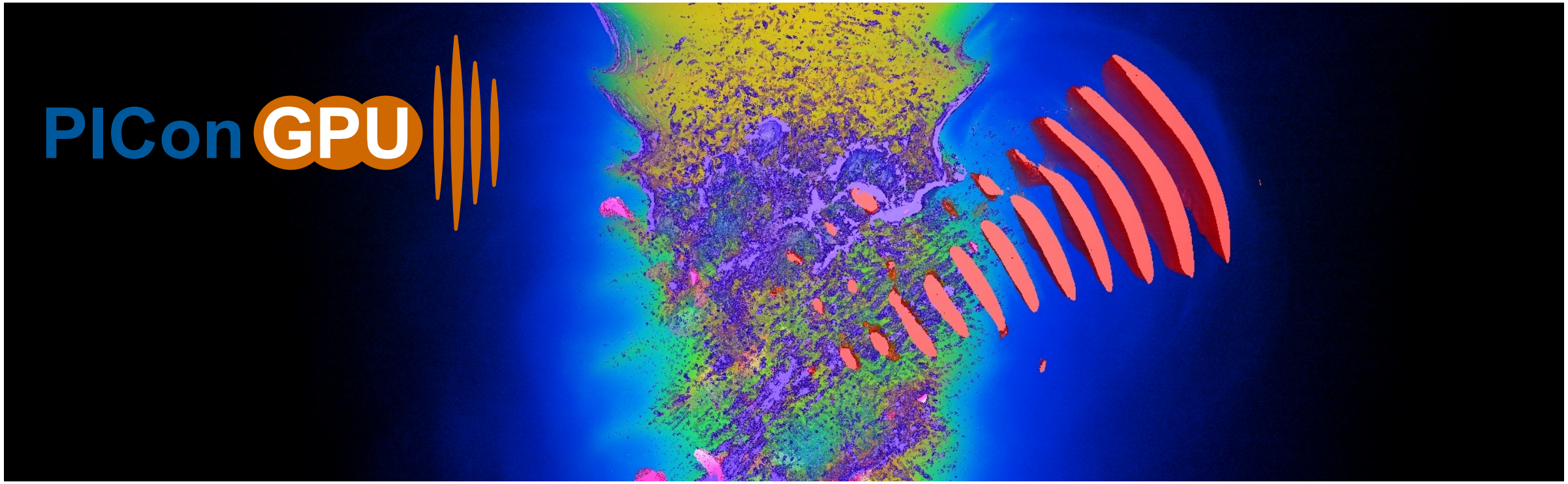
PLASMA PEPSC

HZDR
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

PIConGPU



PIConGPU

Introduction, Concepts and use of Libraries

HZDR · FWKT · Dr. Richard Pausch · r.pausch@hzdr.de · www.hzdr.de

DRESDEN concept

PLASMA PEPSC

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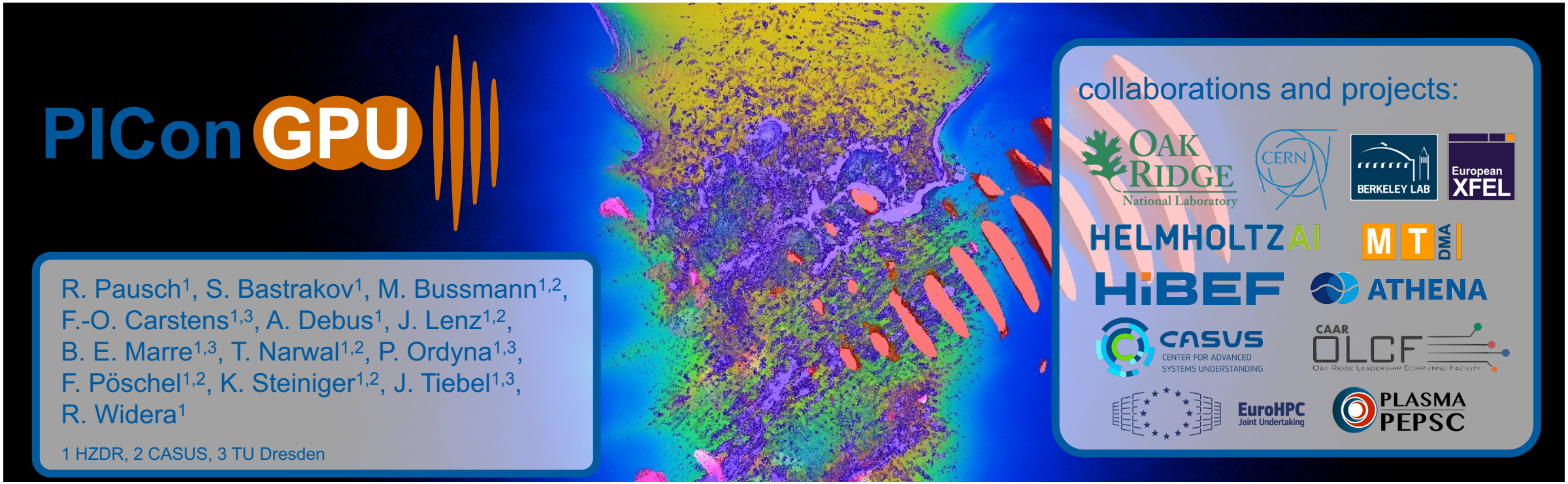

R. Pausch[1], S. Bastrakov[1], M. Bussmann[1,2], F.-O. Carstens[1,3], A. Debus[1], J. Lenz[1,2], B. E. Marre[1,3], T. Narwal[1,2], P. Ordyna[1,3], F. Pöschel[1,2], K. Steiniger[1,2], J. Tiebel[1,3], R. Widera[1]

1 HZDR, 2 CASUS, 3 TU Dresden

PIConGPU

Introduction, Concepts and use of Libaries

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DRESDEN concept

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Laser Plasma Physics at HZDR

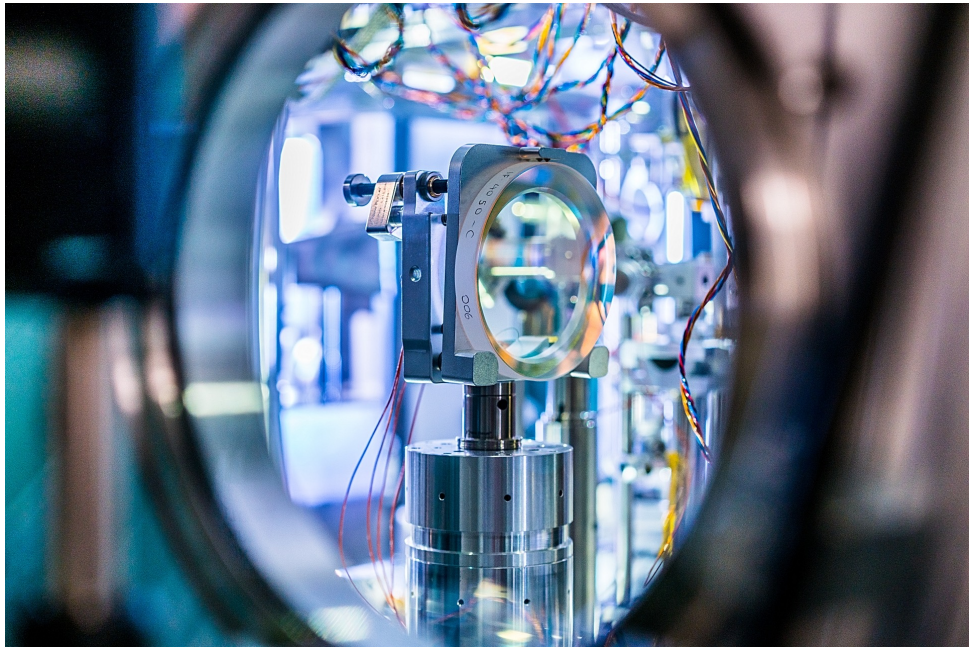
What are we using PIConGPU for?

DRESDEN
concept

Laser Plasma Acceleration

Compact particle accelerators with high power lasers

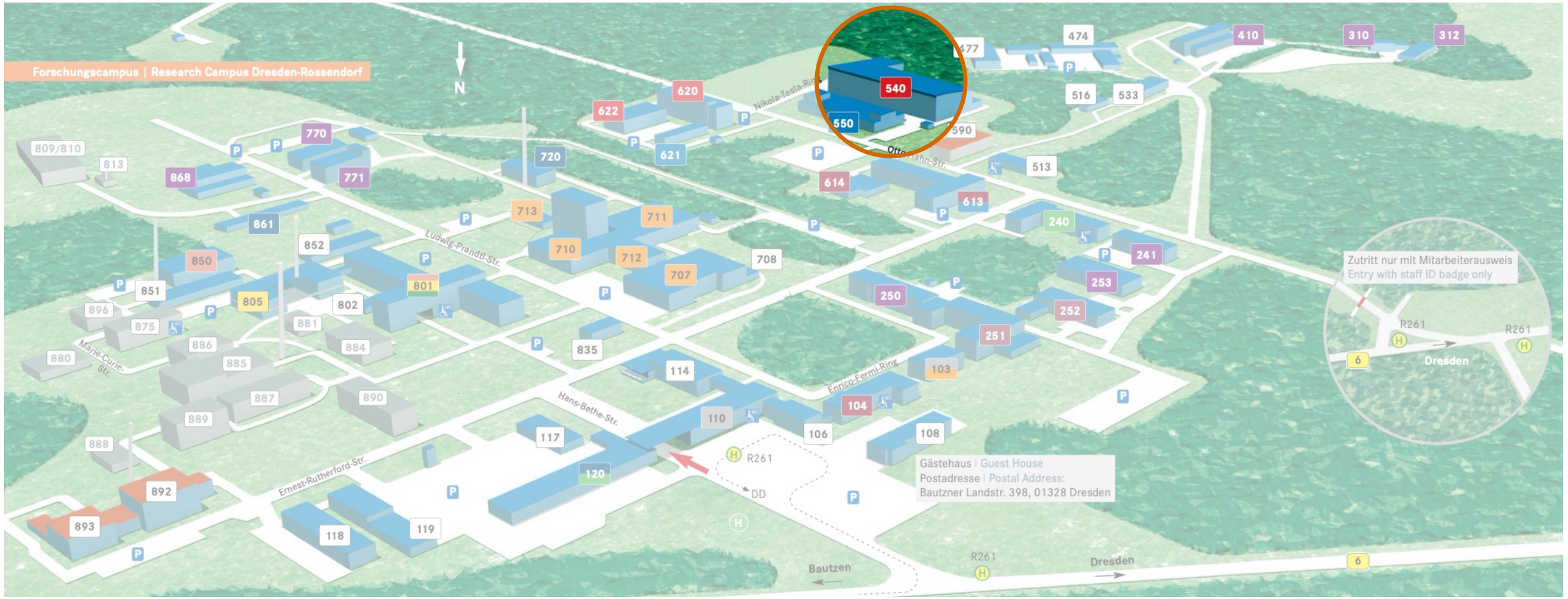
short high-power laser pulses → focused on a plasma to accelerate particles



PIConGPU PLASMA PEPSC DRESDEN concept SCIENCE AND INNOVATION CAMPUS HZDR

Laser Plasma Acceleration

Compact particle accelerators with high power lasers

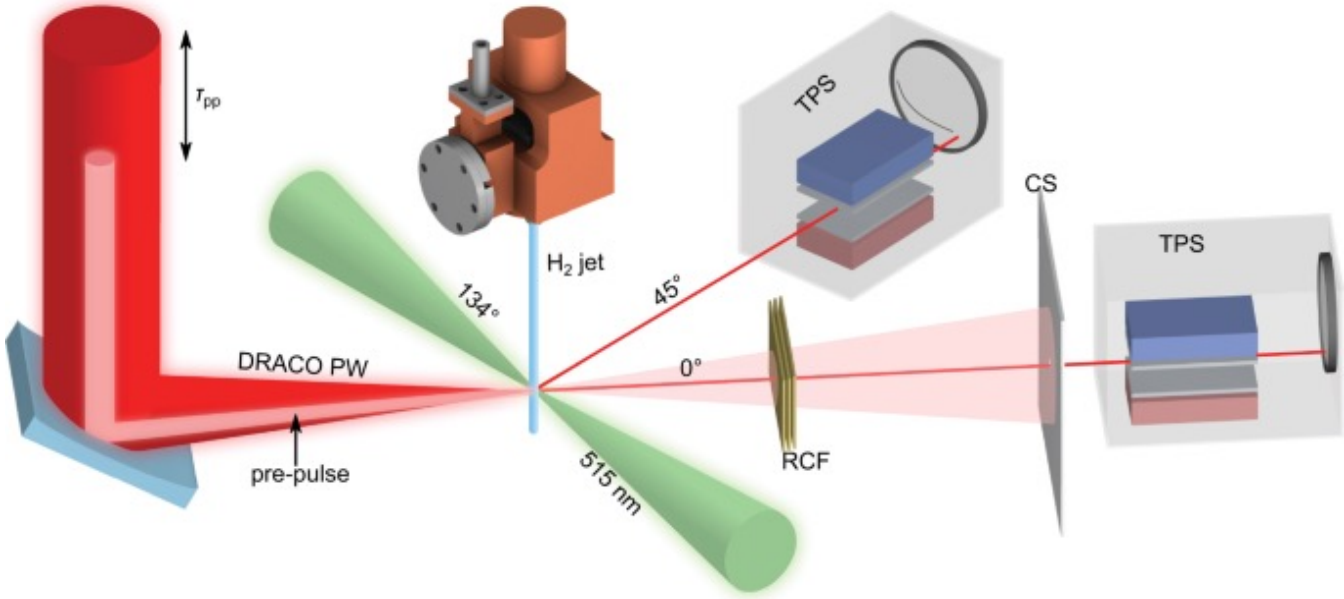


Laser Proton acceleration using a cryogenic hydrogen jet

Laser Proton acceleration using a cryogenic hydrogen jet

a near-critical, debris-free target to efficiently accelerate protons

- cryogenic hydrogen jet provides:
  - self-replacing
  - debris-free
  - near-critical target
- up to 80 MeV protons could be achieved
- much easier to diagnose the plasma state



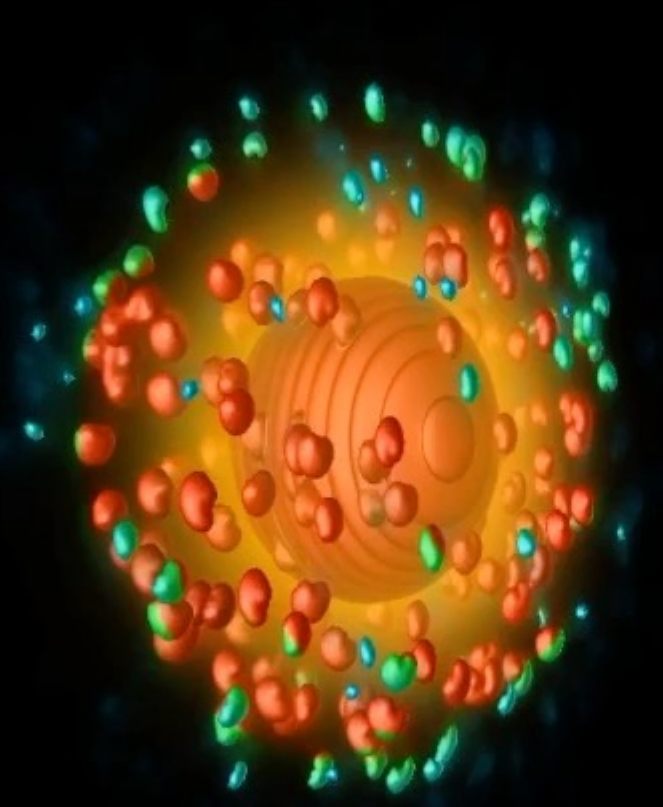
Rehwald, M., Assenbaum, S. Bernert, C. et al.

