HiPACE++: presentation of the code

Maxence Thévenet – DESY

MPA – plasma acceleration

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY.

Plasma acceleration is described by kinetic plasma dynamics

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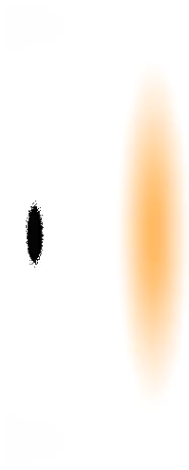

Plasma acceleration is described by kinetic plasma dynamics

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

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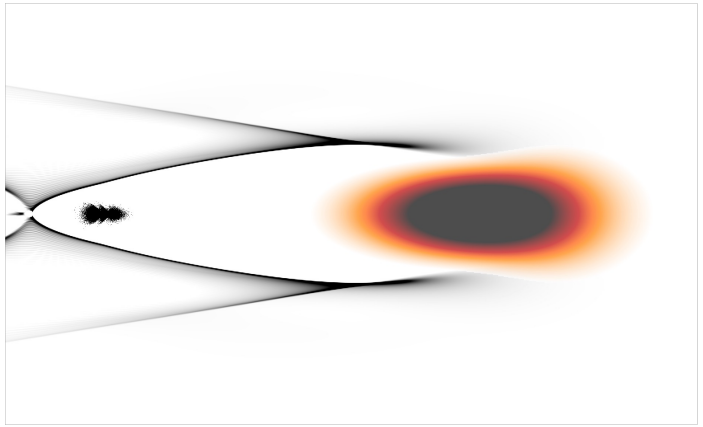
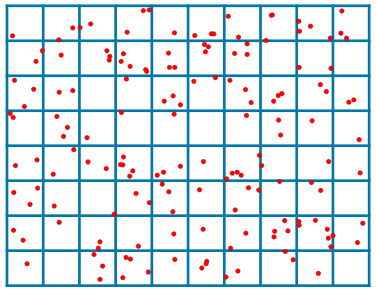
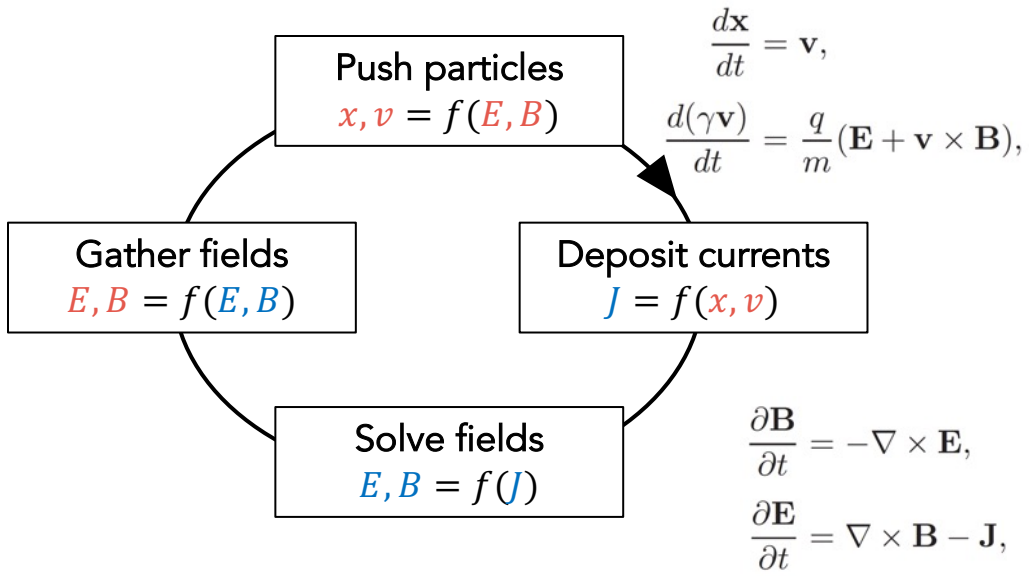




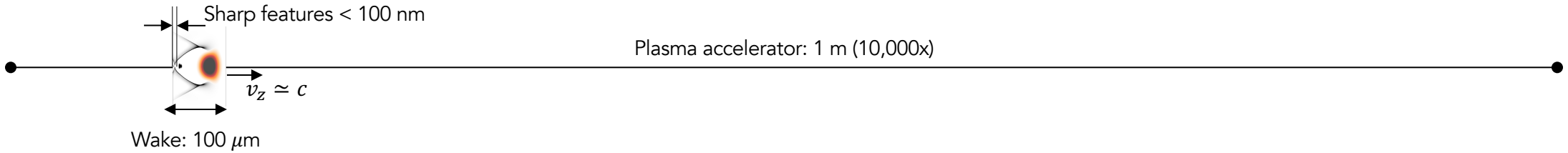
Regular mesh
Macroparticles



- *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

Fast plasma acceleration simulations with quasistatic approximation



Problem: the CFL condition limits the time step to $\Delta t < c\Delta z$

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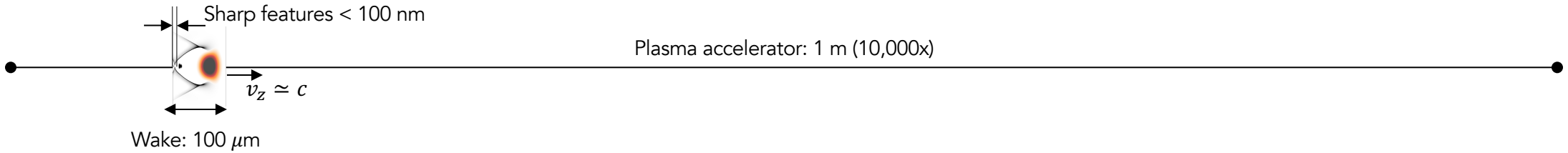

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Two main methods for larger time steps

- **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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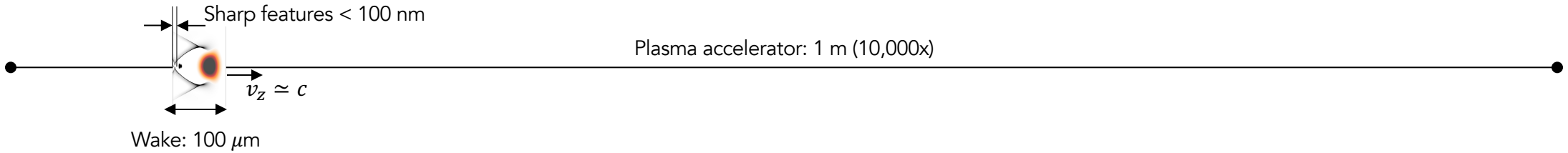

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- **Quasi-static particle-in-cell**
  - Beam & wake: $\boldsymbol{v} \sim c\boldsymbol{e_z}$
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  → No CFL condition, large time step for the beam

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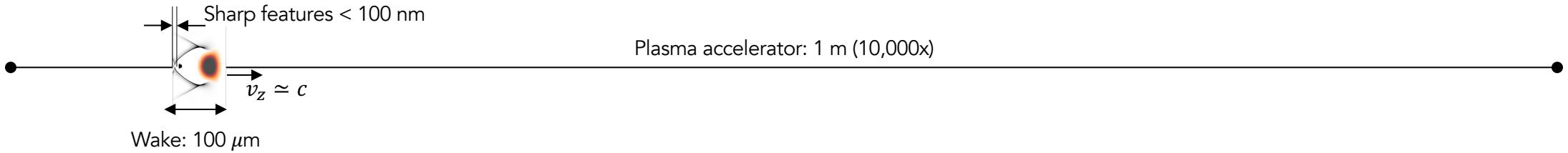

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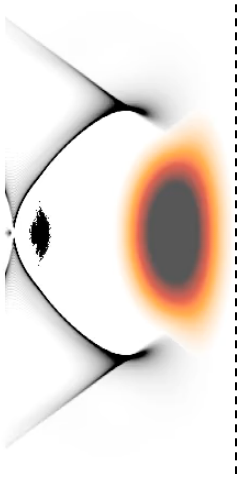

"the fields $\boldsymbol{a}$ and $\boldsymbol{\phi}$ which drive the plasma are expected to change little during a transit time of the plasma through the laser pulse"

"Under the quasistatic approximation, the $\partial/\partial z$ derivatives may be neglected in the electron (fluid) equations"

[P. Sprangle et al., PRL 64, 17 (1990)]

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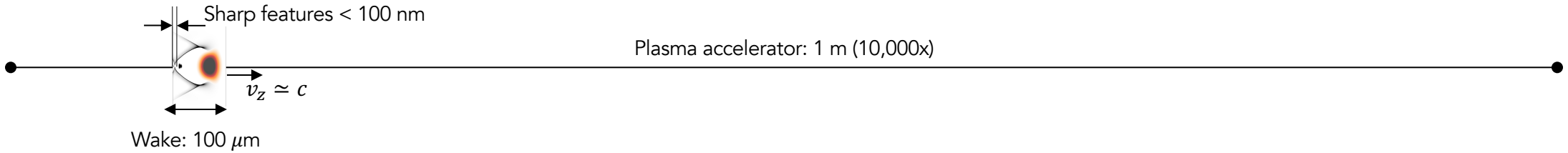

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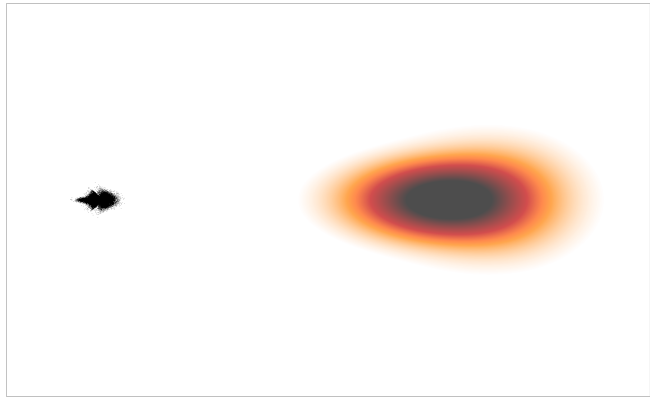
In QS PIC, plasma and laser/particle beams are treated differently



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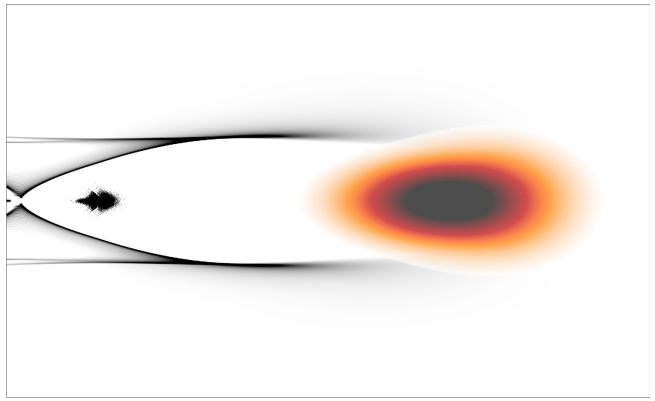

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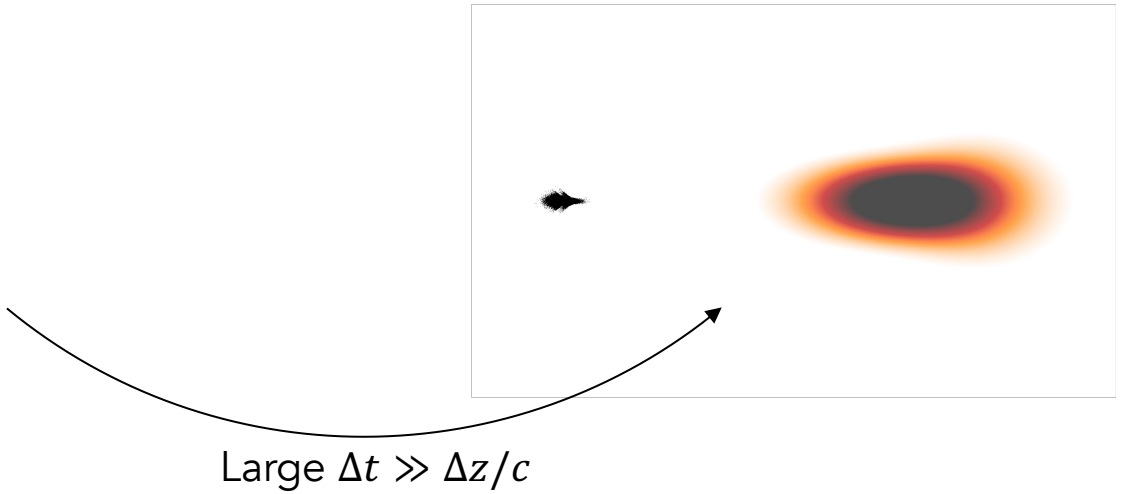

