Mainstreaming Start-to-End Realistic Simulations in Plasma Acceleration Research

Maxence Thévenet – DESY

Theory & simulation for plasma acceleration

MPL

DESY: S. Diederichs, A. Ferran Pousa, A. Sinn, J. Osterhoff, A. Martinez de la Ossa, S. Jalas, M. Kirchen, R. Shalloo, X. Hui, M. Formela, S. M. Mewes, J. M. Garland, M. Huck, H. Jones, G. Loisch, A. R. Maier, T. Parikh, S. Wesch, J. C. Wood

BERKELEY LAB: C. Benedetti, J.-L. Vay, A. Huebl, R. Lehe, A. Myers, W. Zhang, C. B. Schroeder

UNIVERSITY OF OSLO: C. A. Lindstrøm, P. Drobniak, J.B.B.Chen

JCU: G. J. Boyle

LOA: I. Andriyash

UNIVERSITY OF OXFORD: R. D'Arcy

cea: L. Fedeli

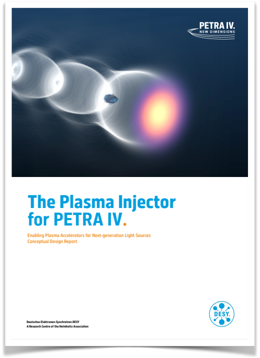
HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

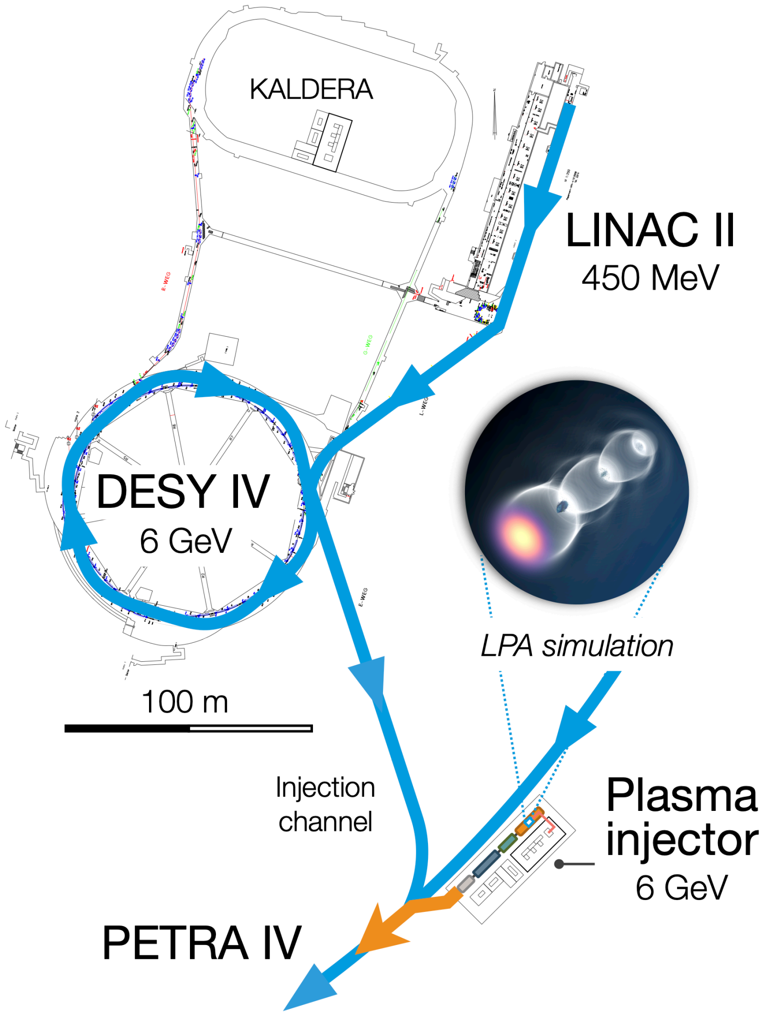
DESY.

Plasma acceleration involves multiple physical models

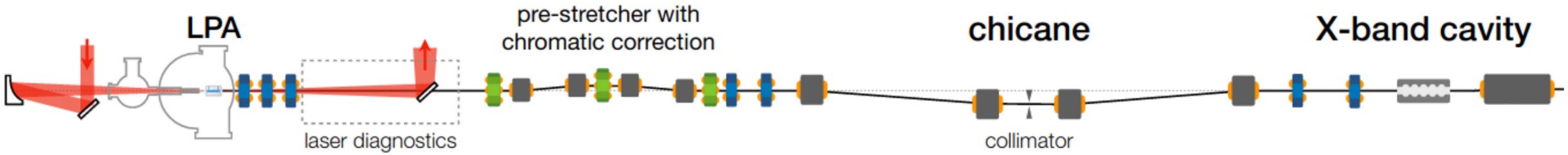
Example: study for the plasma injector for PETRA IV

- A. Martinez de la Ossa et al., The Plasma Injector for PETRA IV: Conceptual Design Report **https://doi.org/10.3204/PUBDB-2024-06078**
- S. A. Antipov *et al.* Design of a prototype laser-plasma injector for an electron synchrotron **PRAB** 24.11 (2021)
- A. Ferran Pousa *et al.,* Energy Compression and Stabilization of Laser-Plasma Accelerators **PRL** 129, 094801 (2022)
- P. Winkler *et al.* Active energy compression of a laser-plasma electron beam **Nature** 1-4 (2025)