Ultra-short pulse laser acceleration of protons to 80 MeV from cryogenic hydrogen jets tailored to near-critical density

Nat Commun 14, 4009 (2023)

DOI: 10.1038/s41467-023-39739-0

Electron acceleration with laser wakefield acceleration (LWFA)



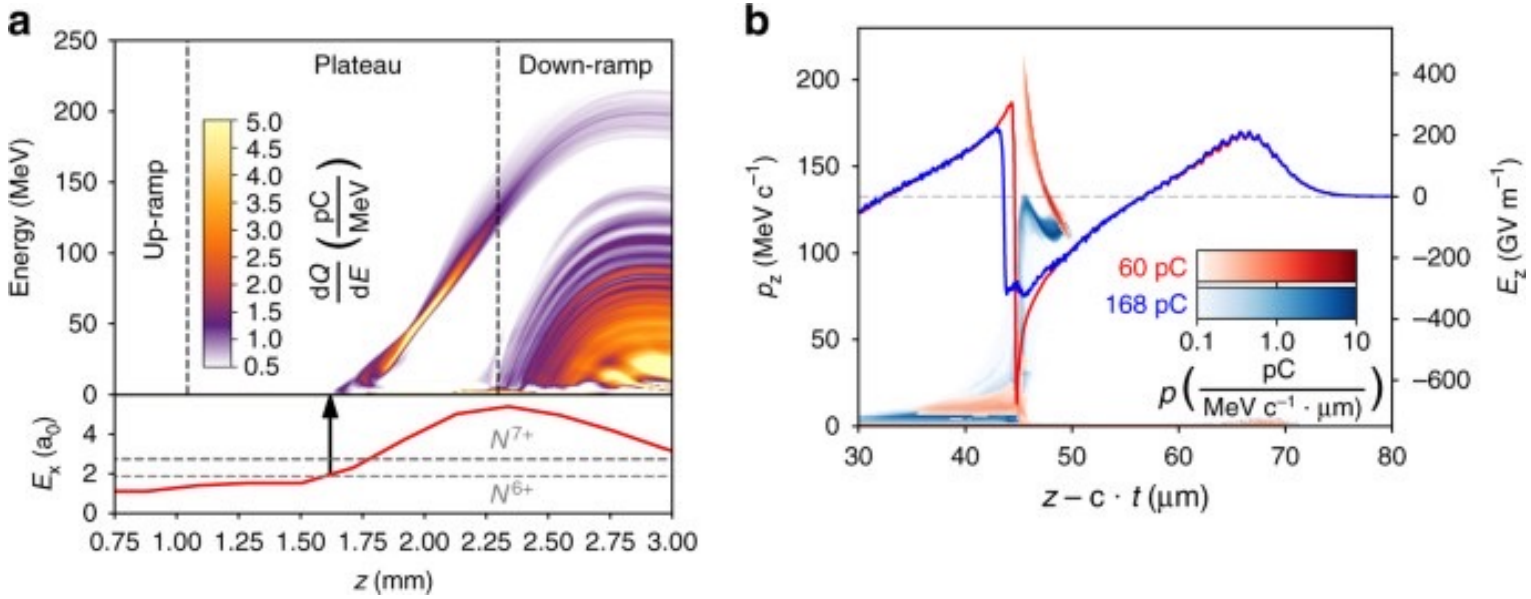
summit

ISAAC PIConGPU

Electron acceleration with laser wakefield acceleration (LWFA)

electrons ride a plasma wave and are accelerated following the laser pulse

- short pulse laser creates wake
- electrons surf wake and accelerate
- various forms of injection
  - self-injection
  - ionization injection
  - downramp injection
  - …
- variety of further applications developed



Couperus, J.P., Pausch, R., Köhler, A. et al

Demonstration of a beam loaded nanocoulomb-class laser wakefield accelerator

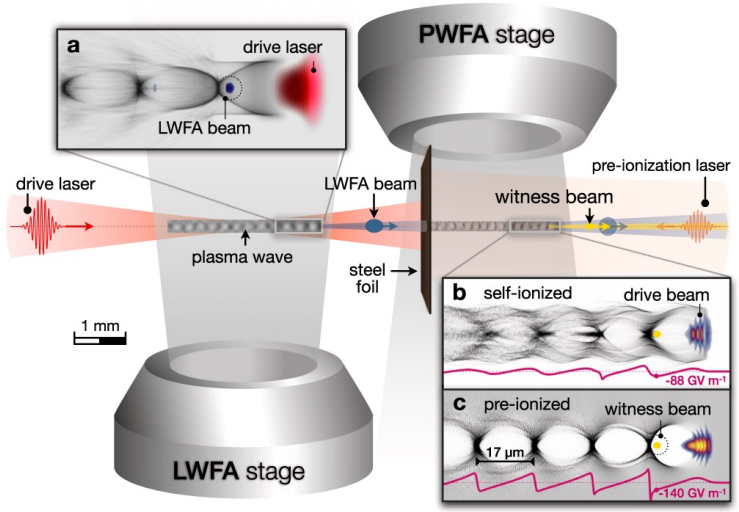
Nat Commun 8, 487 (2017)

DOI: 10.1038/s41467-017-00592-7

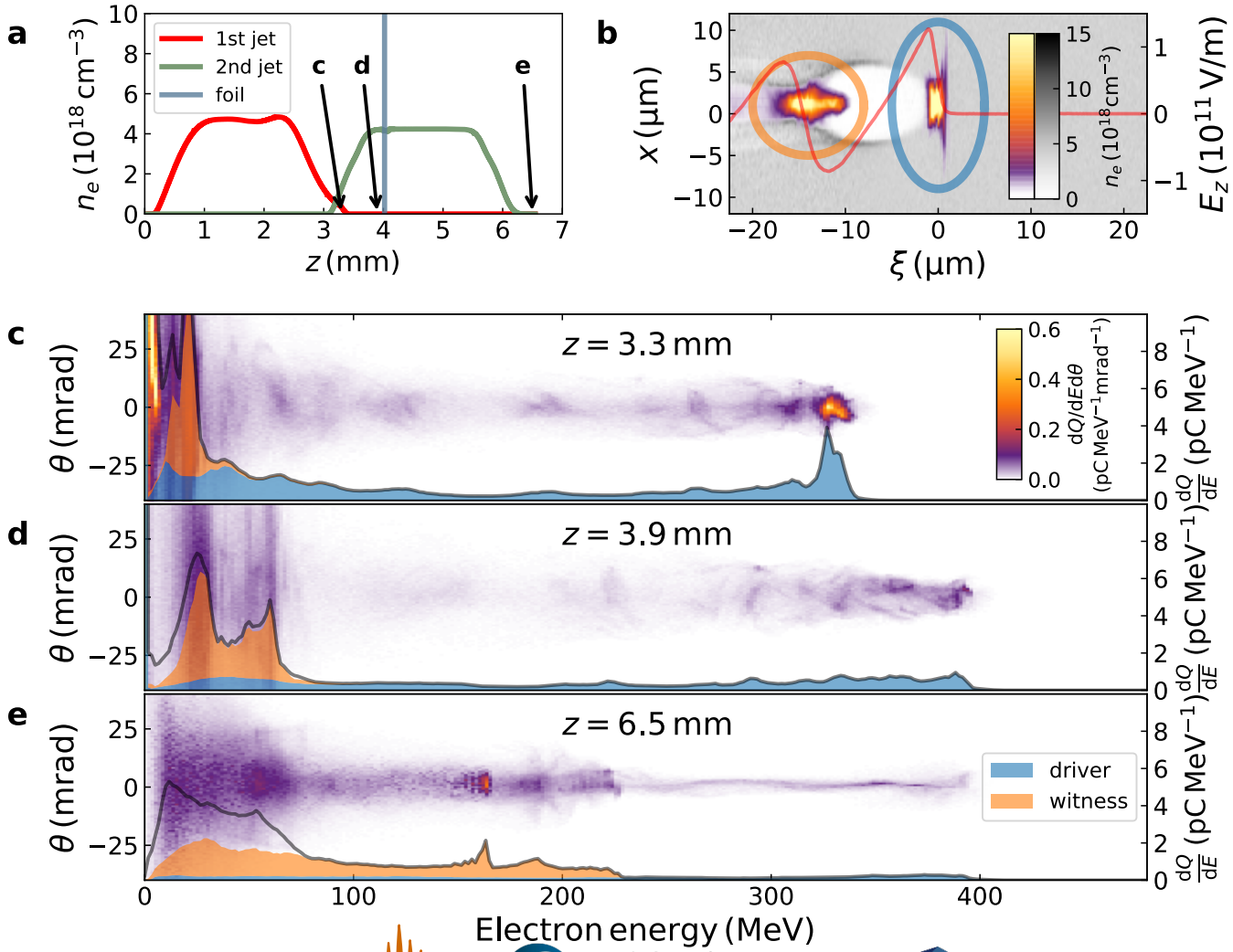
Using these unprecedented beams for first table-top PWFA …

First start-to-end simulation of LWFA|PWFA hybrid accelerator

- first compact plasma wakefield accelerator (PWFA)
- first start-to-end hybrid simulations
- simulation enabled understanding the origin of the witness beam

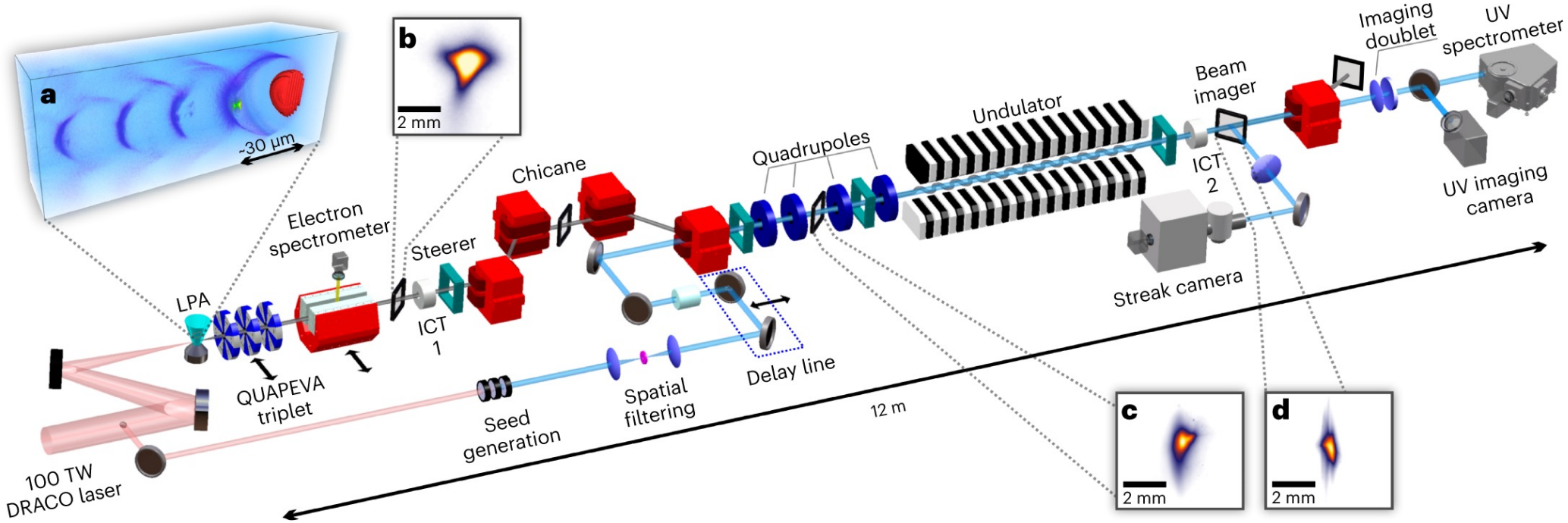


Kurz, T., *et al. Nature Commun* 12, 2895 (2021)



… and for the first seeded FEL driven by LWFA electrons

Going beyond standard FEL simulations by using particle-in-cell simulations as input

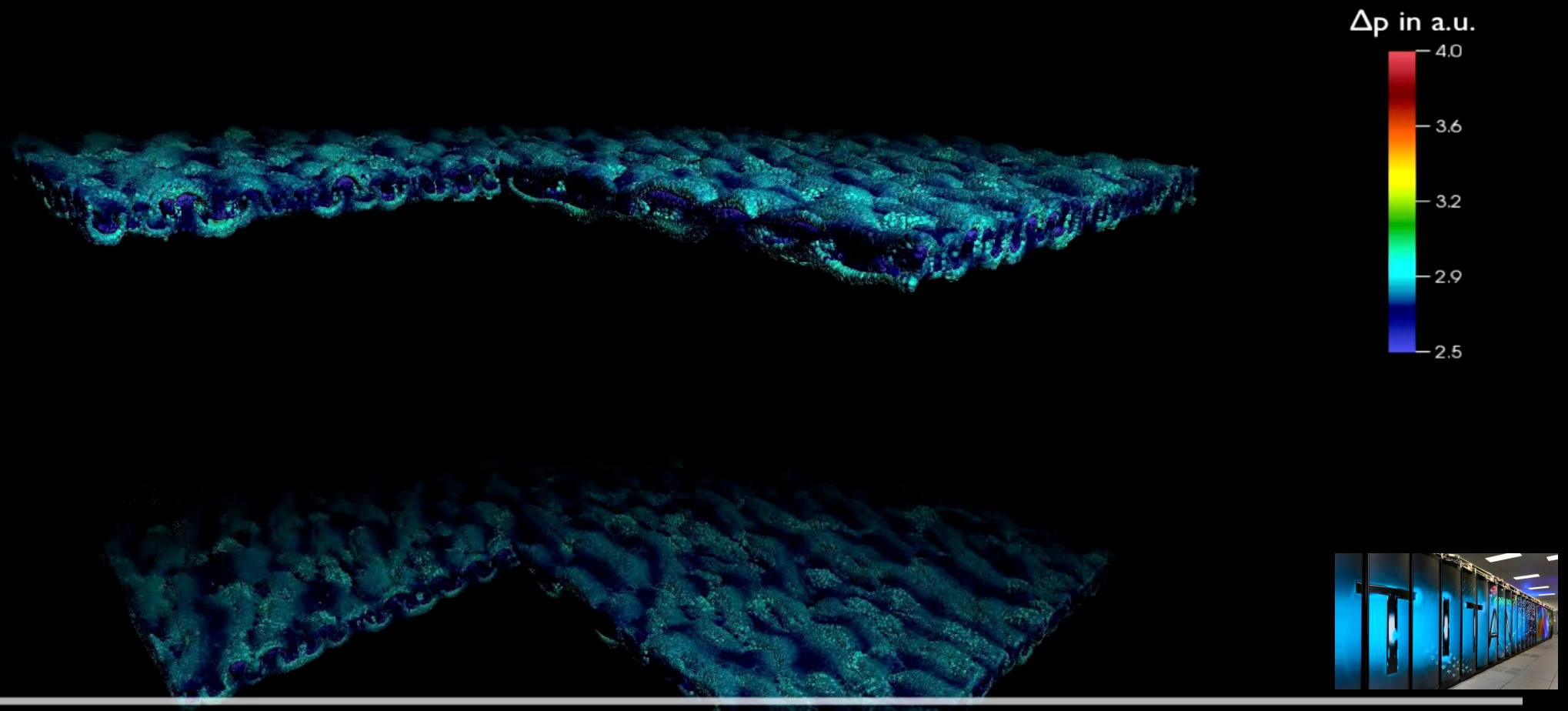


Labat, M., *et al. Nature Photon.* 17, 150–156 (2023)

Radiation from interstellar jets (KHI)

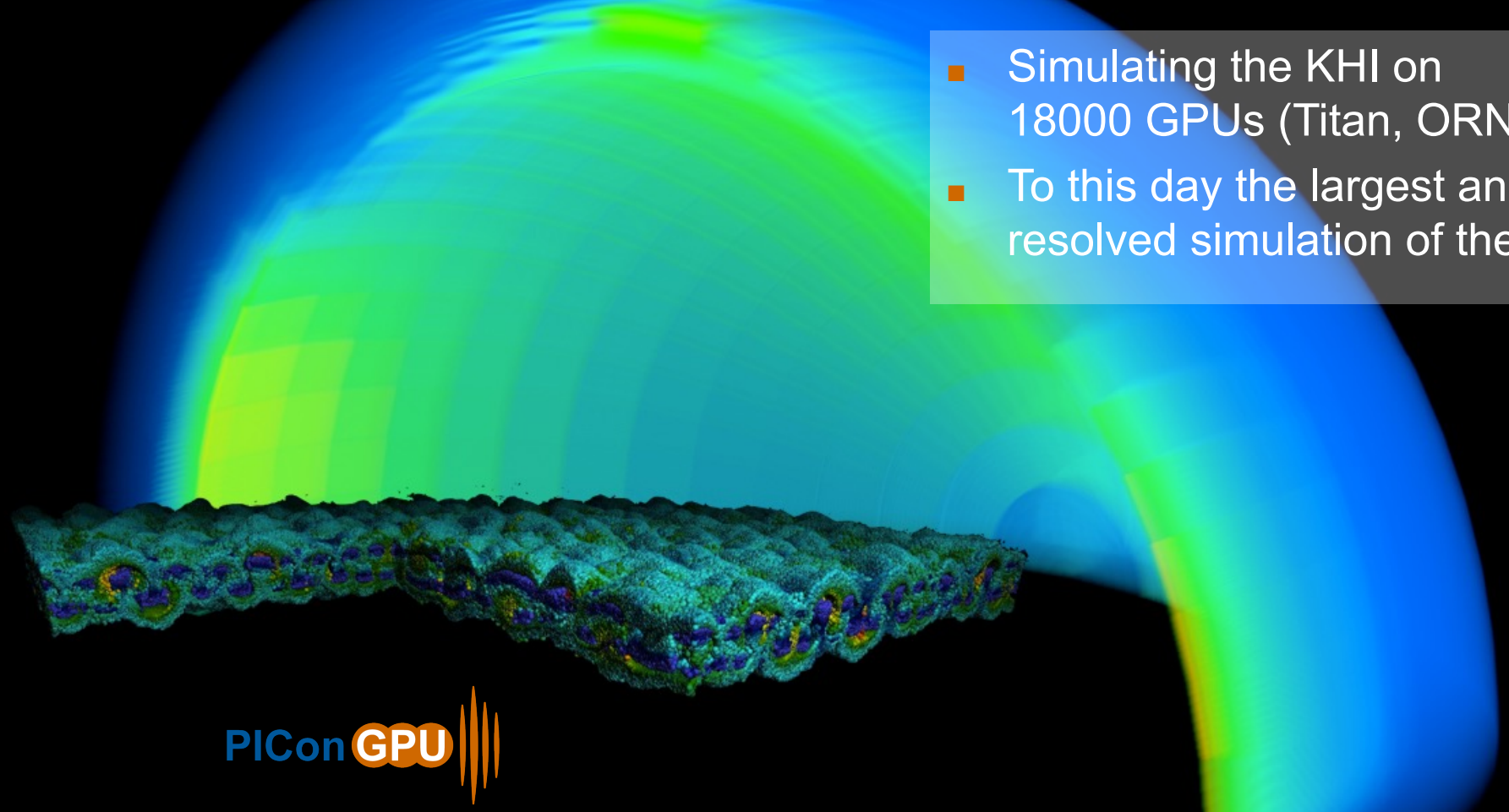
Correlating changes in polarization to the onset of plasma instabilities

