Plasma acceleration and modern computing practices at DESY

Maxence Thévenet – DESY

Second DMLab meeting, DESY, Hamburg, 12/12/2022

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

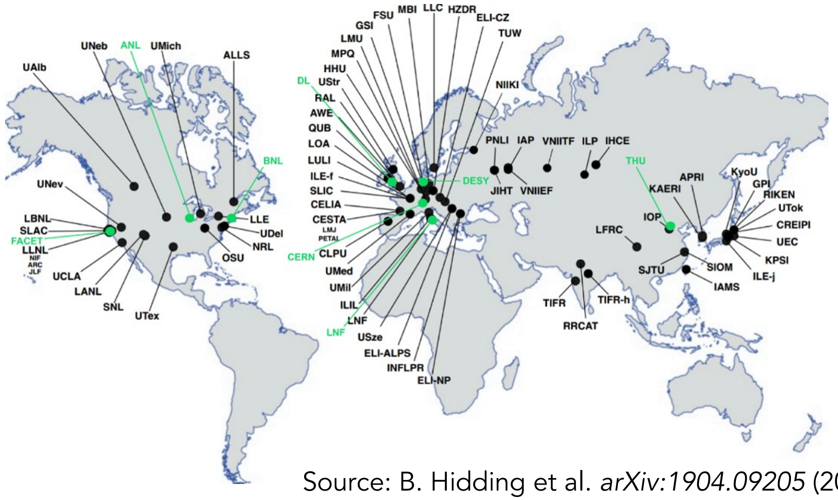
Particle accelerators are large devices

Jens Osterhoff in the XFEL tunnel

- Enable research in biology, medicine, chemistry, HEP, etc.
- Kinetic energy: $\mathcal{E}_k \propto L \times E_z$
- Conventional accelerators limited to $E_z < 100$ MV/m

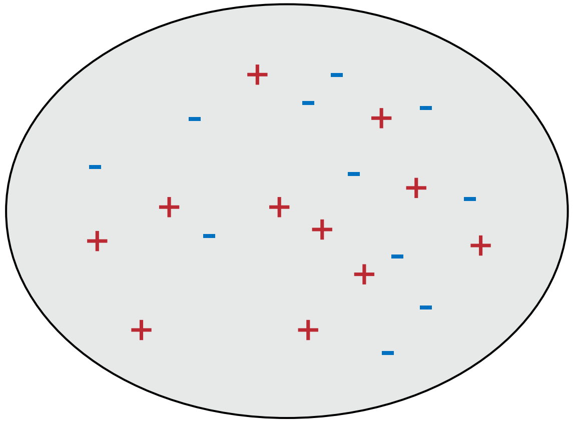
Plasma acceleration $E_z > 10$ GV/m → 100x more compact

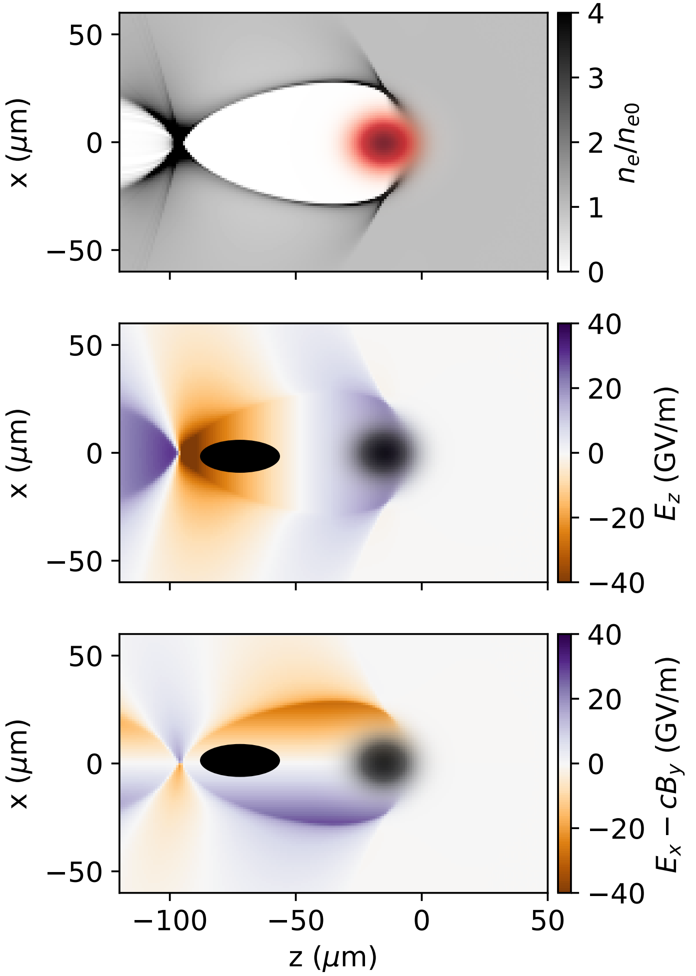
Applications from MeV to TeV energy ranges
- X-ray sources, high-energy physics
- Democratize accelerator-based sources