Plasma acceleration involves multiple physical models



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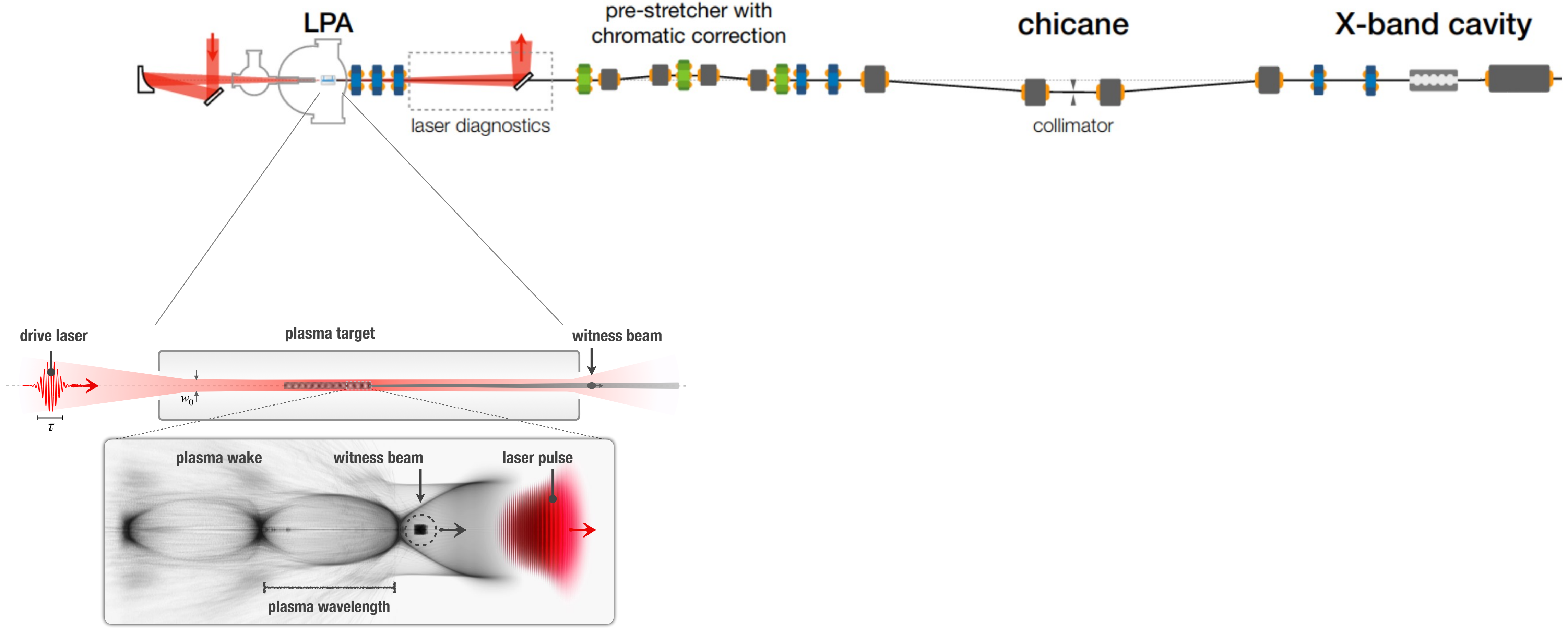
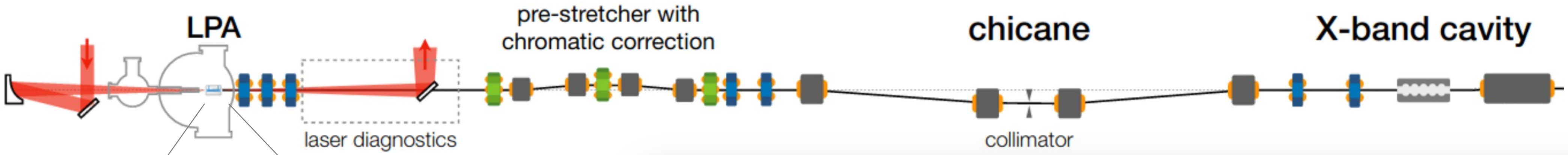
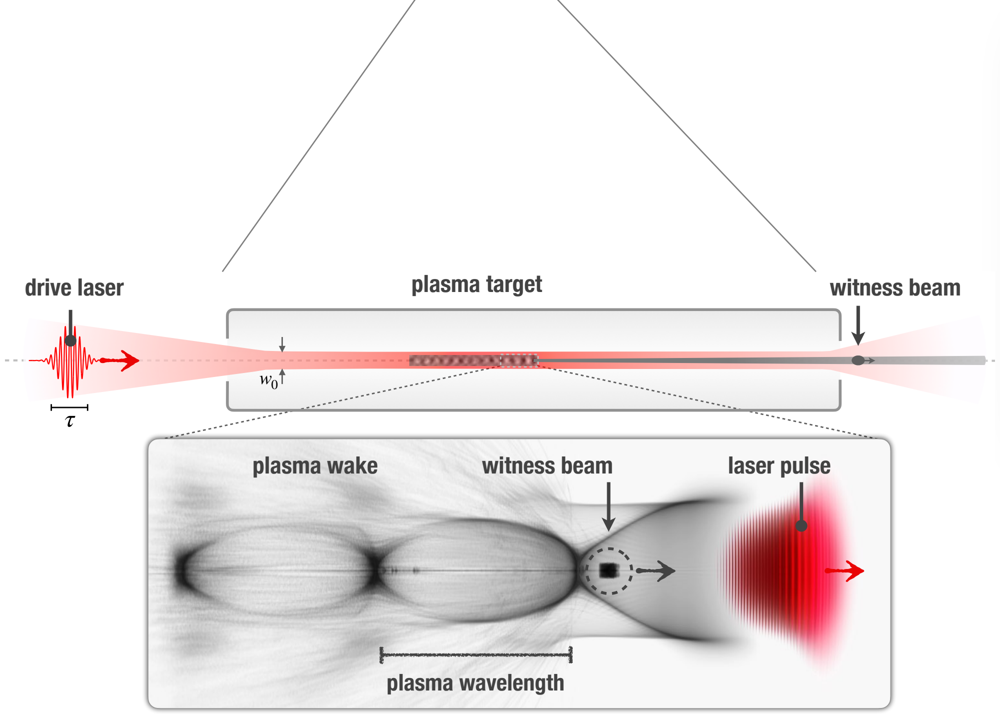
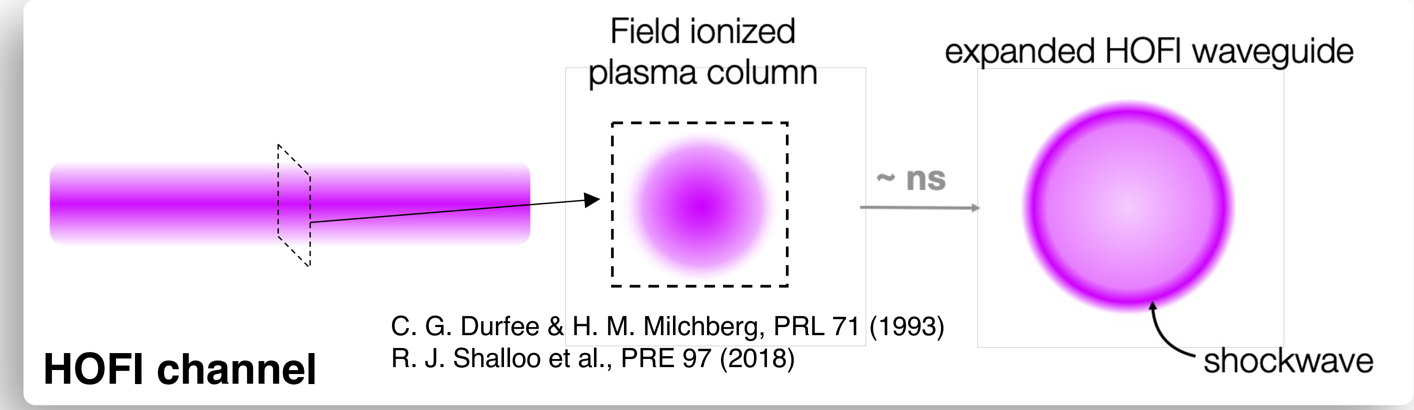


