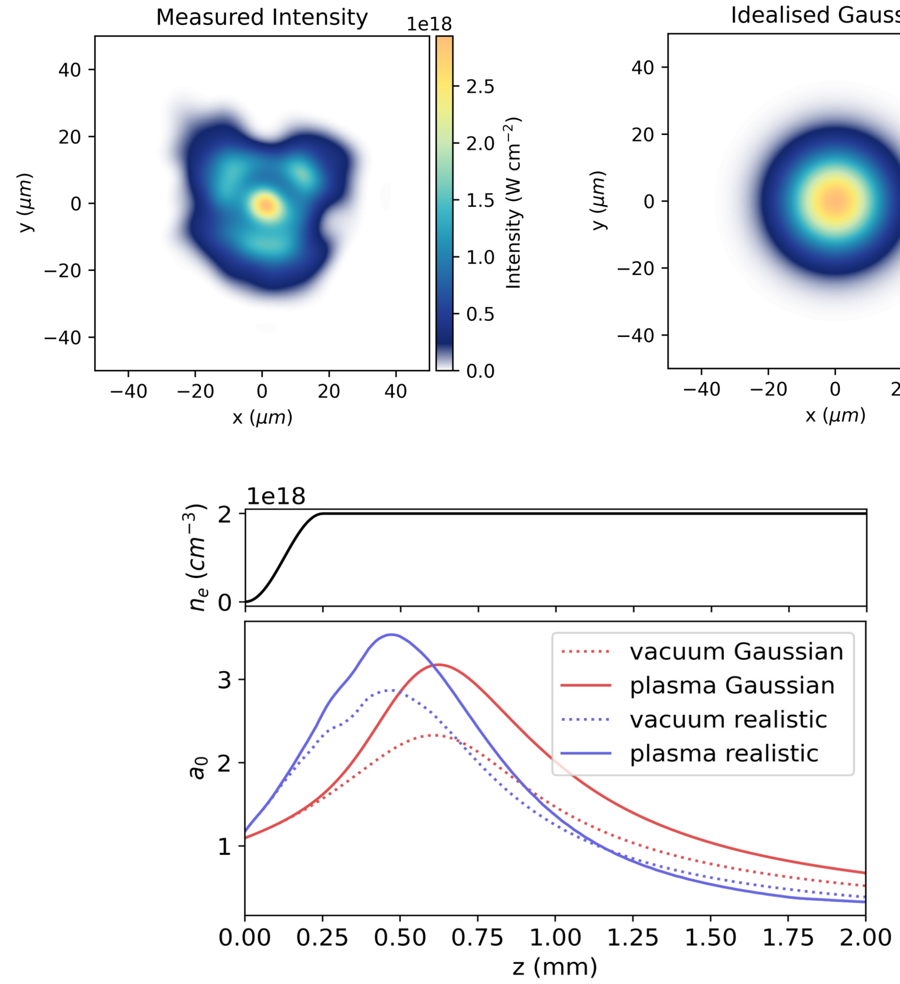
Acknowledgements

DESY. Severin Diederichs, Ángel Ferran Pousa, Alexander Sinn

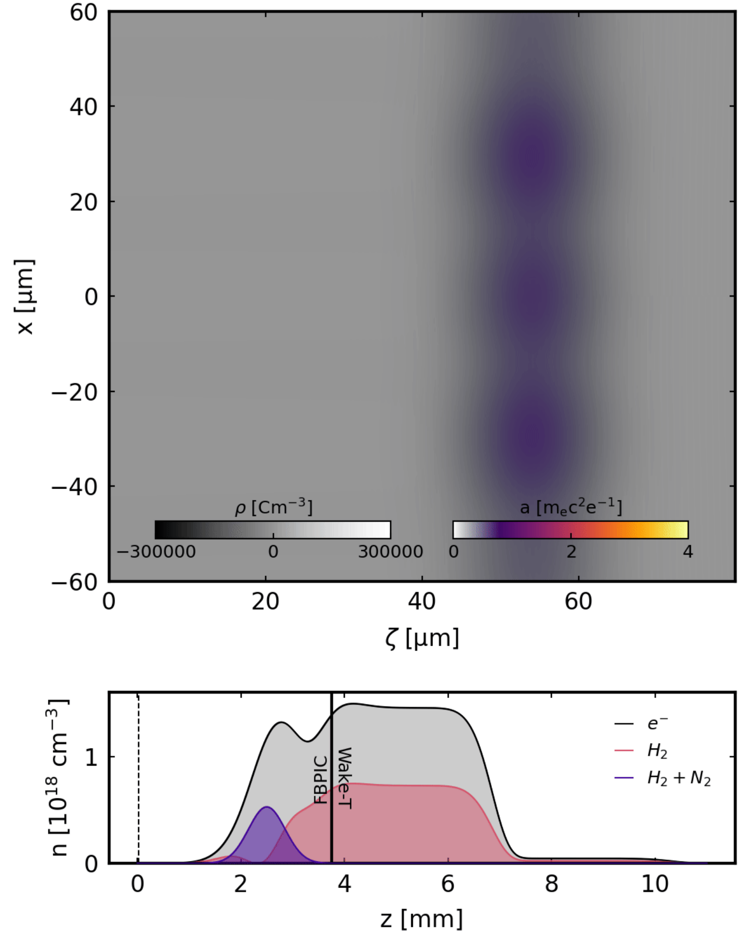
BERKELEY LAB Carlo Benedetti, Axel Huebl, Rémi Lehe, Andrew Myers, Weiqun Zhang, Jean-Luc Vay

LASY: LAser manipulations made eaSY

From experiment to simulation



From simulation to simulation



https://github.com/LASY-org/LASY
https://lasydoc.readthedocs.io/en/latest/

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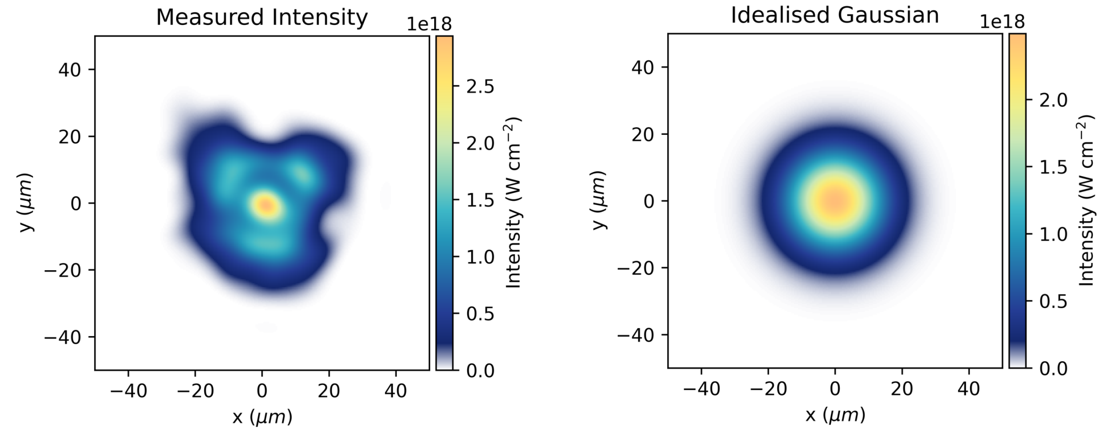

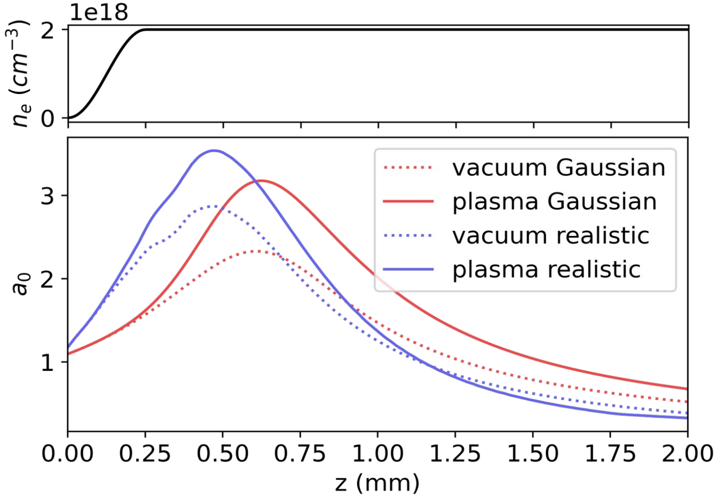

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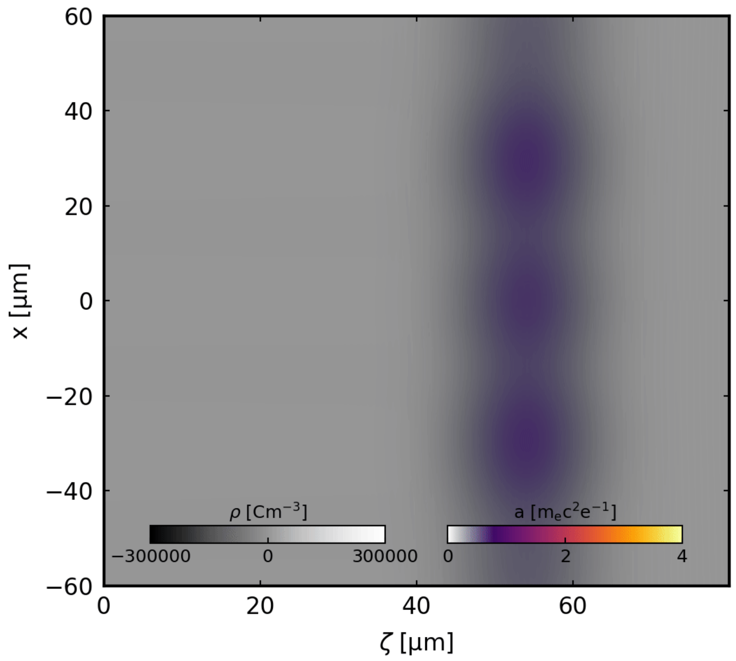
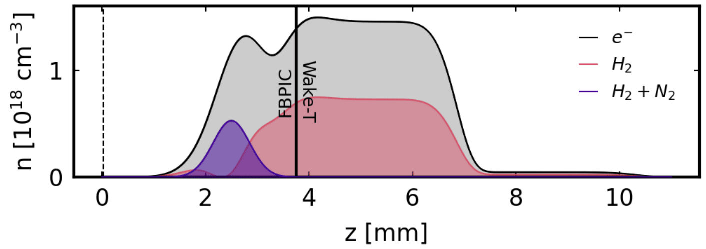




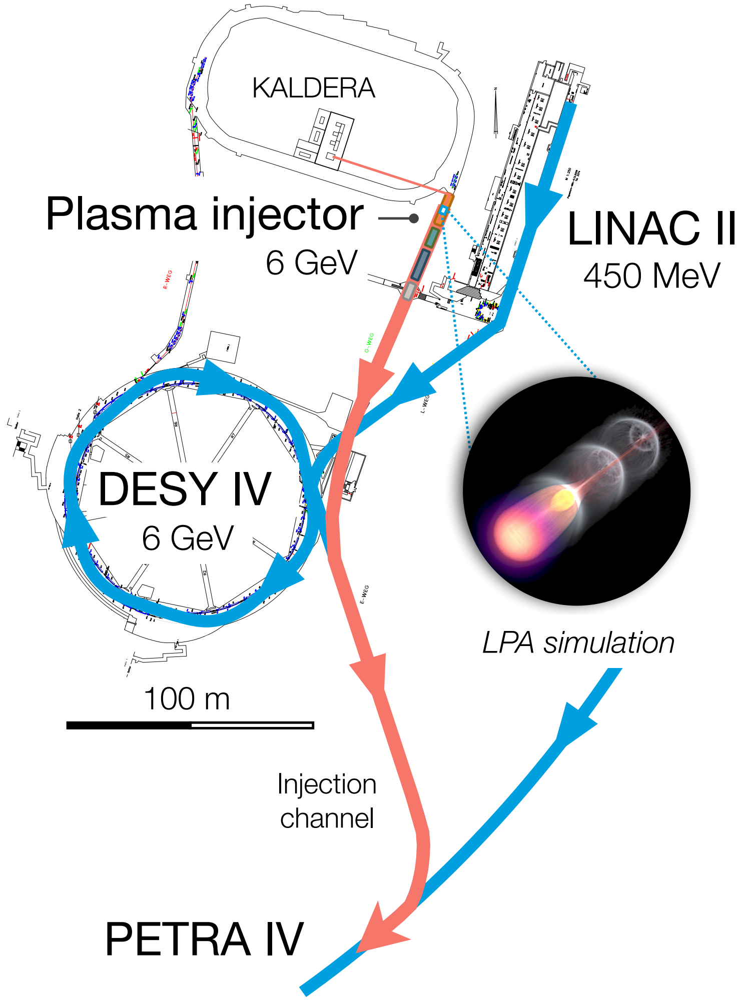
Come see poster #381 (yesterday)

https://github.com/LASY-org/LASY
https://lasydoc.readthedocs.io/en/latest/

A plasma injector for PETRA IV (PIP4)

The team

I. Agapov, S. Antipov, R. Brinkmann, A. Ferran Pousa, S. Jalas, L. Jeppe, M. Kirchen, W. P. Leemans, A. R. Maier, <u>A. Martinez de la Ossa</u>, J. Osterhoff, R. Shalloo, M. Thévenet, P. Winkler



