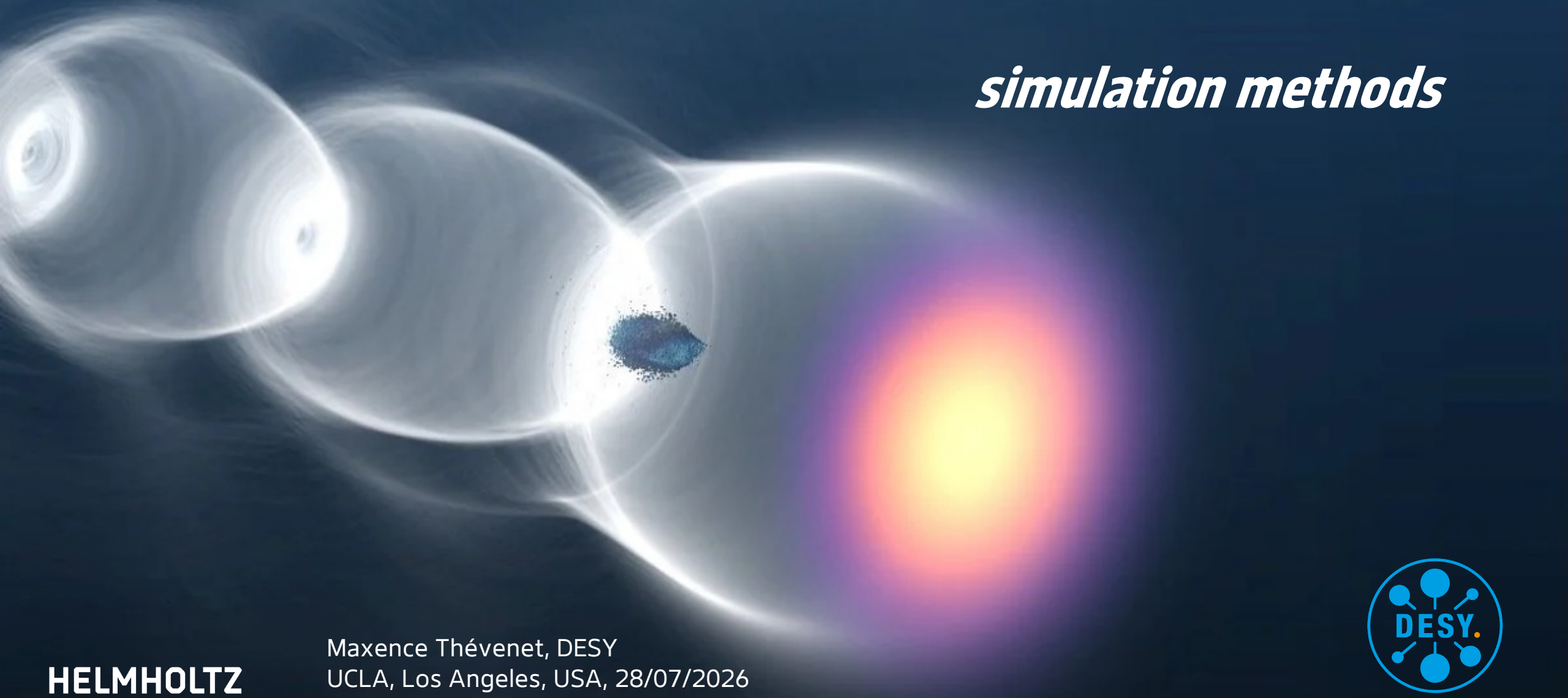


THE PLASMA INJECTOR FOR PETRA IV

simulation methods



HELMHOLTZ

Maxence Thévenet, DESY
UCLA, Los Angeles, USA, 28/07/2026



Plasma acceleration group MPL



Andi Maier
group leader

Wim Leemans
division director



Paul Winkler
Coordinator
Plasma Injector



Manuel Kirchen
Team Leader
High Average
Power LPA