Plasma acceleration involves multiple physical models

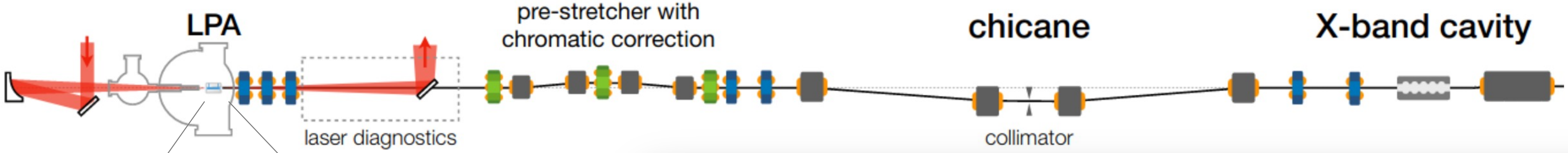


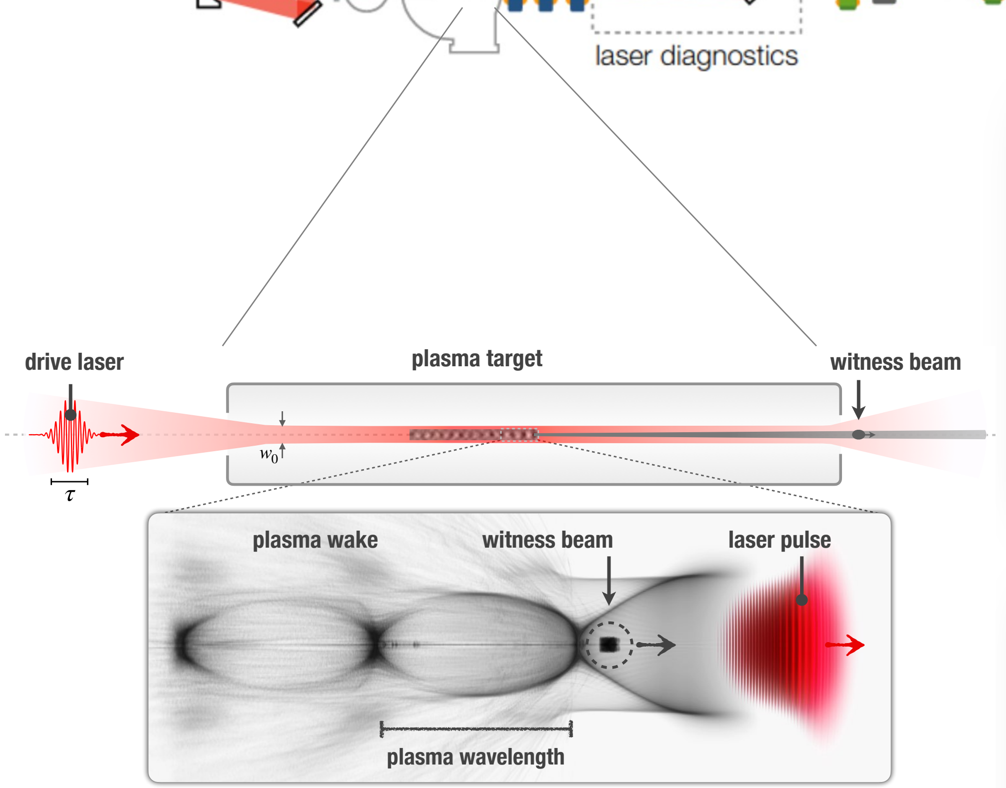


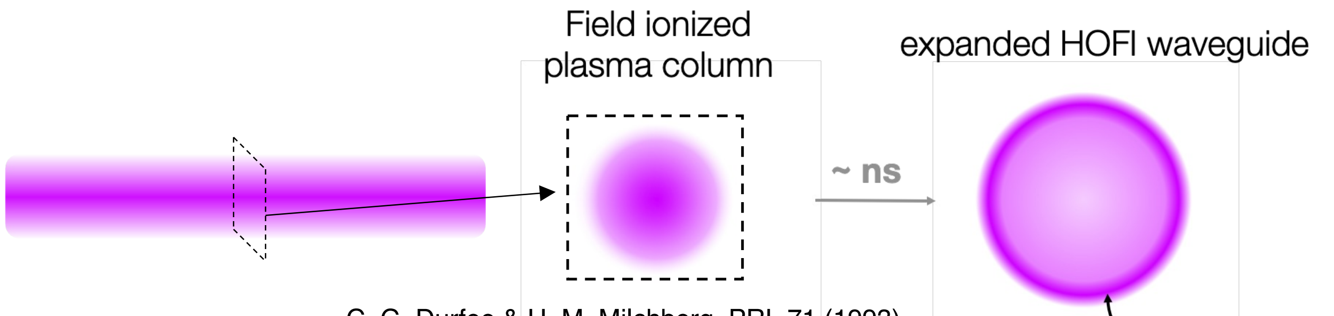


C. G. Durfee & H. M. Milchberg, PRL 71 (1993)
R. J. Shalloo et al., PRE 97 (2018)

Plasma acceleration involves multiple physical models







HOFI channel

C. G. Durfee & H. M. Milchberg, PRL 71 (1993)
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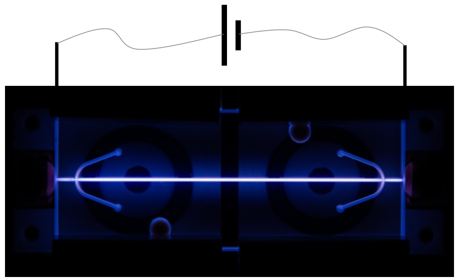
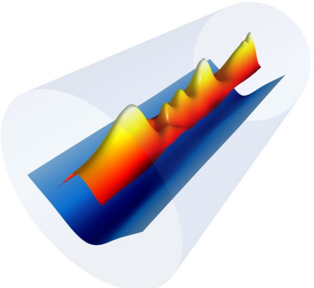




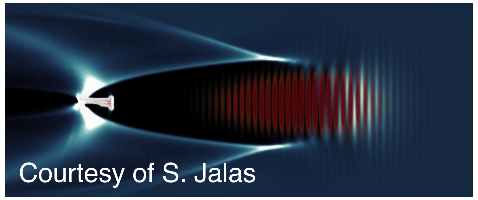
Discharge capillary

D. J. Spence & S. M. Hooker, Phys. Rev. E 63, 015401 (2000)
A. J. Gonsalves et al., *PRL 122, 084801 (2019)*

Accurate simulations requires interfacing tools together

LPA

FBPIC

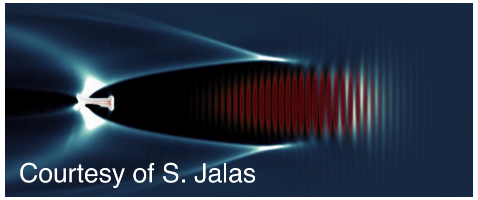

Courtesy of S. Jalas

Accurate simulations requires interfacing tools together

Realistic laser

LPA

FBPIC



Courtesy of S. Jalas

Accurate simulations requires interfacing tools together

Laser
Gas profile

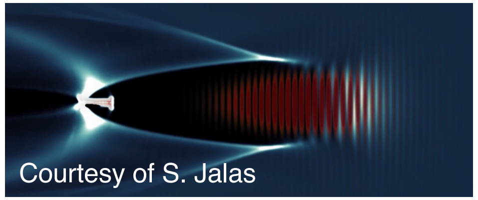
Density & temperature

Laser ionization → HOFI expansion

Plasma density

Realistic laser → LPA

FBPIC



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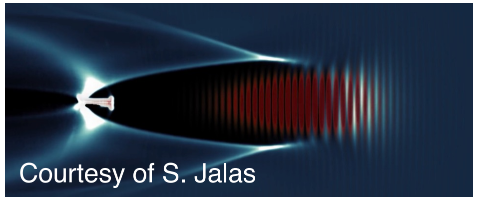