[1] https://www.desy.de/research/facilities__projects/petra_iv
[2] M. Kirchen *et al. PRL* 126.17 (2021); LUX PI: A. R. Maier
[3] S. Antipov *et al.*, *24, PRAB 111301* (2021)
[4]A. Ferran Pousa et al. *PRL 129, 094801* (2021)

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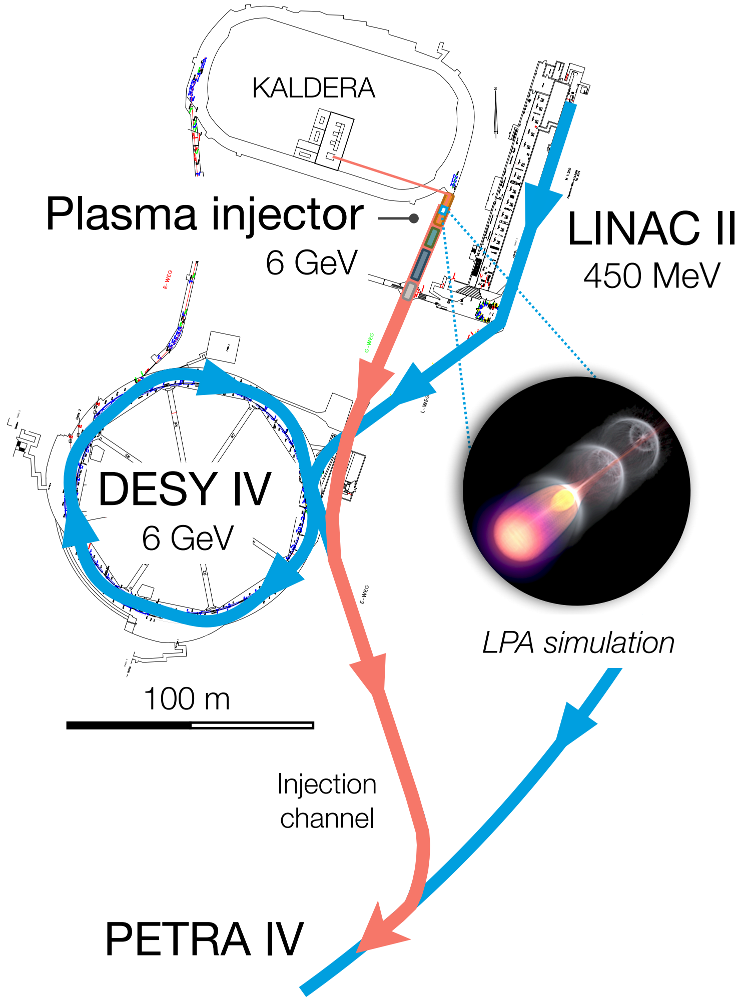
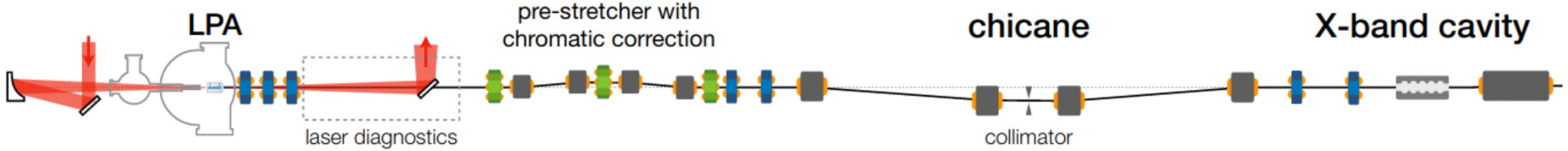
Come see poster #169 (today)





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Acknowledgements

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Thank you for your attention

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY.

QS PIC even captures depletion

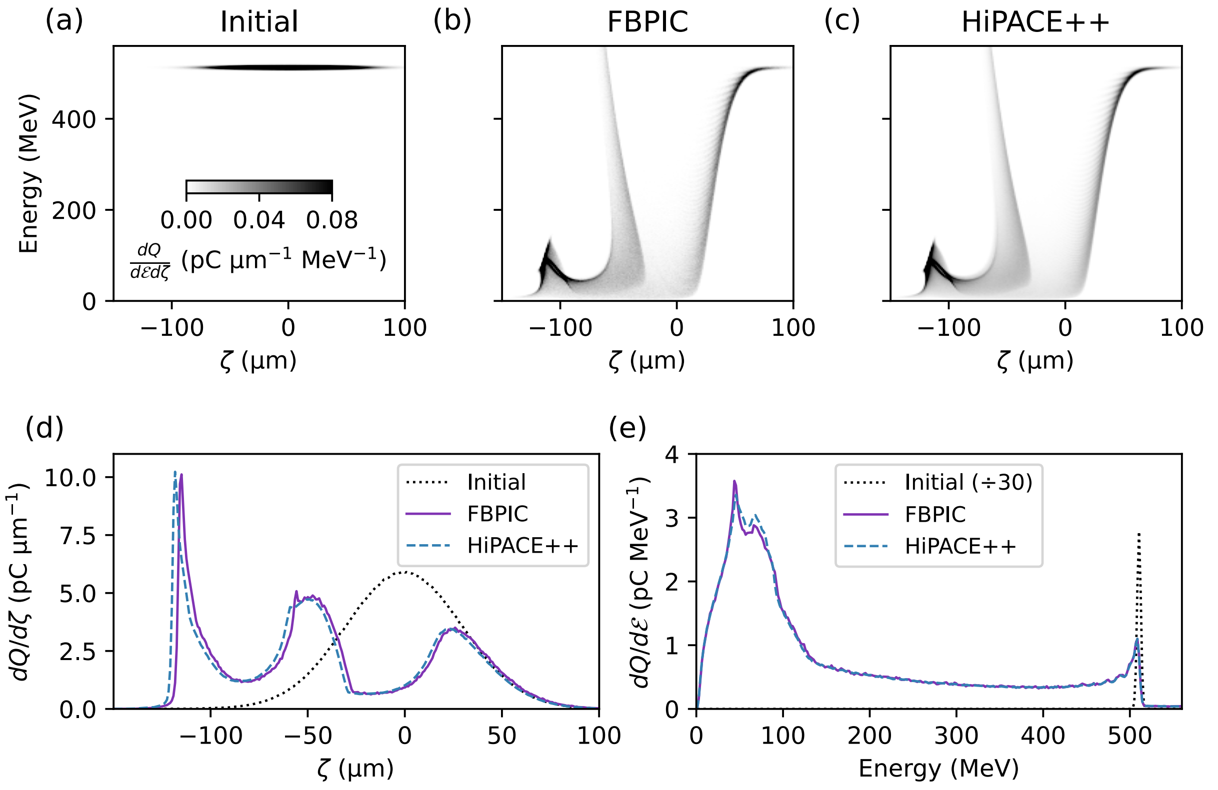


Figure 1: Longitudinal phase-space of the initial beam (a) and final beam from simulations using HiPACE++ (b) and FPBIC (c) along the co-moving variable $\zeta = s - ct$, with s being the longitudinal coordinate, t the time, and c the speed of light in vacuum. The longitudinal charge distribution (d) and the energy spectrum (e) show good agreement between the different PIC codes.

```
amr.n_cell = 4095 4095 3072

my_constants.Lramp = 0.025
my_constants.Lplateau = .3
my_constants.n0 = 3.7e22

max_step = 15000
hipace.max_time = (0.2+Lramp)/clight
diagnostic.output_period = 200

hipace.depos_order_xy = 2
hipace.dt = adaptive
hipace.nt_per_betatron = 10
hipace.dt_max = 1.e-13

geometry.coord_sys   = 0                  # 0: Cartesian
geometry.is_periodic = true  true  false  # Is periodic?
geometry.prob_lo     = -350.e-6 -350.e-6 -250.e-6  # physical domain
geometry.prob_hi     =  350.e-6  350.e-6  110.e-6

beams.names = beam

beam.position_mean = 0. 0. 0.
beam.position_std = 15.e-6 15.e-6 30.e-6
beam.injection_type = fixed_weight
beam.num_particles = 10000000
beam.total_charge = 443.e-12
beam.u_mean = 0. 0. 1000.
beam.u_std = .7 .7 4.

plasmas.names = plasma
plasma.density(x,y,z) = "if(z>0, if(z<Lramp,n0*0.5*(1.-cos(pi*z/Lramp)),n0), 1.e-20)"
plasma.ppc = 1 1
plasma.element = electron

diagnostic.diag_type = xz
```

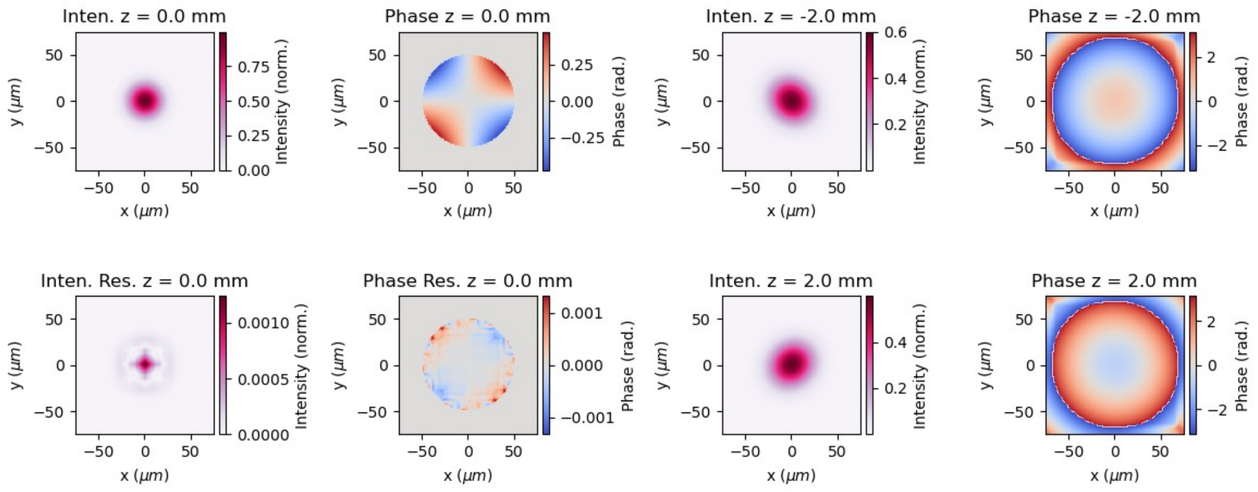
LASY: LAser manipulation made eaSY

- *Realistic/measured laser profiles are critical*
- Workflow can be cumbersome, with efforts duplication
- LASY aims at making this easy
- Contributors from DESY, LBNL, LOA, CEA, and more

```
from lasy.laser import Laser
from lasy.profiles.gaussian_profile import GaussianProfile

profile = GaussianProfile(wavelength, pol, energy, w0, tau, t_peak)
laser = Laser(dim, lo, hi, npoints, gaussian)
laser.propagate(-100.e-6)
laser.write_to_file('laser_file')
```

- Written in Python
- Envelope model
- Support RZ (azimuthal modes) & XYZ
- Measured or analytic profiles
- Read/write openPMD standard, envelope or field
- Propagator powered by Axiprop (I. Andriyash)
- Utils (Gerchberg-Saxton algorithm, etc.)