Time: $27\,\omega^{-1}_{pe}$



Radiation from interstellar jets (KHI)

Correlating changes in polarization to the onset of plasma instabilities



- Simulating the KHI on 18000 GPUs (Titan, ORNL)
- To this day the largest and best-resolved simulation of the KHI

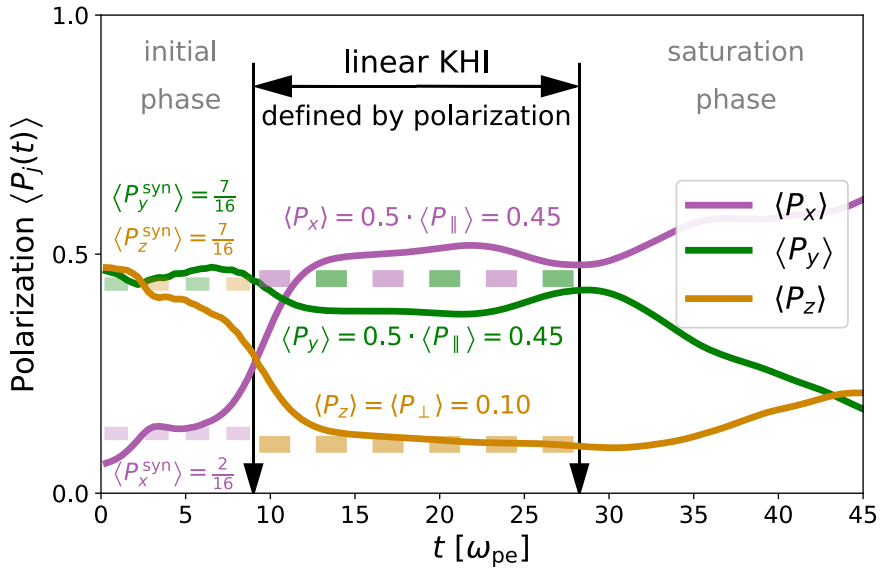
PIConGPU

Pausch, R., et al. PRE 96(1) 013316 (2017)
Bussmann, M., Pausch, R., et al. Proc. of. SC13 pp. 5.1-5.12 (2013)
Huebl, A., Pausch, R. et al. IEEE Trans. on Plas. Sci., 42(10), 2638–2639 (2014)

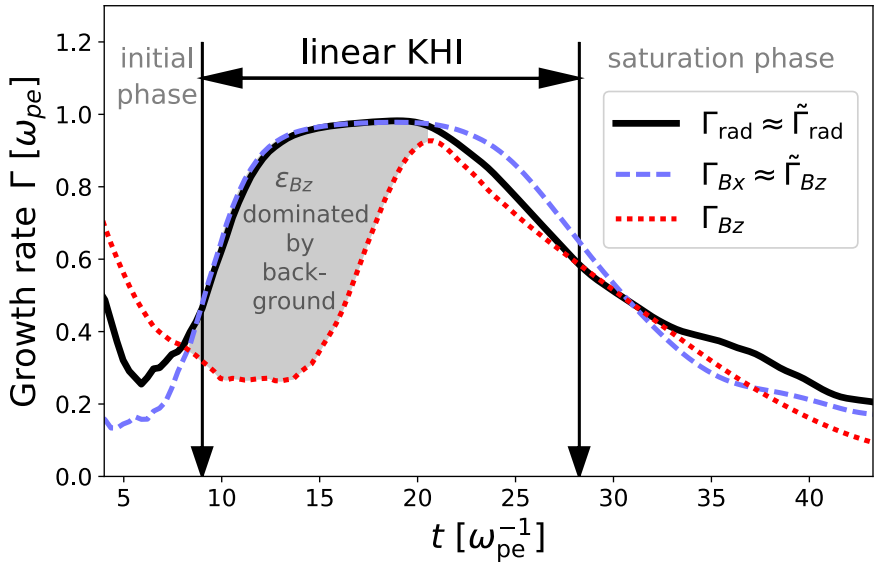
Radiation from interstellar jets (KHI)

Correlating changes in polarization to the onset of plasma instabilities

time evolution of radiation shows characteristic polarization



The growth of the radiation intensity allows determining the growth of the instability.



Pausch, R., et al. PRE 96(1) 013316 (2017)
Bussmann, M., Pausch, R., et al. Proc. of. SC13 pp. 5.1-5.12 (2013)
Huebl, A., Pausch, R. et al. IEEE Trans. on Plas. Sci., 42(10), 2638–2639 (2014)

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Particle-in-cell codes

An introduction on how PIConGPU works

DRESDEN
concept

Why do we need particle-in-cell simulations?

The Vlasov–Maxwell system of equations

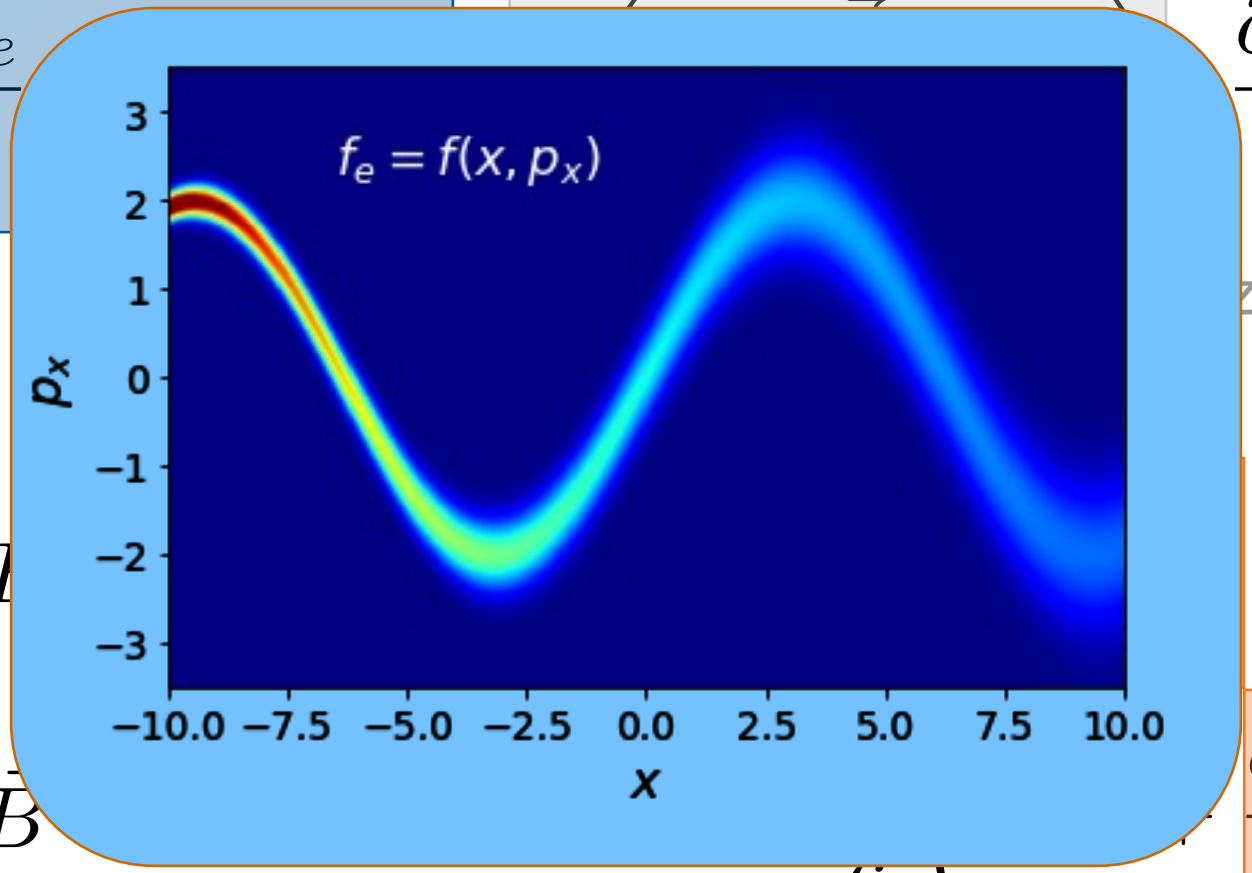
$$\frac{\partial f_e}{\partial \vec{p}} = 0$$

$$\vec{\nabla} \cdot \vec{E}$$

$$\vec{\nabla} \cdot \vec{B}$$

$$c \left(\frac{\partial \vec{E}}{\partial t} \right)$$

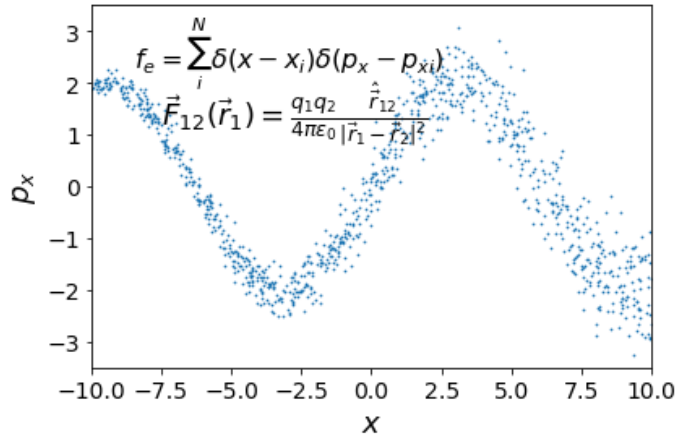
time evolution



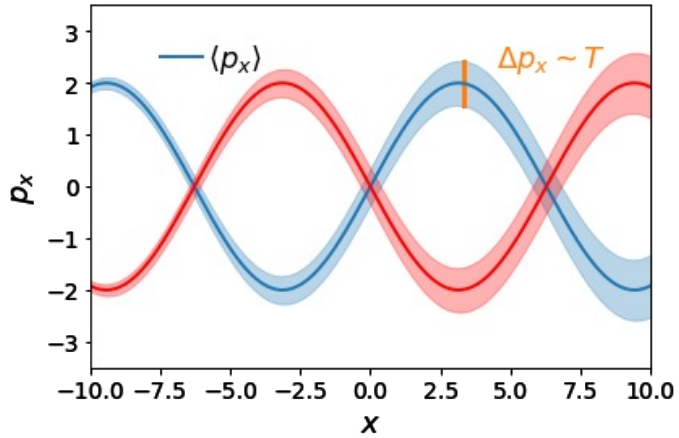
How does a particle-in-cell code work?

How could one solve the Vlasov-Maxwell equations?

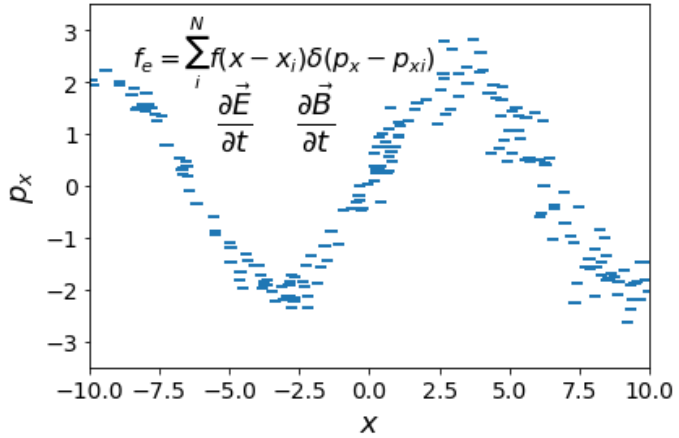
molecular dynamics (MD)



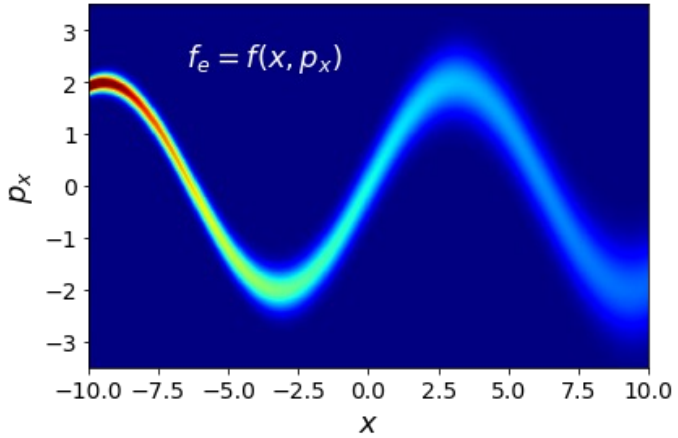
magneto-hydrodynamics (MHD)



particle-in-cell (PIC)



Vlasov-solver



How does a particle-in-cell code work?

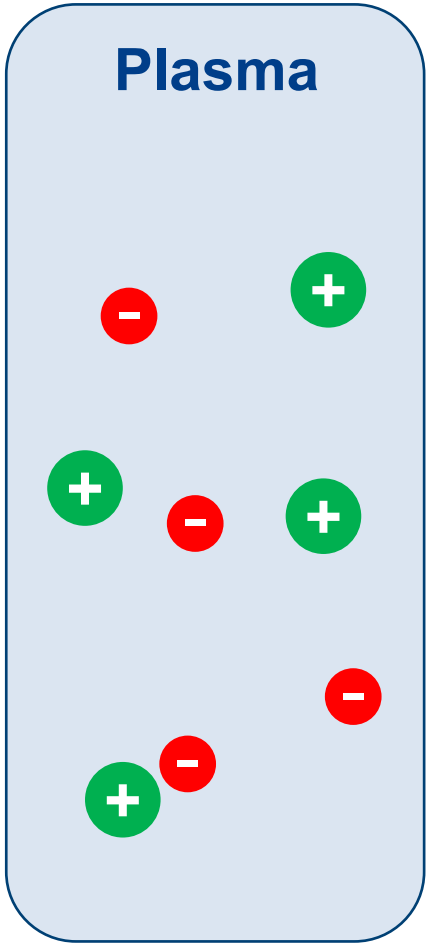
the particle-in-cell method (time evolution)

Maxwell equations

Freely moving charges generate electromagnetic fields.

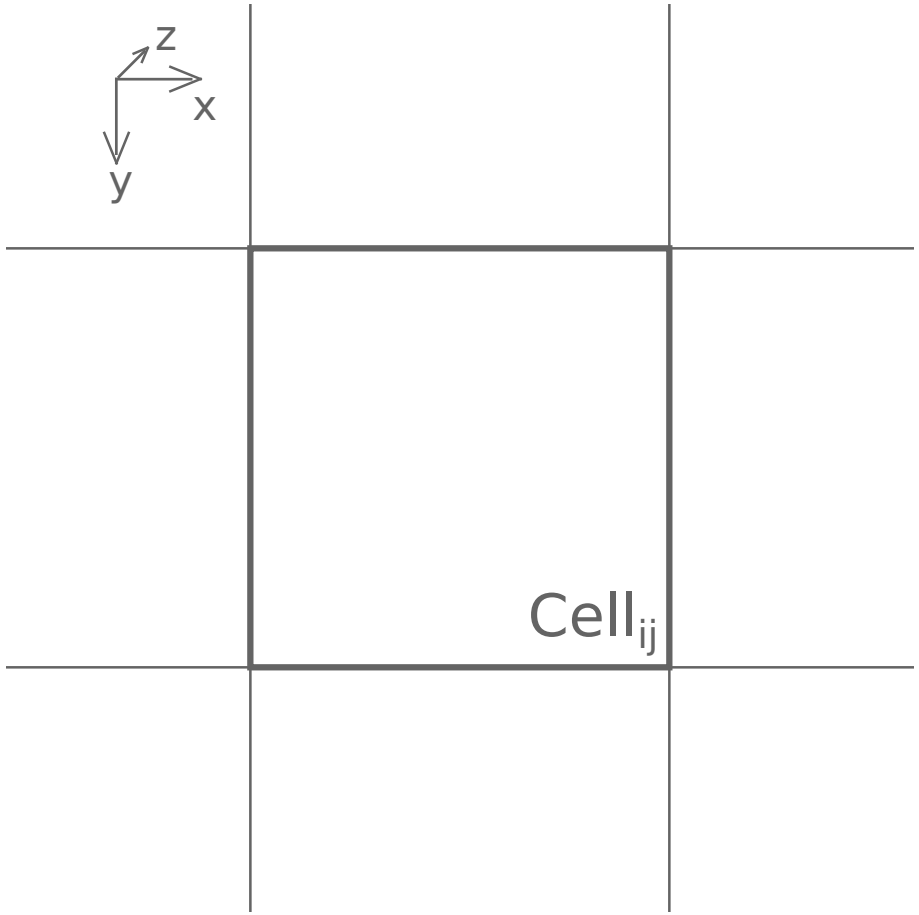
Lorentz force

These fields cause forces to act on the charged particles.



How does a particle-in-cell code work?