Source: B. Hidding et al. *arXiv:1904.09205* (2019)

Plasma acceleration: an alternative to conventional technologies





Wake ~ λ_p ~ 100 μm
Propagation ~ mm-m distance

T. Tajima, J. M. Dawson. *PRL* 43.4 (1979)

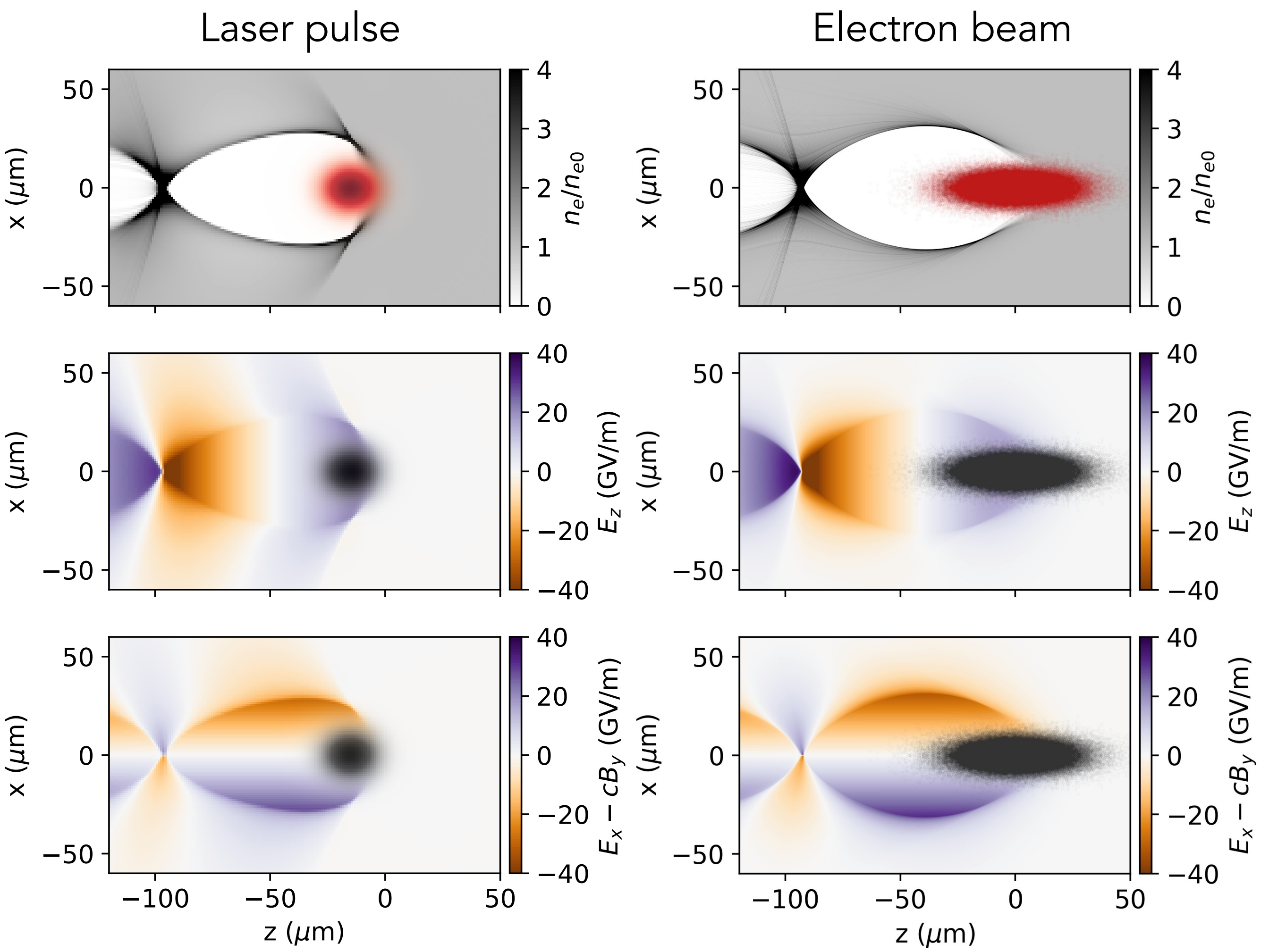
The wake can be driven by a particle beam or a laser pulse