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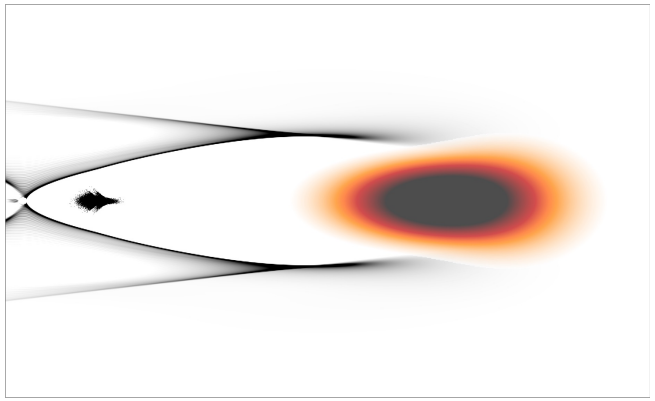

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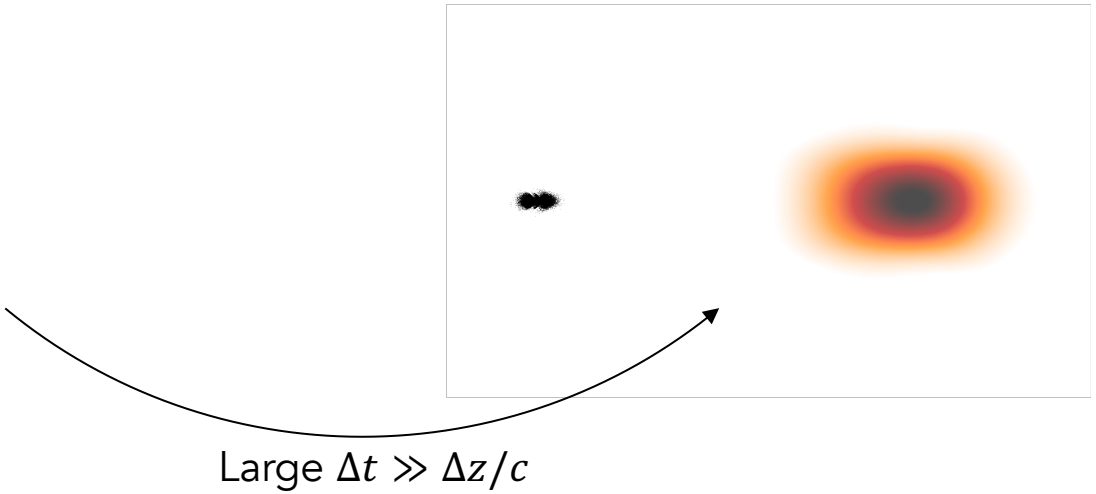

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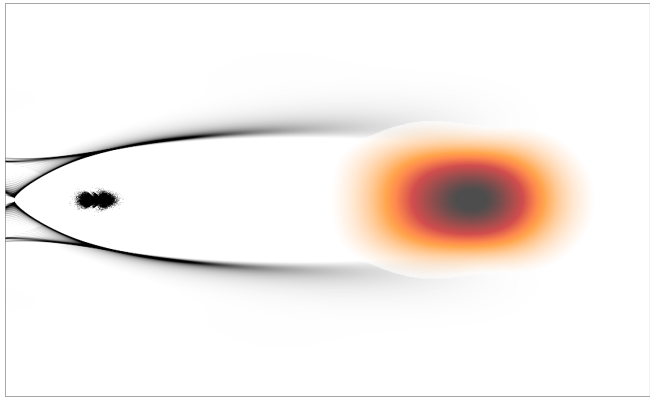

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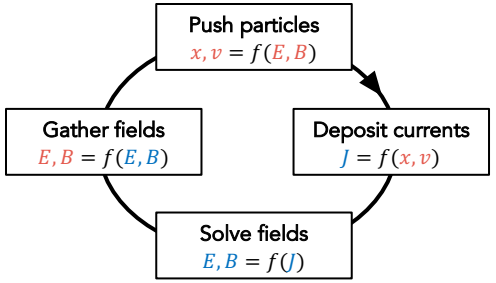

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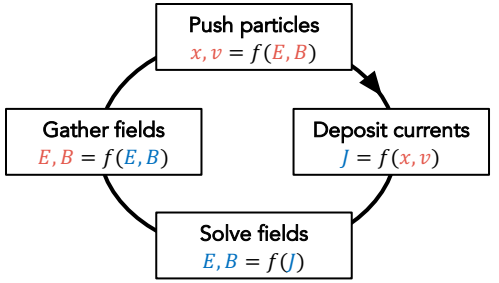
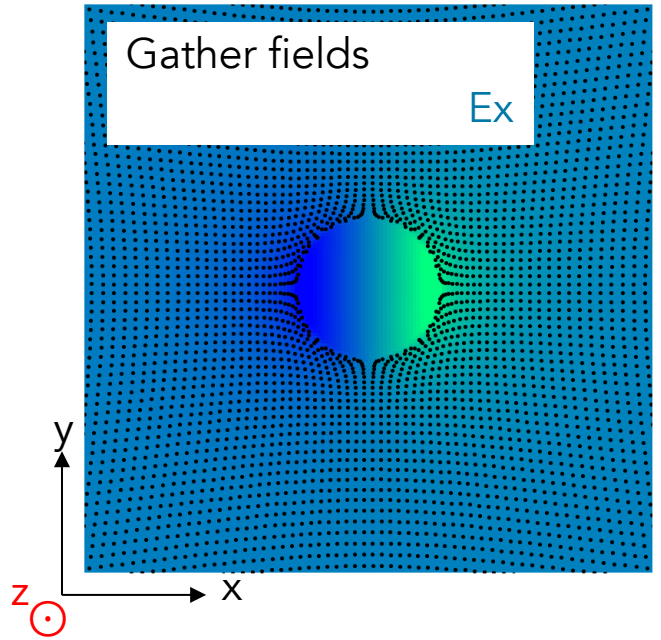


2D slice
Field & particles



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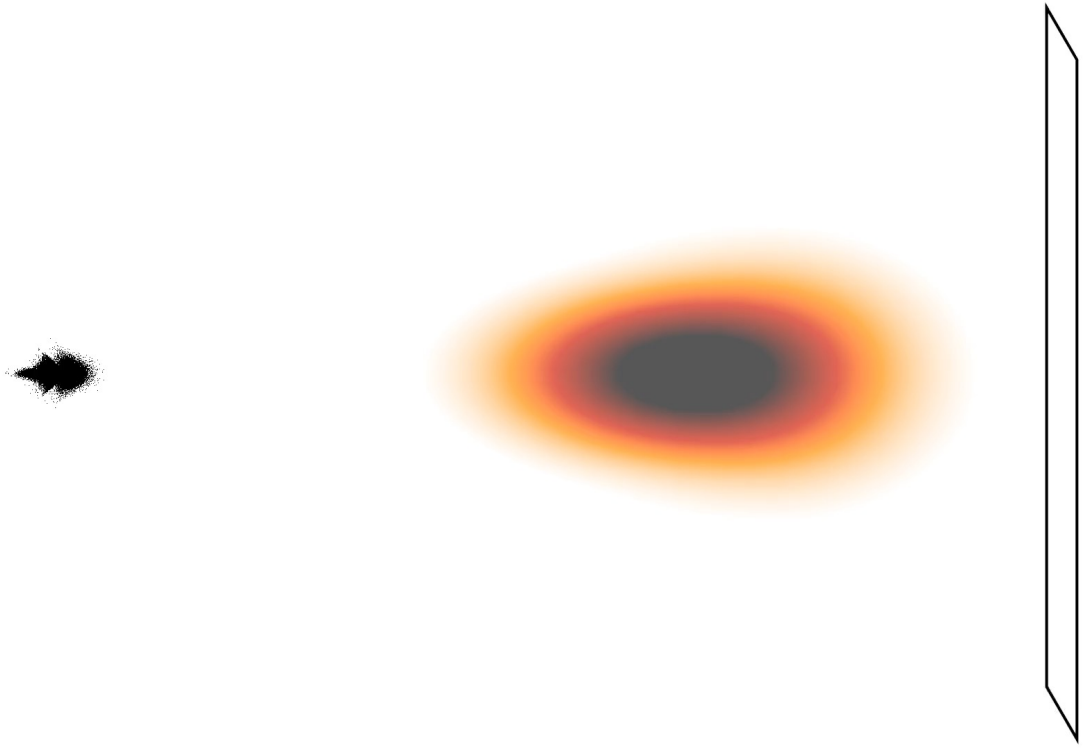

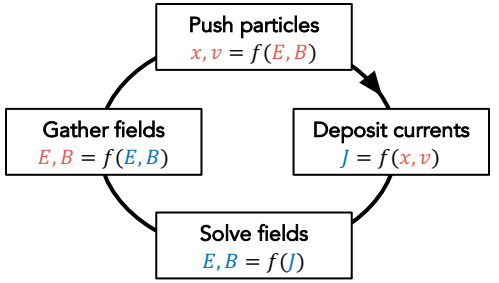

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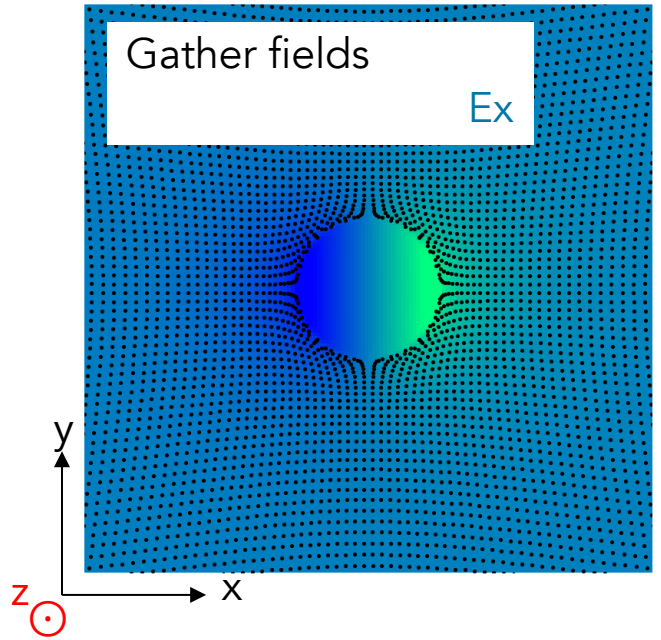

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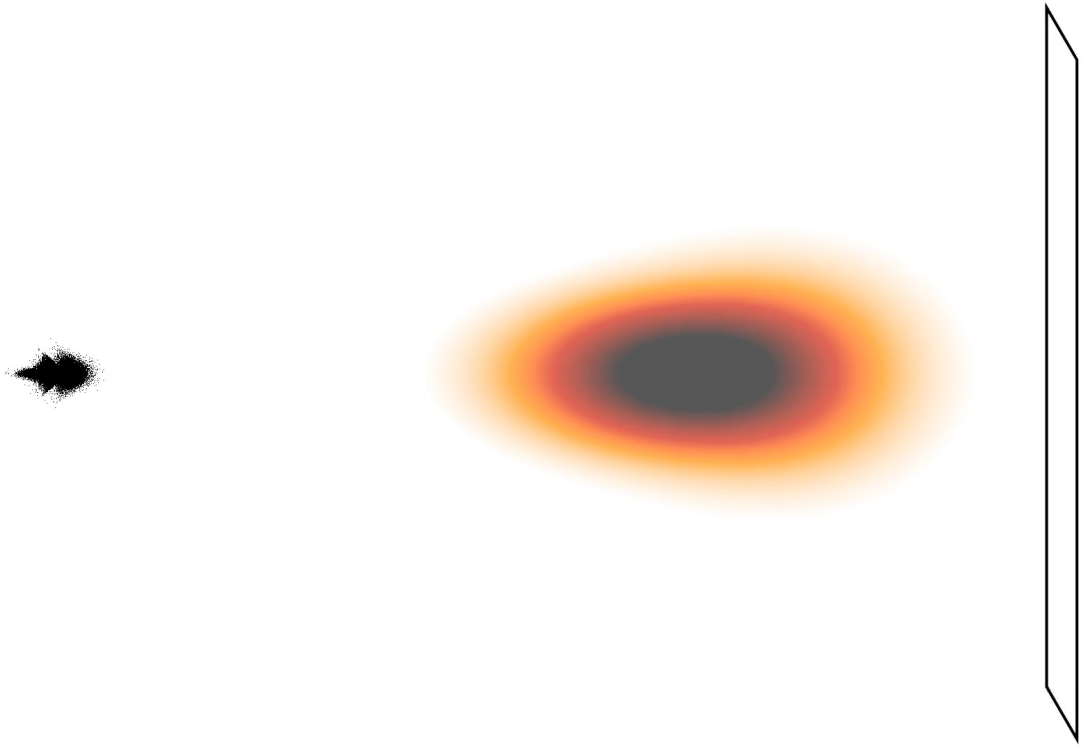