[2] L. T. Dickson et al., Phys. Rev. Accel. Beams 25, 101301 (2022)

https://github.com/LASY-org/LASY
https://lasydoc.readthedocs.io/en/latest/

Plasma acceleration is described by kinetic plasma dynamics

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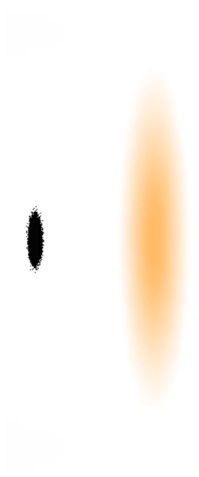


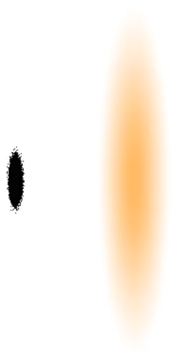
$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E},$$

$$\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \mathbf{J},$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{v},$$

$$\frac{d(\gamma \mathbf{v})}{dt} = \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}),$$

Plasma acceleration is described by kinetic plasma dynamics



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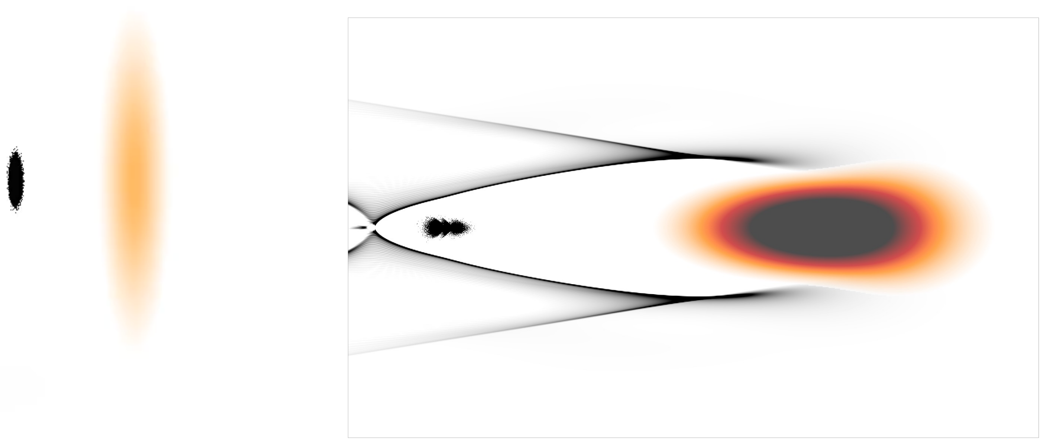
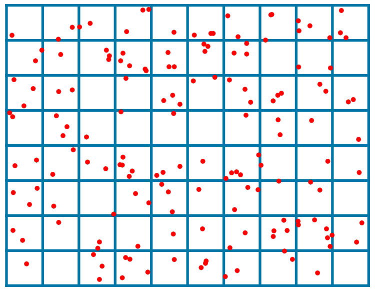
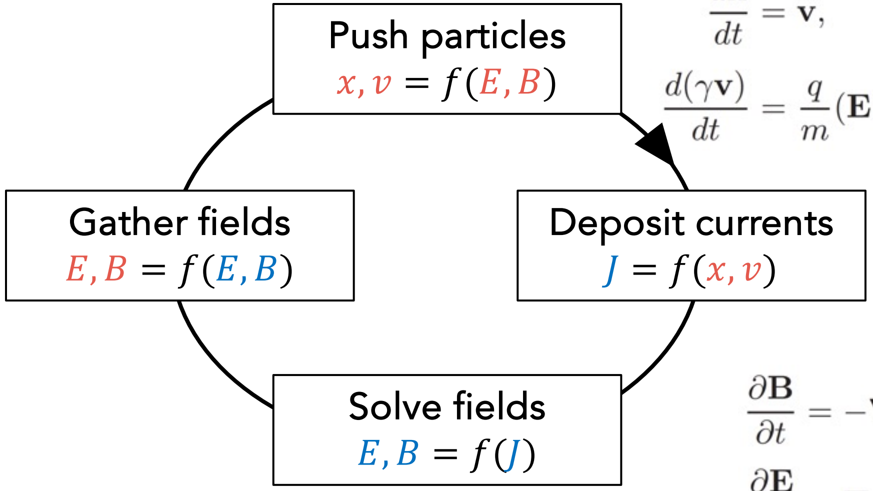
Plasma acceleration is described by kinetic plasma dynamics





Regular mesh
Macroparticles



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$$\frac{d(\gamma\mathbf{v})}{dt} = \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B}),$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E},$$
$$\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \mathbf{J},$$

- *Lagrangian* description of plasma, *Eulerian* description of fields
- Physics can be added
- Time step limited by CFL condition: $\Delta t \simeq \frac{\Delta z}{c}$

→ 3D (EM) PIC simulations of plasma acceleration are very expensive

Recent advances improved accuracy of the field solver

$$\nabla_\perp^2 \psi = -\frac{1}{\epsilon_0}\left(\rho - \frac{1}{c}j_z\right)$$

$$E_x - c\,B_y = -\partial_x \psi$$

$$E_y + c\,B_x = -\partial_y \psi$$

$$\nabla_\perp^2 E_z = c\mu_0\left(\partial_x j_x + \partial_y j_y\right)$$

$$\nabla_\perp^2 B_x = \mu_0\left(-\partial_y j_z + \partial_\zeta j_y\right)$$

$$\nabla_\perp^2 B_y = \mu_0\left(\partial_x j_z - \partial_\zeta j_x\right)$$

$$\nabla_\perp^2 B_z = \mu_0\left(\partial_y j_x - \partial_x j_y\right)$$

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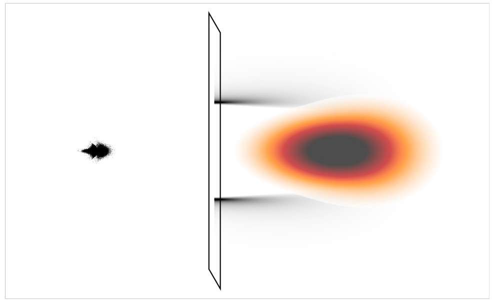

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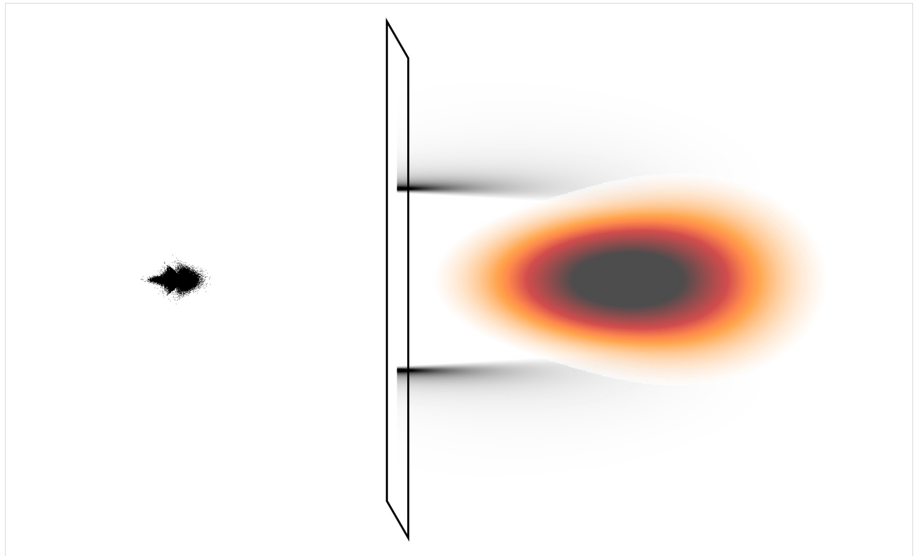
$$\nabla_\perp^2 B_z = \mu_0 \left(\partial_y j_x - \partial_x j_y\right)$$

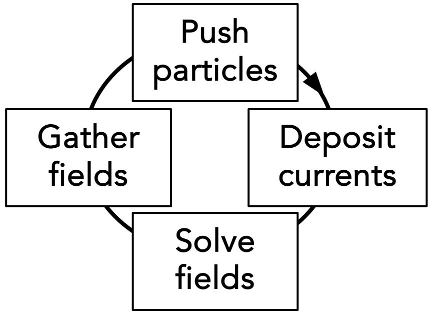
Source terms $\boldsymbol{\partial_\zeta j_{x/y}}$ are difficult to obtain

- **predictor-corrector solver**: *the old one*
  - [Mora & T. Antonsen, Phys. Plasmas (1997), W. An et al., JCP (2013)]
  - Not very stable
- **explicit solver**: *the new one*
  - [T. Wang et al., Phys. Plasmas (2017), P. Baxevanis & G. Stupakov, PRAB (2018), T. Wang, et al. PRAB 25.10 (2022)]
  - Analytic integration of the source term
  - Gives a screened Poisson equation, solved with multigrid solver

$$\boxed{\nabla_\perp^2 B_\perp - \frac{n^*}{1+\psi} B_\perp = -[e_z \times S]}$$

Mesh Refinement in HiPACE++

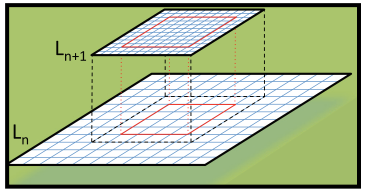




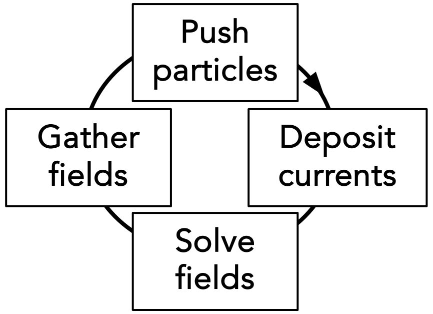
- Deposit beam and plasma densities $\rho, \vec{J}$
- Solve Poisson fields $(E_x - cB_y, E_y + cB_x, E_z. B_z)$
- Deposit beam and plasma source terms S_x, S_y
- Explicit solve $(B_x. B_y)$
- Advance plasma particles by 1 slice $(-\Delta\zeta)$
- Advance beam particles by 1 time step $(+\Delta t)$

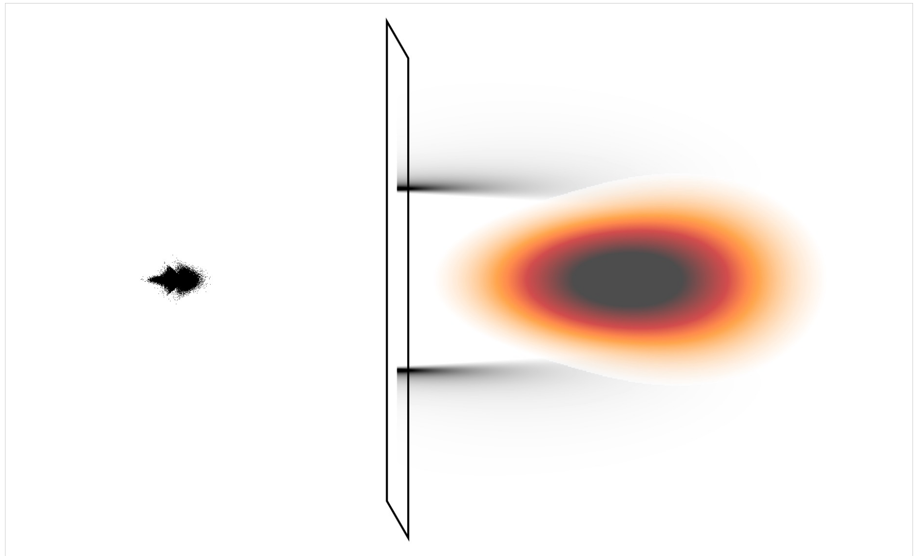
Mesh Refinement in HiPACE++

- MR in electrostatic PIC



J.-L. Vay et al., Comput. Sci. & Disc. 5, 014019 (2012)





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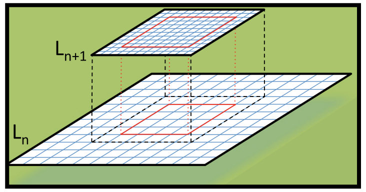
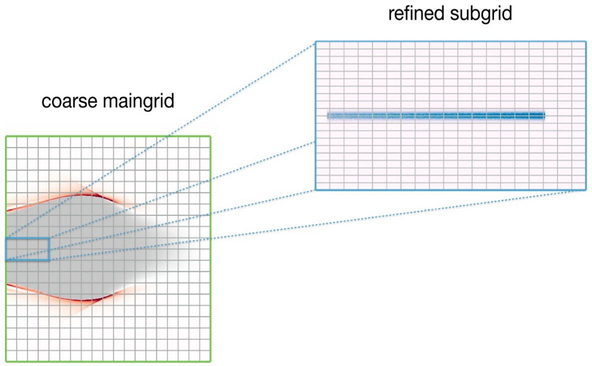
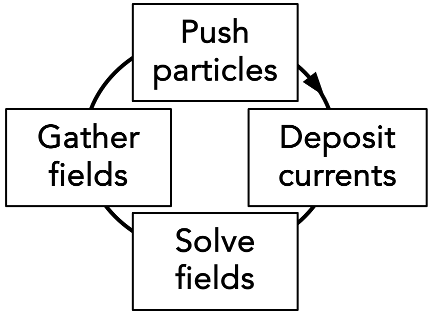
Mesh Refinement in HiPACE++

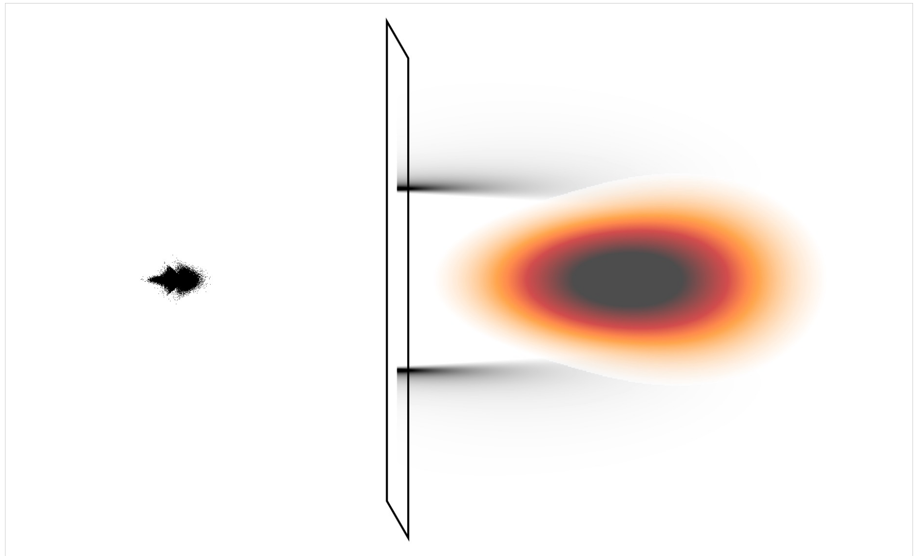
- MR in electrostatic PIC
- MR with quasi-static PIC, no crossing





J.-L. Vay et al., Comput. Sci. & Disc. 5, 014019 (2012)	T. J. Mehrling et al., IEEE, AAC (2018)