Electron beam

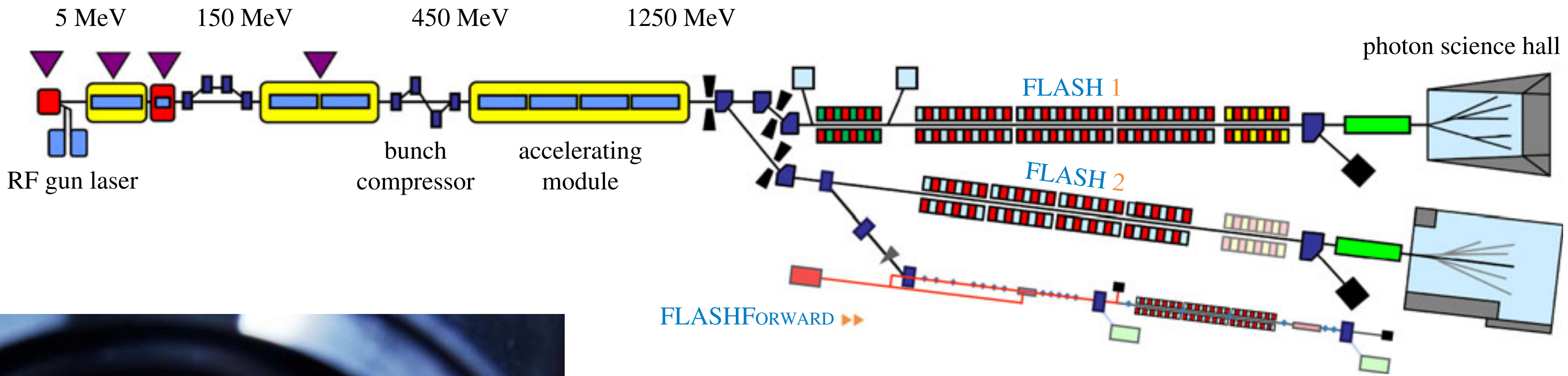
- $L < \lambda_p$
- $\boldsymbol{v} \sim c\boldsymbol{e_z}$
- $\rho, \boldsymbol{J} \rightarrow \boldsymbol{E}, \boldsymbol{B}$

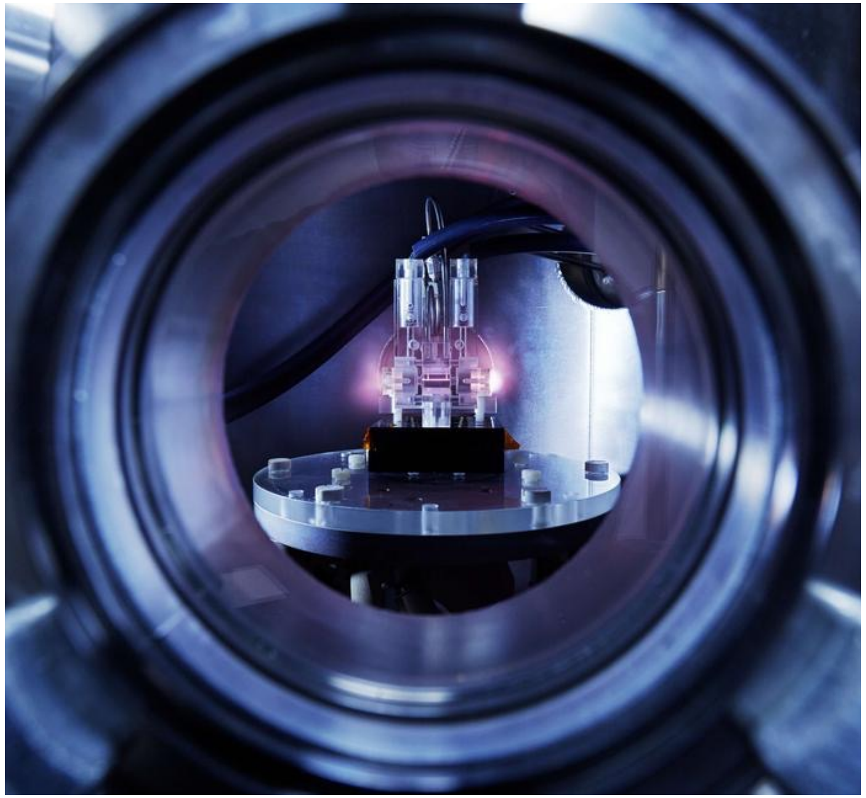
Laser pulse

- Ultrashort (fs): $L < \lambda_p$
- Ultraintense: $a_0 = \frac{eE_0}{m_e\omega c} \sim 1$
- Ponderomotive force: $\boldsymbol{F_p} = -\frac{1}{2m_e\bar{\gamma}}\boldsymbol{\nabla}\overline{|qA_x^2|}$



Beam-driven wakefield acceleration (FLASHForward, DESY)