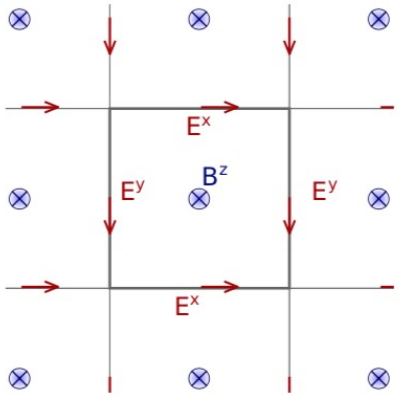
Discretizing the Maxwell equations on a grid



- Finite Difference Time Domain (FDTD) method
- common algorithm: **Yee-solver**
- defines Yee-grid
- staggered grid for higher numeric accuracy

How does a particle-in-cell code work?

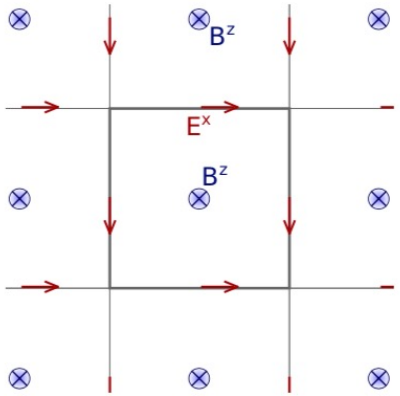
Discretizing the Maxwell equations on a grid



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

$$\Rightarrow -\nabla^{+} \times \mathbf{E}$$

$$\frac{\partial}{\partial t}\mathbf{B}^{z}_{ij} = -\left(\mathbf{E}^{y}_{i+1j} - \mathbf{E}^{y}_{ij}\right)/\Delta x + \left(\mathbf{E}^{x}_{ij+1} - \mathbf{E}^{x}_{ij}\right)/\Delta y$$



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

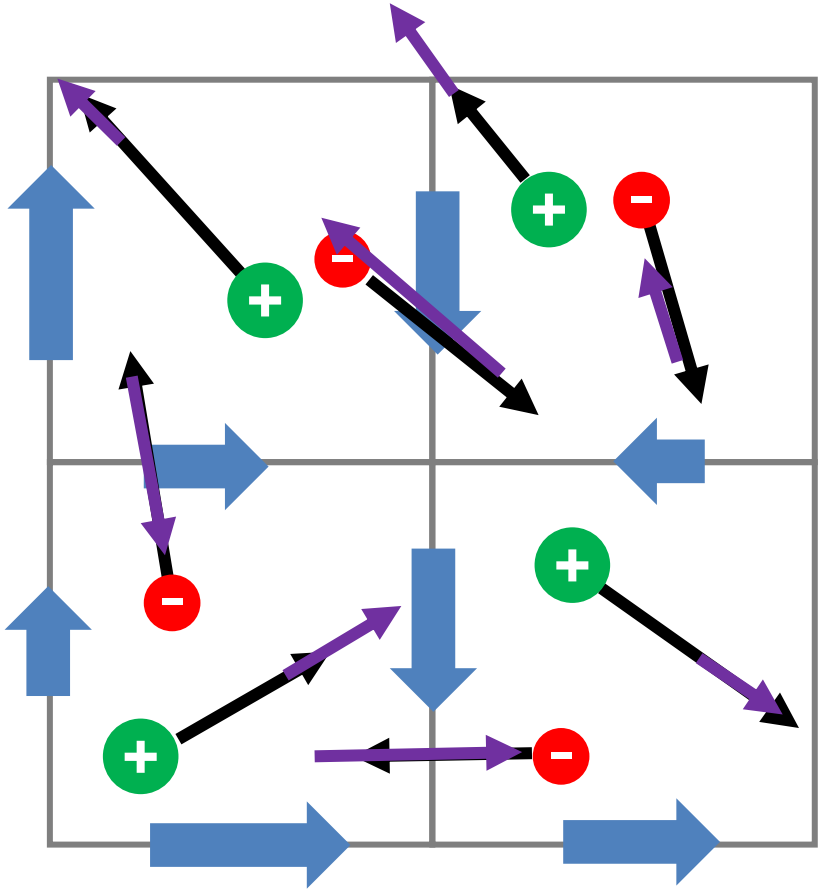
$$\Rightarrow +\nabla^{-} \times \mathbf{B}$$

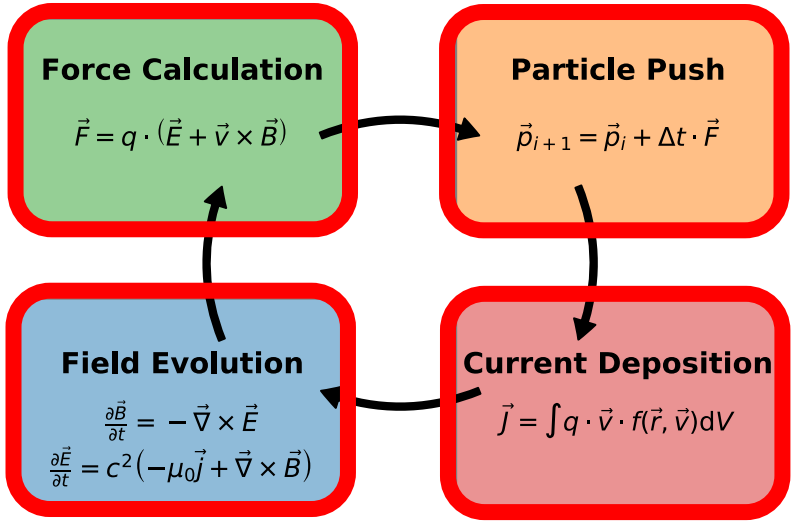
$$\frac{\partial}{\partial t}\mathbf{E}^{x}_{ij} = +\left(\mathbf{B}^{z}_{ij} - \mathbf{B}^{z}_{ij-1}\right)/\Delta y$$

- Yee stencils
- better schemes exits
- Lehe, AOFDT,CKC, spectral solver, …
- interaction with current highly important

How does a particle-in-cell code work?

the PIC cycle





- one complete cycle corresponds to one time step.
- repeated cycles allow simulating longer time durations.
- local operations only: well suited for parallelization.

Real experiments need really large simulations

The need for large scale simulations equals the need for fast simulations

high resolution

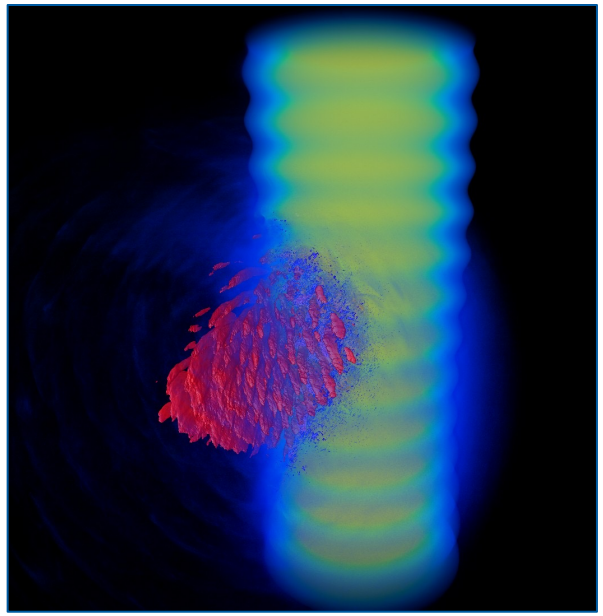
3D
(no symmetry)

long duration

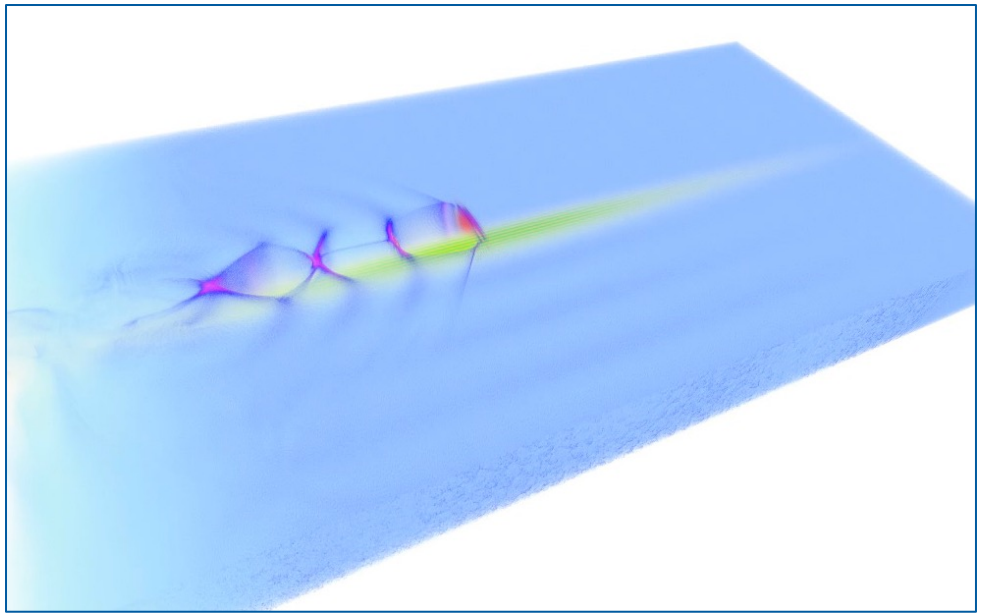
TB of data

complex models

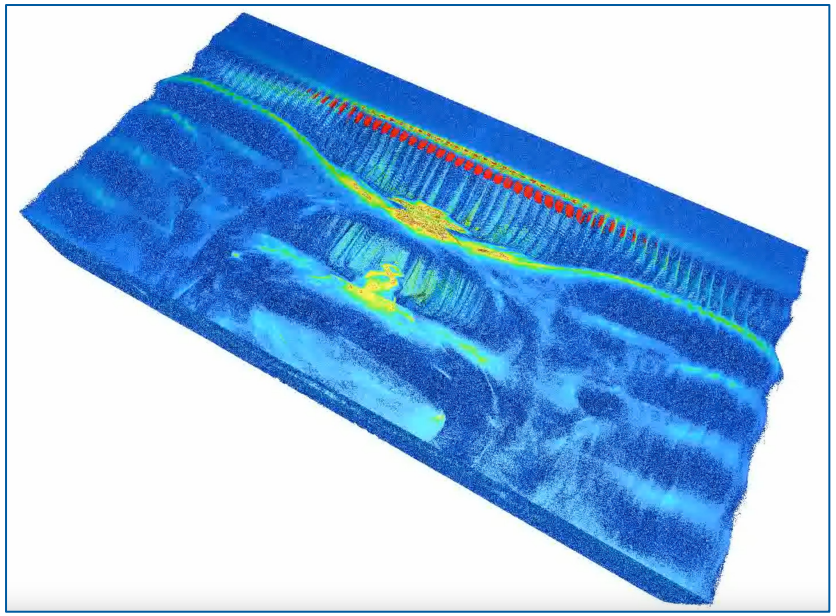
cryogenic hydrogen jet



electron acceleration with probe pulse



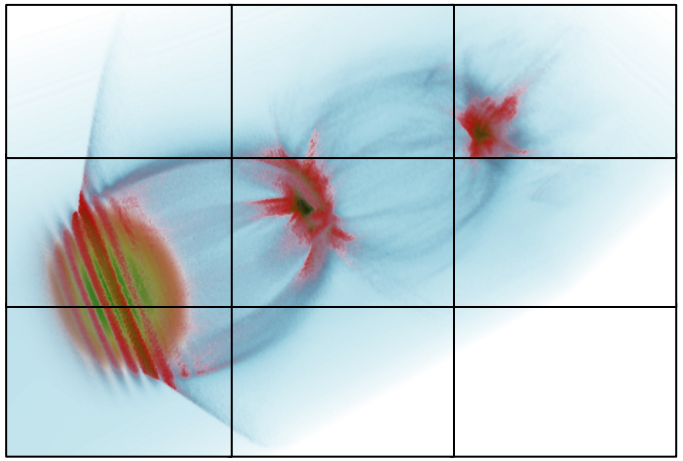
TWEAC



PIConGPU PLASMA PEPSC DRESDEN concept SCIENCE AND INNOVATION CAMPUS HZDR

How does PIConGPU reach its fast performance?

Domain decomposition – distributing spatial subregions into different computers



PIConGPU

HPC Compute Node | HPC Compute Node | HPC Compute Node

HPC Compute Node | HPC Compute Node | HPC Compute Node

HPC Compute Node | HPC Compute Node | HPC Compute Node

PIConGPU PLASMA PEPSC DRESDEN concept SCIENCE AND INNOVATION CAMPUS HZDR

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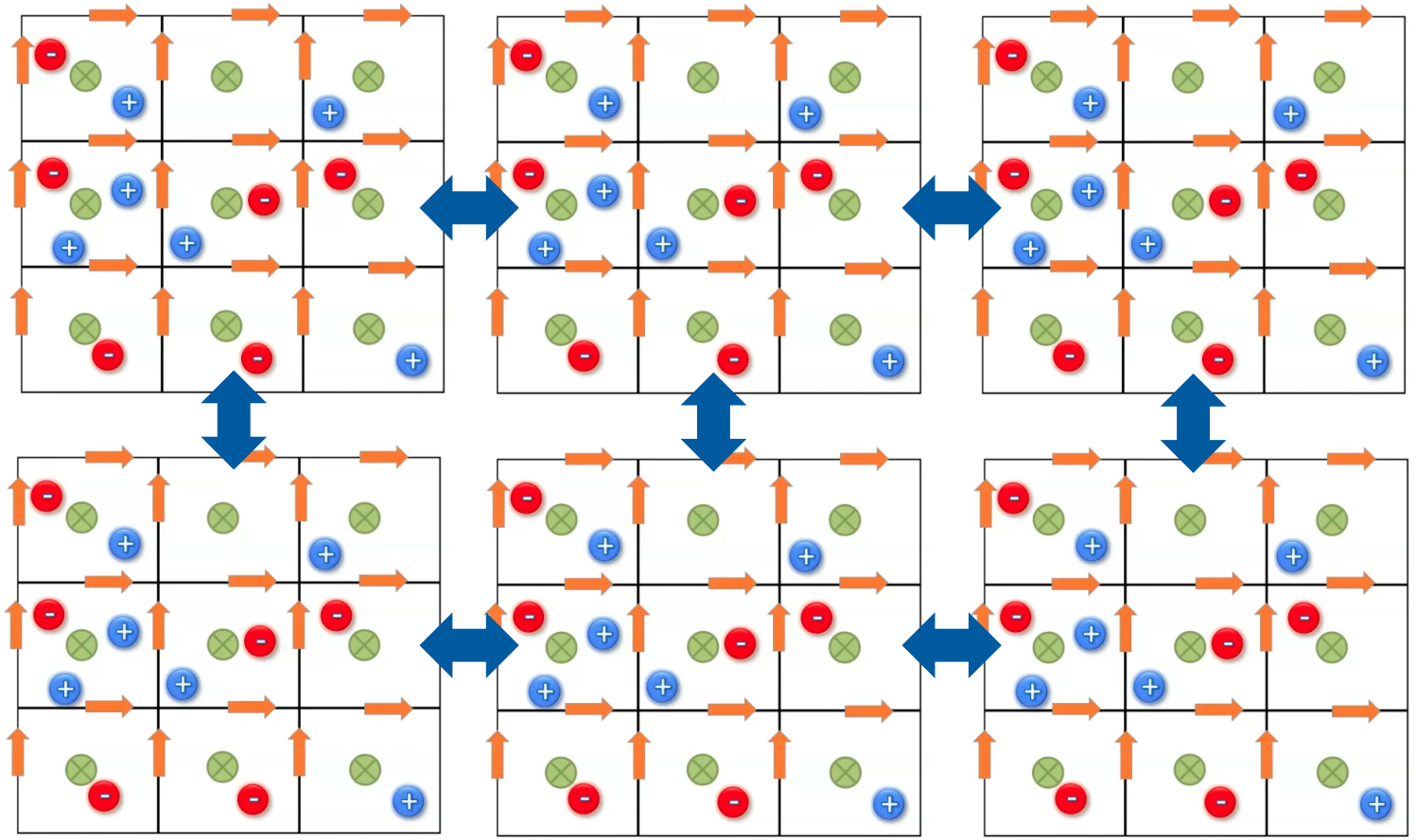
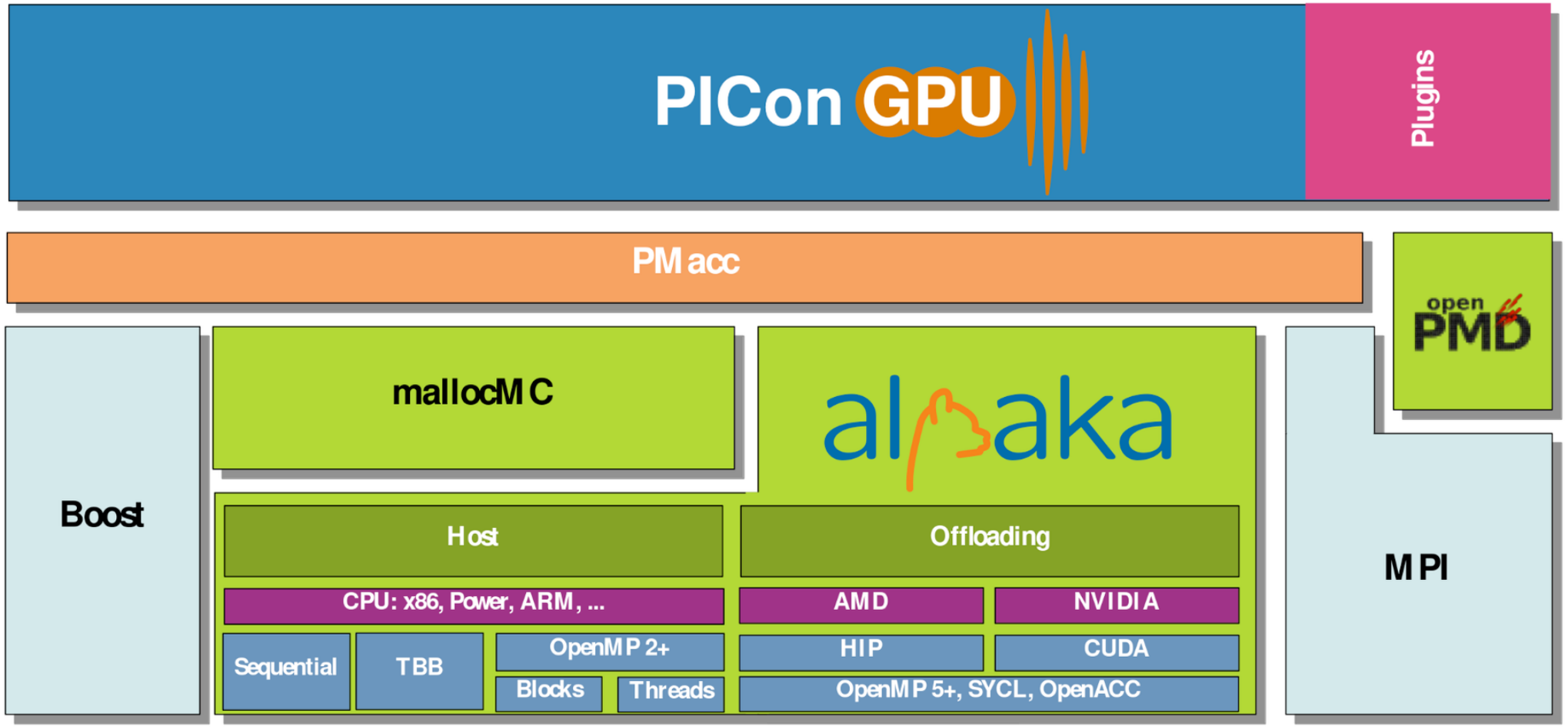