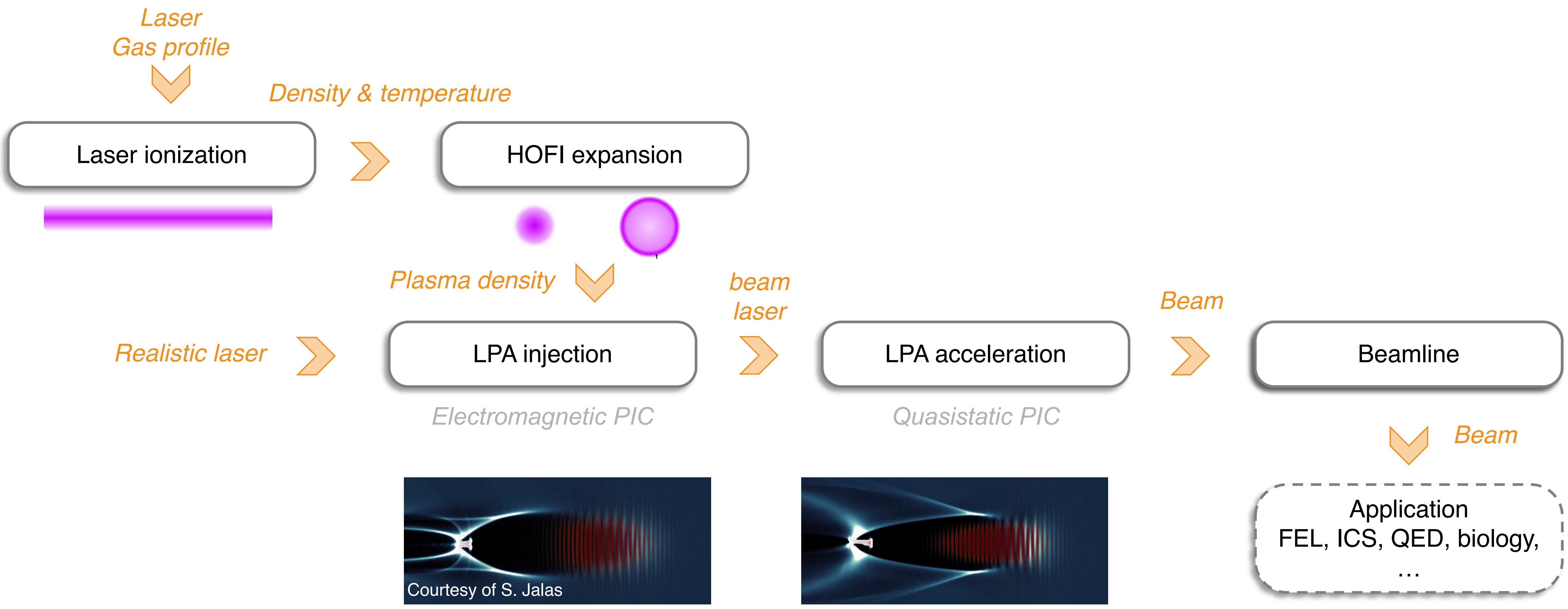
Beam

Beamline

Beam

Application
FEL, ICS, QED, biology,
…

Accurate simulations requires interfacing tools together



Accurate simulations requires interfacing tools together

Requirements

- ➢ Simulation tools
  - Laser propagators
  - Kinetic plasma
  - Fluid plasma
  - Beam dynamics
- ➢ Data transfer
  - electron beam
  - plasma profile
  - laser pulse (exp./sim.)
  - ad-hoc quantities

Laser
Gas profile

Laser ionization

Density & temperature

HOFI expansion

Plasma density

Realistic laser

LPA injection

Electromagnetic PIC

beam
laser

LPA acceleration

Quasistatic PIC

Beam

Beamline

Beam

Application
FEL, ICS, QED, biology,
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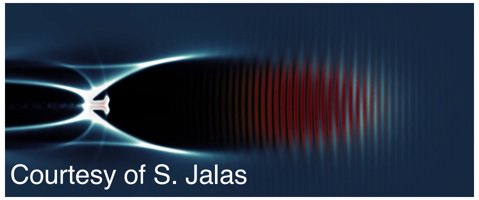

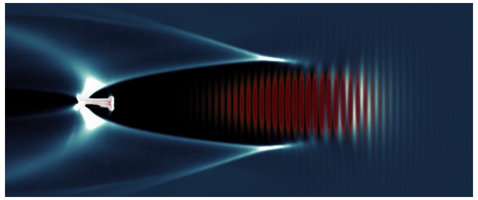

General approach to simplify start-to-end workflows

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- ***Build upon community work***
- ***Independent codes + helpers***

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openPMD

Open standard for Particle Mesh Data

LBNL & CASUS https://github.com/openPMD

PIConGPU
WarpX
HiPACE++
<your code>

→ openPMD →

- ✓ ***Archive***
- ✓ ***Analyze***
- ✓ ***Exchange***
- ✓ ***Interface***

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- ✓ ***Archive***
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- ✓ ***Interface***

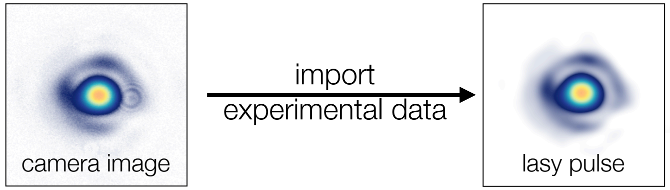
LASY

LAser manipulations made eaSY

https://github.com/LASY-org/lasy

poster by R. Shalloo

- Simulation to simulation
- Experiment to simulation



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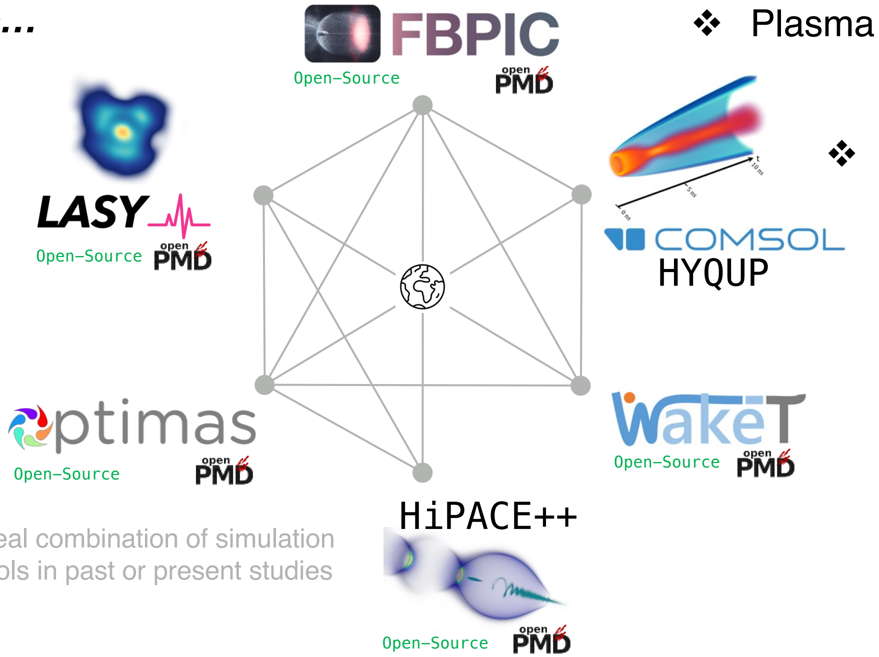
Start-to-end studies are enabled by an interconnected ecosystem

Simulate wakefield acceleration and more…



Real combination of simulation tools in past or present studies

- ❖ Plasma source tailoring
- ❖ Realistic experimental profiles
- ❖ Plasma recovery for repetition rate
- ❖ Parallel Bayesian optimization

BLAST BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT

… harnessing the fastest supercomputers

https://github.com/AngelFP/Wake-T
https://github.com/Hi-PACE/hipace
https://github.com/fbpic/fbpic
https://github.com/optimas-org/optimas
https://github.com/LASY-org/lasy

Highlights

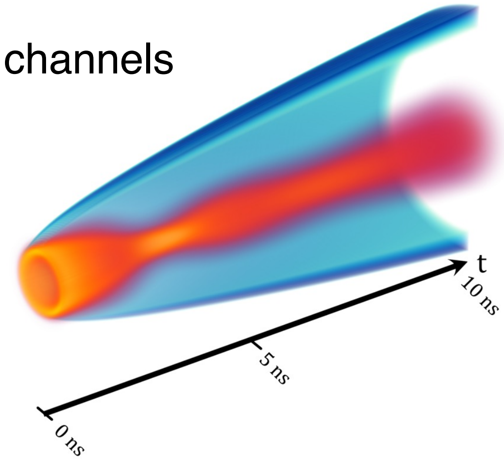
- ➢ Affordable **multi-stage** simulations in RZ and 3D with *Wake-T* & *HiPACE++* at **5-nm resolution** using **mesh refinement**.
- ➢ Easy **code handshakes** with broad adoption of **openPMD standard** and library *LASY*, including **plasma source tailoring** with *HYQUP*.
- ➢ Support studies at DESY and worldwide with **open-source** codes *FBPIC*, *Wake-T* in **scalable Bayesian optimization** with *Optimas*.
- ➢ Harness the **latest GPUs** with *FBPIC* and address **Exascale computing** with *HiPACE++*.