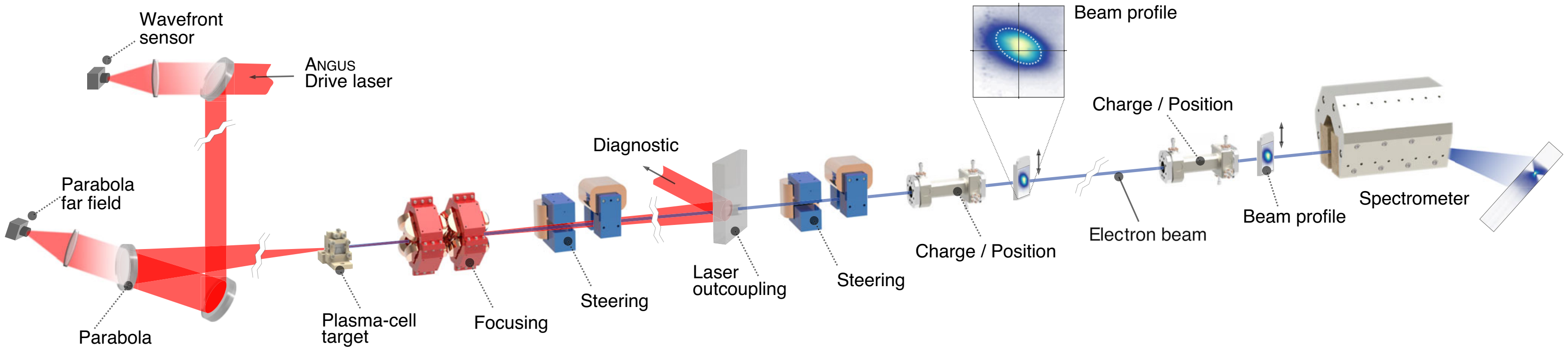


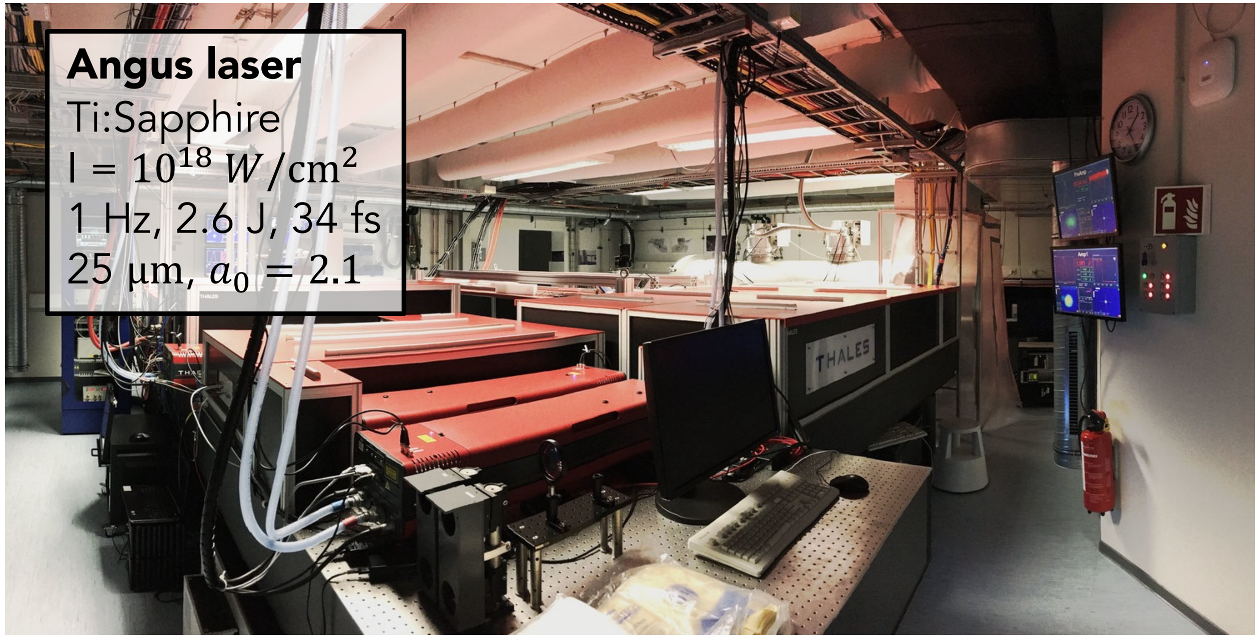
FLASH electron beam
1 GeV, 1 nC

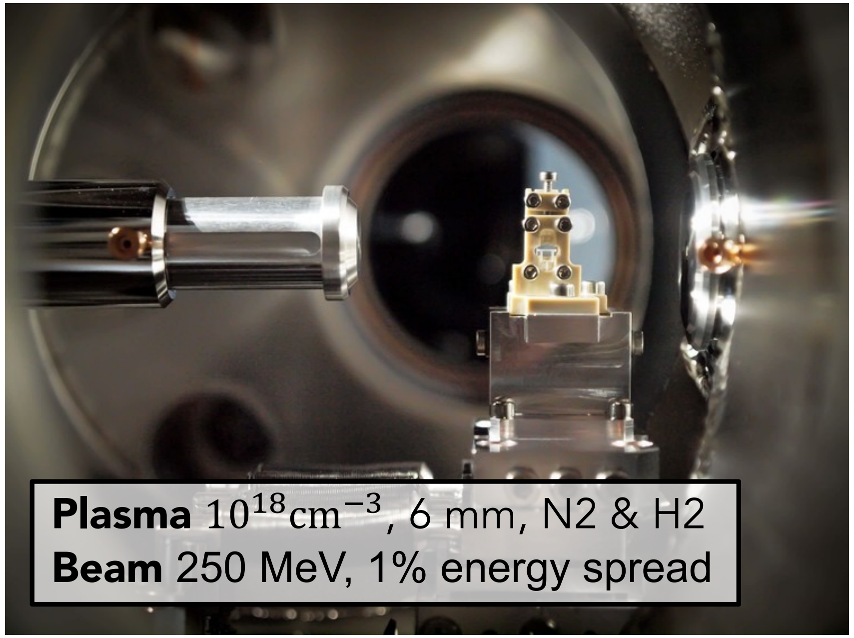
Plasma
10^{15} - 10^{17} cm^{-3}, 5-20 cm long