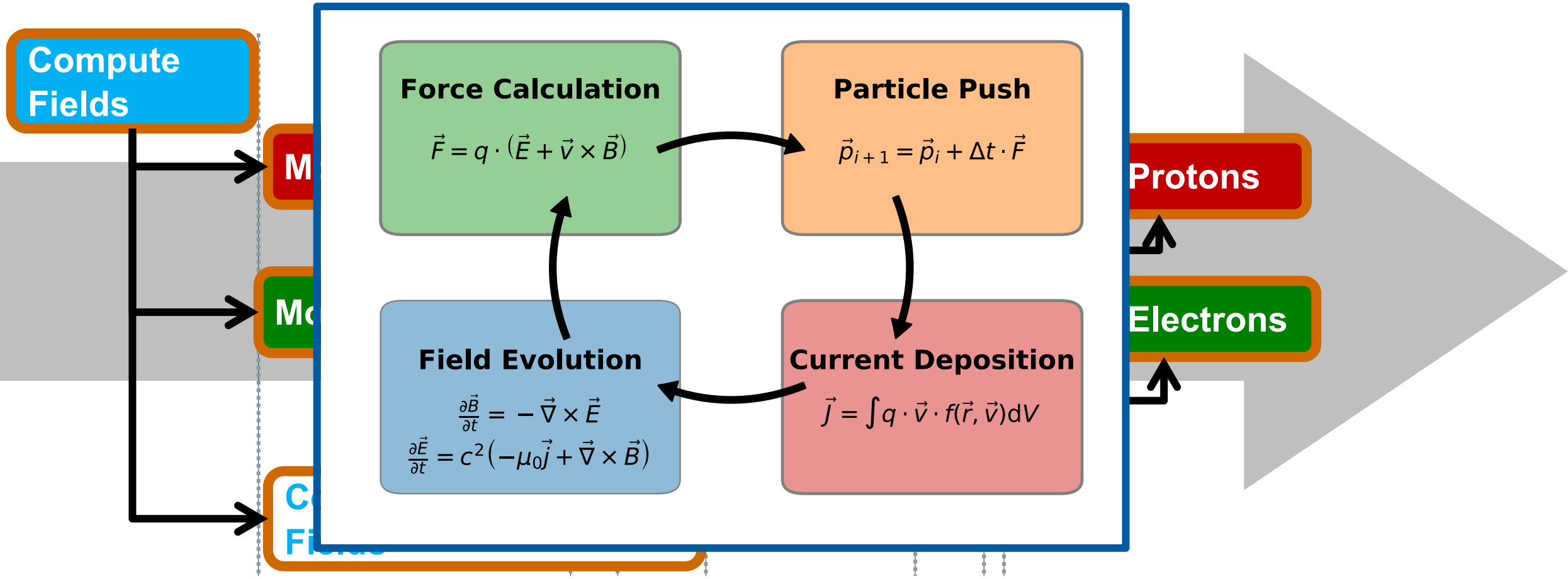
How does PIConGPU reach its fast performance?

Abstractions of data structures and algorithms in libPMacc



How does PIConGPU reach its fast performance?

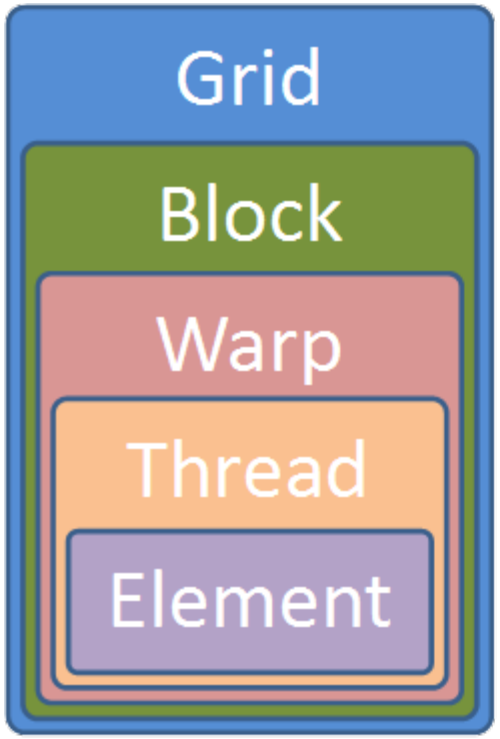
Handling data exchange – asynchronous communication and execution for the rescue



Quick recap: alpaka

How does the alpaka hardware abstraction work?

Data parallelism in modern hardware:



- **Grid** whole parallel task
- **Block** fully independent part of the grid
- **Warp** group of synchronous threads
- **Threads** executed concurrently
- **Elements** sub-thread, sequential lock-step

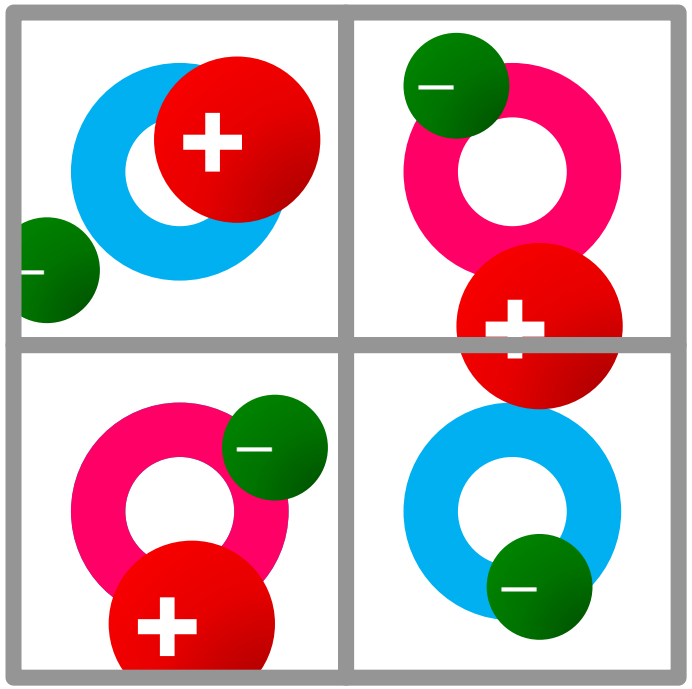
alpaka

Zenker E. et al. (2016) IEEE Xpress DOI:10.1109/IPDPSW.2016.50
Zenker E. et al. ISC (2016) ISC High Performance DOI:10.1007/978-3-319-46079-6_21
Matthes A. et al., (2017) ISC High Performance (pp 496-514) DOI: 10.1007/978-3-319-67630-2_2

PIConGPU PLASMA PEPSC DRESDEN concept SCIENCE AND INNOVATION CAMPUS HZDR

How does PIConGPU reaches its fast performance?

Domain decomposition – fields and particles

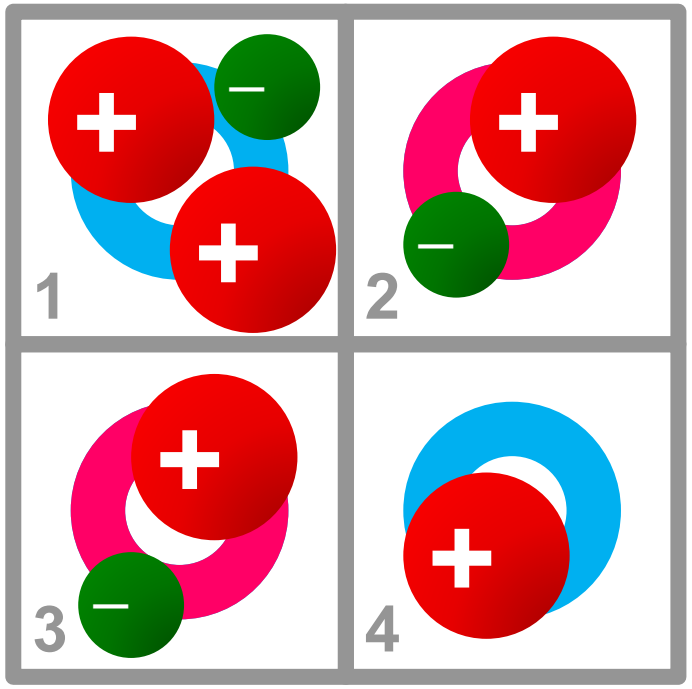


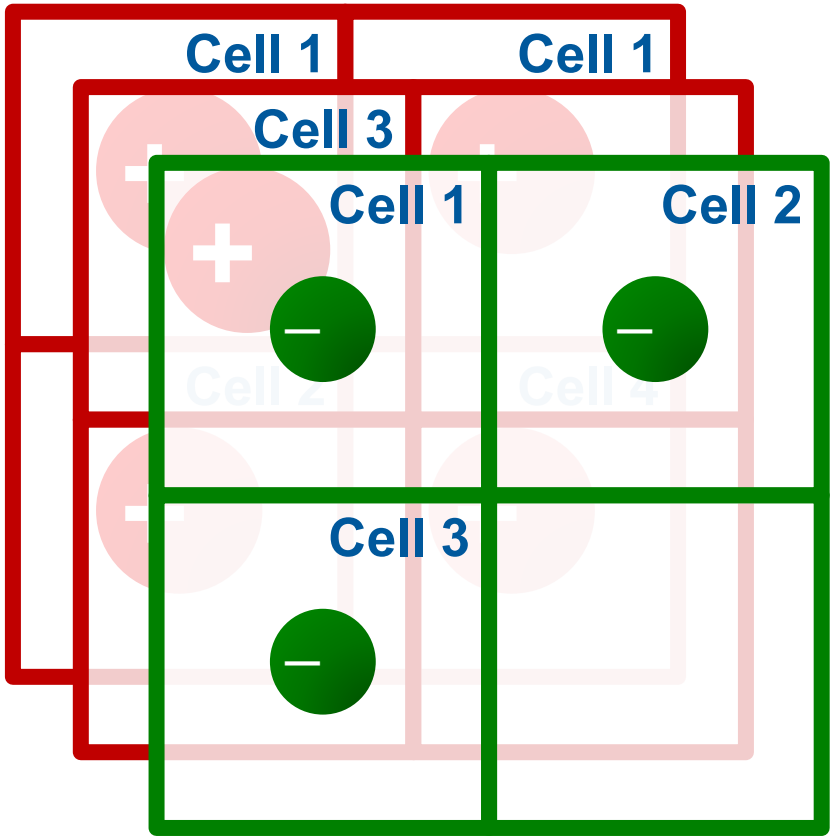
Field Domain

Particle Domain

How does PIConGPU reaches its fast performance?

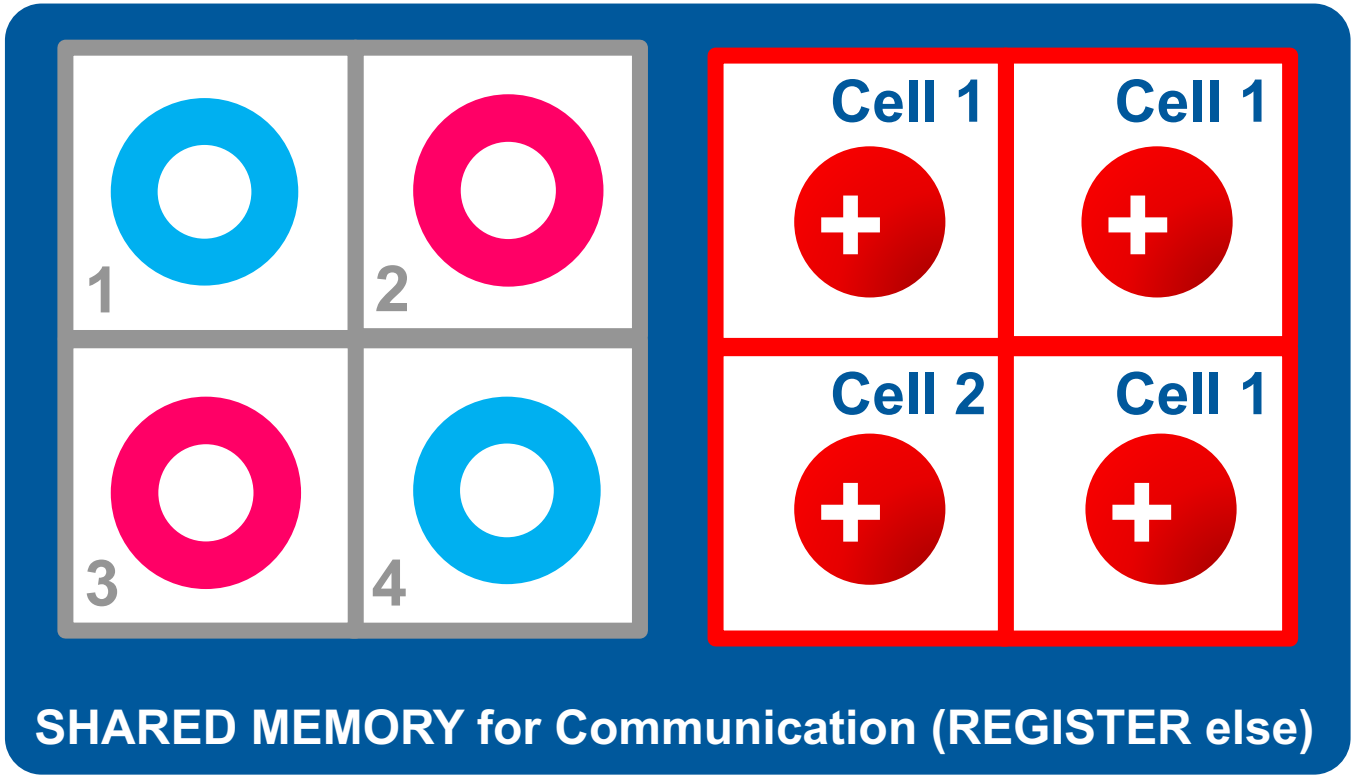
Domain decomposition – fields and particles – adding particles





How does PIConGPU reaches its fast performance?