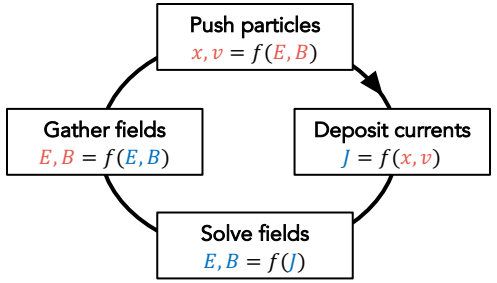

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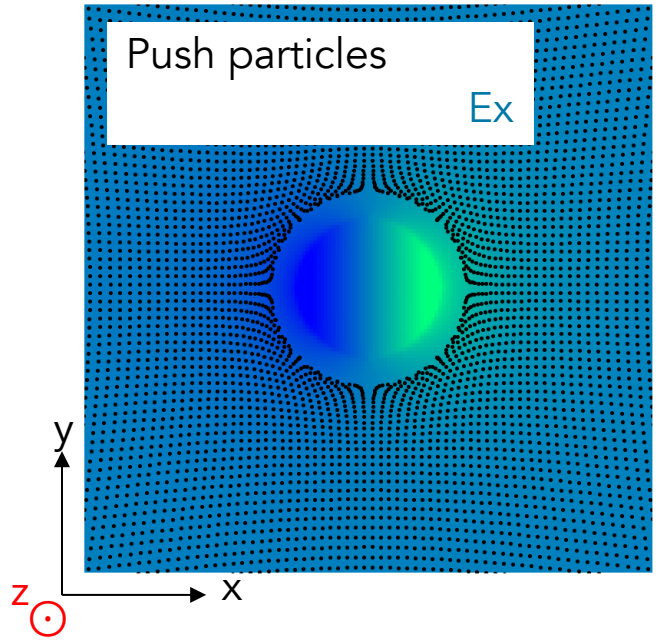

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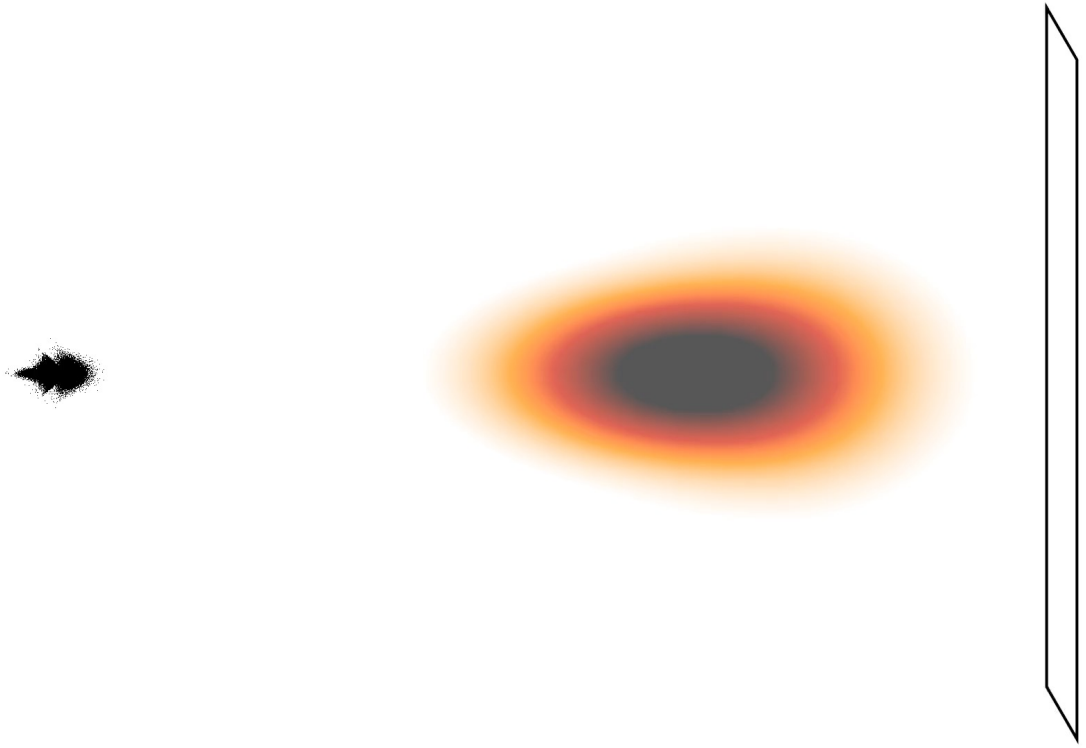

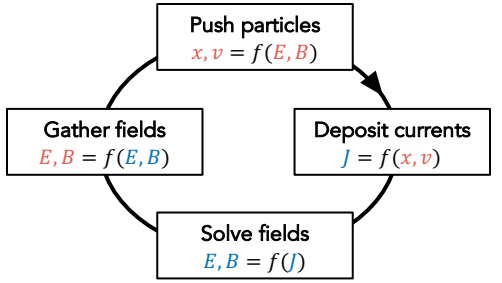

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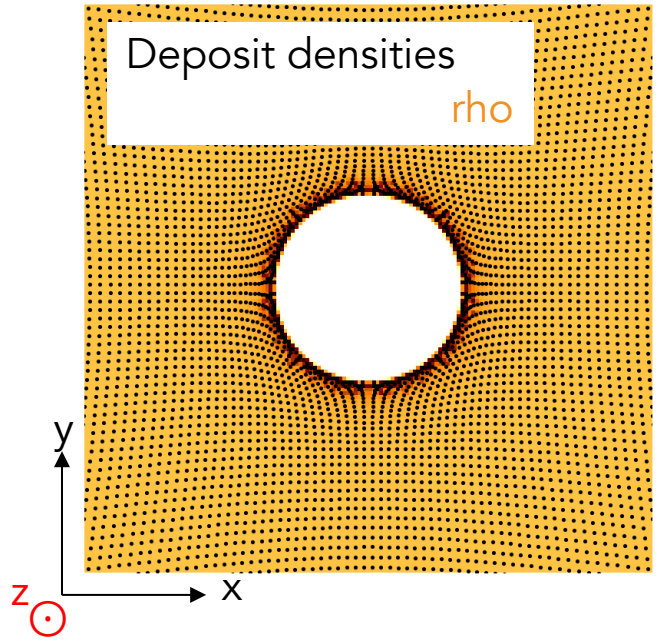

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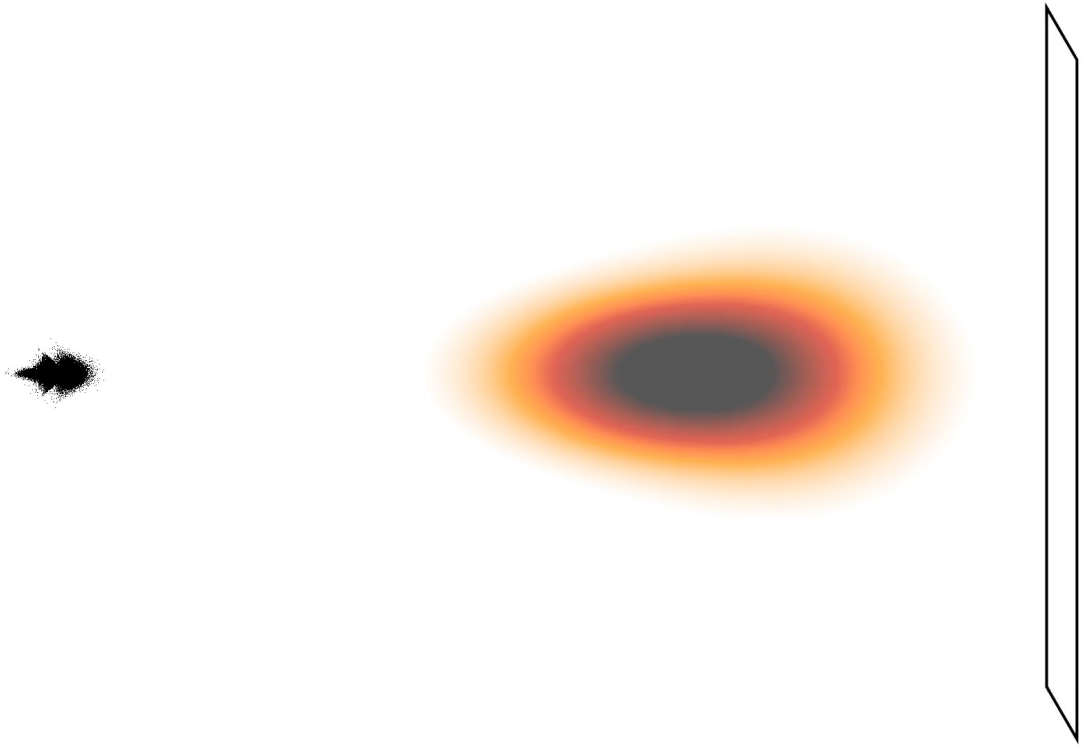

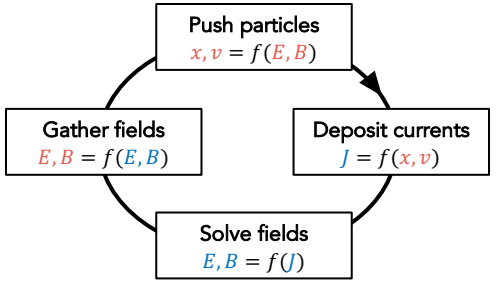

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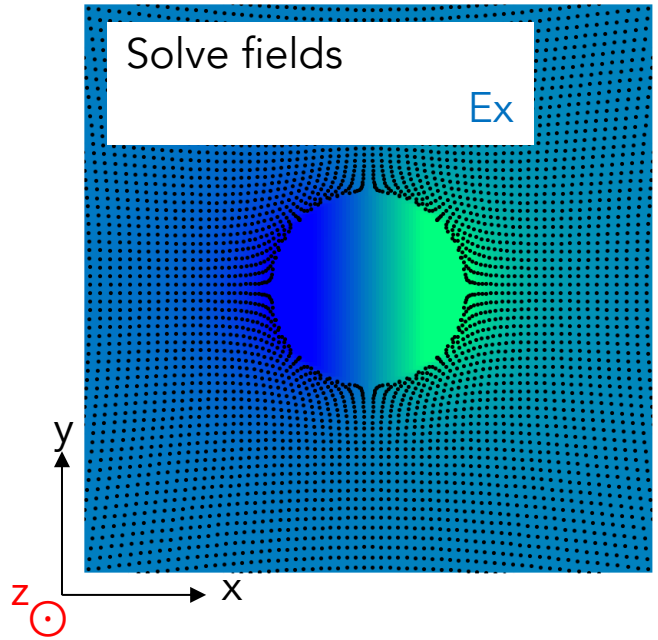

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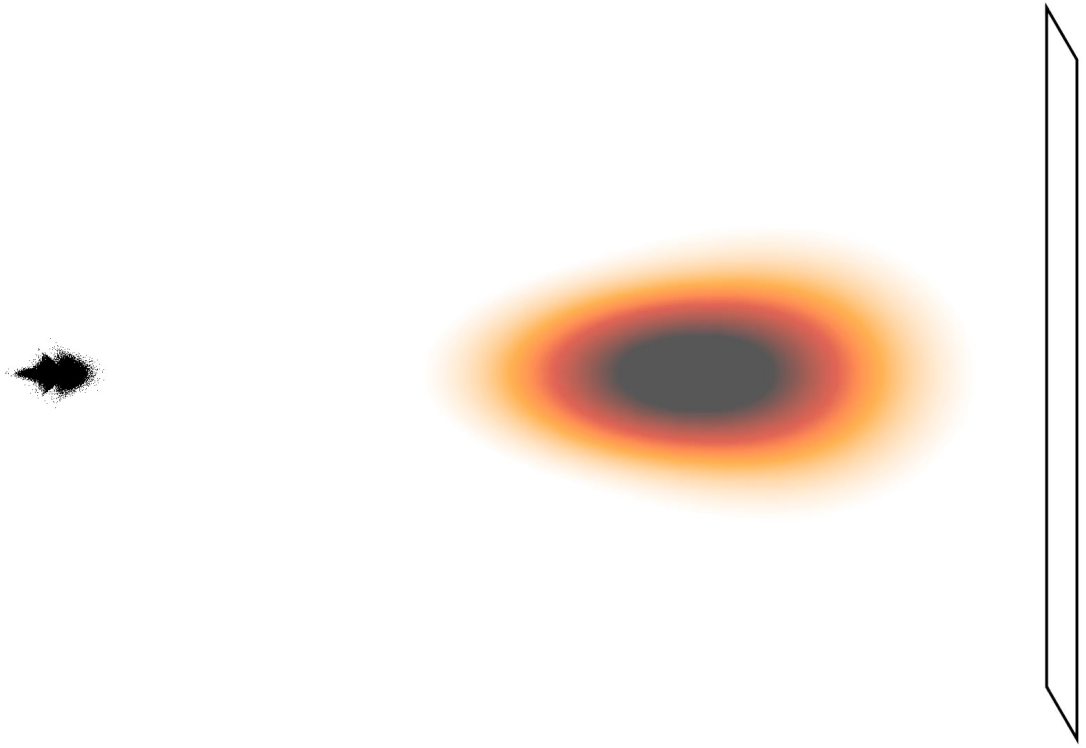