High-quality acceleration

Laser-driven Wakefield Acceleration (LUX, DESY)



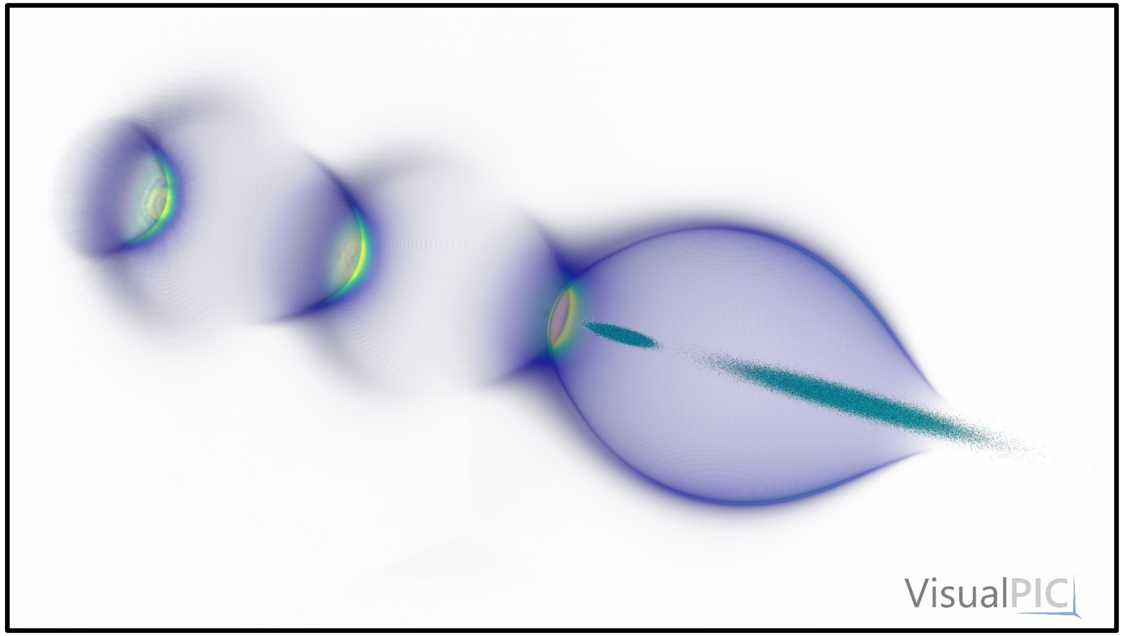




Courtesy of Sören Jalas, UHH, DESY

LUX

Wrapping up on the physics of plasma acceleration

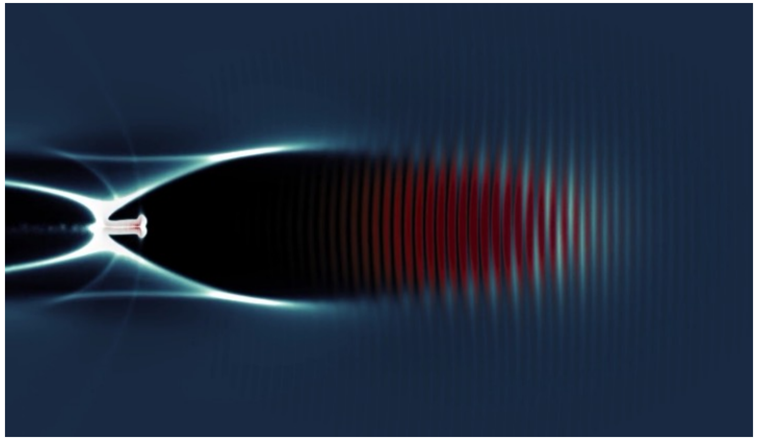


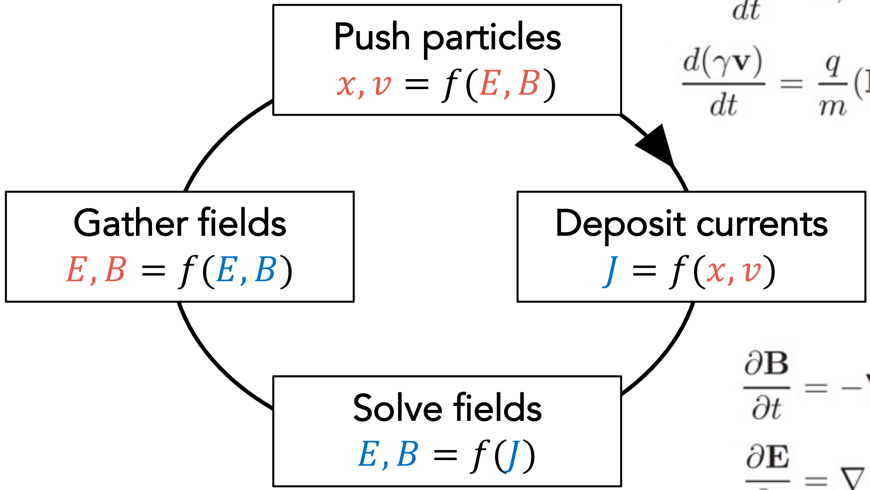
[1] J. Faure et al. *Nature* 431.7008 (2004)
[2] S. Mangles et al. *Nature* 431.7008 (2004)
[3] C. G. R. Geddes et al. *Nature* 431.7008 (2004)
[4] A. J. Gonsalves et al. PRL 122, 084801 (2019)
[5] W. Wang et al. *Nature* 595.7868 (2021)
[6] A. Maier et al. Phys. Rev. X 10, 031039 (2020)
[7] R. D'Arcy et al. *Nature* 603.7899 (2022)

- Strong accelerating fields $E_z \sim 10s\ \mathrm{GV/m}$
- Laser-driven or beam-driven
- Accelerated electron beams are inherently ultrashort (fs)

- Demonstrated
  - Mono-energetic electron beams [1-3]
  - Acceleration up to 8 GeV [4]
  - FEL driven by a laser plasma accelerator [5]
- Remaining challenges
  - Stability [6]
  - Repetition rate [7]
  - Staging
- But: non-linear process → numerical simulations are crucial

Particle-in-cell is the method of choice for wakefield simulations



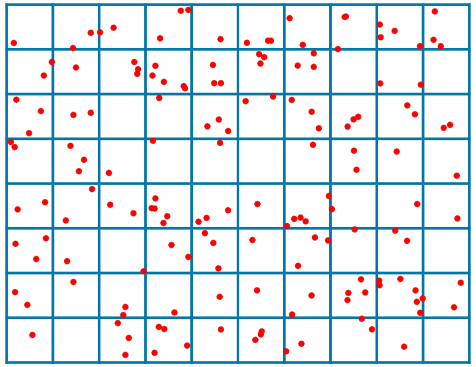


$$\frac{d\mathbf{x}}{dt} = \mathbf{v},$$

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

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