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Mesh Refinement in HiPACE++

Severin Diederichs

Alexander Sinn

- MR in electrostatic PIC
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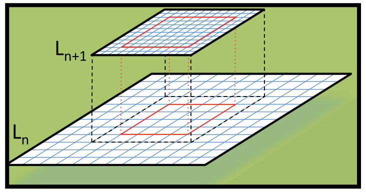
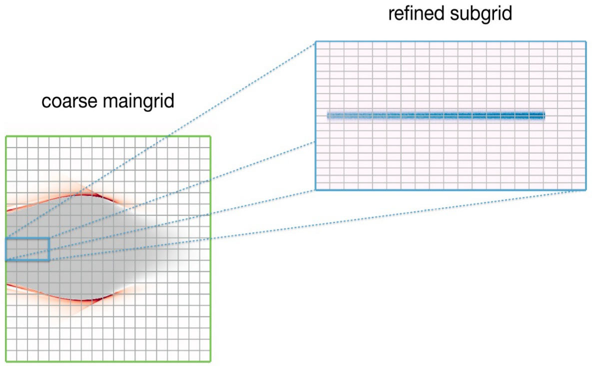
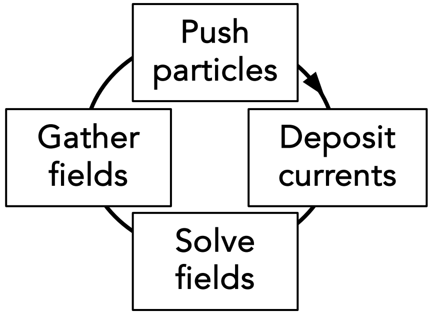
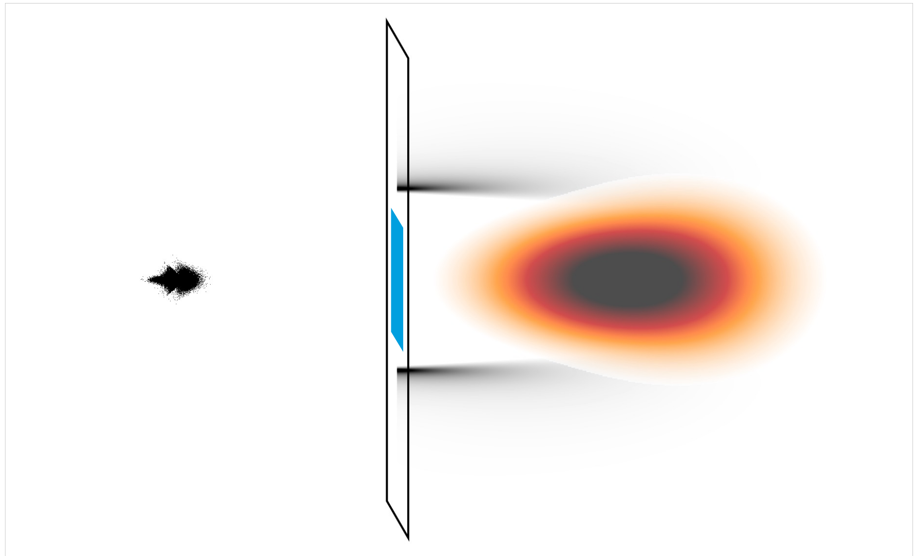




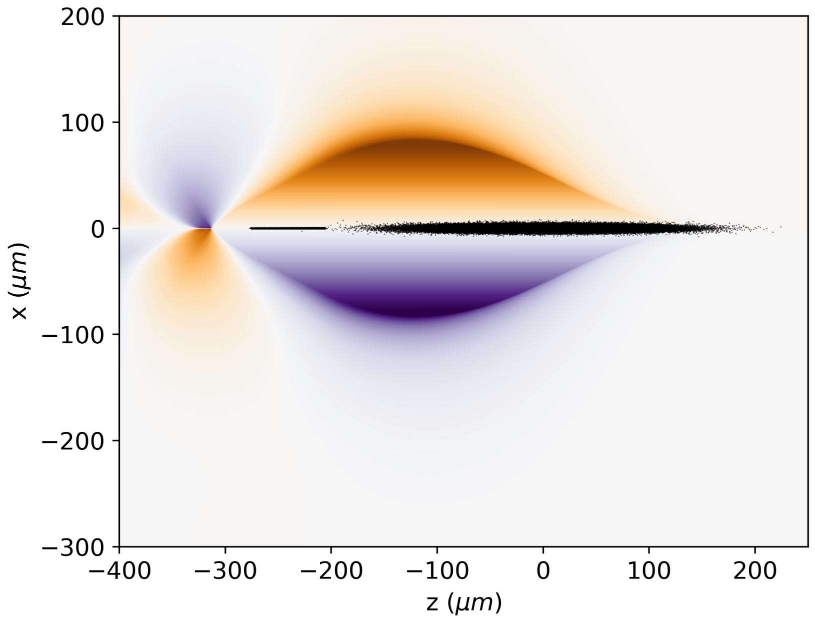
J.-L. Vay et al., Comput. Sci. & Disc. 5, 014019 (2012)	T. J. Mehrling et al., IEEE, AAC (2018)

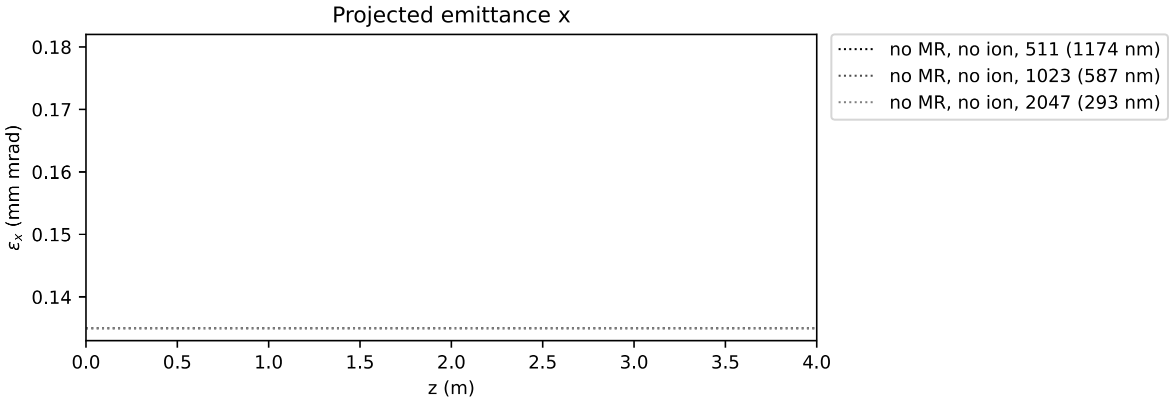




- Deposit beam and plasma densities $\rho, \vec{J}$
  on all levels
- Solve Poisson fields $(E_x - cB_y, E_y + cB_x, E_z. B_z)$
  BC on fine patch, solve, Interpolate in ghost cells
- Tag by level
- Deposit beam and plasma source terms S_x, S_y
  on all levels
- Explicit solve $(B_x. B_y)$
  BC of source and B, solve
- Advance plasma particles by 1 slice $(-\Delta\zeta)$
- Advance beam particles by 1 time step $(+\Delta t)$

Converged simulations in collider-relevant range are ~~feasible~~ cheap





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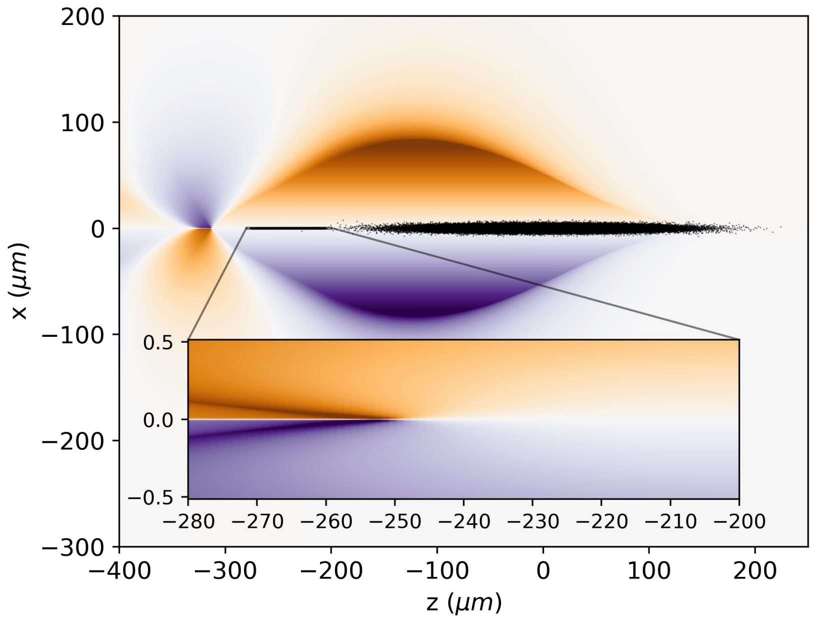

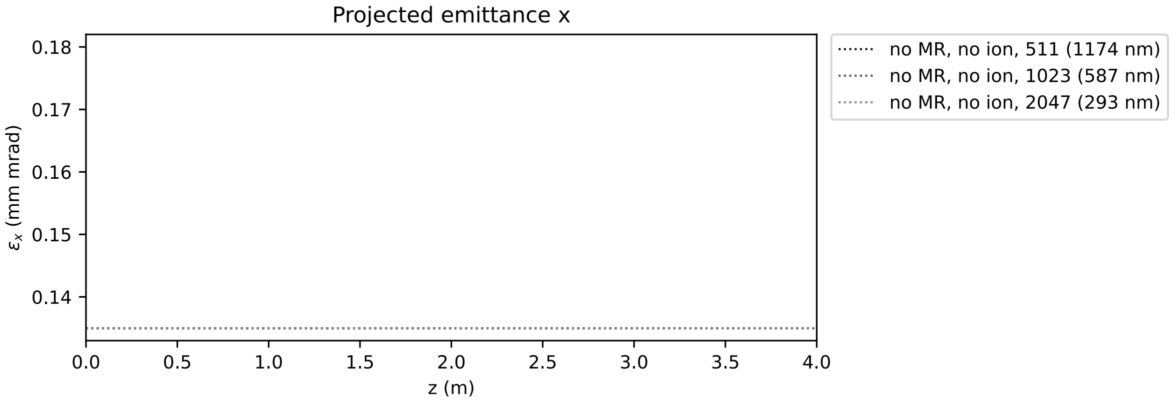

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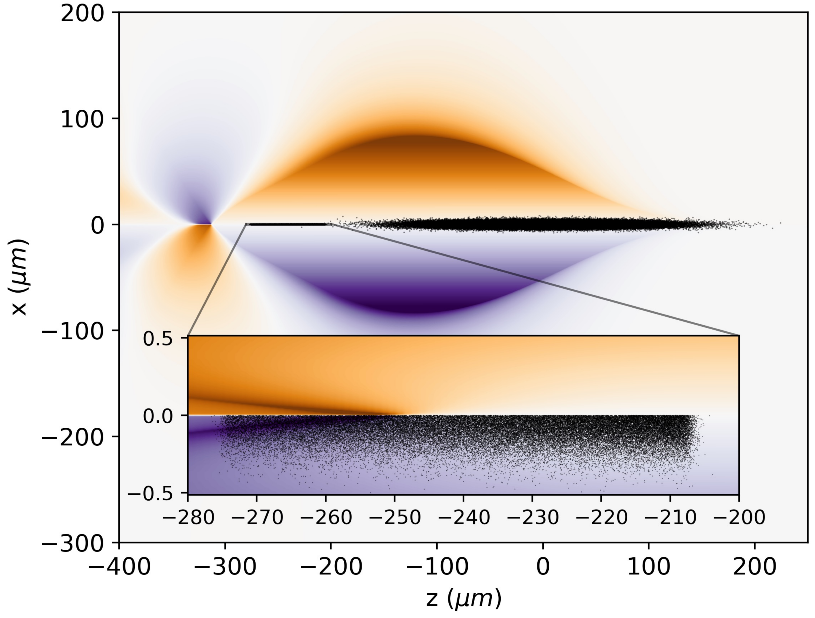