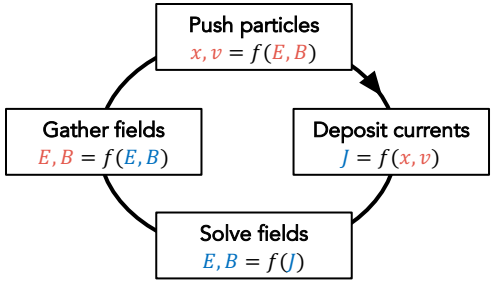

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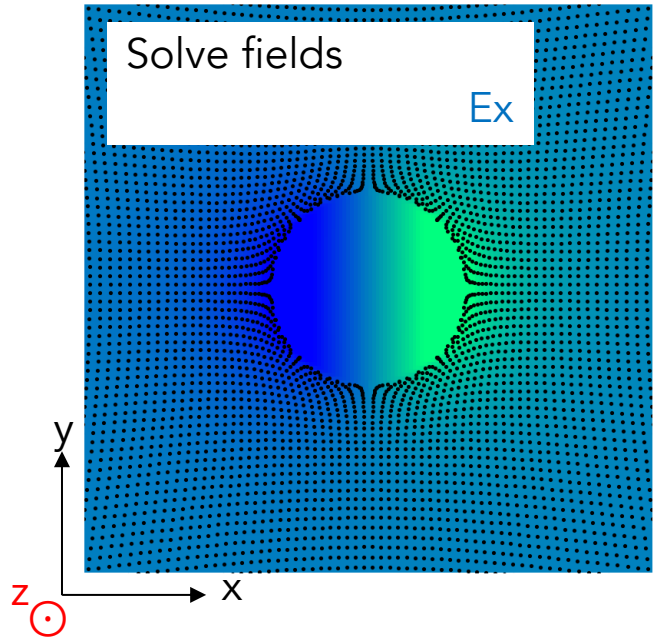

- All PIC operations occur on the 2D transverse domain
- Plasma particles are advanced in ζ (z), not in time
- (specific to HiPACE++: beams and lasers also advanced in the swipe)
- A simulation does $\boldsymbol{n_t \times n_z}$ PIC iterations on domain $\boldsymbol{n_x \times n_y}$
- (EM PIC: does $\boldsymbol{n_t}$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

Recent advances improved accuracy of the field solver

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

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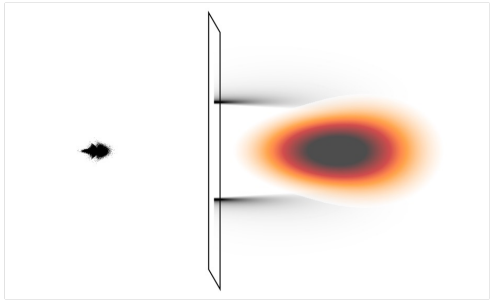

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Source terms $\partial_\zeta j_{x/y}$ are difficult to obtain

- 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. Suakov, 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

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

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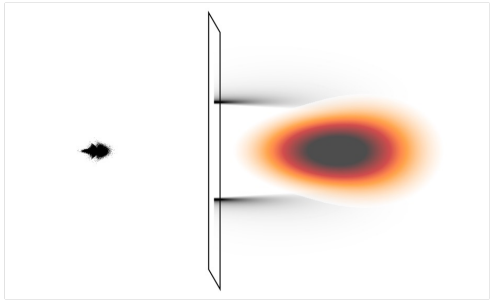

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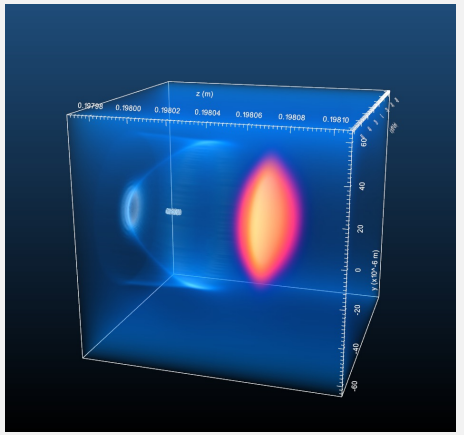
WakeT

Wakefield particle Tracker [1]

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



→ **Realistic 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)
[2] C. Benedetti et al., PPCF 60 014002 (2018)
[3] P. Baxevanis and G. Stupakov, PRAB 21 (2018)

→ Ask Ángel

Accelerated computing dominates supercomputing

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,194.00	1,679.82	22,703
2	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,220,288	309.10	428.70	6,016
4	**Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA Italy	1,824,768	238.70	304.47	7,404
5	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096

https://www.top500.org/lists/top500/2023/06/

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Equipped with GPUs:

Top500 33/50

Green500 46/50

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Equipped with GPUs:

Top500	33/50
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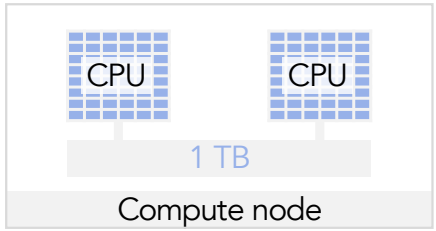
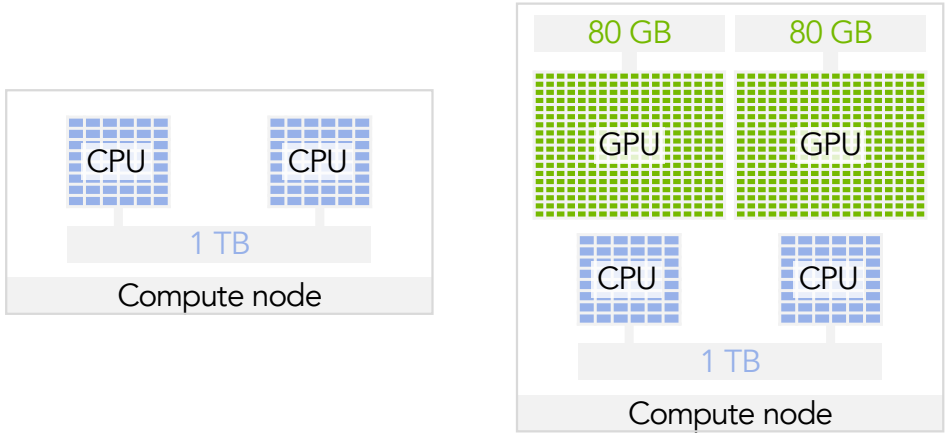
- GPUs meant for rendering, adopted by HPC
- Strong trend in HPC & scientific computing towards GPU (fast and energy-efficient)
- Trend driven by AI, here to stay

Accelerated computing dominates supercomputing



Accelerated computing dominates supercomputing



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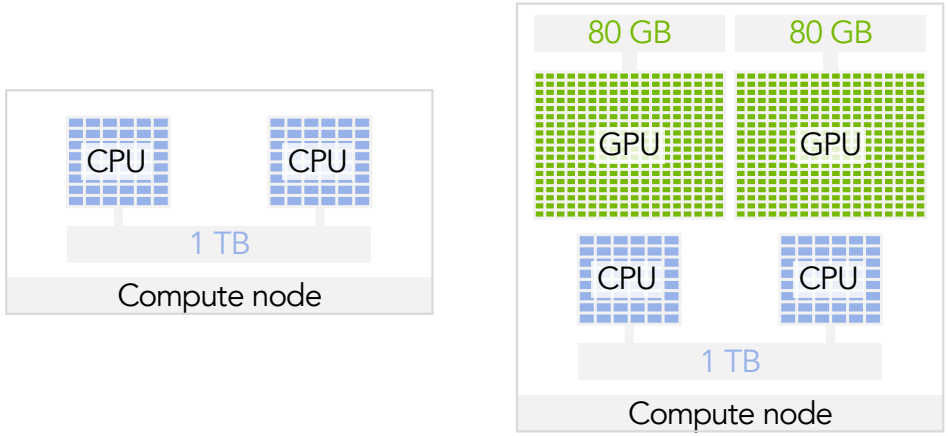
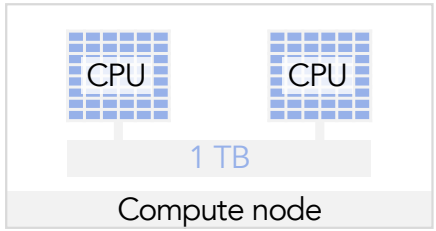


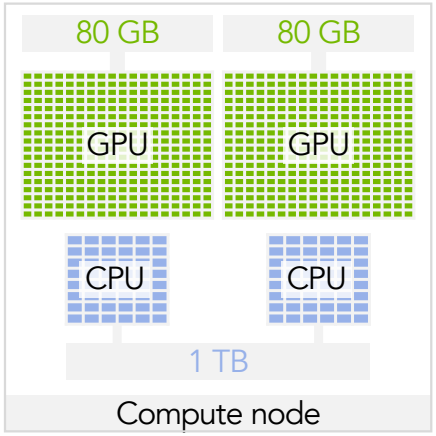
- What changes?
  - Many slow cores → expose parallelism
  - Modest memory available

- Performance-portability
  - In particular GPU computing
  - Portability layer (Kokkos, Alpaka, RAJA) C++

- Open Source & Open Repository
  - Software can be freely used, modified and shared
  - Encourages flexible, modular code
  - Favor good dependency graph rather than duplication

Accelerated computing dominates supercomputing





CPU

```
for(int i=0; i<N; i++){
    xp[i] += 1.;
}
```

GPU (CUDA)

```
kernel(int* xp) {
    int i = blockIdx.x *
            blockDim.x
            + threadIdx.x;
    if (i<N) xp[i] += 1.; }
kernel<<<N, 256>>>(xp);
```

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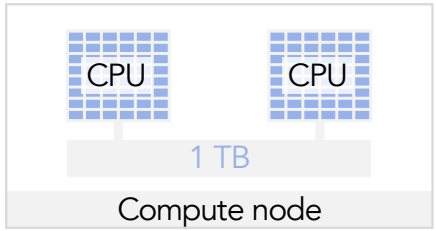

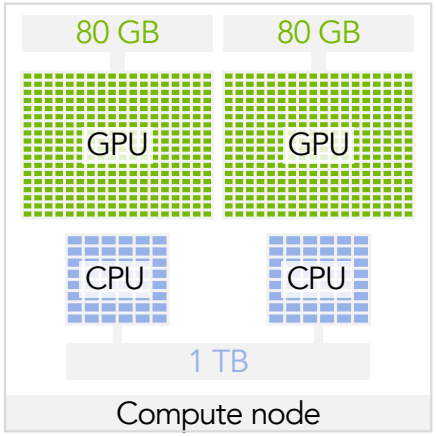

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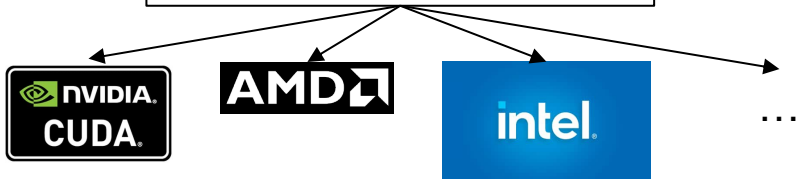
Any platform

```
ParallelFor( N,
    [=] (int i) {
        xp[i] += 1.;
    }
);
```



HiPACE++ – The Team

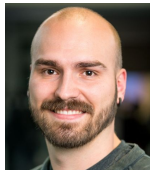
Advanced algorithms and high-performance computing for fast and energy-efficient 3D simulations of plasma acceleration – for everyone


Maxence Thévenet (lead)


Severin Diederichs


Alexander Sinn

DESY – MPA


Axel Huebl


Rémi Lehe


Jean-Luc Vay

LBNL – AMP

ECP *project WarpX*


Andrew Myers


Weiqun Zhang

LBNL – AMCR

Developers of AMReX


Carlo Benedetti

LBNL – BELLA

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

DESY. BERKELEY LAB

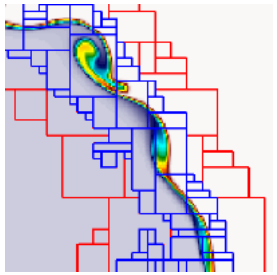
HiPACE++ – The Code

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

- **Modern HPC standard**
  - Modern C++, Python for pre- and post-processing
  - Cmake build systems, supports various compilers (Clang, GCC, Intel)
  - Open-source, documented, versioning system (1 per month), CI