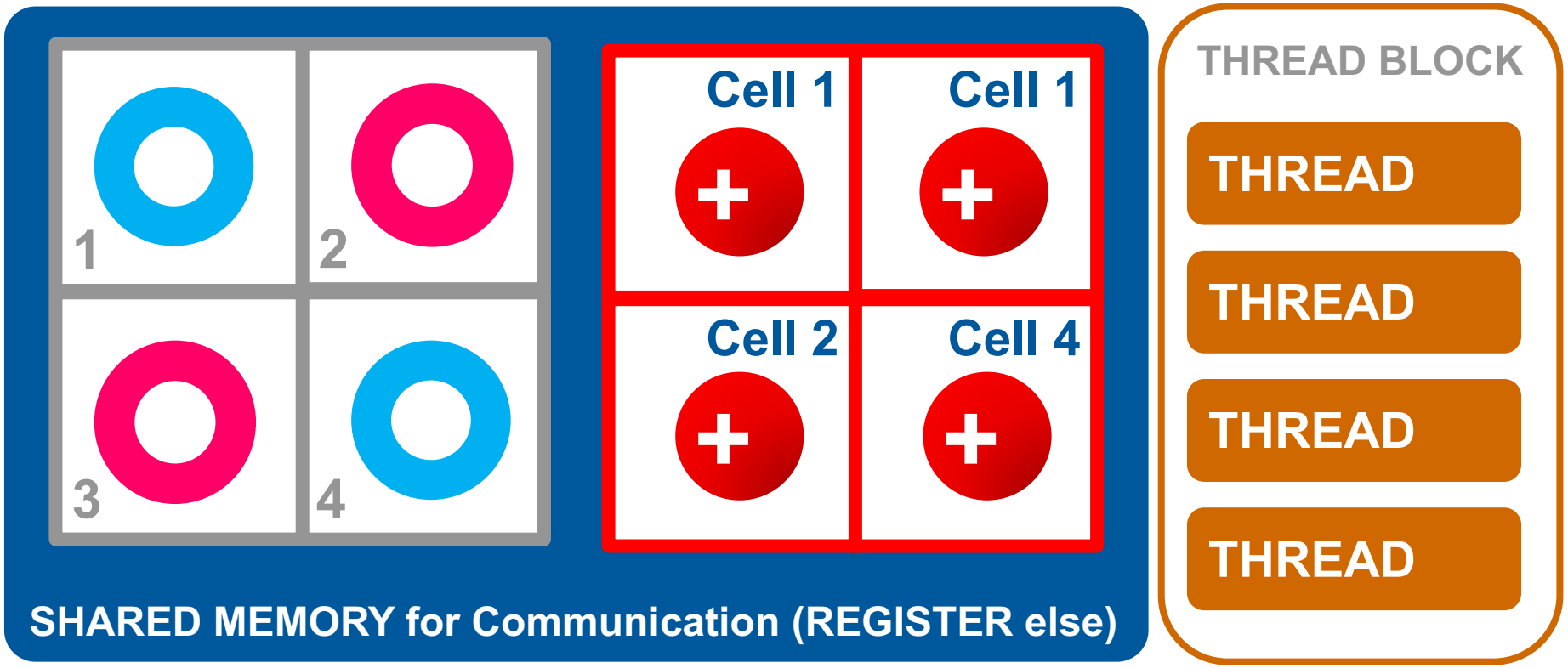
Domain decomposition – using register/shared memory for efficient data handling



How does PIConGPU reaches its fast performance?

Domain decomposition – using register/shared memory for efficient data handling

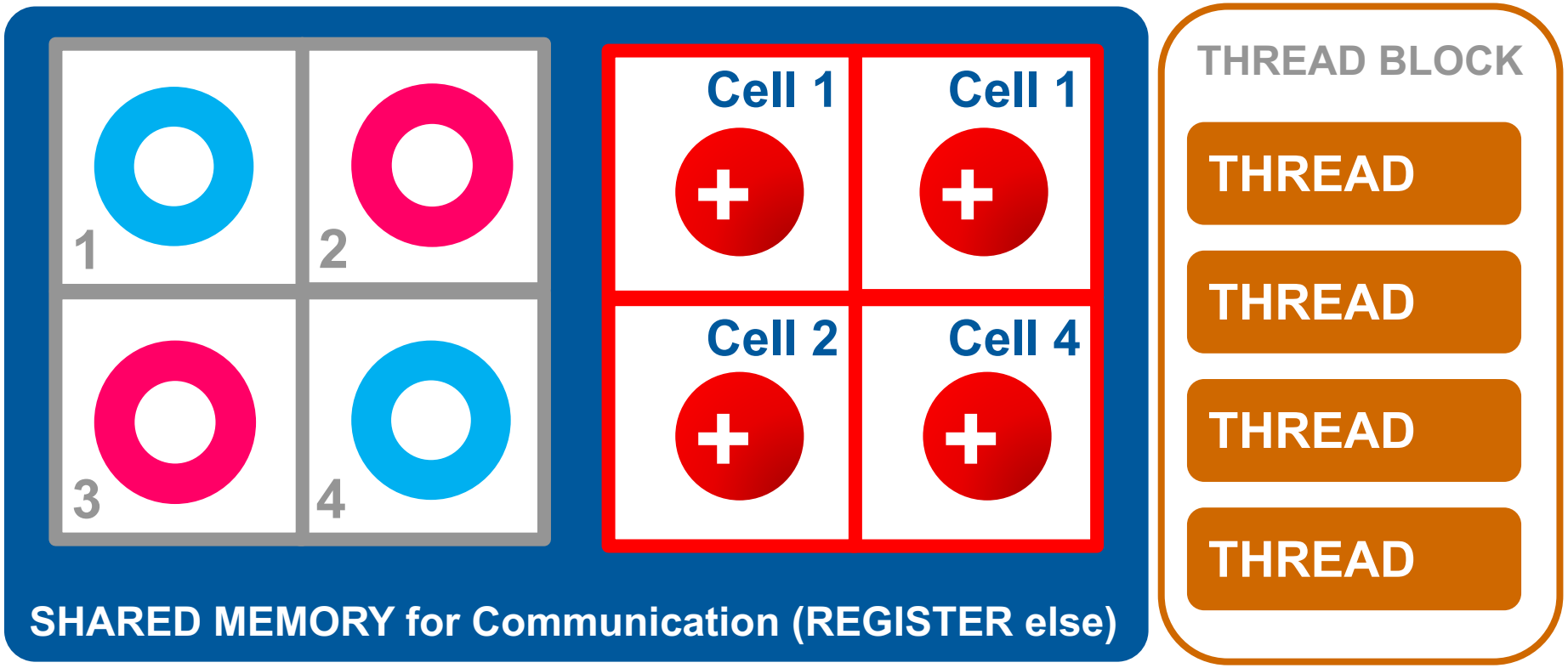
Cell-wise Threading



How does PIConGPU reaches its fast performance?

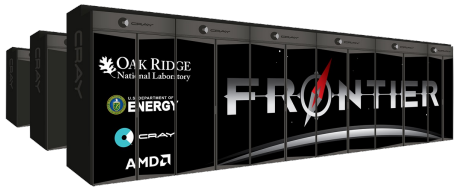
Domain decomposition – using register/shared memory for efficient data handling

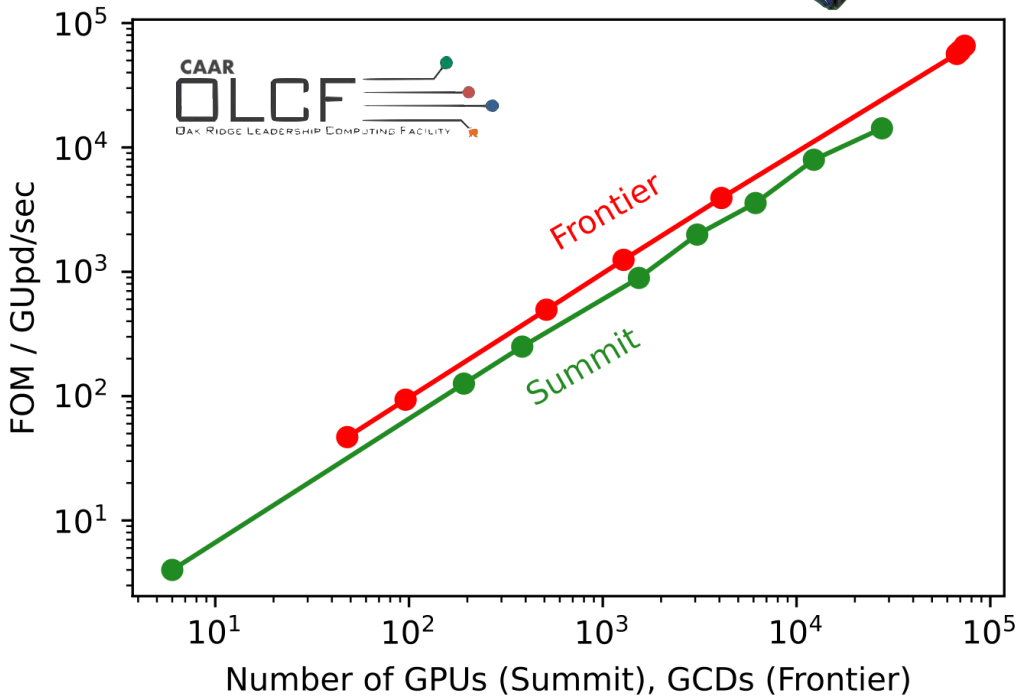
Particle-wise Threading

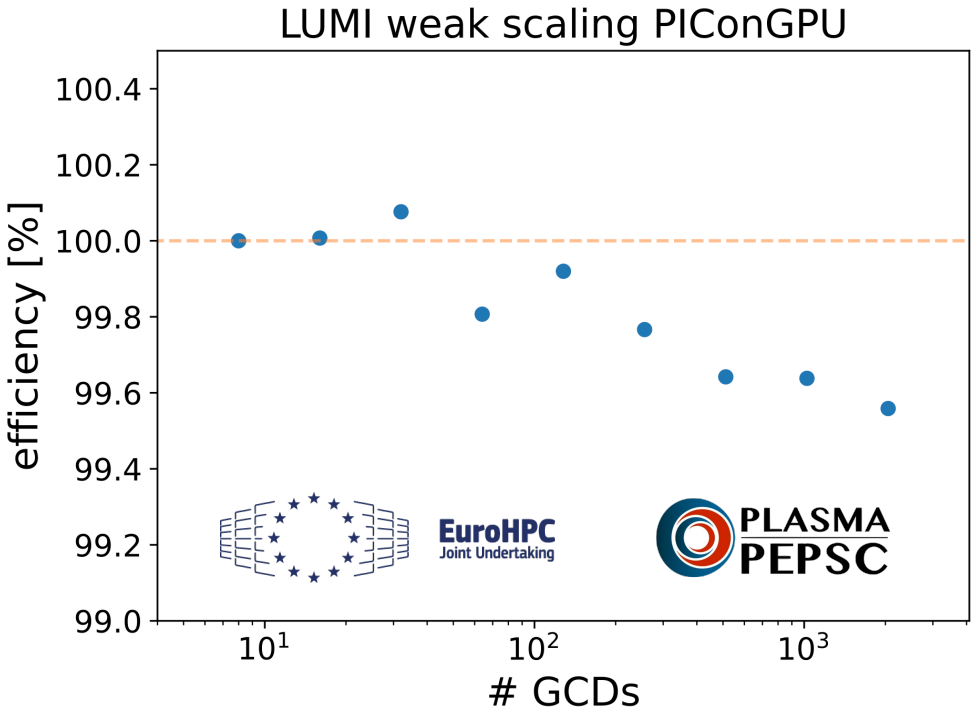


How fast is PIConGPU's performance?

Scaling runs on the largest HPC systems in the world







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HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

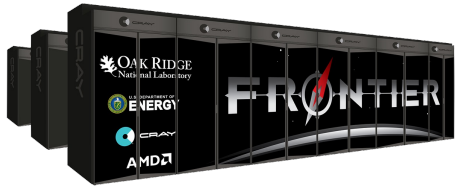
Fast, Faster, File-system full

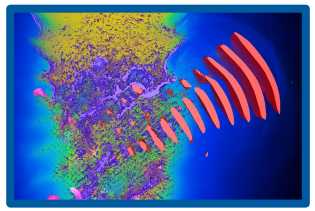
Why in-situ data analysis and models are the future

DRESDEN
concept

What to do with this high performance?

Going beyond “just” large simulation: complex in-situ data analysis

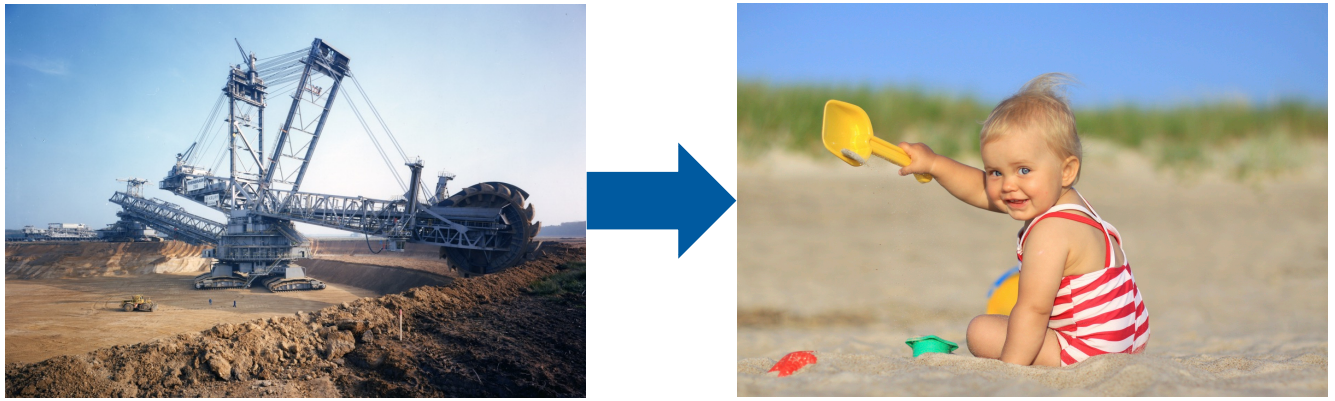




128 nodes = 1024 GPUs
with 64 GB RAM each
at >10 Hz iteration rate

0.6 PetaByte / s
0.1TB/s GPU to GPU 16GB/s internode

file System: 679 PB
full in 100s – or 1000 iterations
but simulation runs 15x longer



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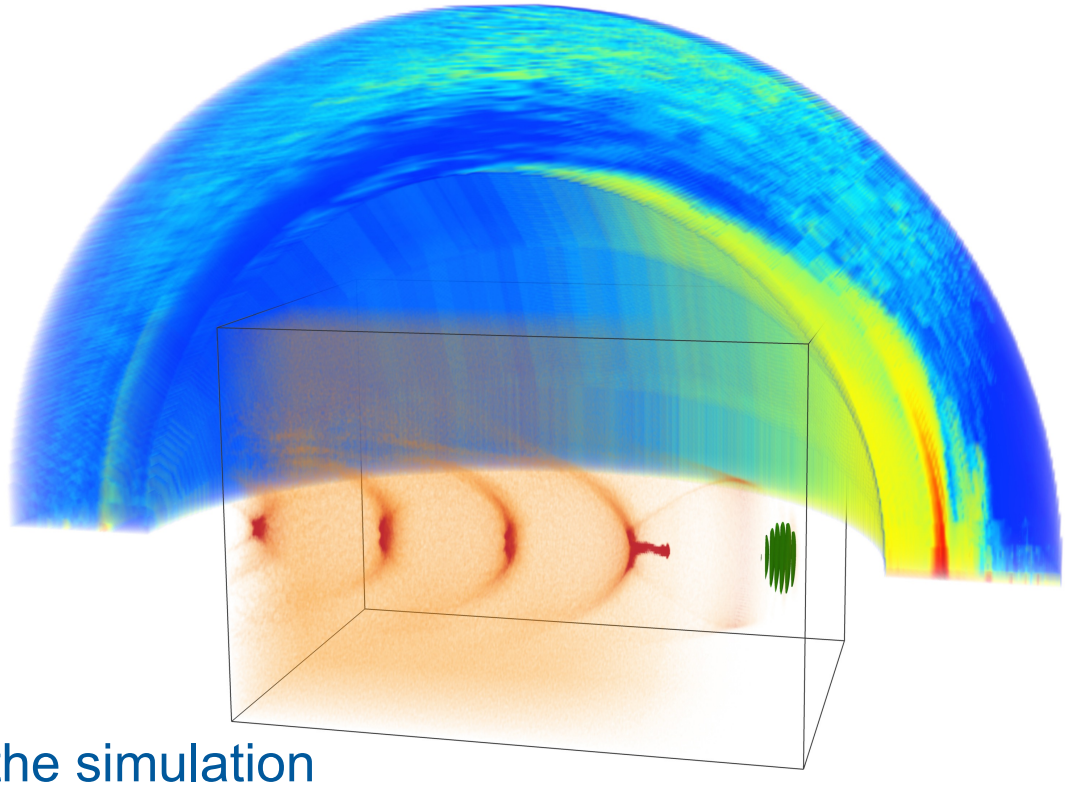
What to do with this high performance?