Guido Palmer
Team Leader
Laser
Development



Rob Shalloo
Team Leader
High Energy LPA



Maxence Thévenet
Team Leader
Theory & Simulations



Jon Wood
Team Leader
Beam-Driven
Plasma Acceleration

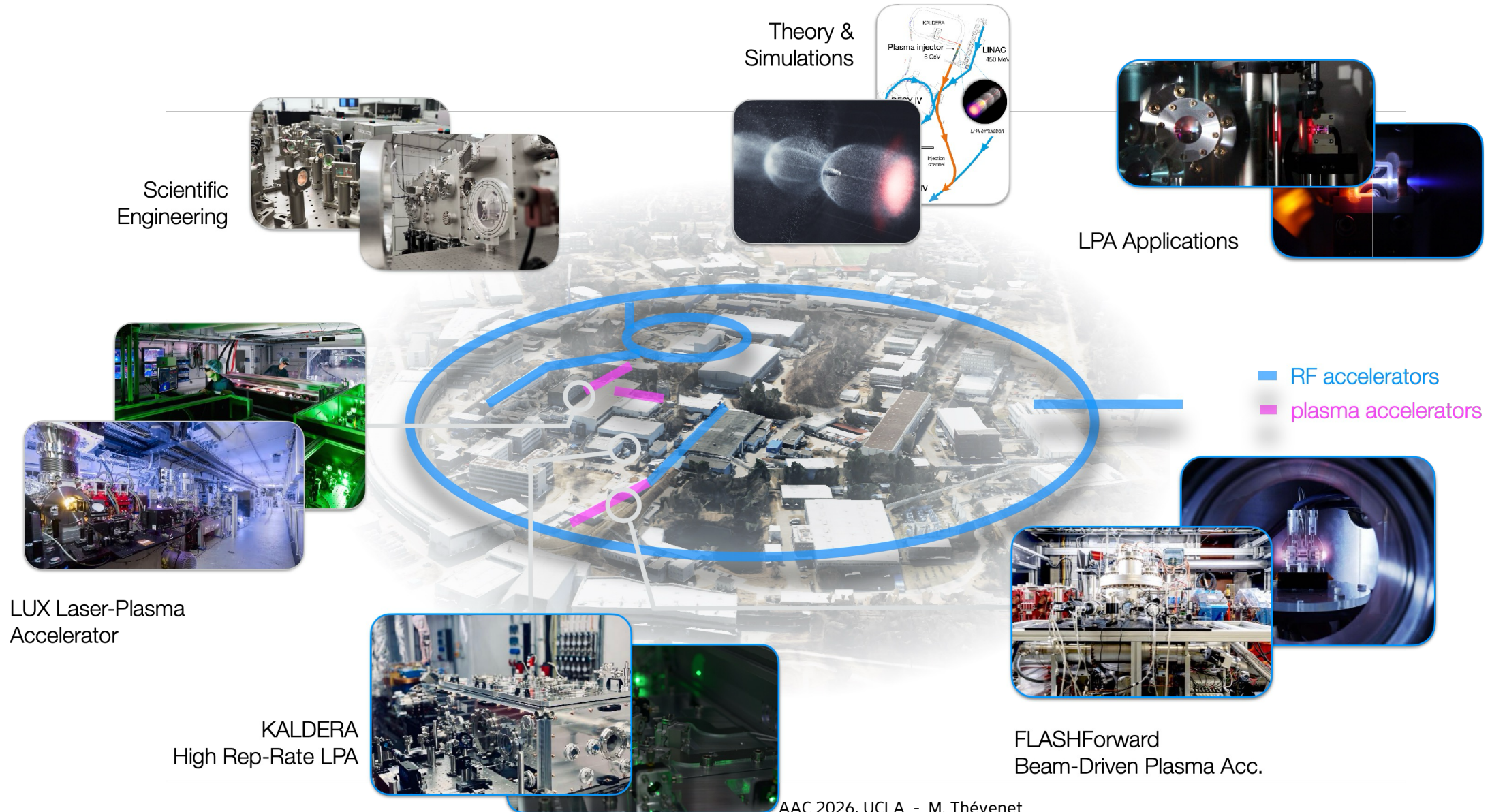


Lutz Winkelmann
Team Leader
Scientific
Engineering



Andi Walker
Coordinator
Scientific
Infrastructure