- **Built on strong libraries**
  - Build on AMReX – Adaptive Mesh Refinement at eXascale for data structures & portability
  - Build on openPMD-api for I/O

- **Meant for inter-operability**
  - OpenPMD standard
  - Shares the ecosystem with WarpX and others: BLAST
  - Beams and laser readers and writers



amrex

https://github.com/Hi-PACE/hipace
https://hipace.readthedocs.io
S. Diederichs et al., *Comput. Phys. Comm.* 278: 108421 (2022)

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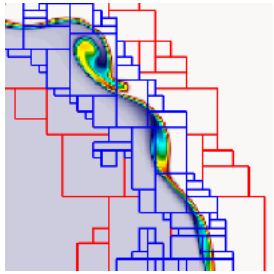

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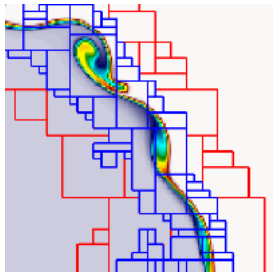

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HiPACE++ – The Capabilities

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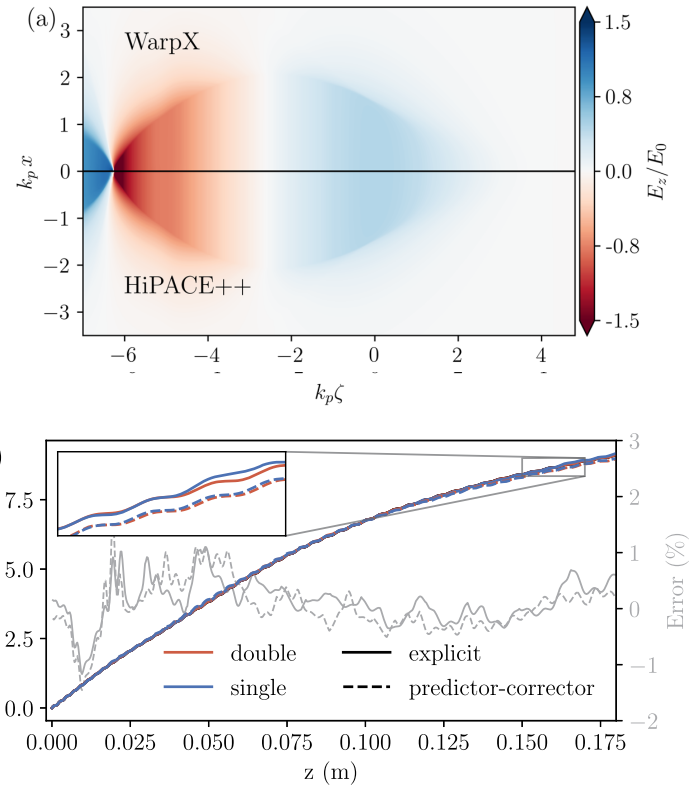
➢ Physics

- Laser and particle beam drivers
- Two unit systems (*SI* and *normalized*)
- Multi-physics (binary collisions, field ionization, radiation reaction)
- SALAME algorithm for automatic beam loading

➢ Numerics

- Single or double-precision
- Explicit solver (and predictor-corrector loop)
- Runs on various architectures (NVIDIA GPUs, AMD GPUs, most CPUs)
  Used on laptops, gaming GPUs, LUMI, Perlmutter, JUWELS Booster, etc.
- Considerable speedup over CPU-only
- Builds on Linux, Windows, MacOS
- Adaptive time step
- In-situ diagnostics



	4 GPUs	1024 CPU cores
Runtime (seconds)	6	556
Cost (node-hours)	6	11900

Used in (a few) scientific publications

R. D'Arcy et al., **Nature** 603.7899 (2022)
S. Diederichs et al., **PRAB** 25.9 (2022)
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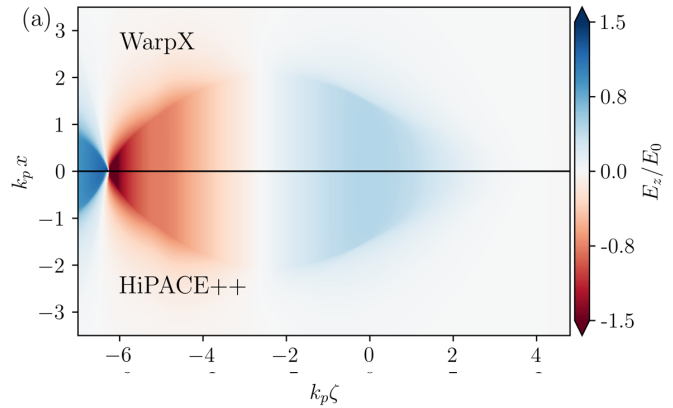

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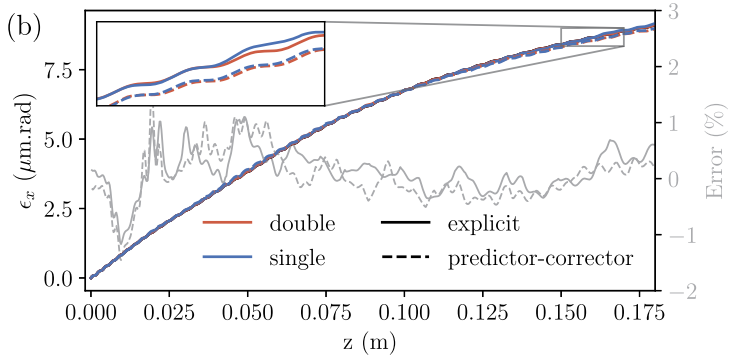

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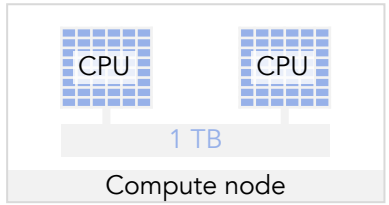
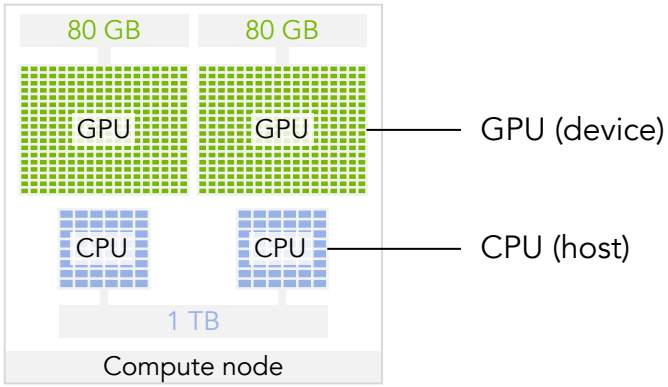
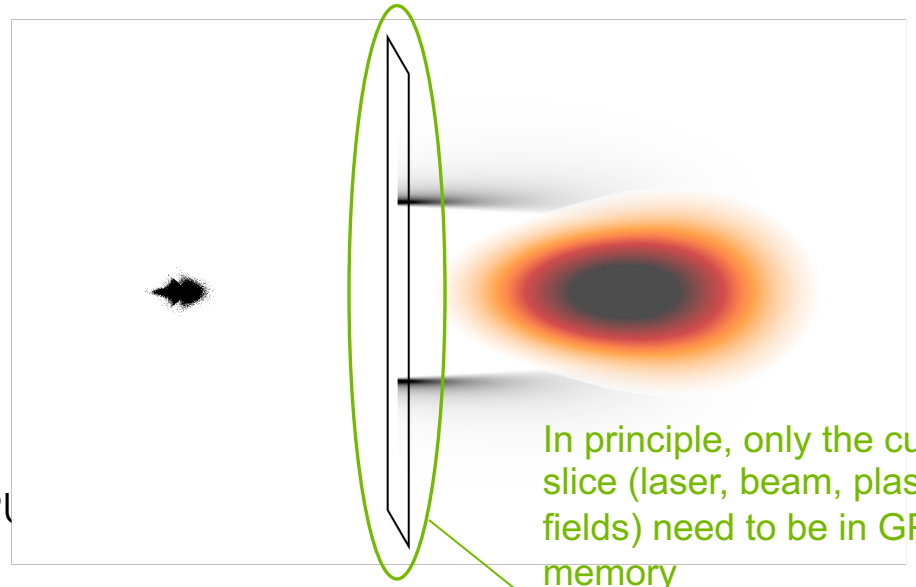
Quasi-static PIC is well-suited for GPU computing





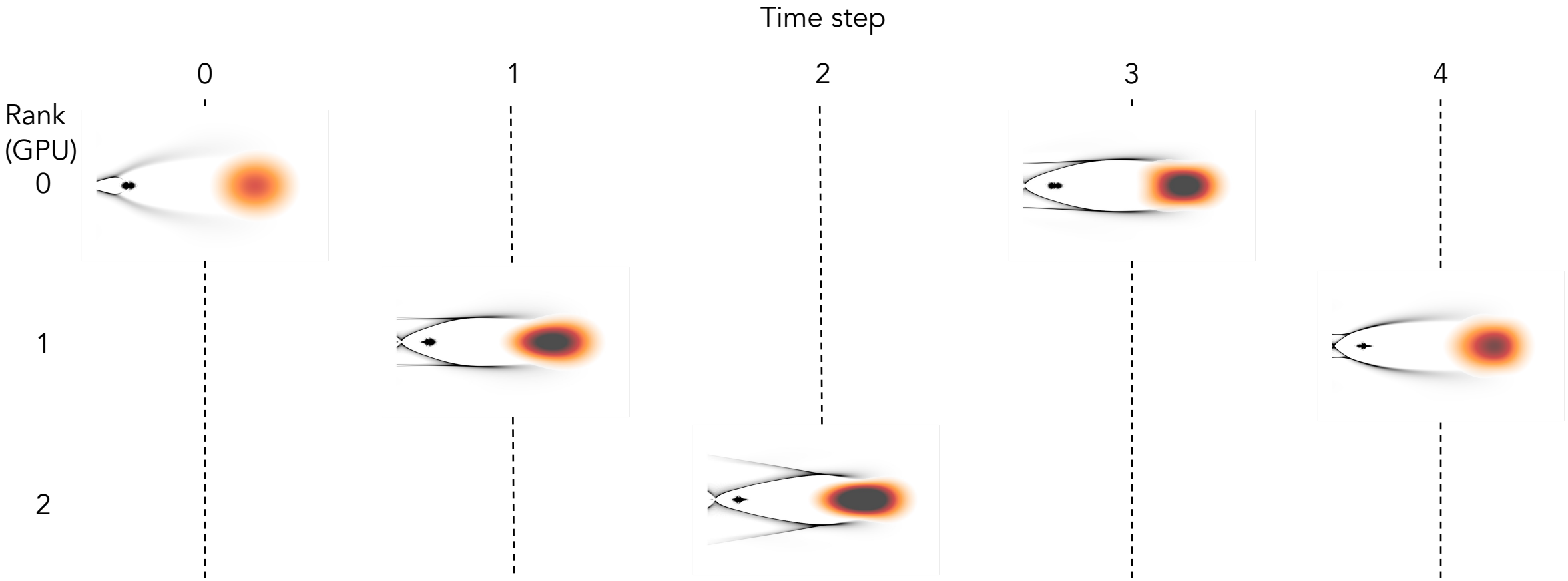


- Massive parallelism: Particle-in-cell can be ported efficiently to GPU
  - PIConGPU (HZDR, Germany), WarpX (LBNL, USA)
  - > millions of cells and particles
  - Main challenge: particle-grid exchanges
- Modest high-bandwidth memory: Only 1 slice in device memory
  - In reality, currently full particle driver
  - High transverse resolution (8000^2) on a single GPU → no comms
  - Parallelization in longitudinal direction

Parallelization: the new (old?) pipeline algorithm

Transverse parallelization:
- None on GPU
- OpenMP on CPU

Longitudinal parallelization: MPI (Message Passing Interface)
- $n_{ranks} < n_{slices}$ ($4 \times n_{slices}$ currently in HiPACE++)
- $n_{ranks} \leq n_{steps}$