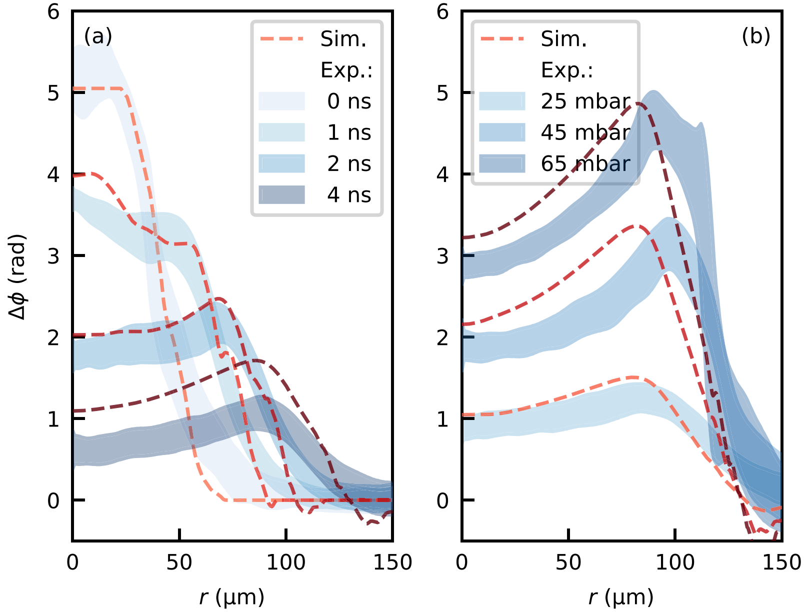
Codes are being developed to address the needs

➢ **COMSOL - HYQUP.** plasma fluid dynamics

- Hydrodynamic Optical-Field-Ionized (HOFI) channels

  M. Mewes et al. PRR 5, 033112 (2023)





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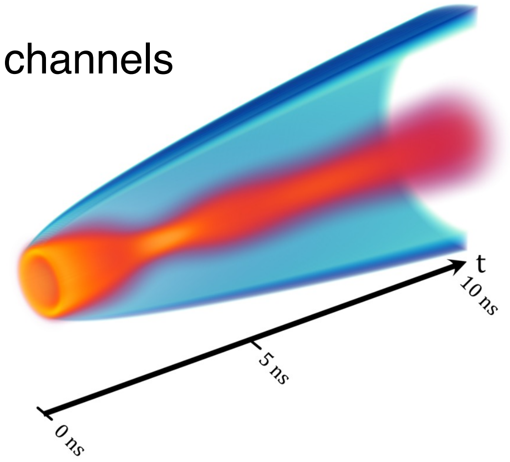
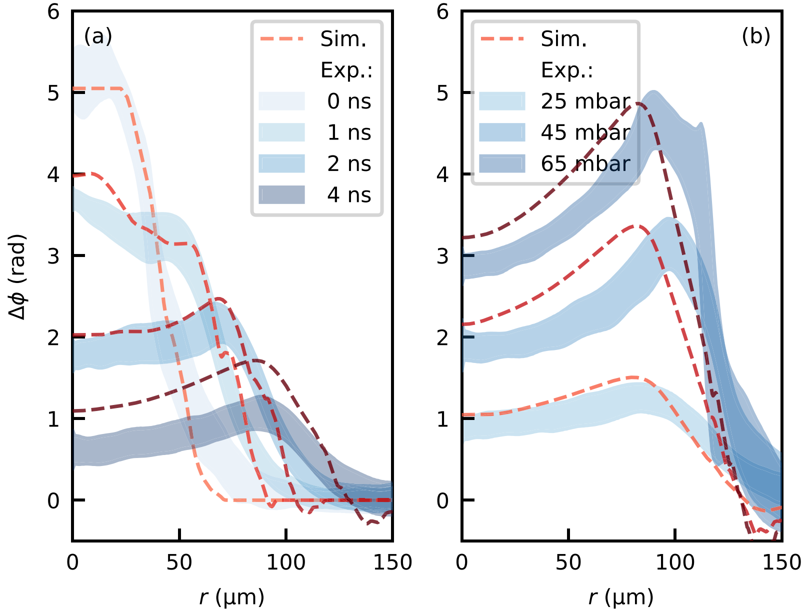
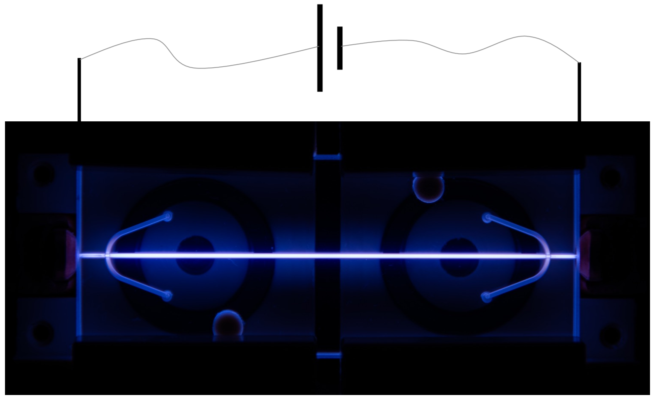
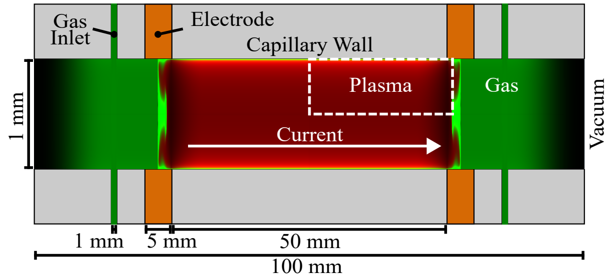


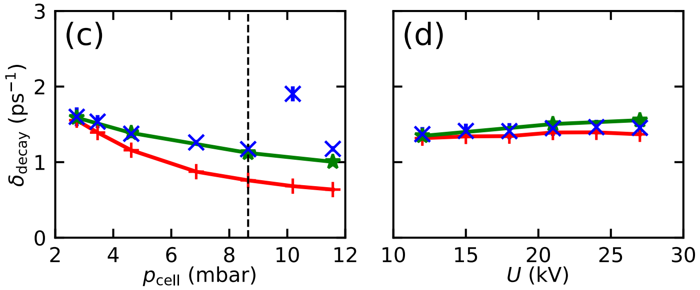


- Plasma discharge capillary

  M. Mewes et al. *in review (2025)*







Benchmarks in the ADVANCE lab at DESY

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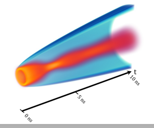
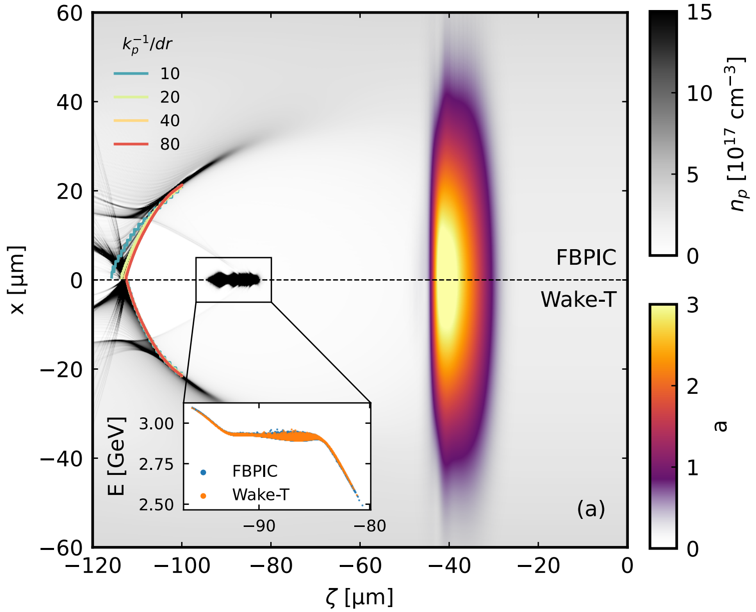