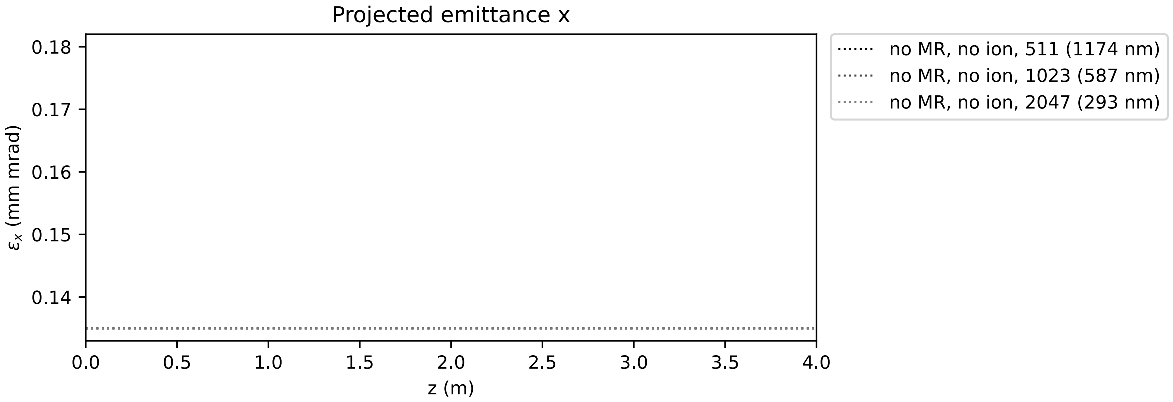

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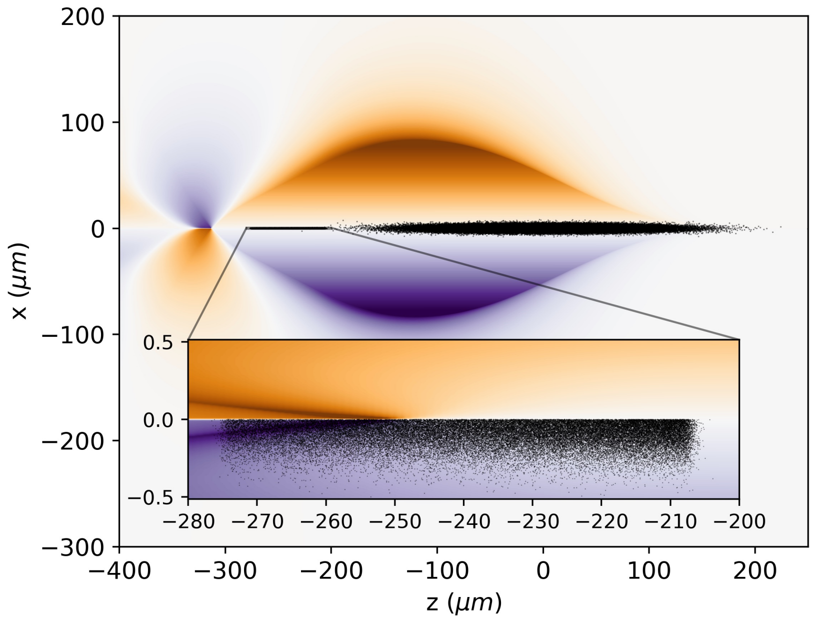

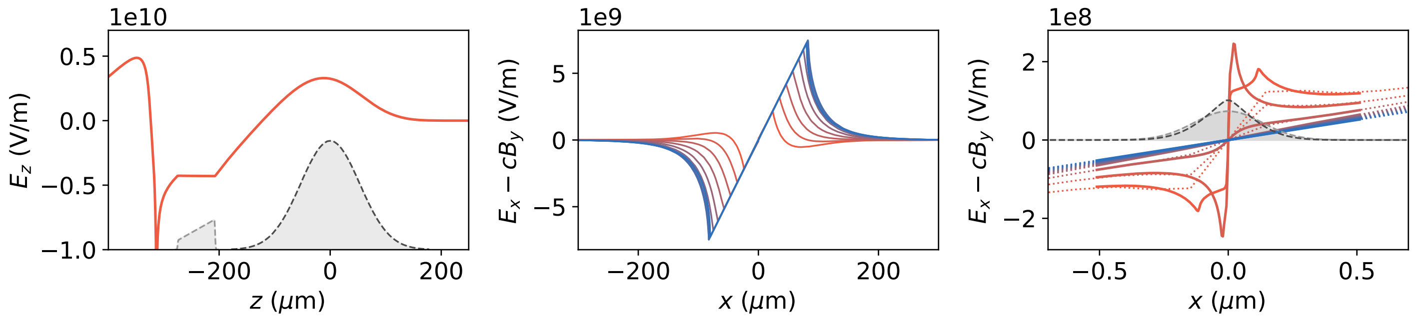

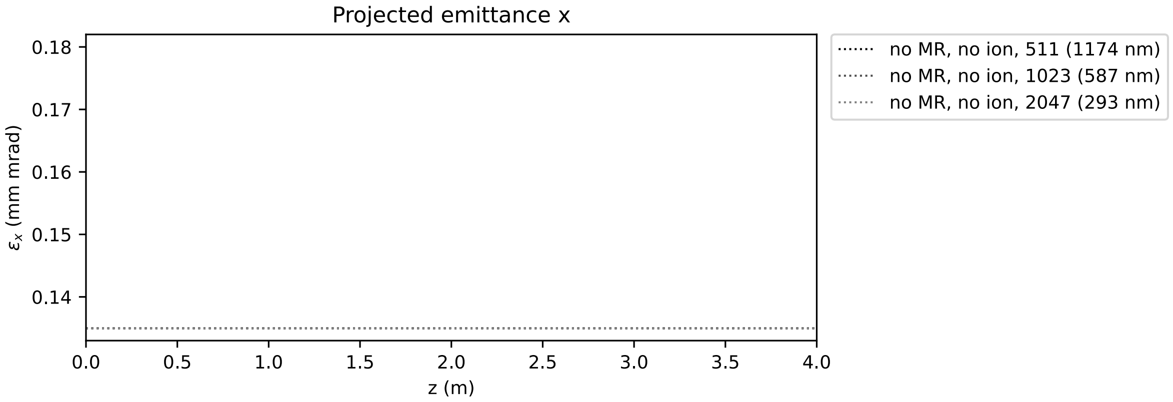

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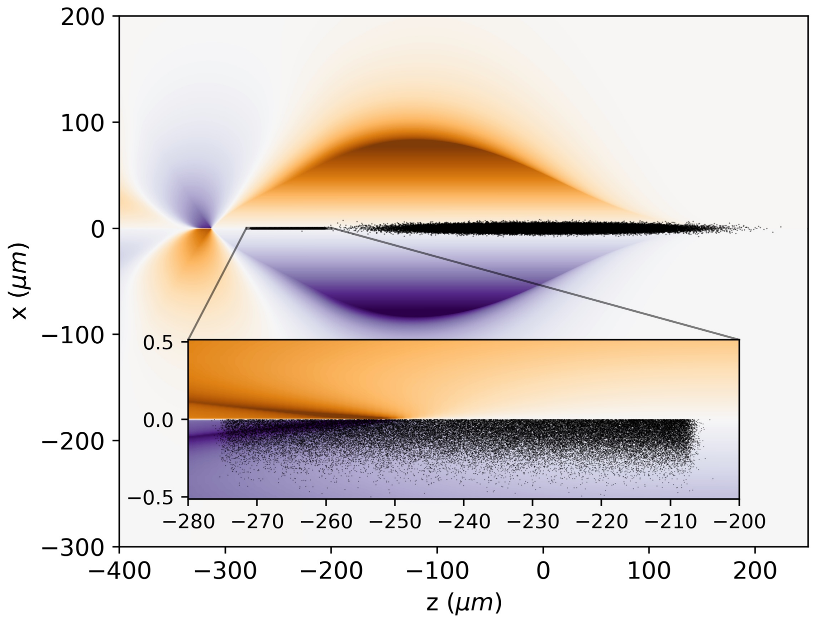

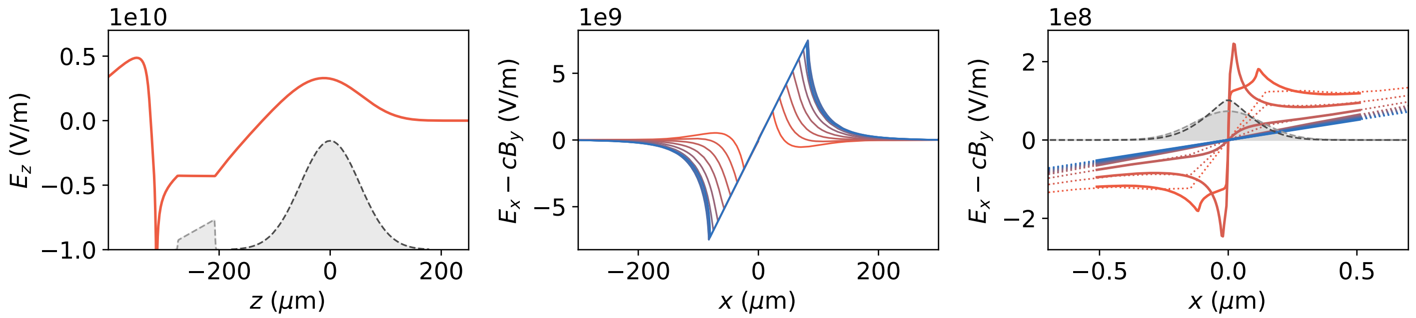

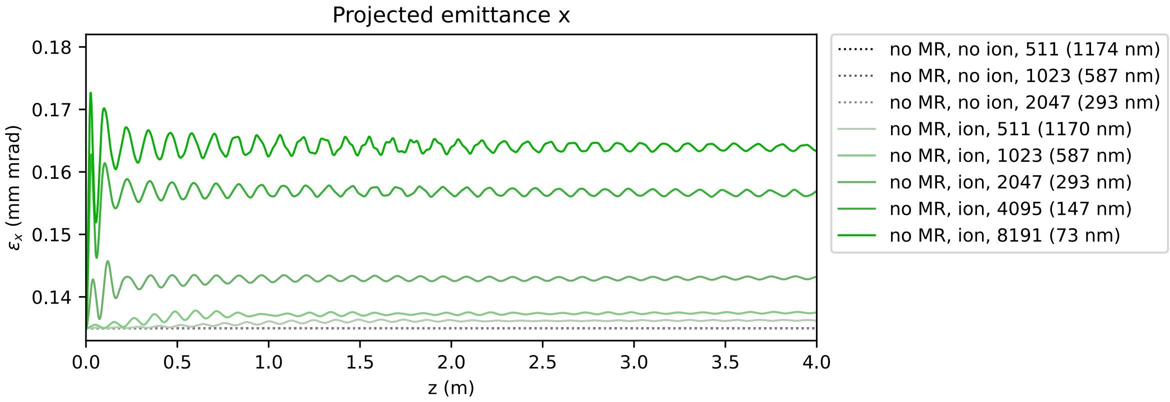

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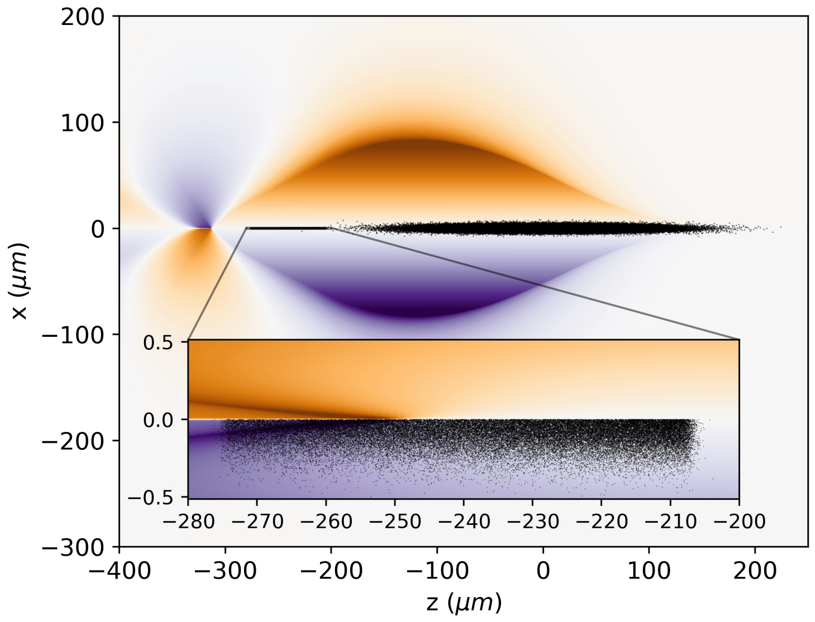