Going beyond “just” large simulation: complex in-situ data analysis

In-situ radiation plugin

- spectra range from **IR to x-ray**
  Pausch, R., et al. NIMA 740, 250-256 (2014)
- resolves **coherent** and **incoherent** radiation **simultaneously**
  Pausch, R., et al. NIMA 909, 419-422 (2018)
- includes **polarization** properties
  Pausch, R., et al. PRE 96(1) 013316 (2017)
- resolves **temporal evolution** of spectra
  Pausch, R., et al. Proc. of IPAC MOPRI069 (2014)
- computes radiation of all **billions of particles** in the simulation
  Bussmann, M., Pausch, R., et al. Proc. of. SC13 pp. 5.1-5.12 (2013)



$$\frac{\mathrm{d}^2 W}{\mathrm{d}\,\Omega\,\mathrm{d}\,\omega} = \frac{1}{16\pi^3 \varepsilon_0 c} \left| \sum_{k=1}^{N_p} \int_{-\infty}^{+\infty} q_k \cdot \frac{\vec{n} \times \left[\left(\vec{n} - \vec{\beta}_k \right) \times \dot{\vec{\beta}}_k \right]}{\left(1 - \vec{\beta}_k \cdot \vec{n} \right)^2} \cdot \mathrm{e}^{\mathrm{i}\omega \left(t - \vec{n} \cdot \vec{r}_k(t)/c \right)} \,\mathrm{d}\,t \right|^2$$

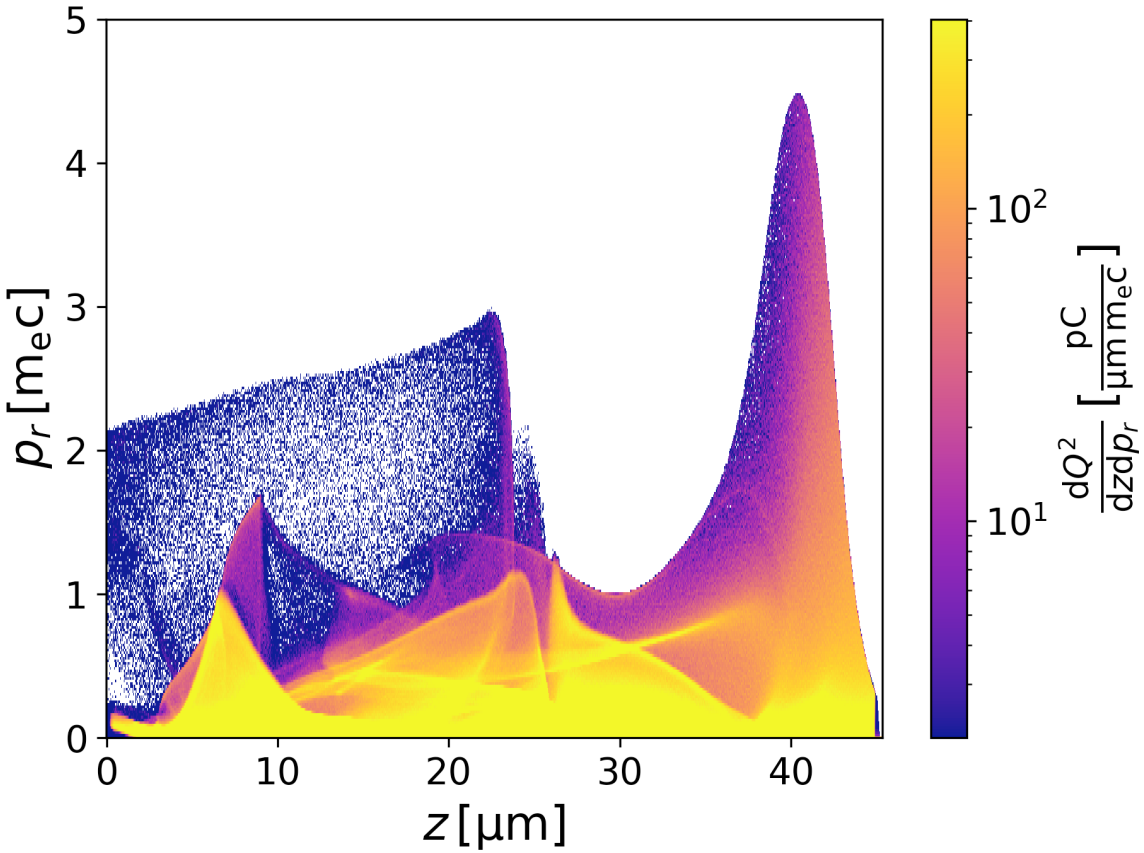
What to do with this high performance?

Going beyond “just” large simulation: complex in-situ data analysis

binning plugin

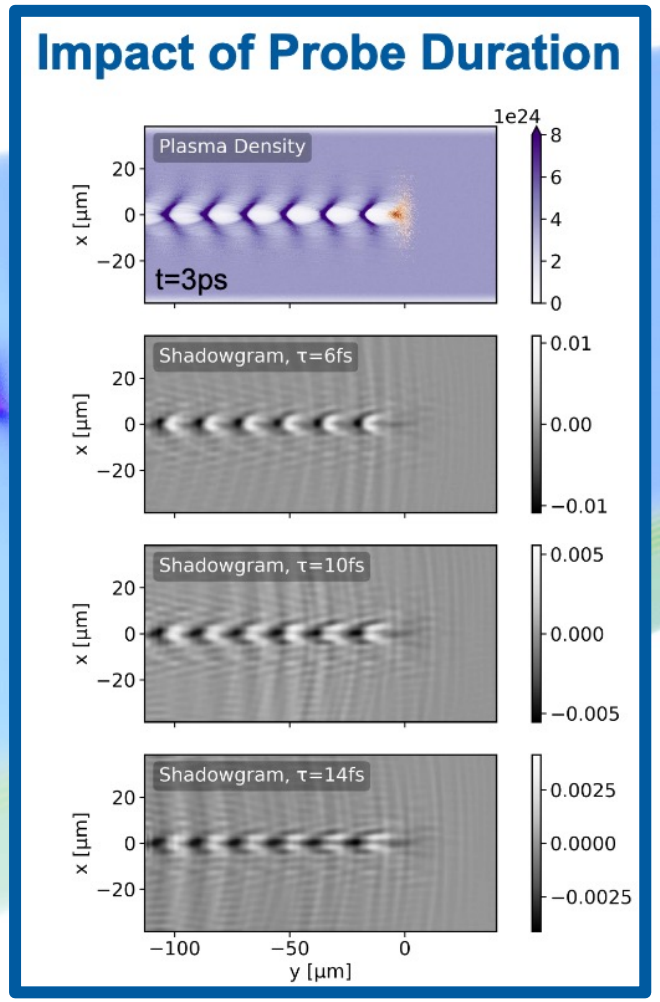
- Ultra flexible **bin quantities**
- automatically **distributed** and **parallelized**
- just **a few lines C++** code

```
/// Axis 2
// Define Functor
auto getMomentumRadial
    = [] ALPAKA_FN_ACC(auto const& domainInfo,
                       auto const& worker,
                       auto const& particle) -> float_X
{
    return picongpu::math::sqrt(
                particle[momentum_][0] * particle[momentum_][0]
                + particle[momentum_][2] * particle[momentum_][2])
        / particle[weighting_];
};
```



What to do with this high performance?

Going beyond “just” large simulation: complex in-situ data analysis



shadowgram plugin

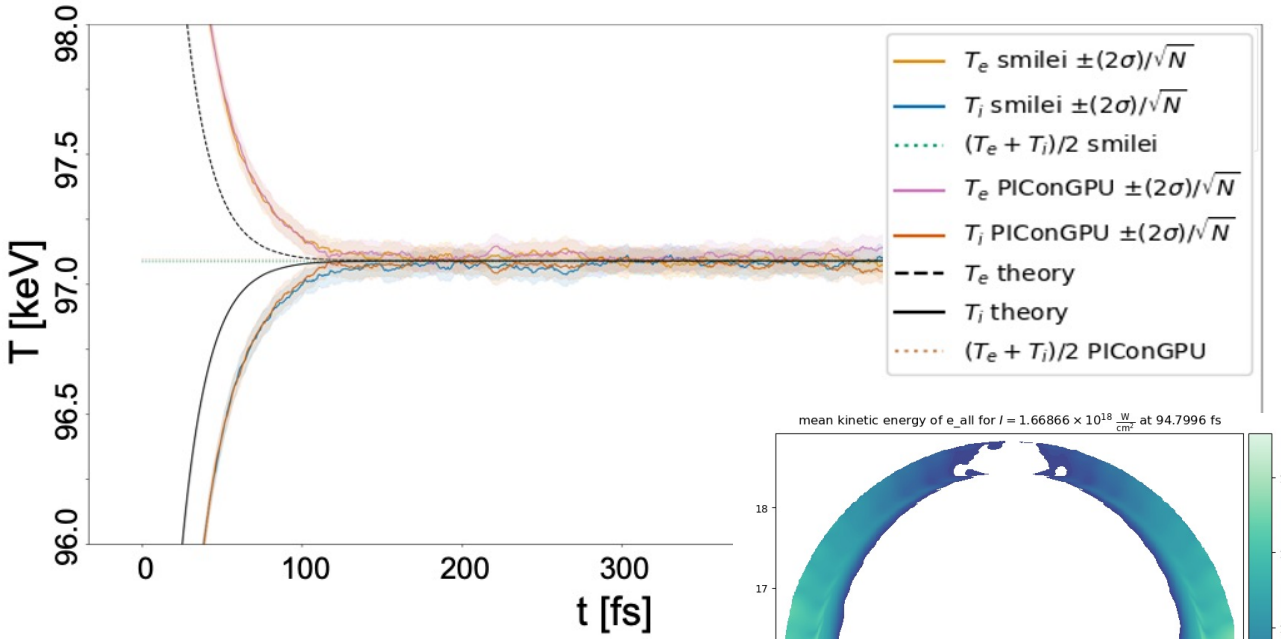
- models **full** probe laser plasma interaction
- automatically performs **Fourier optics** and **predicts experimental image**
- ideally suited to **compare to experiments**

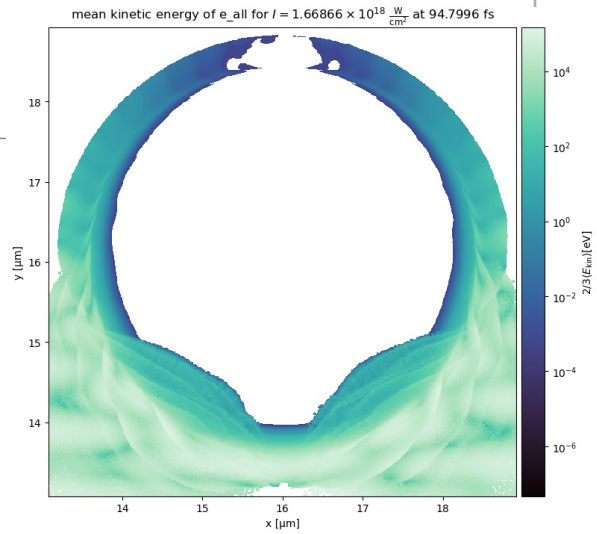
What is new in PIConGPU?

Particle-particle collisions to better model energy transfer in overdense targets

binary collisions

- needed to model **energy transfer** in overdense targets correctly
- collision frequency to much higher than PIC time step:
  one collision per step with **average angle**
- handling various particle weightings via **rejection method** *(Higginson 2020)*
- **code comparison** against Smilei



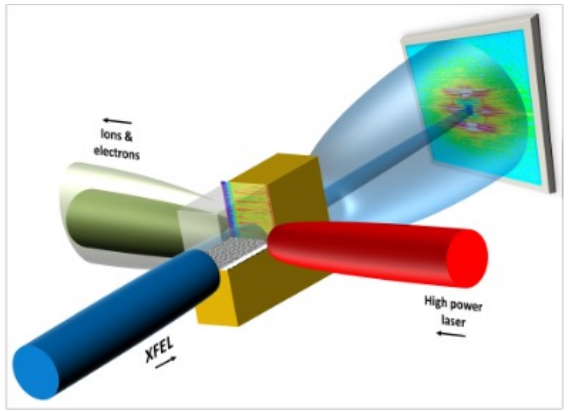


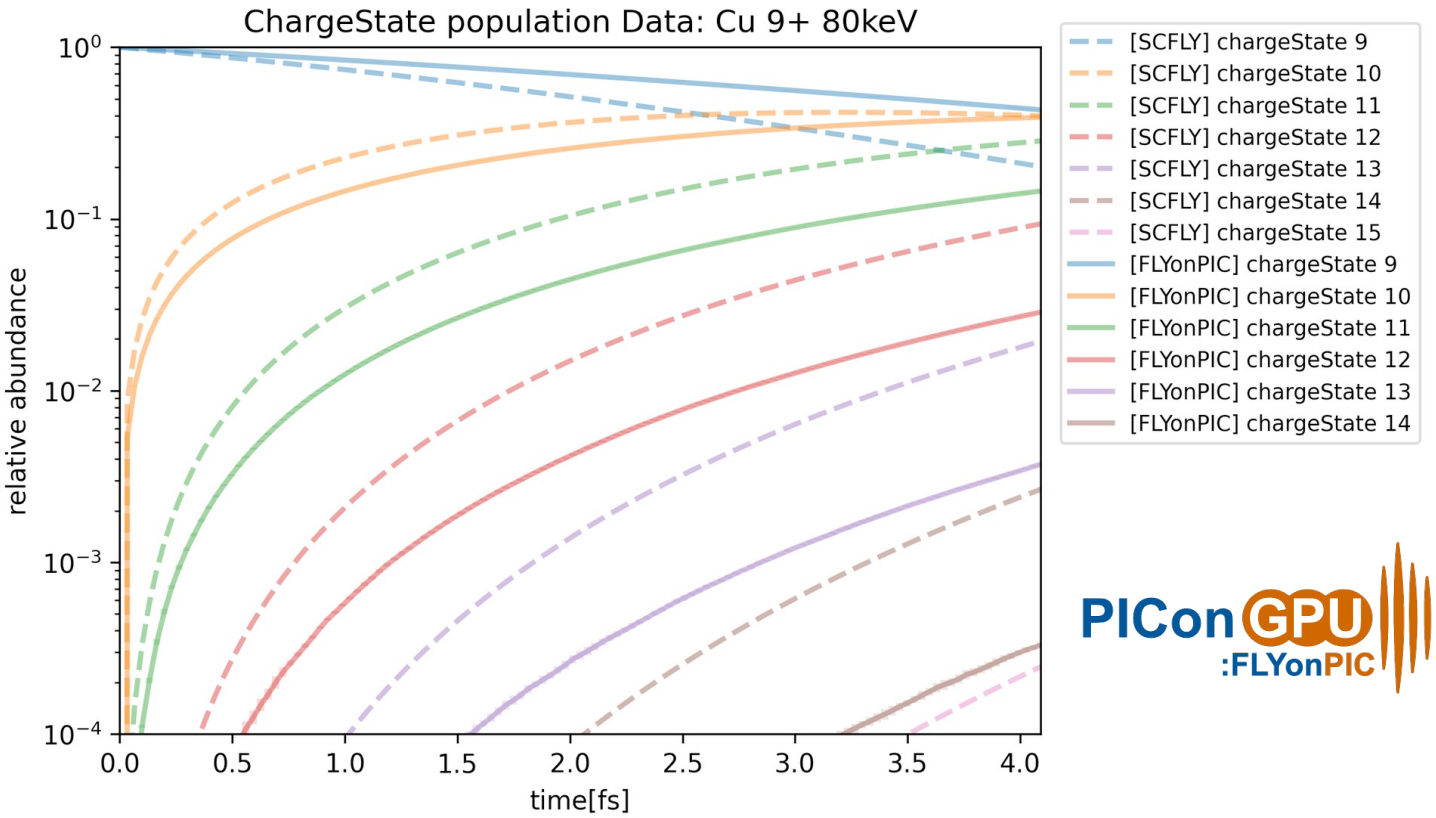
What is new in PIConGPU?

Non-thermal atomic transition for future ion-acceleration and fusion research

atomic physics

- going beyond BSI and ADK
- **non-thermal** atomic transitions
- average atom-state time-depended rate solver
- **code comparison** against SCFly
- Potentially experimentally validate at XFEL



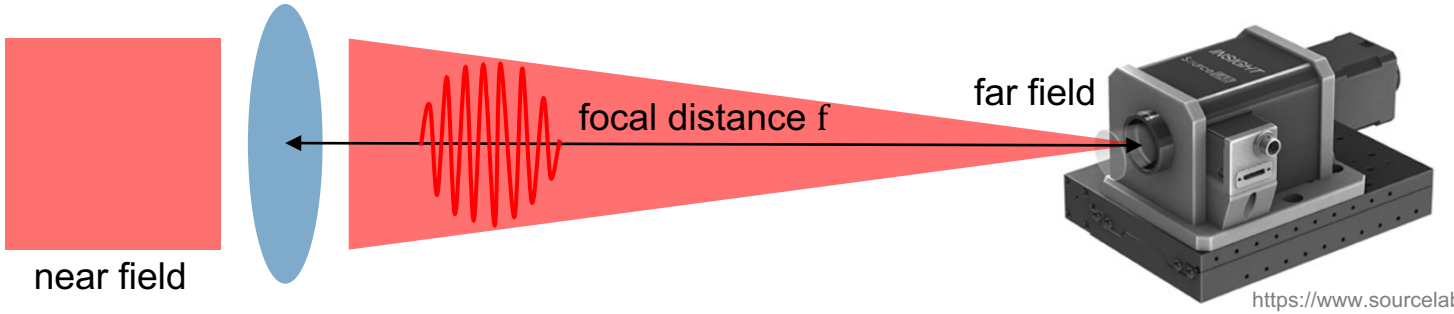


What is new in PIConGPU?