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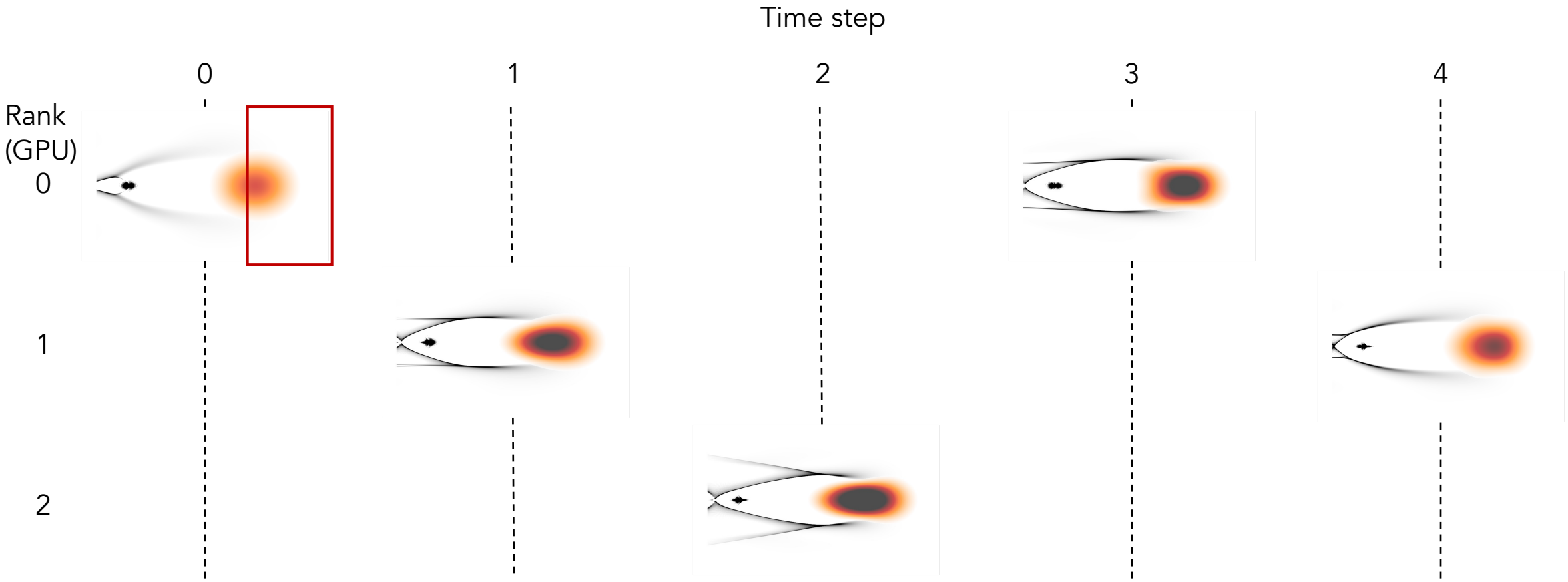

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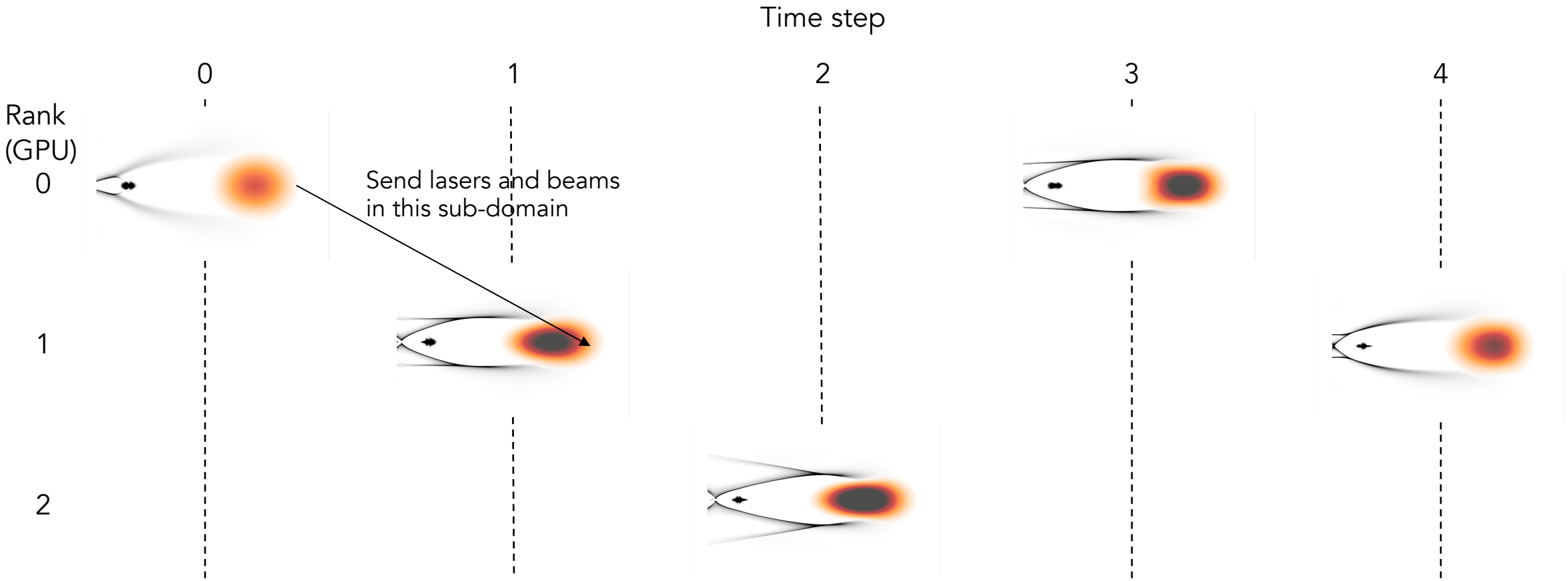

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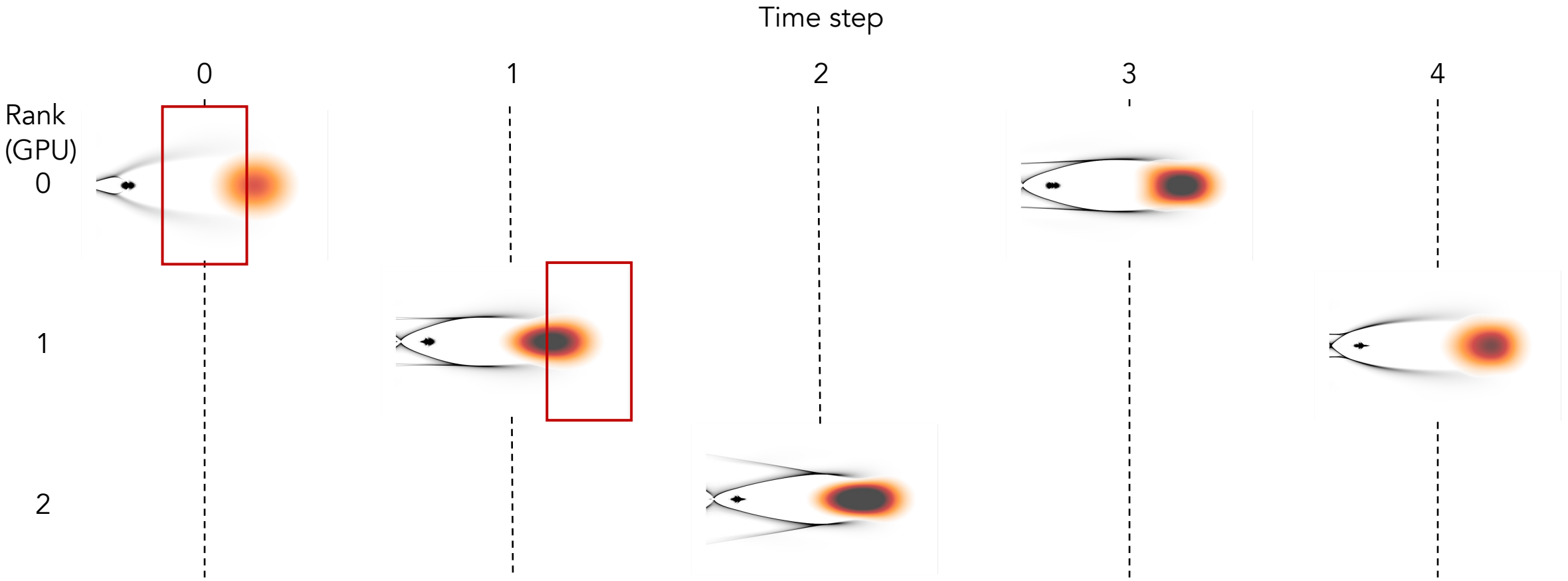

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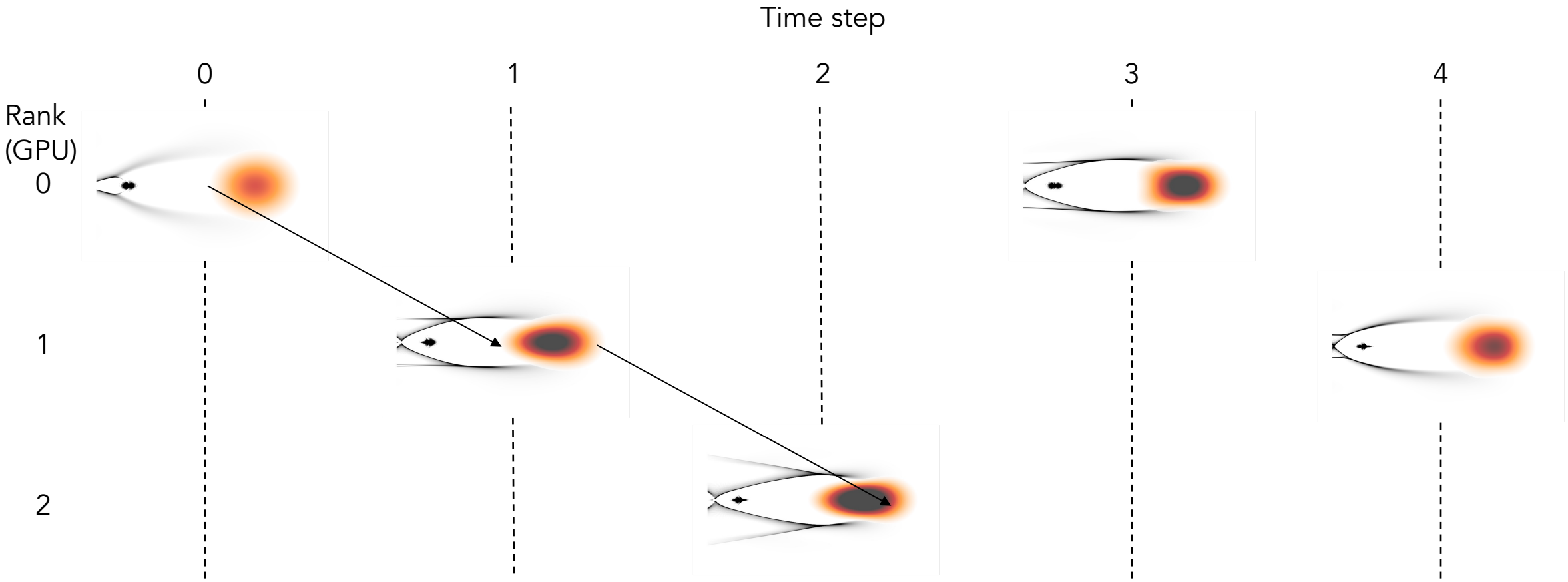

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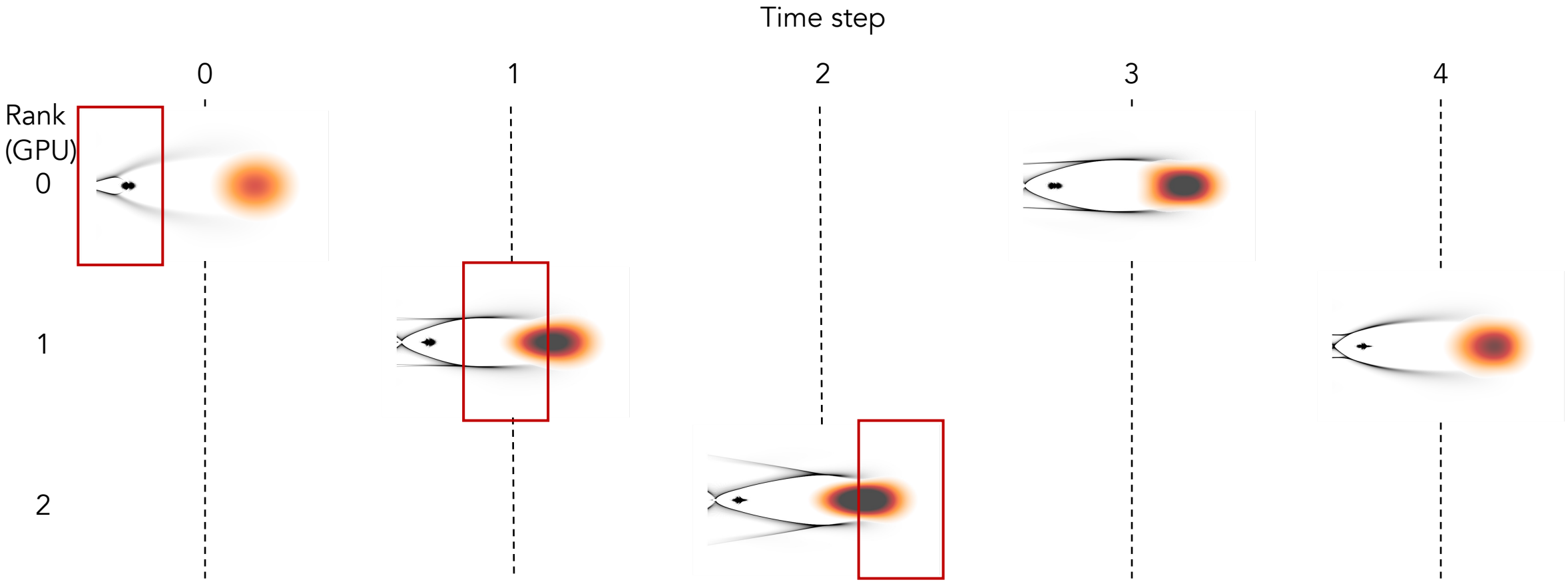