- **Wake-T.** quasistatic & cylindrical wakefield on a laptop

  - 2D (axisymmetric) quasistatic
  - Laser-driven or beam-driven
  - Python, second/minutes on a laptop
  - Adaptive grid & ion motion



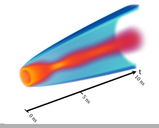
Numerical convergence:
9 hours** on a NVIDIA A100 **GPU

Numerical convergence:
***7 min** on a **CPU** core*

Open-source https://github.com/AngelFP/Wake-T
Ferran Pousa et al., *in preparation*

Codes are being developed to address the needs

➢ **COMSOL - HYQUP.** plasma fluid dynamics



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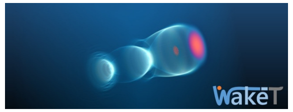
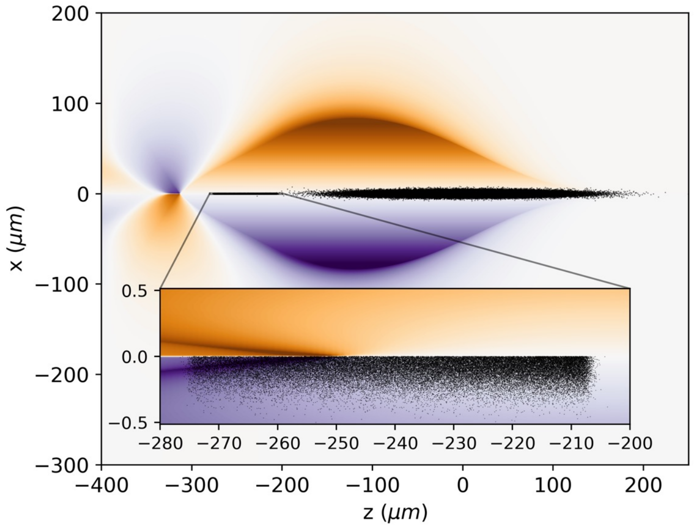


➢ **HiPACE++.** quasistatic PIC in 3D on GPU

- Multi-physics
- C++, laptop to supercomputers
- Mesh refinement

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



Production runs 5 nm resolution take 30 min on 16 GPU-equipped nodes

Codes are being developed to address the needs

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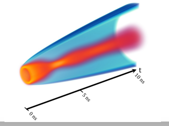

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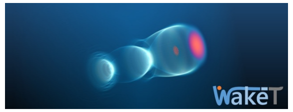
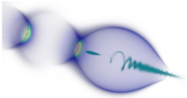
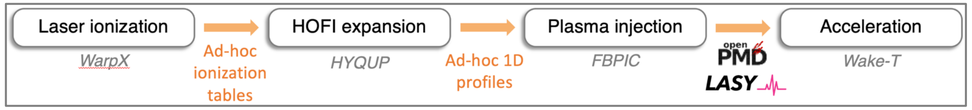


- **HiPACE++.** quasistatic PIC in 3D on GPU

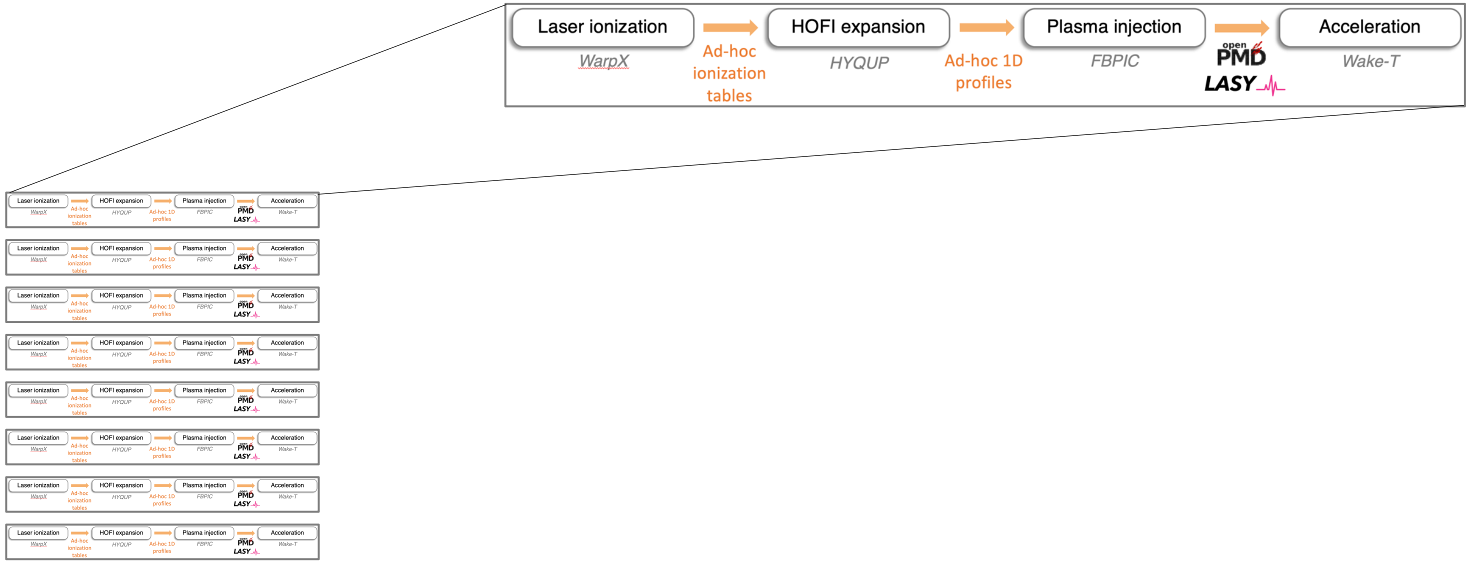


- <u>**Quasi-static codes make challenging simulations very affordable**</u>
    - **5 nanometer** transverse resolution for convergence ion motion
    - Standard HPC allocation allows for **~ 10,000s 3D simulations**