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



Regular grid
Macroparticles

Lagrangian description of plasma
Eulerian description of fields

→ 3D simulations of plasma acceleration are very expensive (1000^3 cells ~ 1 TB)

Particle-in-cell is the method of choice for wakefield simulations

1 m (10,000x)

100 microns

What platform do we run on?
- Top500: 15/20 GPU
- Green500: 19/20 GPU

→ on GPU

Rank	Name	Hardware
1	Frontier TDS	AMD Instinct MI250X
2	Frontier	AMD Instinct MI250X
3	LUMI	AMD Instinct MI250X
4	Adastra	AMD Instinct MI250X
5	ATOS THX.A.B	NVIDIA A100
6	MN-3	Xeon Platinum 8260M
7	SSC-21 Scalable Module	NVIDIA A100
8	Tethys	NVIDIA A100
9	Wilkes-3	NVIDIA A100
10	Athena	NVIDIA A100
11	Phoenix - 2022	NVIDIA A100
12	HiPerGator AI	NVIDIA A100
13	Snellius Phase 1 GPU	NVIDIA A100
14	Perlmutter	NVIDIA A100
15	Karolina, GPU partition	NVIDIA A100
16	MeluXina - Accelerator Module	NVIDIA A100
17	Alex	NVIDIA A100
18	NVIDIA DGX SuperPOD	NVIDIA A100
19	JUWELS Booster Module	NVIDIA A100
20	JURECA Data Centric Module	NVIDIA A100

- Boosted frame method
  J.-L. Vay PRL **98,** 130405 (2007)

- Reduced model: quasi-static approximation (QSA)
  Sprangle, P. et al., *PRL* 64.17 (1990): 2011
  → HiPACE++ at DESY

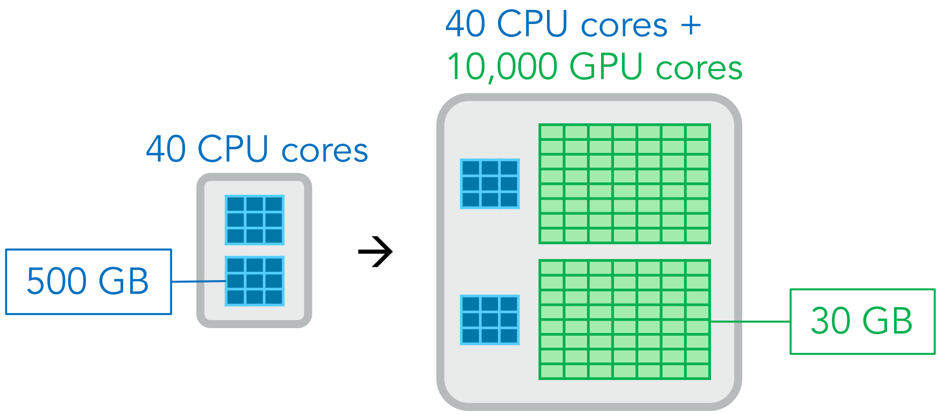
https://www.top500.org/lists/top500/2022/11/