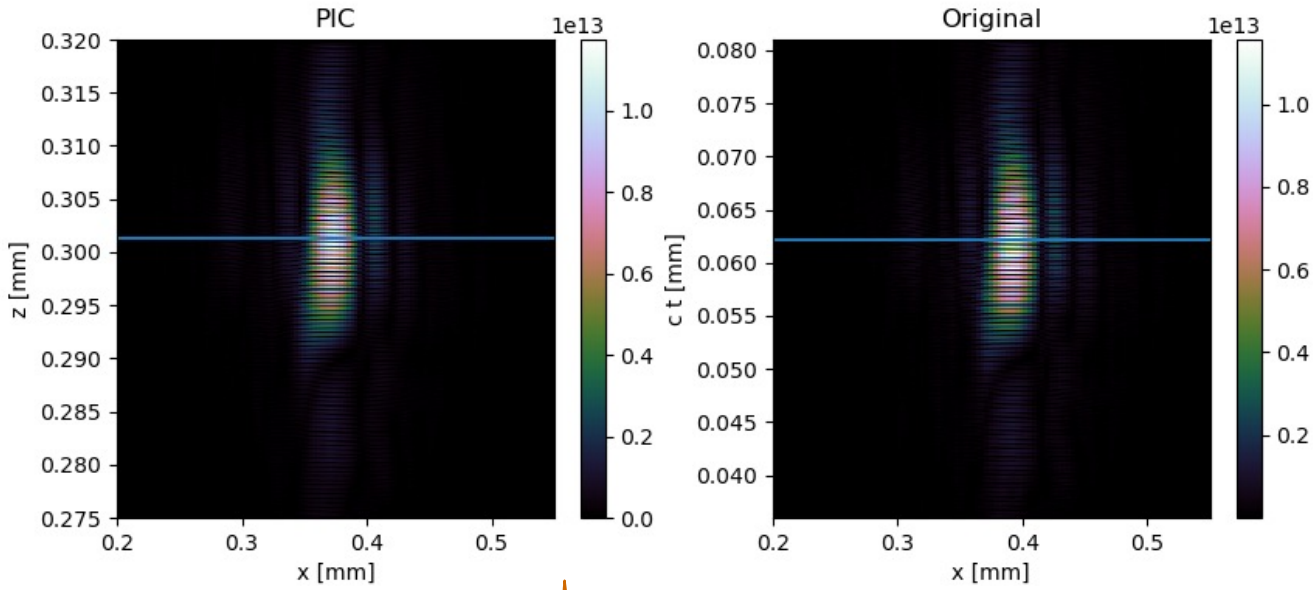
a general method to include complex laser pulses

laser via openPMD

- **real laser** pulses are far from ideal Gaussians
- experimental laser characterization (like **INSIDE**) can measure special and temporal laser profile
- this can be included in PIConGPU via **openPMD laser input**
- also suited for other input
- suited to study influence of non-ideal (real) lasers

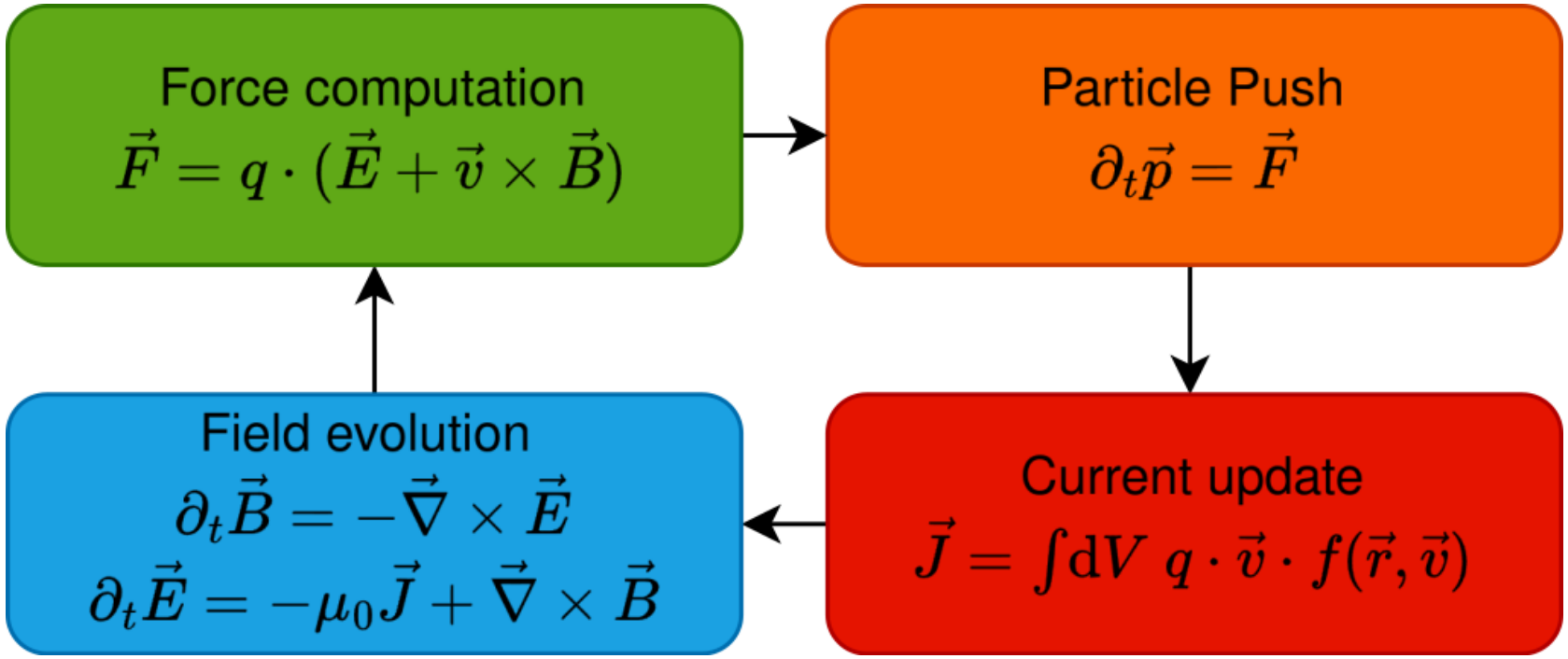


https://www.sourcelab-plasma.com/laser-shaping/beam-shaping-catalog/insight/



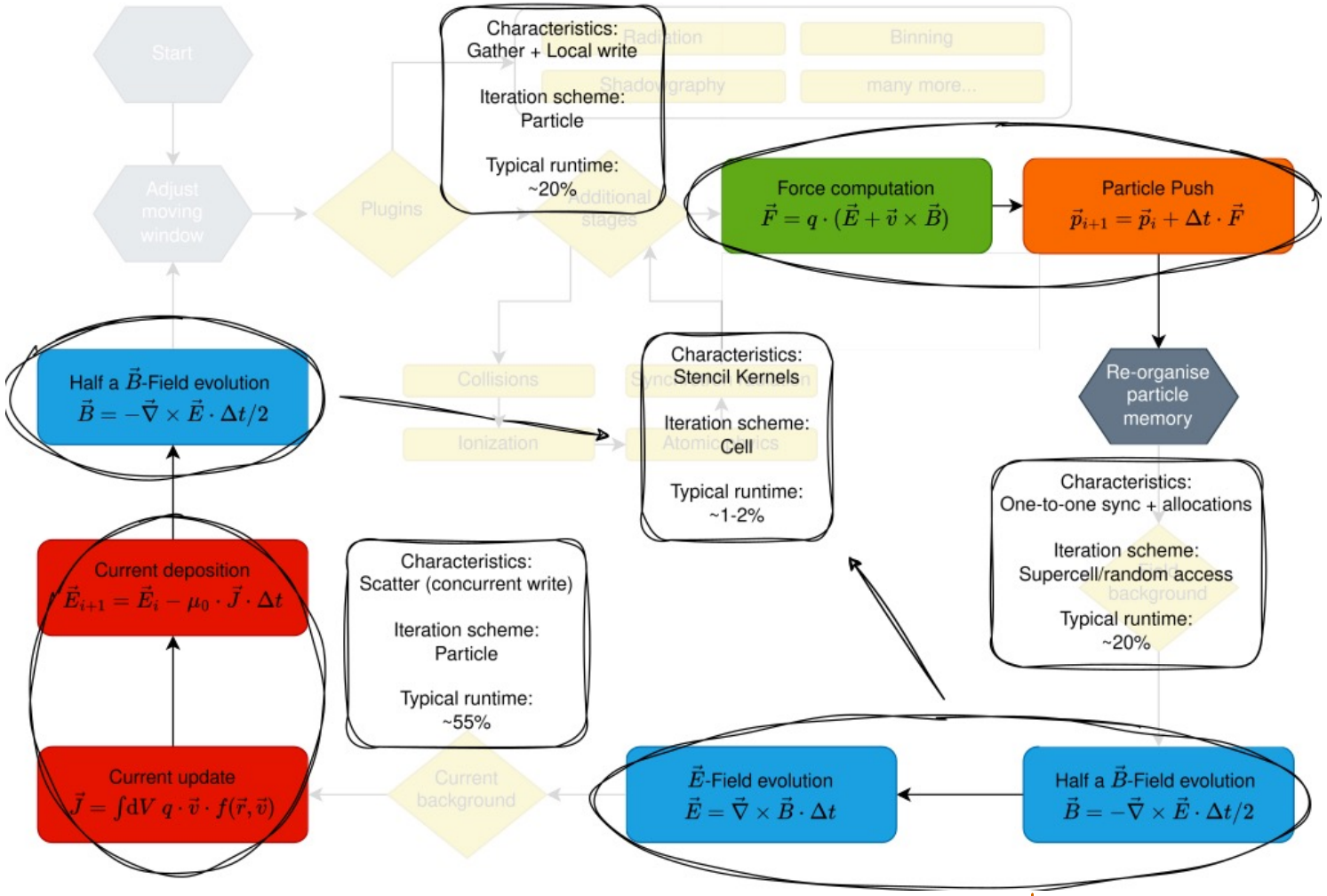
How does it all fit together?

The main PIC-loop in PIConGPU



How does it all fit together?

The main PIC-loop in PIConGPU

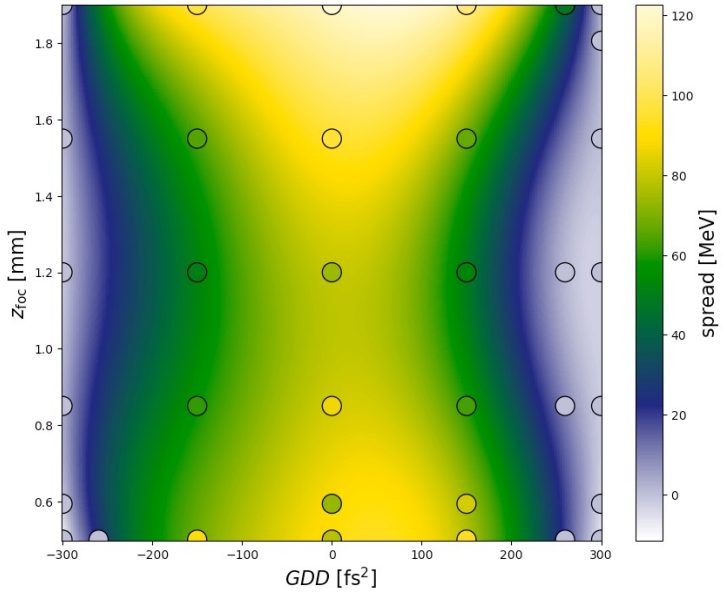


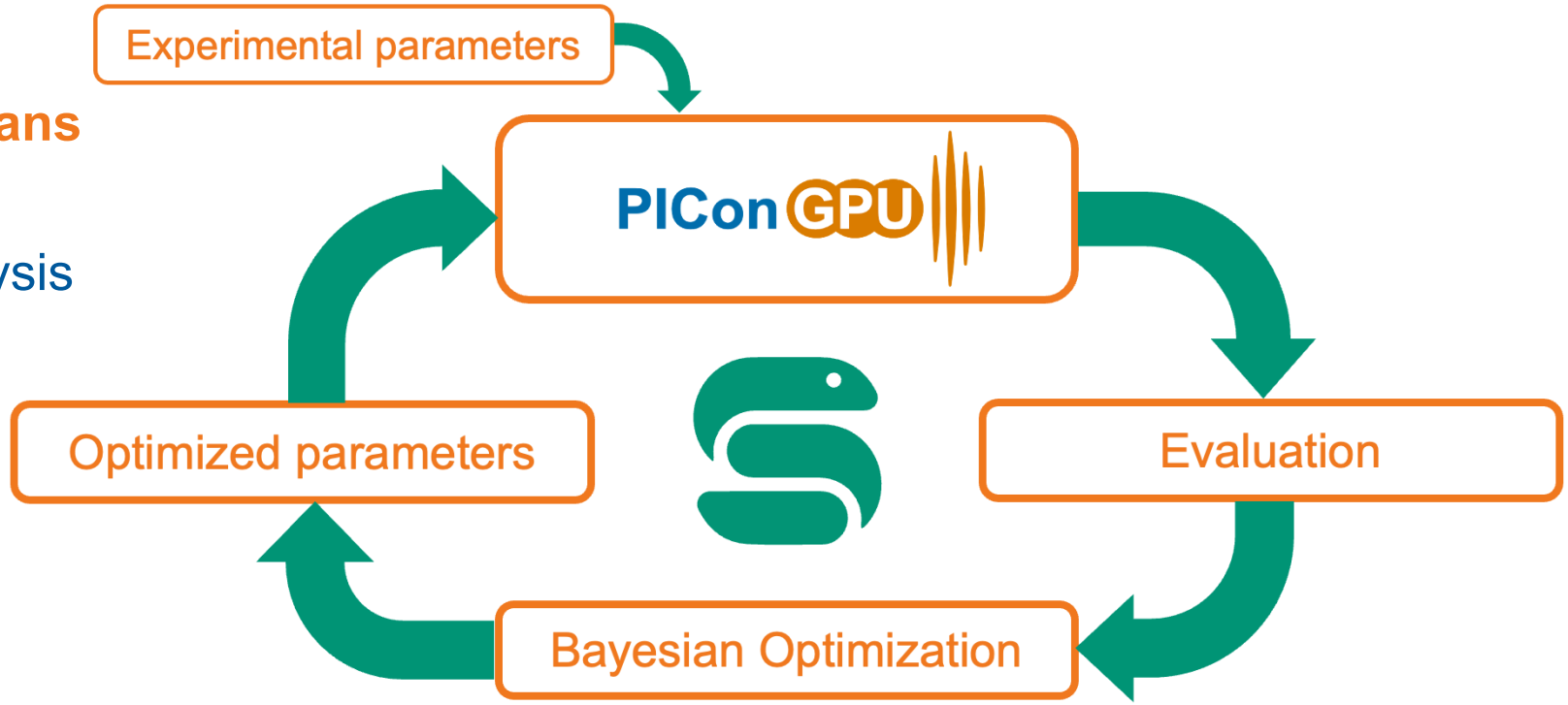
What is new in PIConGPU?

automating the entire many-simulations workflow

automated workflows

- support for **Snakemake**
- **automated parameter scans**
- including all stages:
  compilation, running, analysis





PIConGPU: developed as an open source code

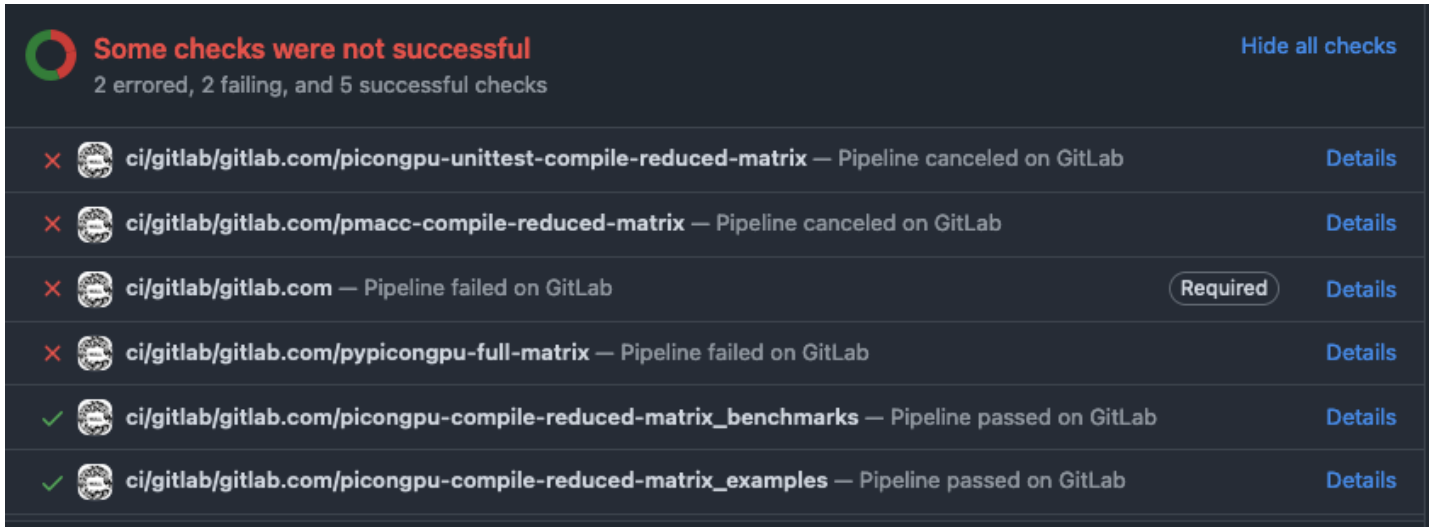
our development is open and relies on open platforms

- fully developed on GitHub
- automated CI tests (on GitHub and GitLab)
- open documentation via readthedocs
- open data via zenodo and rodare
- everybody can ask questions or contribute

zenodo

RODARE
ROSSENDORF DATA REPOSITORY

GitLab




Branch


Discuss


Merge

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Thank you for your attention.

Are there any questions?