Modular framework for ensemble of s2e simulations: Optimas



Modular framework for ensemble of s2e simulations: Optimas



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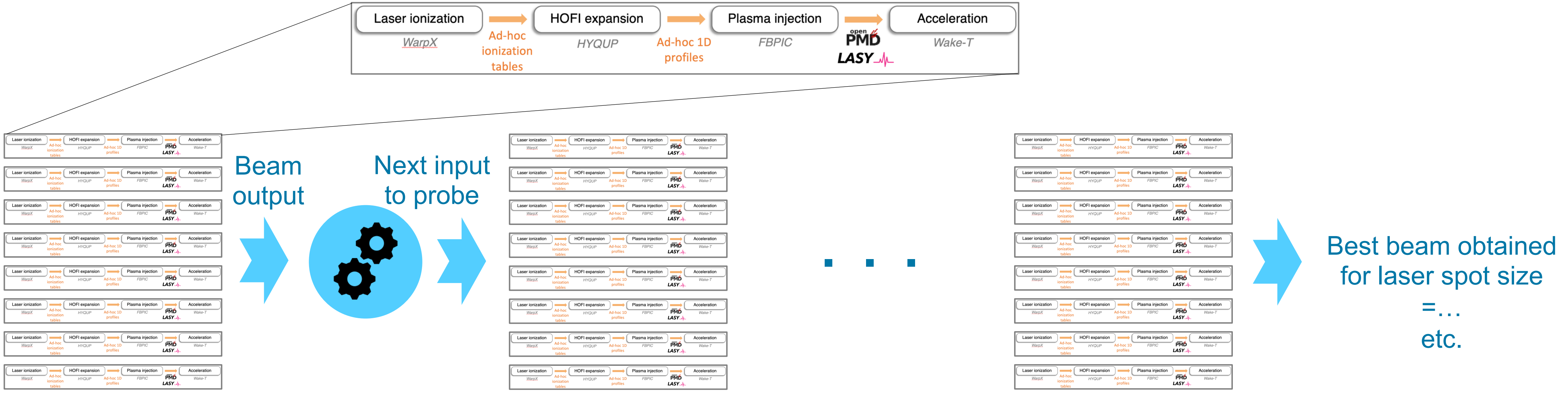

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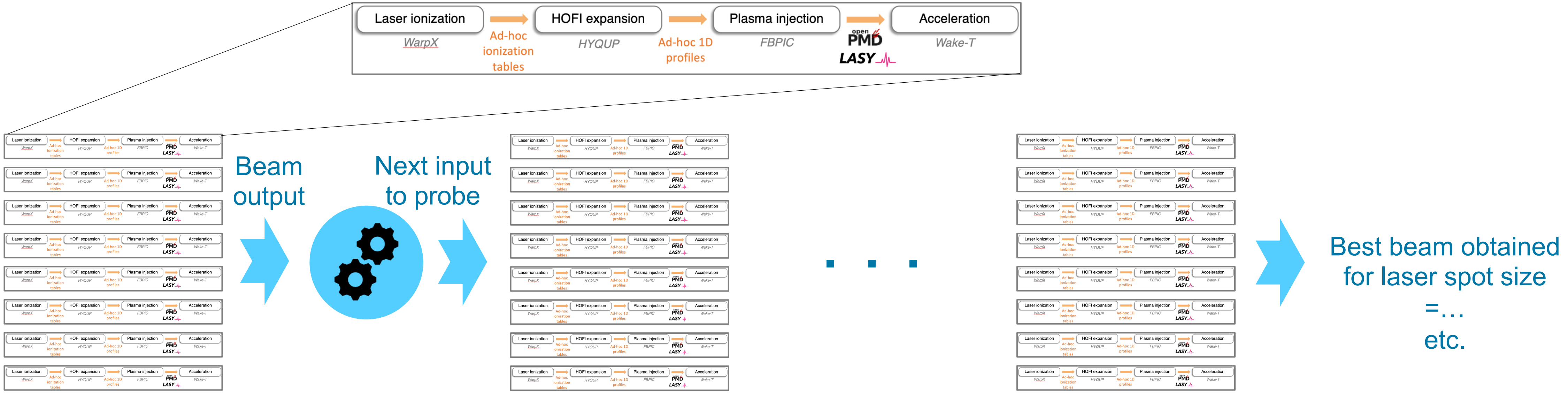
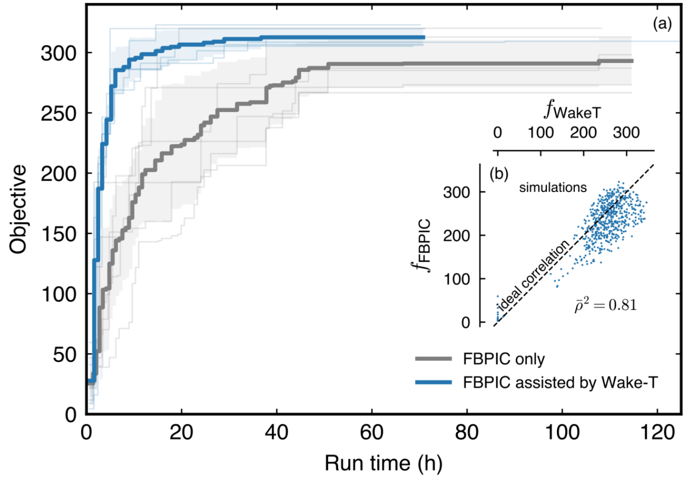




optimas

Optimization **a**t **s**cale

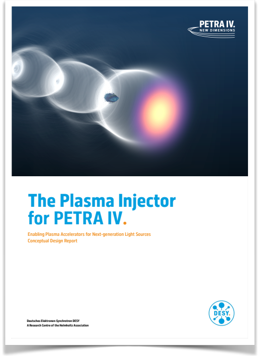
Bayesian Optimization

LBNL, DESY, ANL

https://github.com/optimas-org/optimas

These methods are being used in most of our studies today

- **A. Martinez de la Ossa et al., The Plasma Injector for PETRA IV: Conceptual Design Report**



LPA injection

FBPIC

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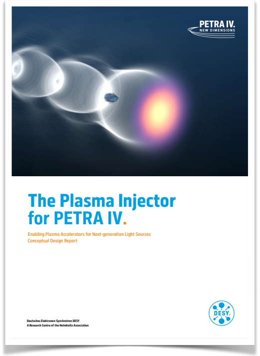

LPA injection → LPA accel.

FBPIC | openPMD LASY | WakeT

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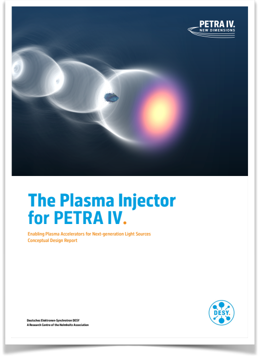

LPA injection → LPA accel. → Beam dyn.

FBPIC | openPMD, LASY | WakeT | Python | Ocelot

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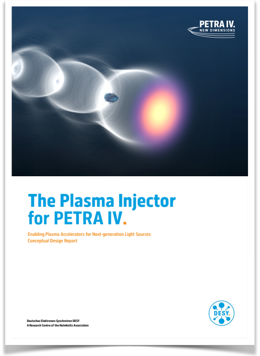

LPA injection → LPA accel. → Beam dyn. → Storage ring

FBPIC

openPMD

LASY

WakeT

Python

Ocelot

Python

Elegant

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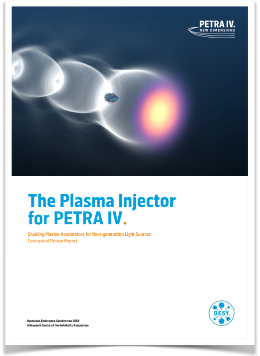

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optimas

LPA injection — FBPIC

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LPA accel. — WakeT

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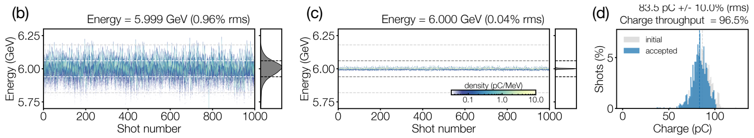
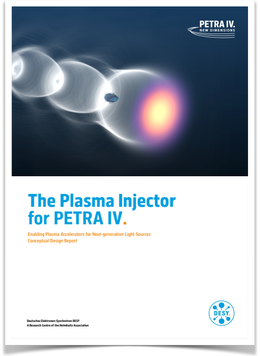
Beam dyn. — Ocelot