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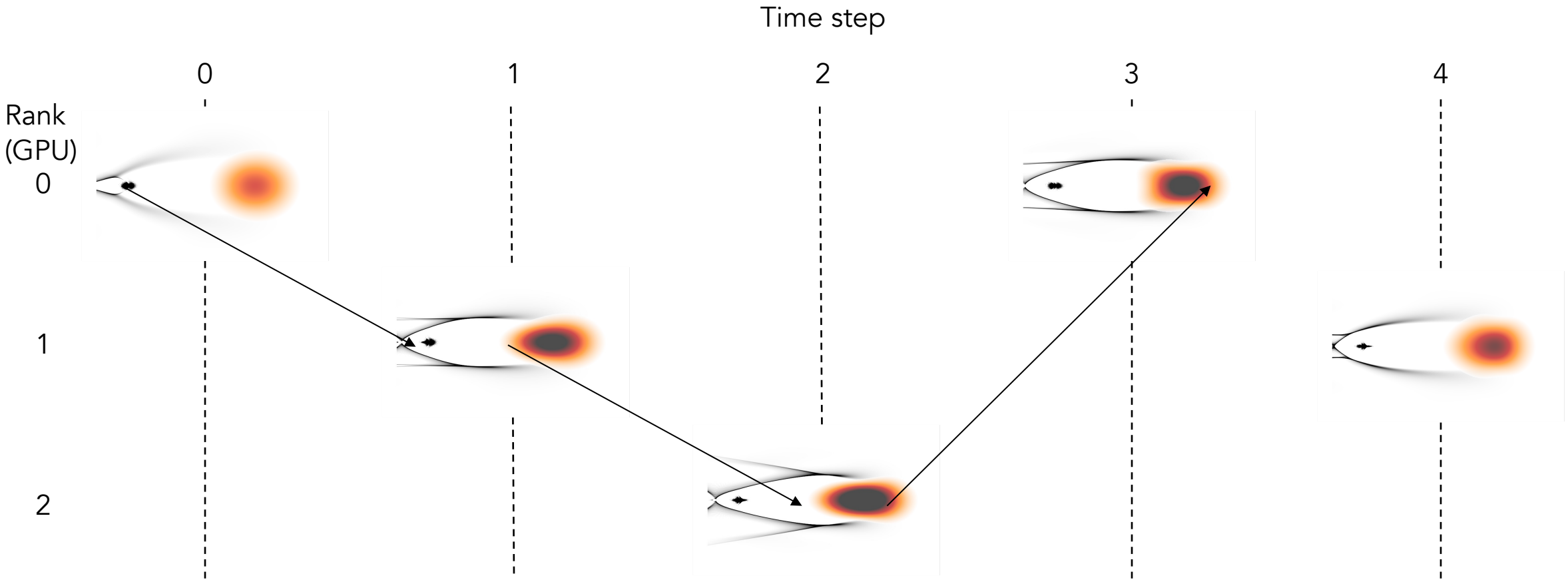

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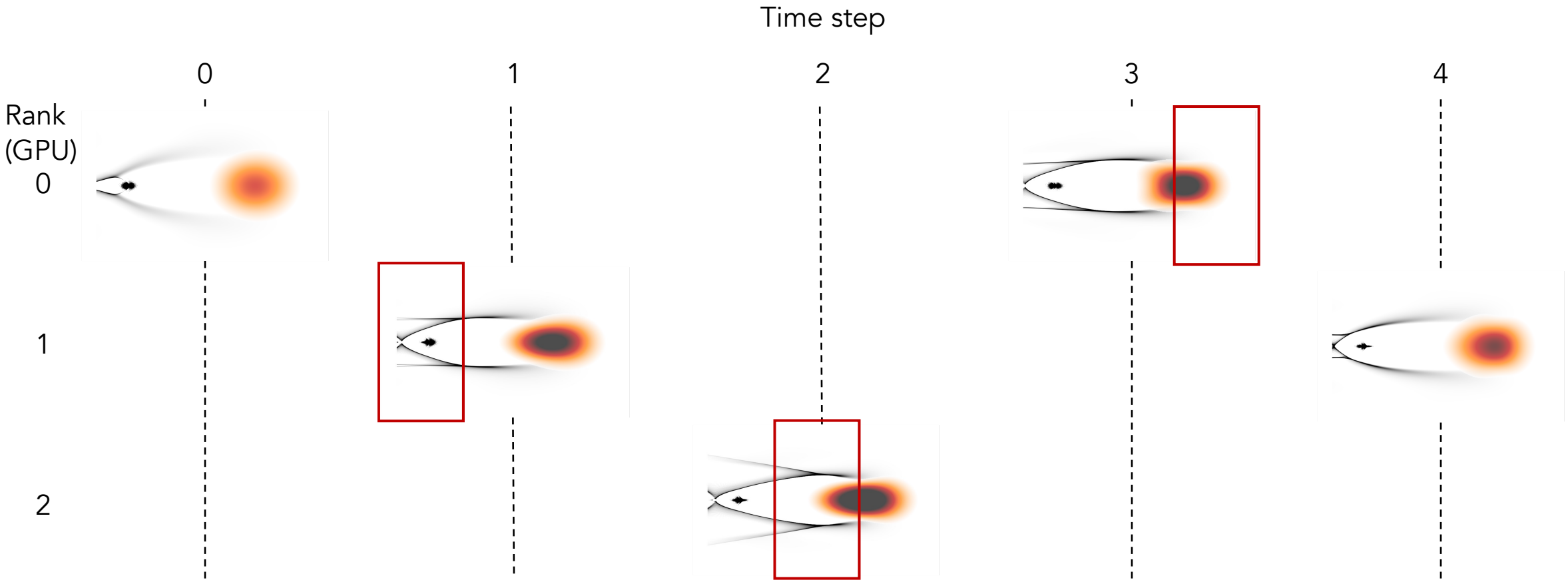

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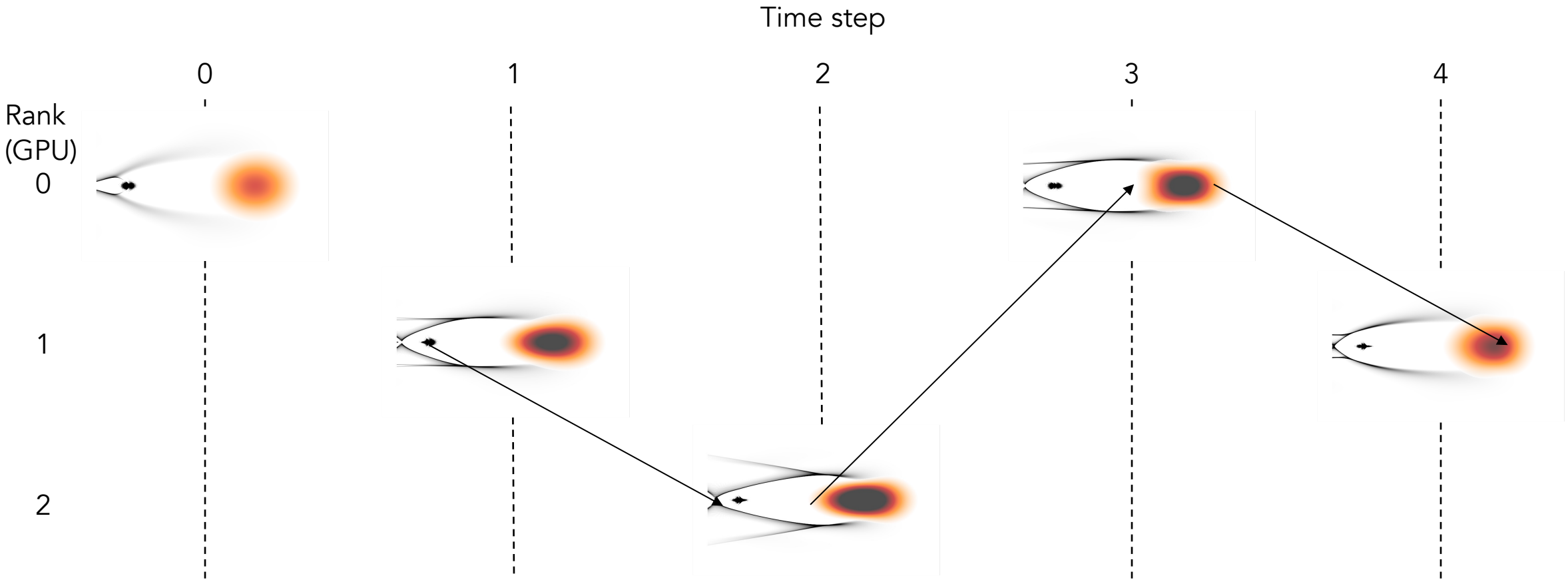
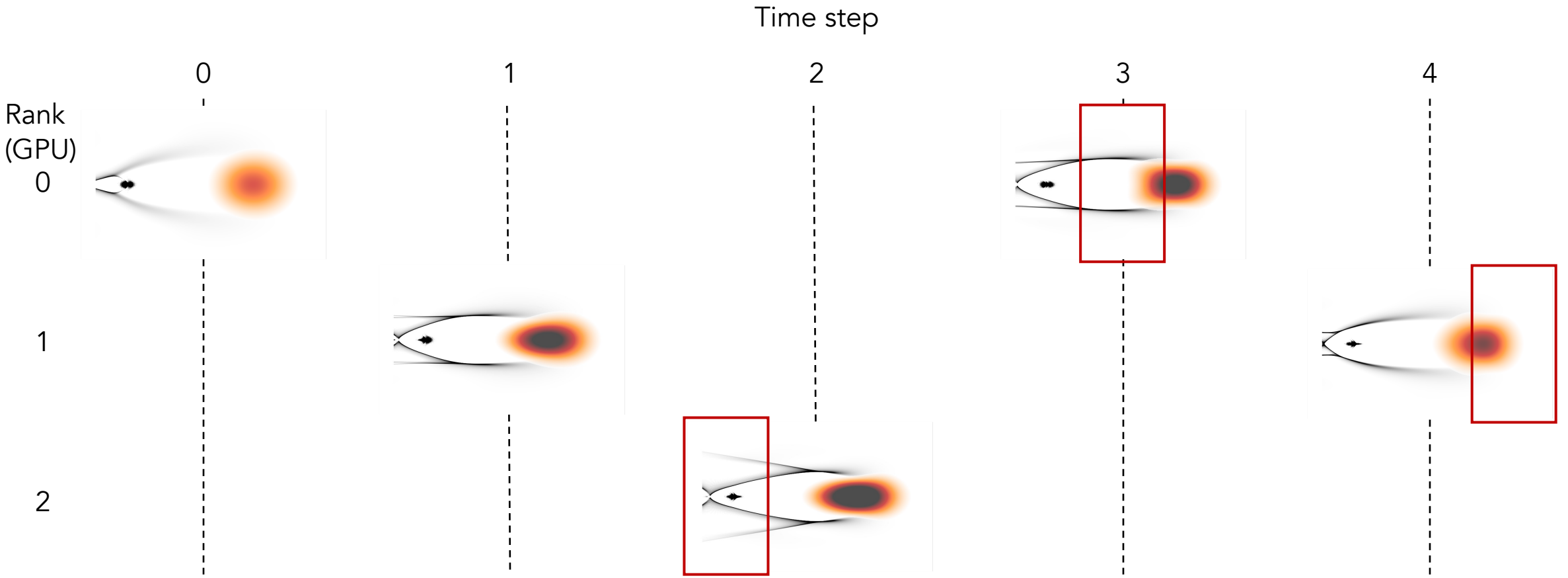