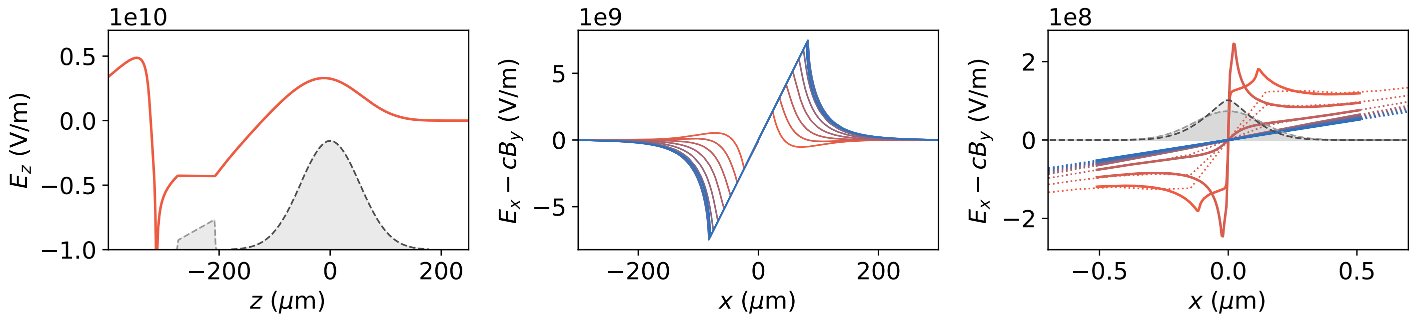

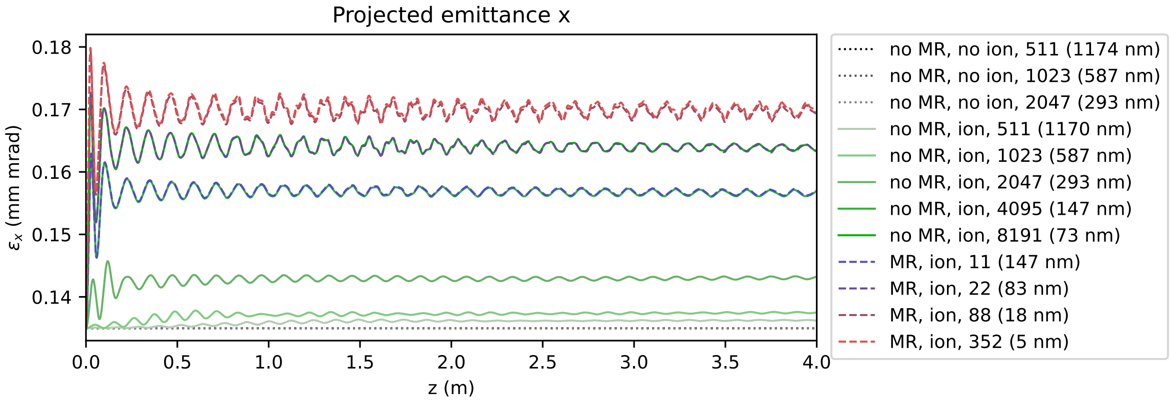

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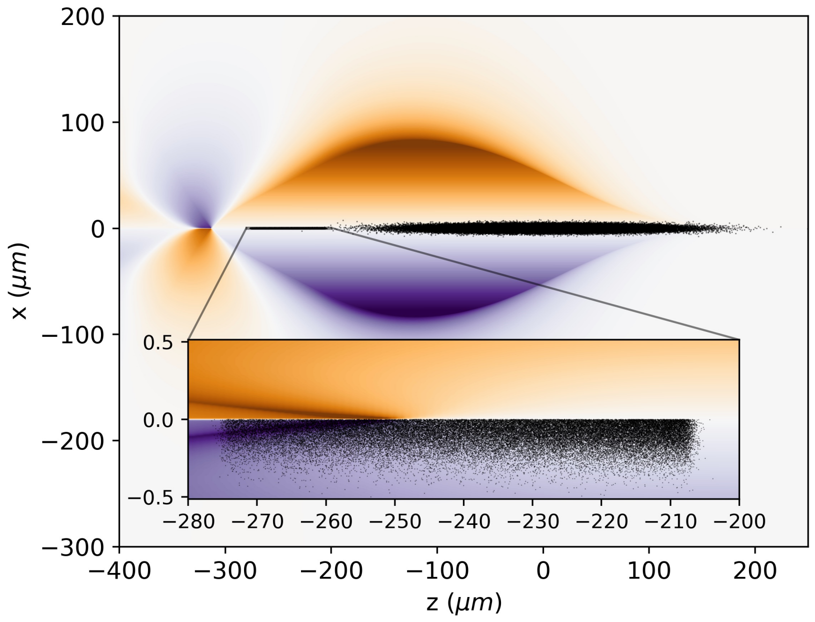

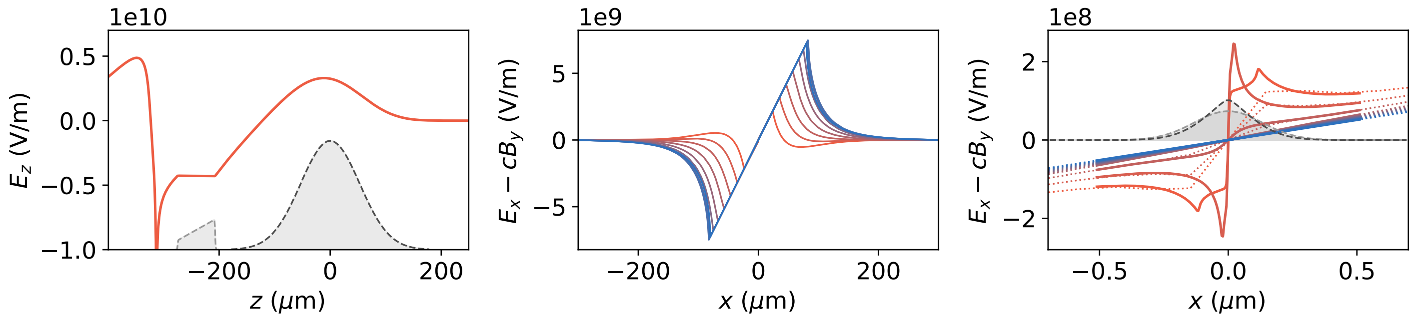

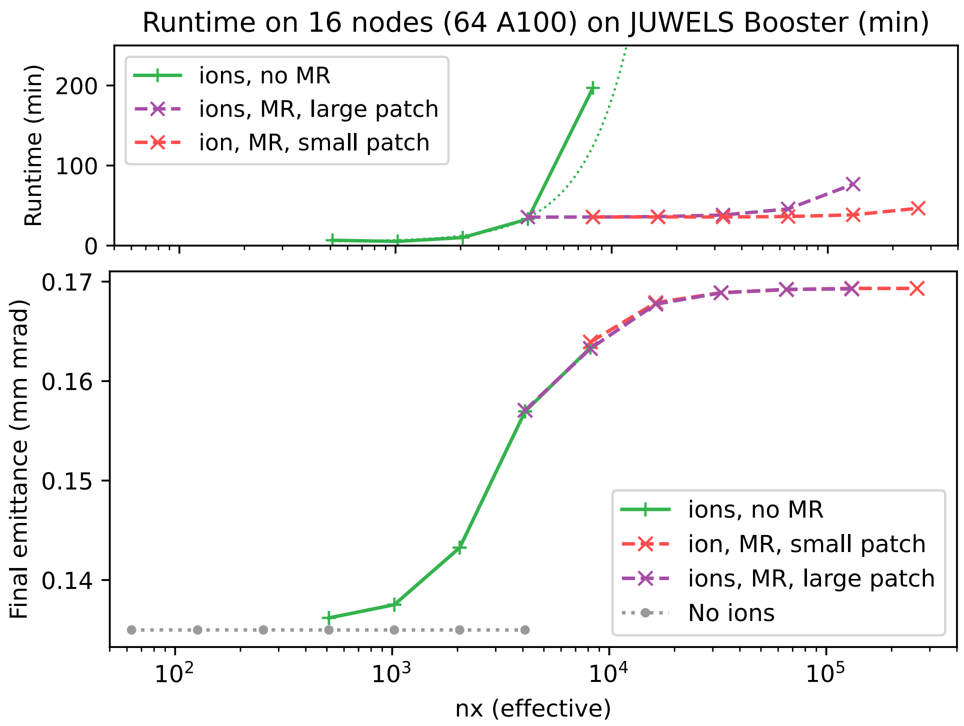

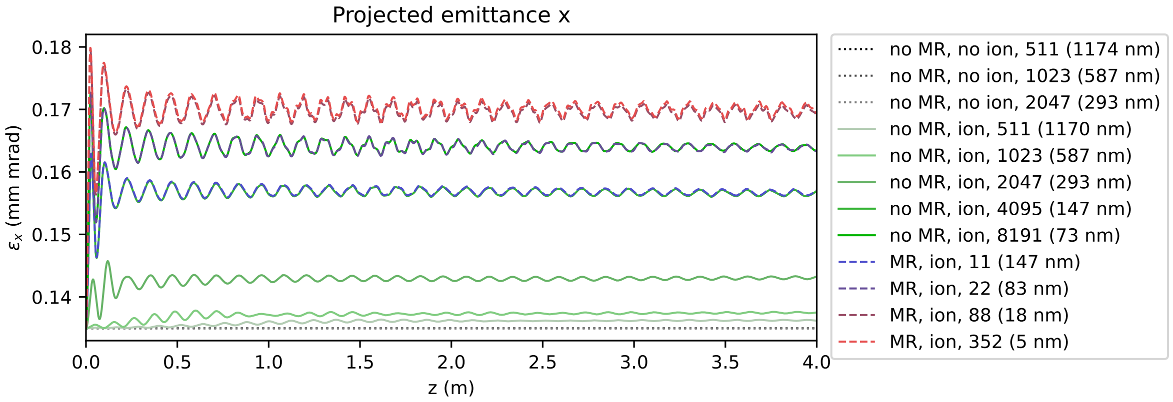

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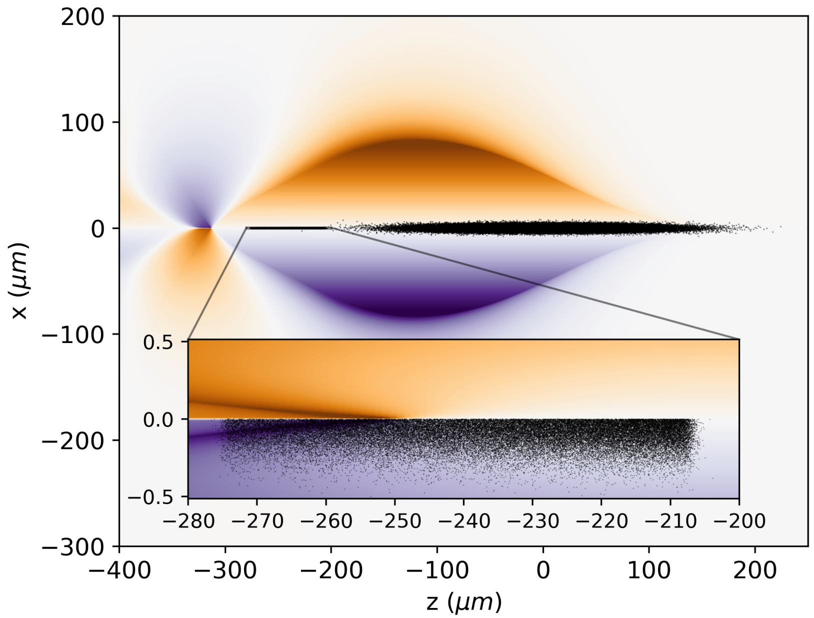
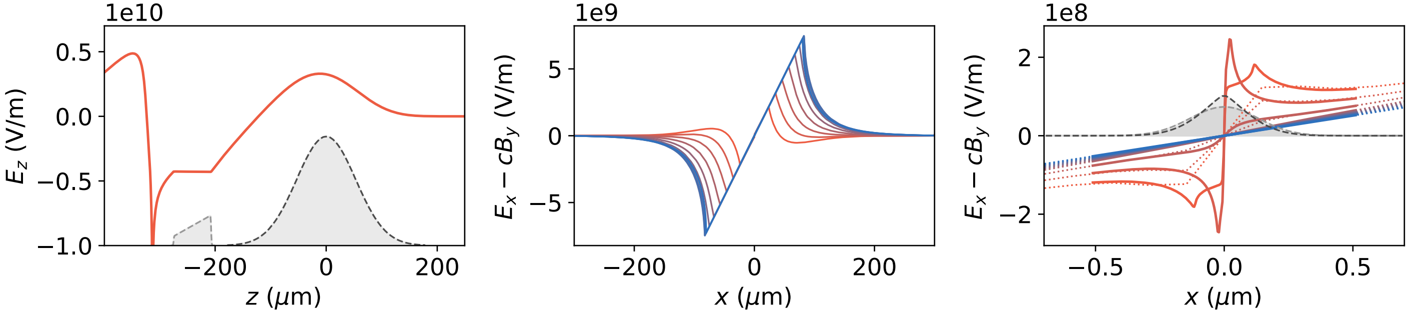
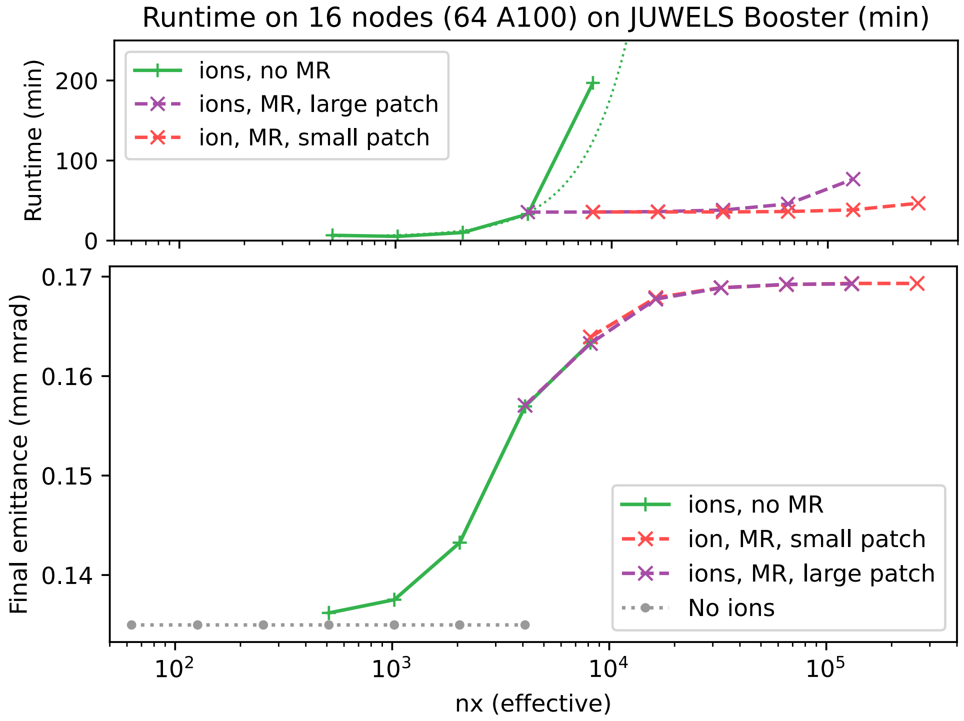
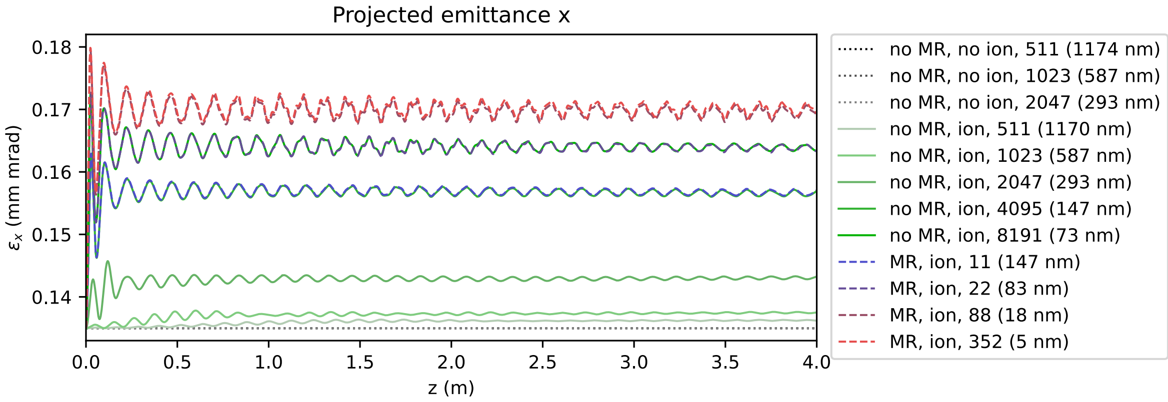