Plasma acceleration at DESY: R&D activities





PIP4 simulation

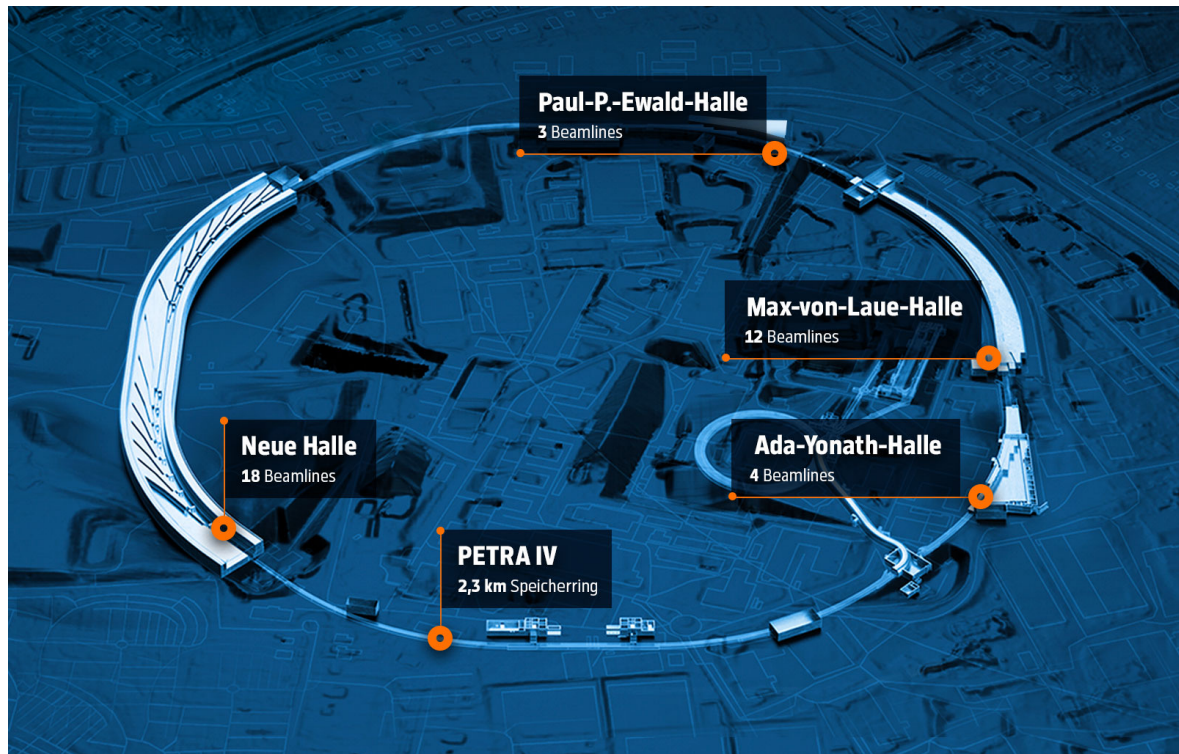
- **The plasma injector for Petra IV**
Science case, Conceptual Design Report, open questions
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3D simulations for misalignment in waveguide
- **How to make the plasma waveguide**
Simulating HOFI + LPA