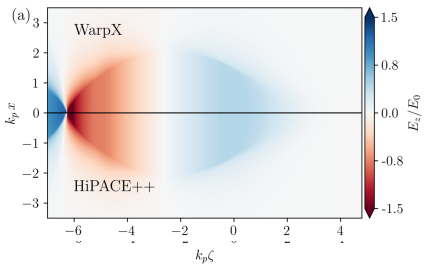
Parallelization: the new (old?) pipeline algorithm

Transverse parallelization:
- None on GPU
- OpenMP on CPU

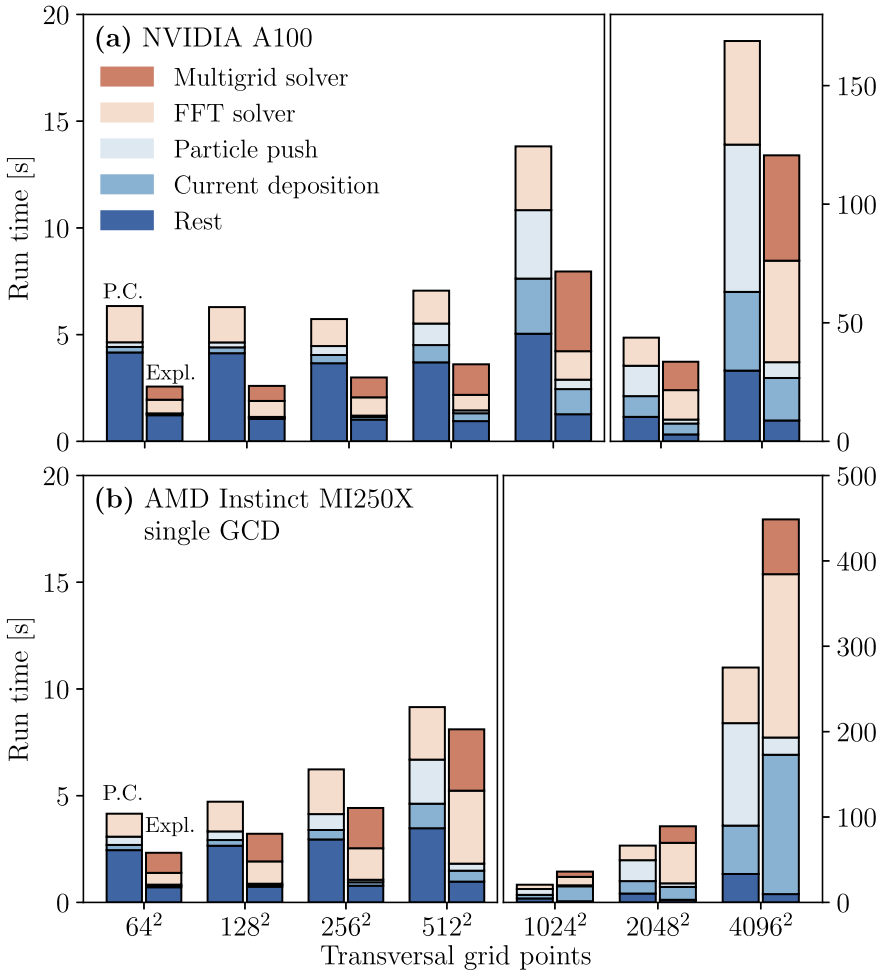
Longitudinal parallelization: MPI (Message Passing Interface)
- $n_{ranks} < n_{slices}$ ($4 \times n_{slices}$ currently in HiPACE++)
- $n_{ranks} \leq n_{steps}$

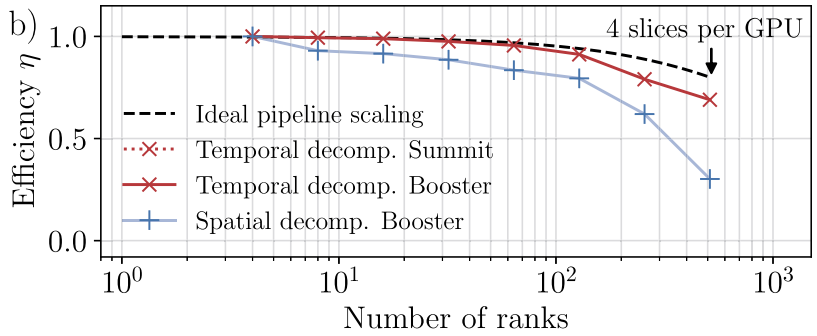


Performance of the code & parallelization



- S. Diederichs et al., *Comput. Phys. Comm.* 278: 108421 (2022)





- Good scaling, good performance and AMD and NVIDIA GPUs
- Relatively old tests, significant speedup since then

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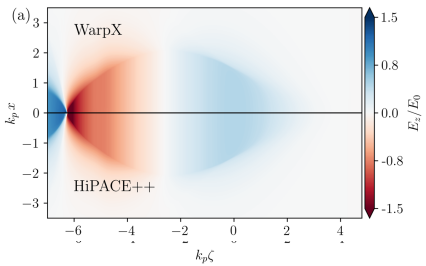

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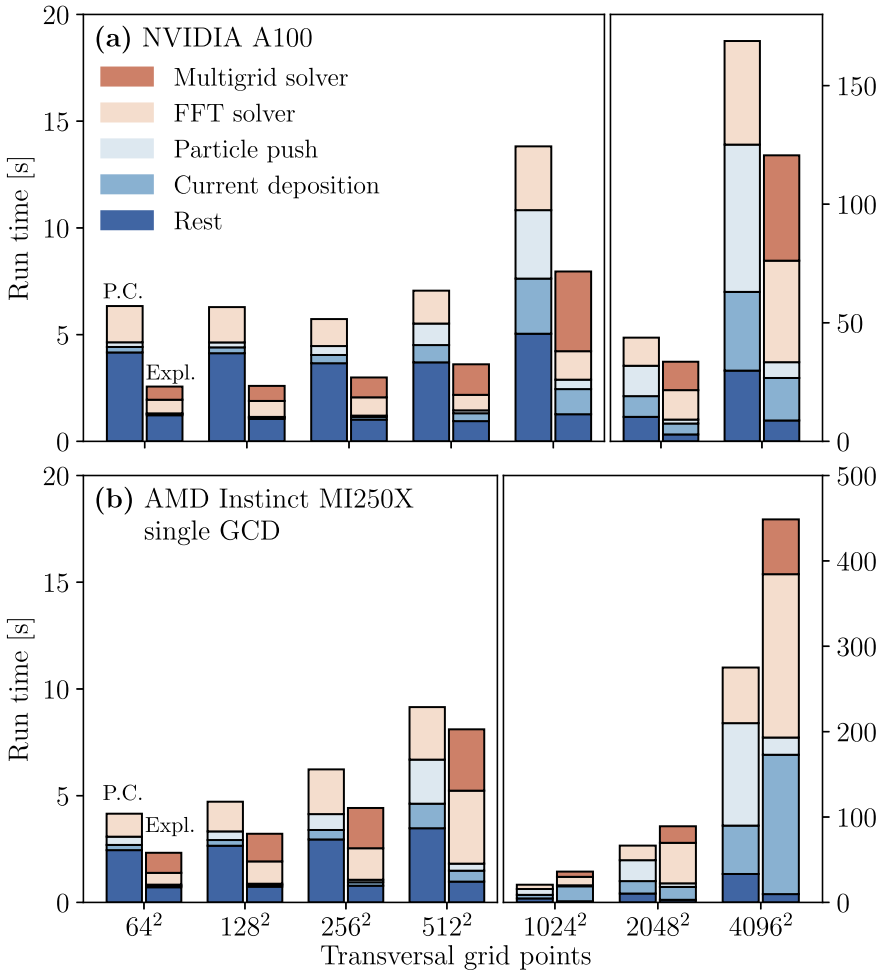

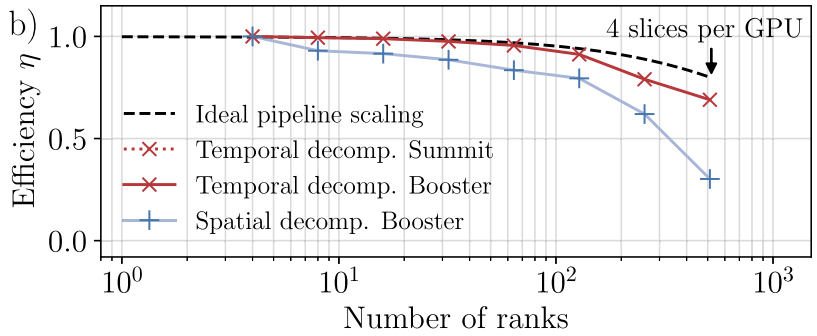

- Good scaling, good performance and AMD and NVIDIA GPUs
- Relatively old tests, significant speedup since then

See presentation by Alex Sinn (#5)

Code usage (illustration)

```
// Provided proper environment

> git clone https://github.com/Hi-PACE/hipace.git

> git checkout v23.05

> cmake -S . -B build -DHiPACE_COMPUTE=CUDA

> cmake --build build -j 16

> ./build/bin/hipace inputs

> mpirun -np 4 ./build/bin/hipace inputs
```

https://hipace.readthedocs.io/en/latest/run/get_started.html

inputs

```
max_step = 300
amr.n_cell = 1024 1024 1024
amr.max_level = 0
hipace.max_time = 0.3/clight
diagnostic.output_period = 1
hipace.dt = adaptive

geometry.is_periodic = true  true  false
geometry.prob_lo     = -250.e-6 -250.e-6 -250.e-6
geometry.prob_hi     =  250.e-6  250.e-6  110.e-6

beams.names = driver
driver.position_mean = 0. 0. 0.
driver.position_std = 2.e-6 2.e-6 30.e-6
driver.injection_type = fixed_weight
driver.num_particles = 1000000
driver.total_charge = .6e-9
driver.u_mean = 0. 0. 1000.
driver.u_std = 2. 2. 10.
driver.do_symmetrize = 1

plasmas.names = electron
electron.density(x,y,z) = 2.e22
electron.ppc = 1 1
electron.u_mean = 0.0 0.0 0.
electron.element = electron

diagnostic.diag_type = xz
```

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See presentation by Severin Diederichs (#4)

inputs

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Conclusion

- HiPACE++: 3D, QS PIC for plasma acceleration
- Advanced methods (pipeline, MG)
- HPC (GPU) computing
- Open-source, documented
- New contributors are welcome!

Perspective

- More physics added
- Goals:
  - multi-stage collider-relevant parameters
  - Target new physics problems
- Advanced algorithms (MR)
- Enjoy the workshop!

Thank you for your attention

Contributions from all HiPACE++ contributors

Conclusion

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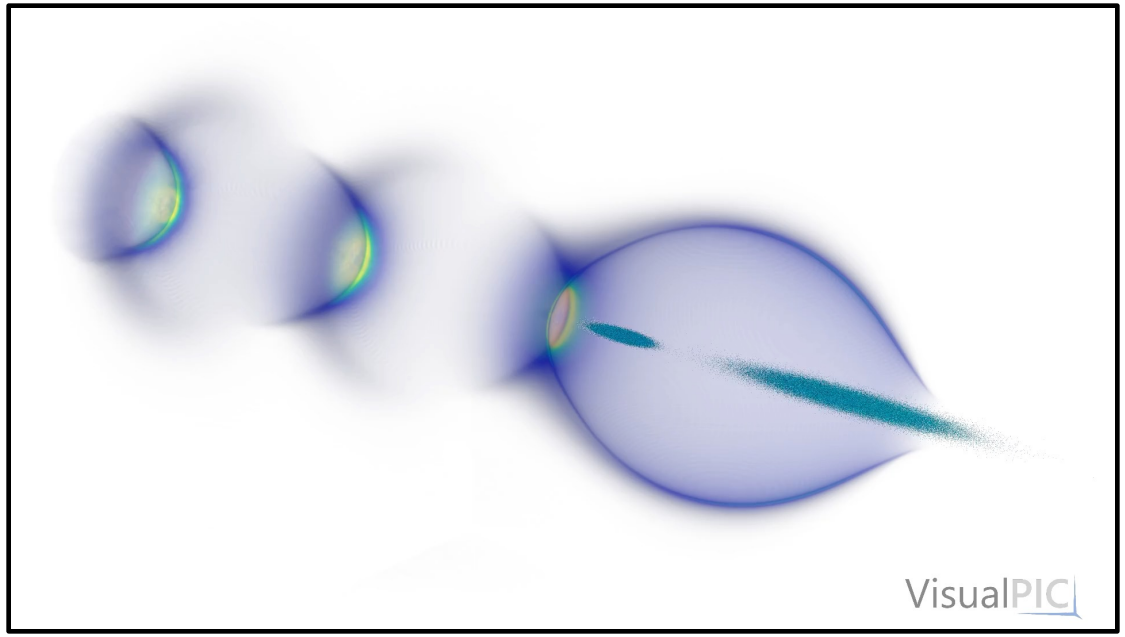

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