PIC codes benefit from modern code practices

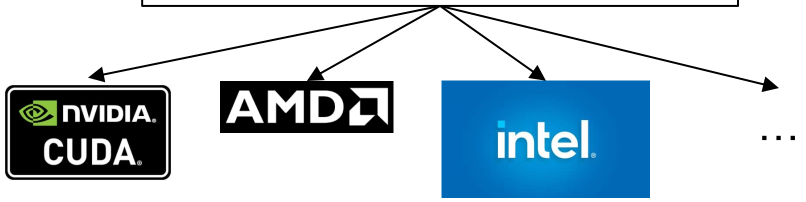
- **Performance-portability**
  - Portability layer (Kokkos, Alpaka, RAJA) C++
- **Open Source & Open Repository**
  - Encourages flexible, modular code
- **Documented**
  - Clear and transparent code

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

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




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



HiPACE++: people and structure

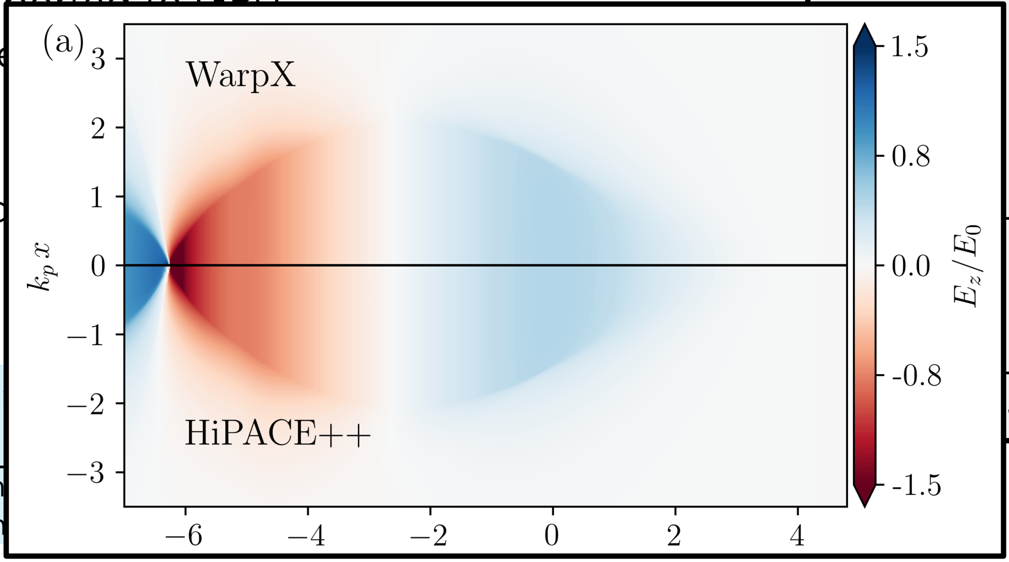
[1] https://github.com/AMReX-Codes/amrex
[2] https://github.com/ECP-WarpX/WarpX
[3] Myers et al., Parallel Comput. 2021
[4] https://github.com/openPMD/openPMD-standard

- Collaboration with the ECP WarpX[2,3] team at LBNL
- On top of AMReX[1] (LBNL): portability
- On top of openPMD-api (HZDR): I/O
- First quasi-static PIC code fully
- High-resolution simulations take

Driving principles

- Open-source, well documented
- Automated testing (CI)
- Adopt community standards
- Performance portability
- Rely on existing libraries

Si
Runtim
Cost (n



HiPACE++

i-static PIC code
ed by DESY & LBNL

/github.com/Hi-PACE/hipace
the BLAST toolkit

tps://hipace.readthedocs.io
s et al., CPC 278, 108421 (2022)

lead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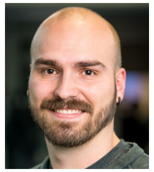
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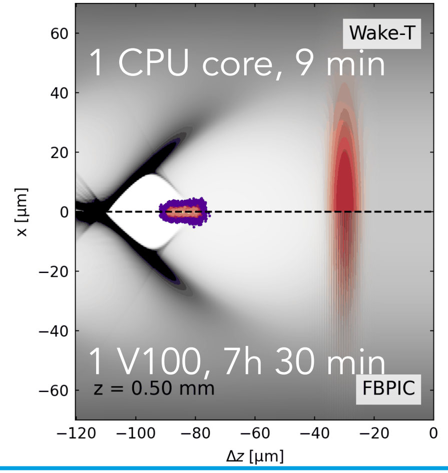
Jean-Luc Vay
LBNL