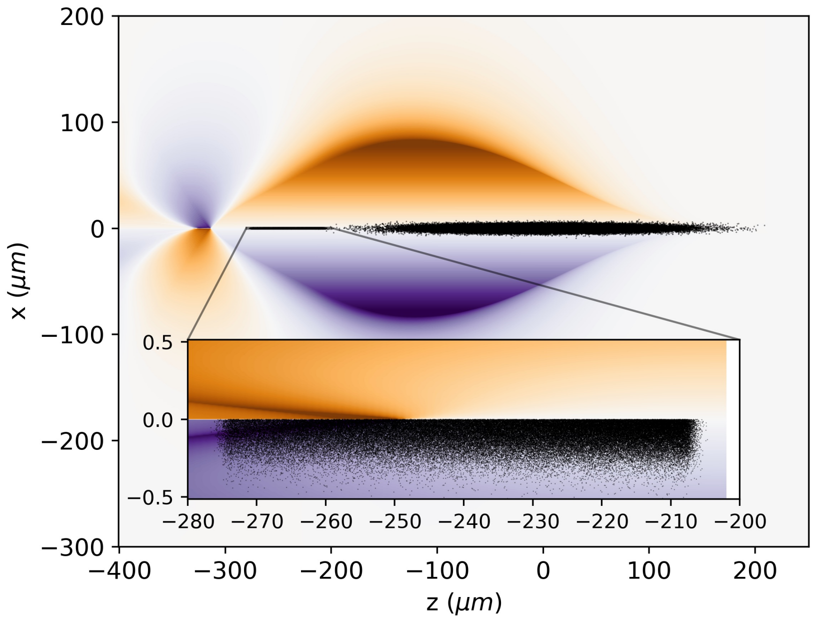






- ➢ Coarse resolution + MR = fine resolution everywhere
- ➢ MR allows for convergence at modest cost

Realistic simulations of collider parameters on a laptop w/ Wake-T



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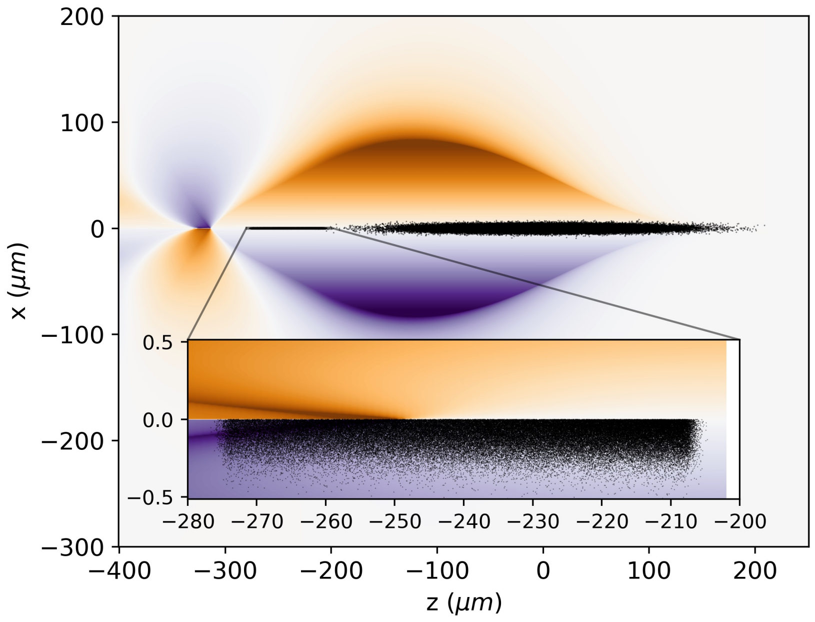

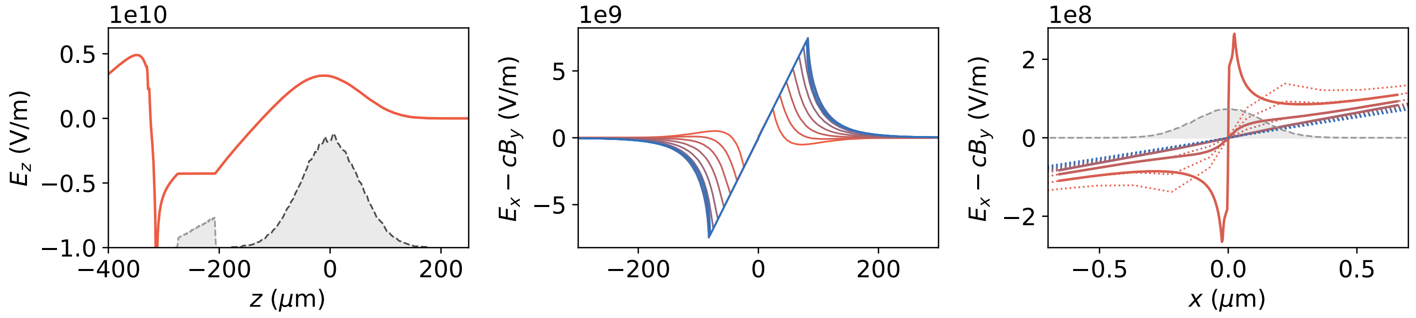

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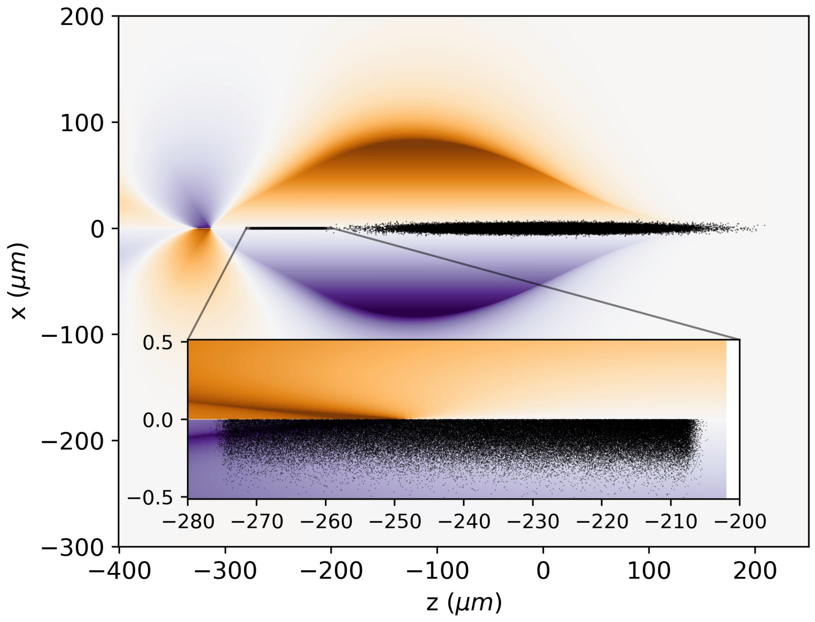

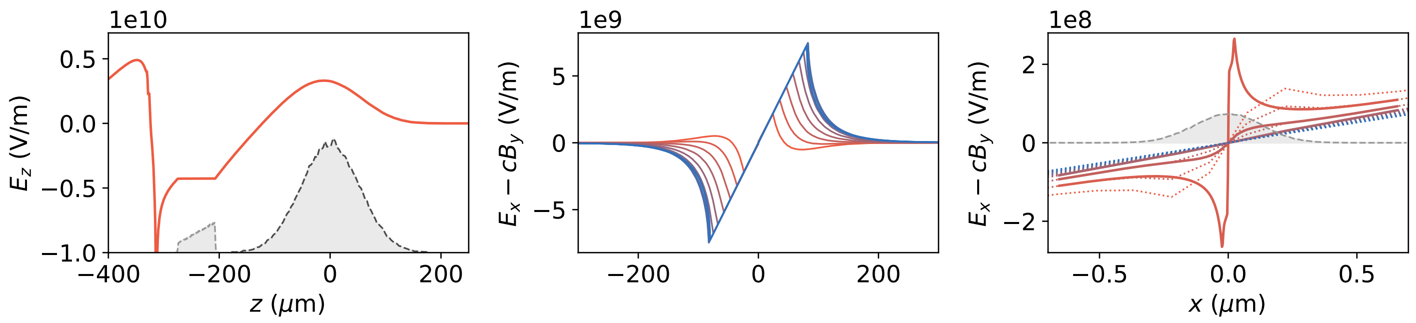

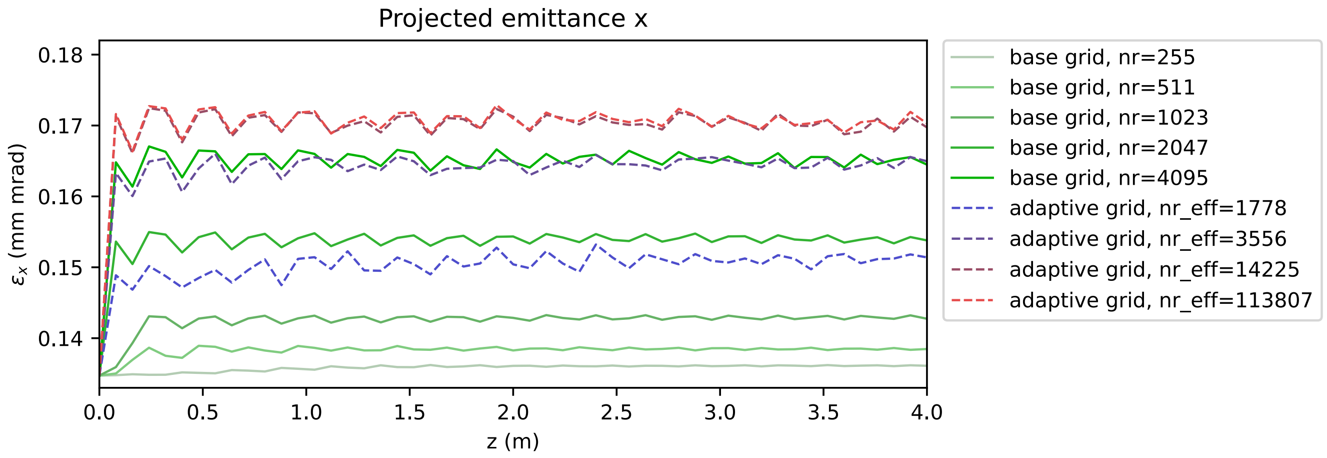

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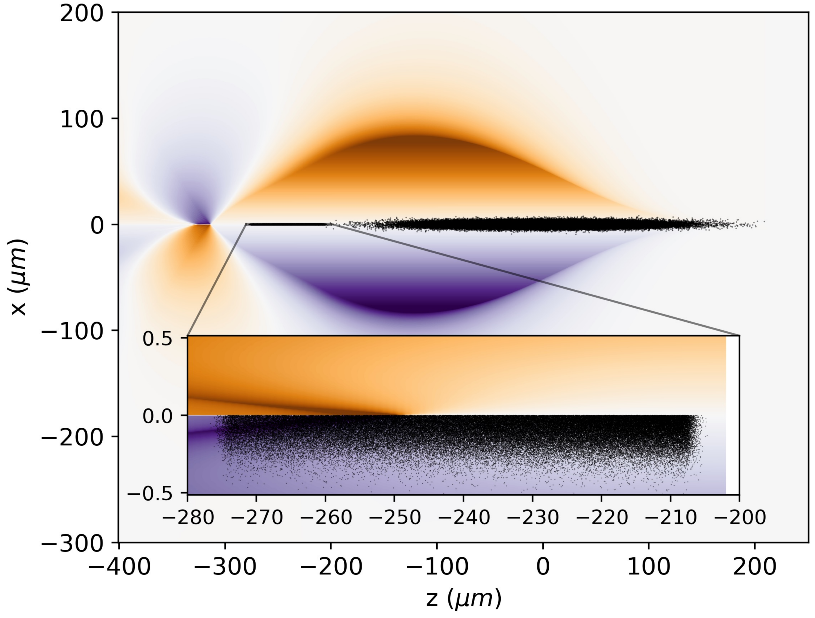