Python

Storage ring — Elegant



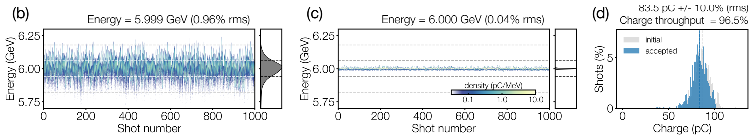
These methods are being used in most of our studies today



- **A. Martinez de la Ossa et al., The Plasma Injector for PETRA IV: Conceptual Design Report**

optimas

LPA injection — FBPIC → openPMD, LASY → LPA accel. — Wake-T → Python → Beam dyn. — Ocelot → Python → Storage ring — Elegant



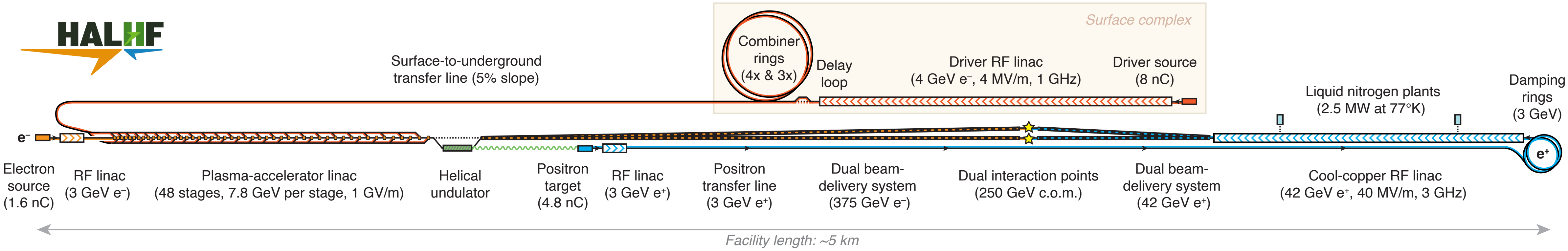
- **Acceleration in HOFI-based LPA**

R. J. Shalloo et al. Controlled Injection in a Laser Plasma Accelerator via an Optically Generated Waveguide Constriction arXiv 2024

optimas

Laser shaping — LASY → openPMD, LASY → Ionization — HiPACE++, WarpX → Python → HOFI hydro. — COMSOL → Python → LPA injection — FBPIC, WarpX → openPMD, LASY → LPA acc. — Wake-T, HiPACE++ → openPMD → Analysis — LASY

Our approach accompanies other efforts in the community



ABEL: The adaptable beginning-to-end linac simulation framework

J. B. B. Chen et al. arXiv:2505.22415 (2025)

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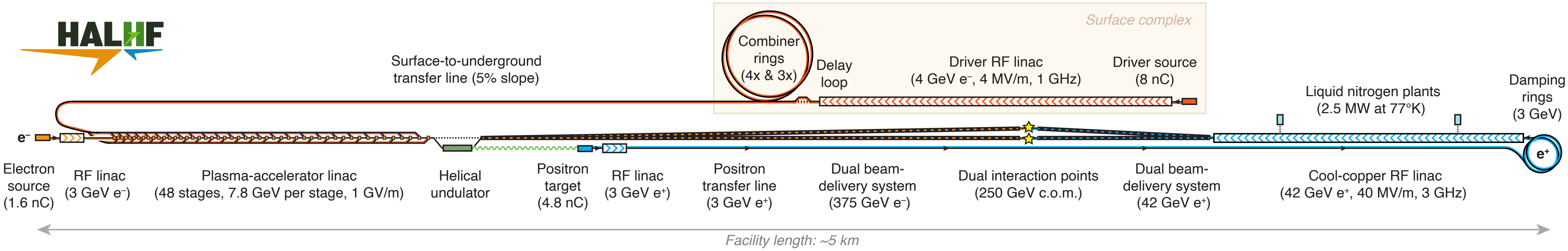

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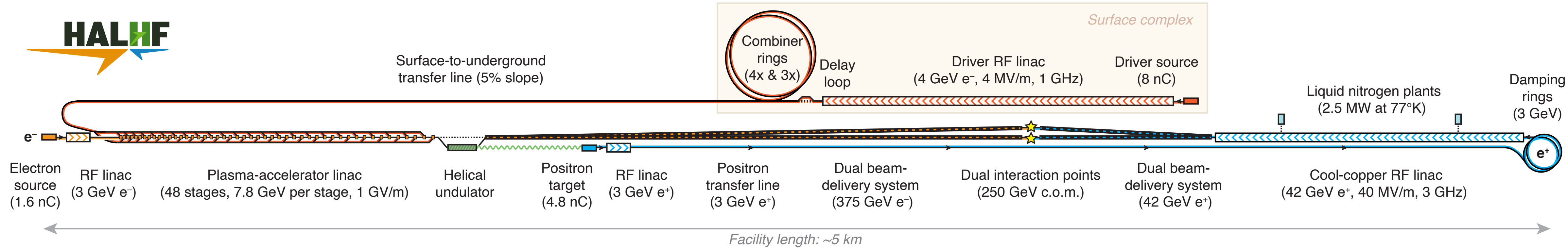

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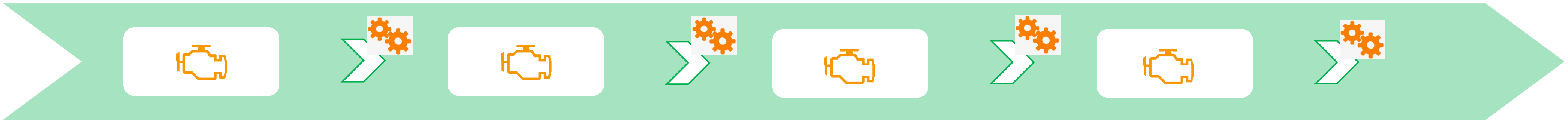

Simulation codes and helper

Thanks to the MPL group at DESY

Andi Maier
group leader

Wim Leemans
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Paul Winkler
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High Average Power LPA

Guido Palmer
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High Energy LPA

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Jon Wood
Team Leader
Beam-Driven Plasma Acceleration

Kris Põder
Team Leader
LPA Applications

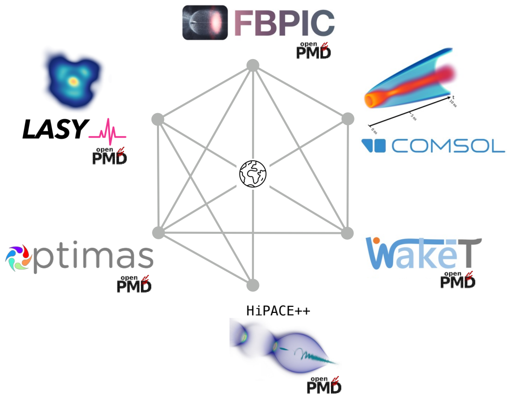
Lutz Winkelmann
Team Leader
Scientific Engineering

Andi Walker
Coordinator
Scientific Infrastructure

Conclusion

- Start-to-end studies are becoming the norm. Often start from experiment.
- Approach with common standard openPMD + targeted libraries LASY & Optimas.
- Modularity important as use cases differ a lot. Very few studies now done with 1 code.
- Compatible with a “backbone” approach e.g. ABEL @ HALHF.
- Next steps: plasma standard, beam manipulation, share methods.
- Don’t worry about the simulation capabilities

Thank you for your attention



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S. Diederichs, A. Ferran Pousa, A. Sinn, J. Osterhoff, A. Martinez de la Ossa, S. Jalas, M. Kirchen, R. Shalloo, X. Hui, M. Formela, S. M. Mewes, J. M. Garland, M. Huck, H. Jones, G. Loisch, A. R. Maier, T. Parikh, S. Wesch, J. C. Wood

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