Modern HPC practices enable more science and collaboration

Driving principles
- Open-source, well documented
- Automated testing (CI)
- Adopt community standards
- Performance portability
- Rely on existing libraries

Develop and combine multiple simulation tools

- Wake-T: lightweight reduced model for 2D simulations (few min on a laptop) – DESY
- FBPIC: LBNL-DESY collaboration for laser wakefield acceleration simulations

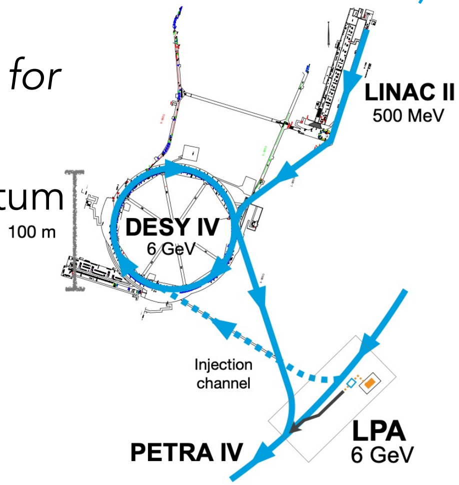


Plasma Injector for Petra IV – PIP4 (A. Martinez de la Ossa)

Petra IV: 2.3 km, 6 GeV storage ring for unprecedented X-ray brightness.

Specs: 6 GeV, > 1 nC/s, 1% momentum acceptance, 10 mm.mrad

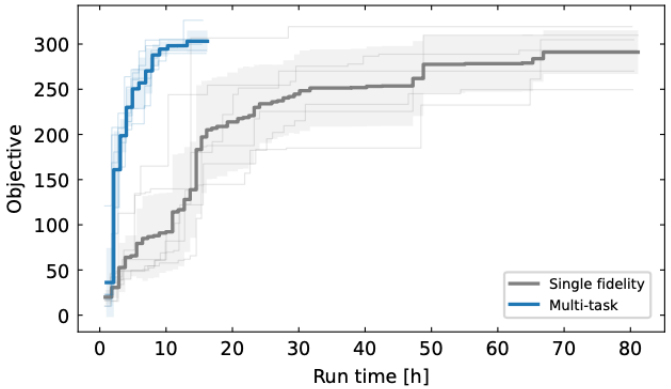
How can the injector be replaced by a LPA?



Implement machine learning for more efficent operation

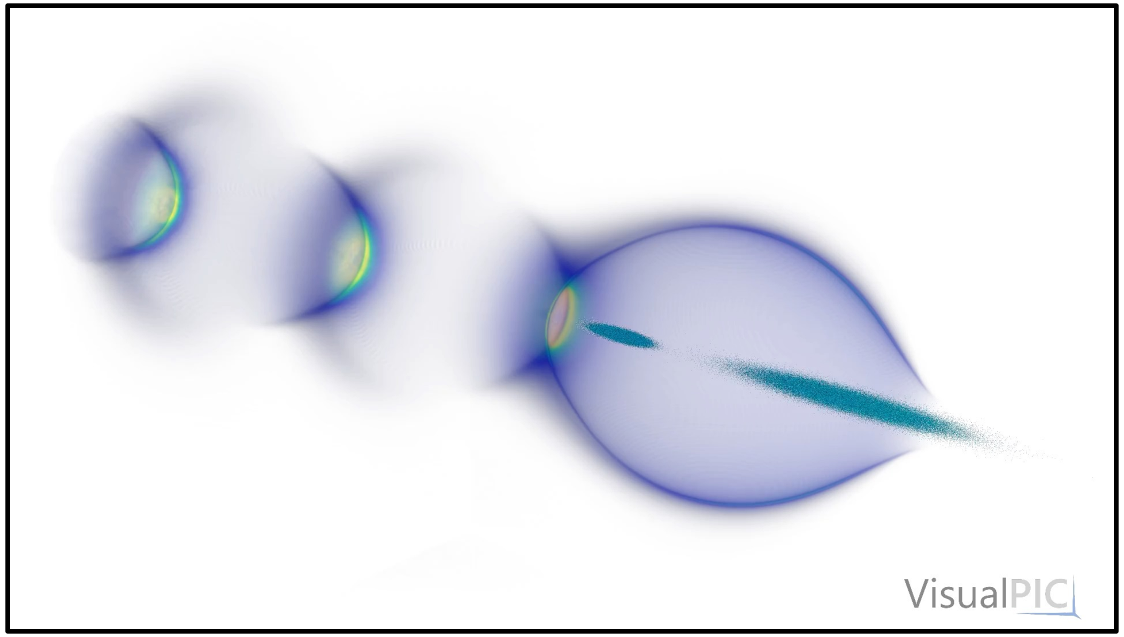
- Parallel Bayesian optimization
- Multi-task BO

(A. Ferran Pousa)



Conclusion & Perspectives

- Plasma acceleration: worldwide effort towards compact accelerators
- Next challenges: stability, repetition rate, staging
- Numerical simulations crucial in plasma acceleration research
- We favor open-source & community standards for more collaboration



Thank you for your attention