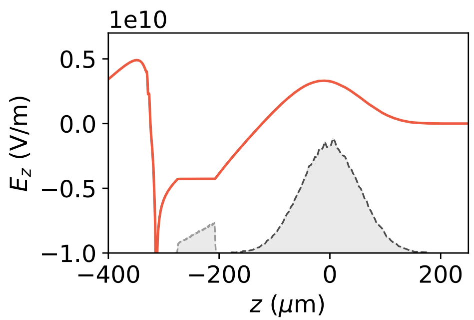

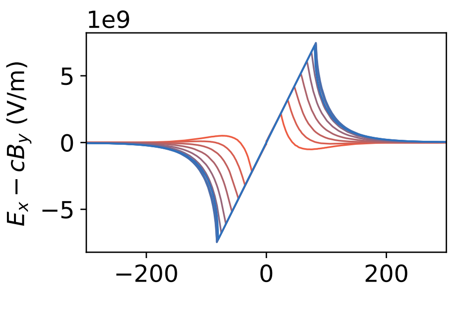

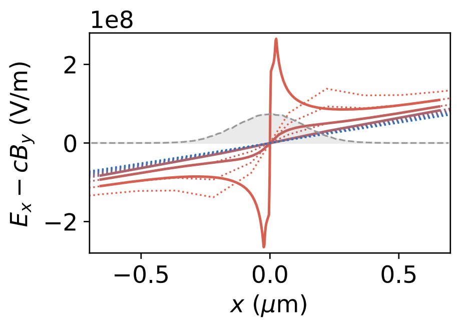

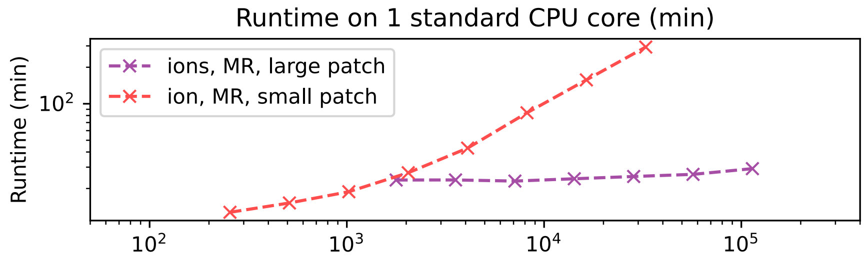

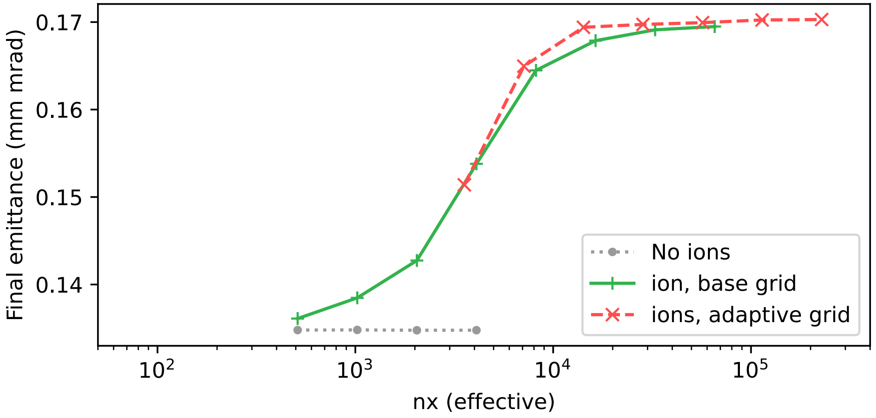

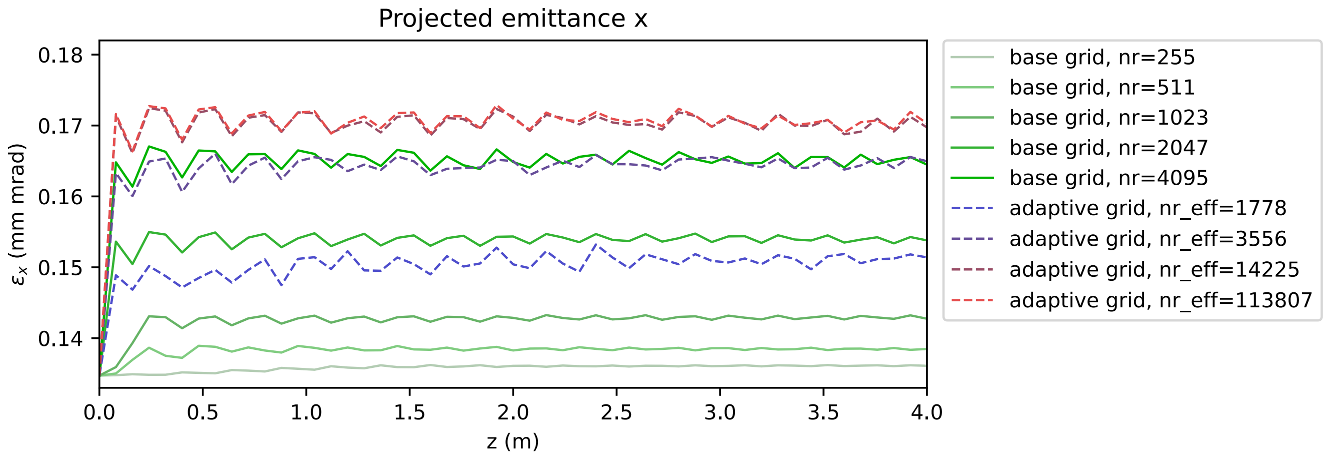

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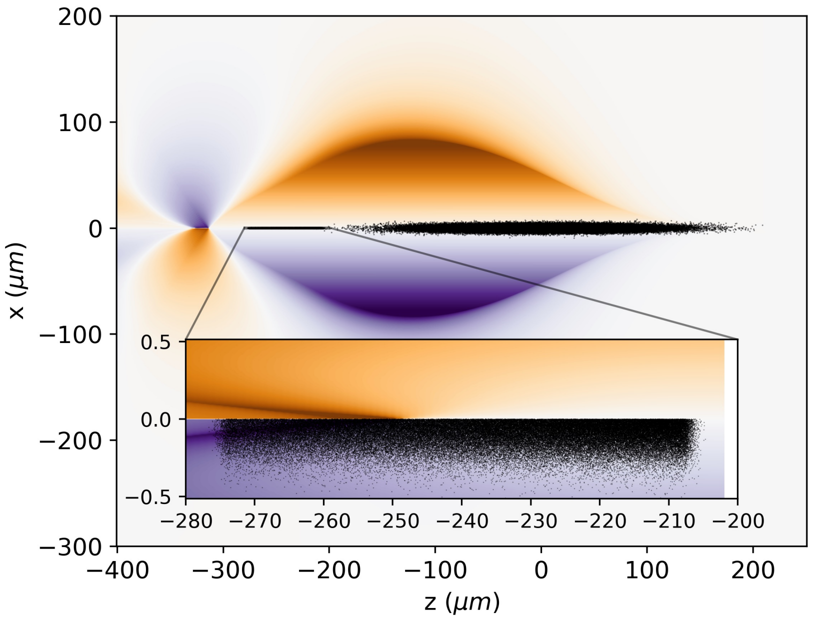

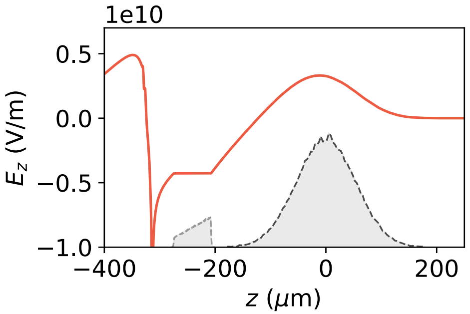

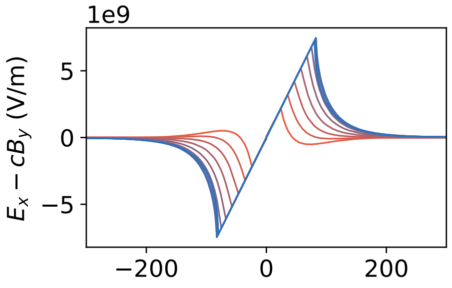

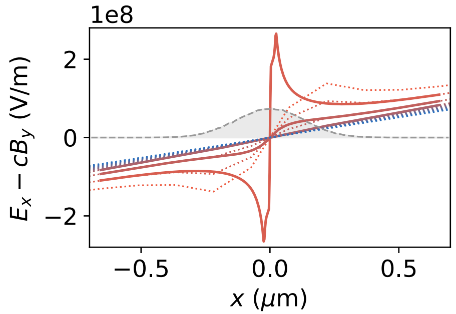

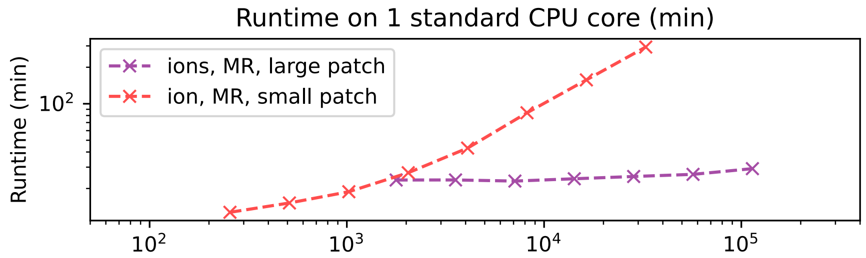

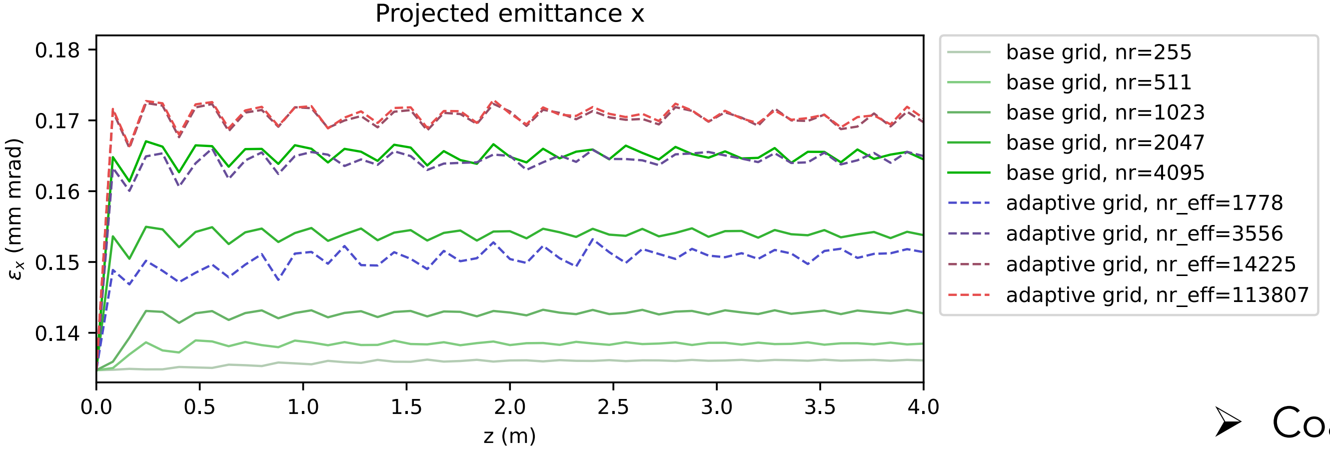

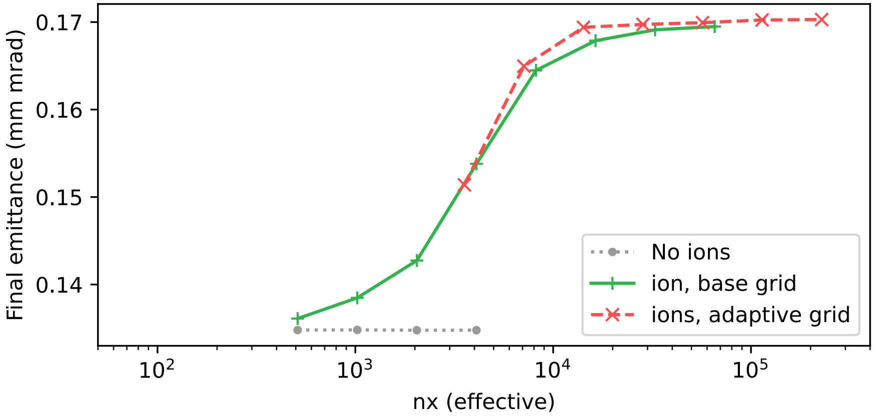

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