Petra IV: next-generation synchrotron source

Upgrade of the 2.3-km Petra III storage ring for synchrotron radiation

Orders-of-magnitude increase in X-ray brightness

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



<https://bib-pubdb1.desy.de/record/426140/files/DESY-PETRAIV-Conceptual-Design-Report.pdf>

https://www.desy.de/research/facilities_projects/petra_iv

Petra IV: next-generation synchrotron source

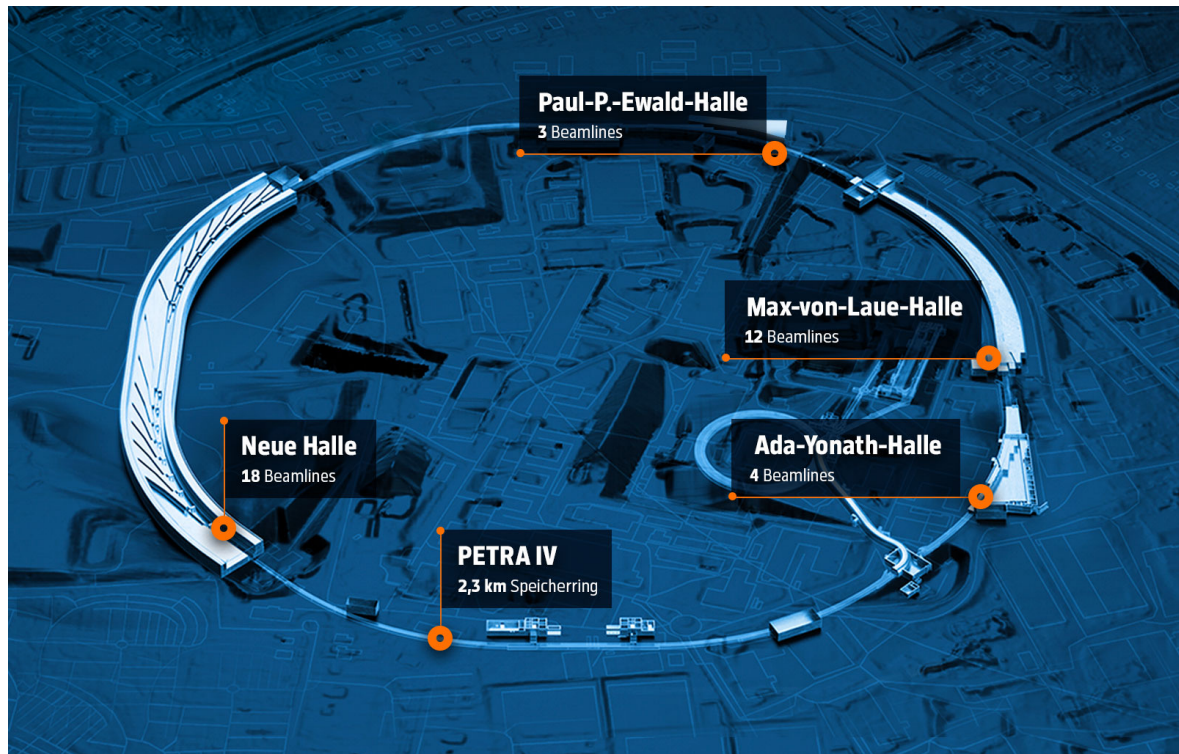


A. Martinez de la Ossa

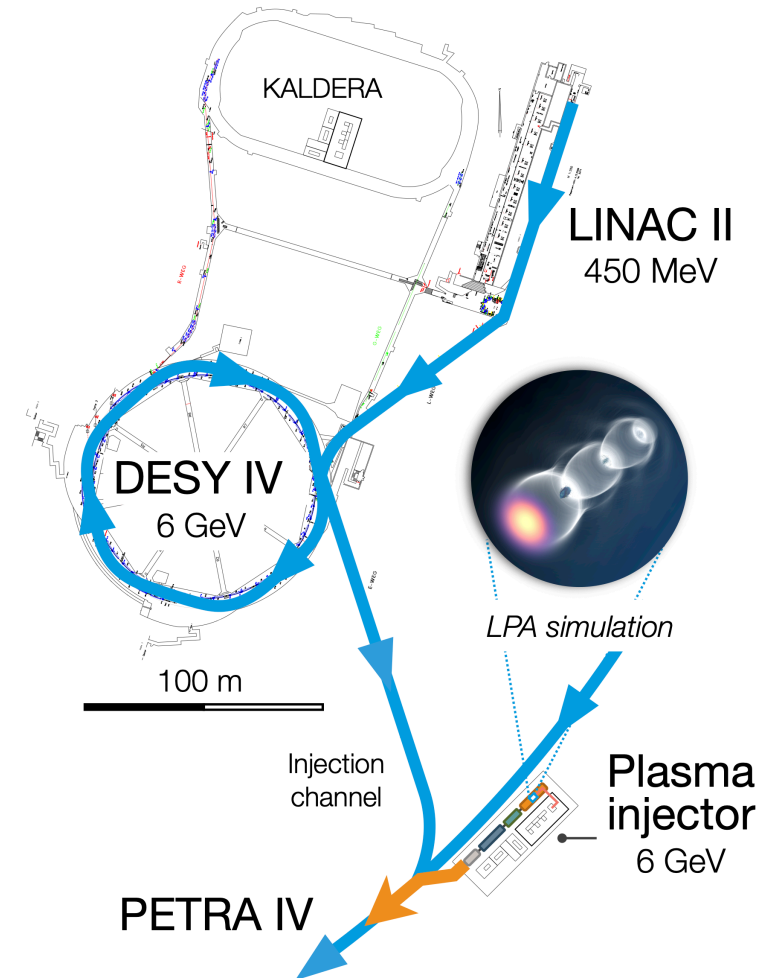
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Can we do it with plasma?



<https://bib-pubdb1.desy.de/record/426140/files/DESY-PETRAIV-Conceptual-Design-Report.pdf>

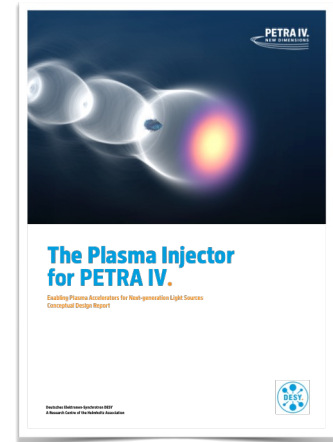
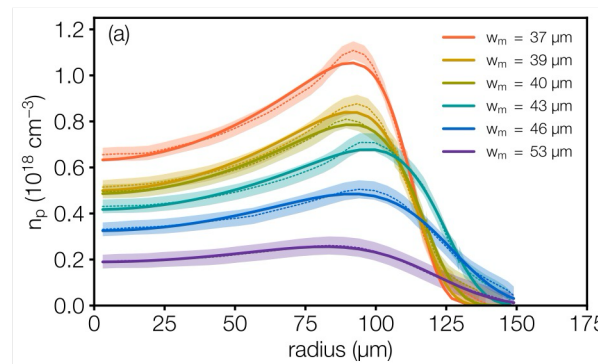
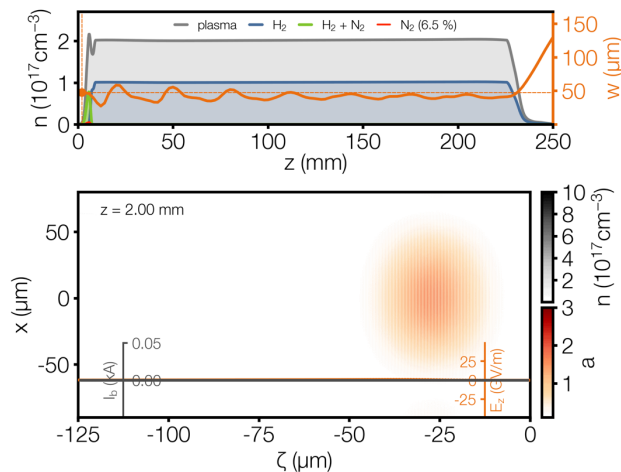
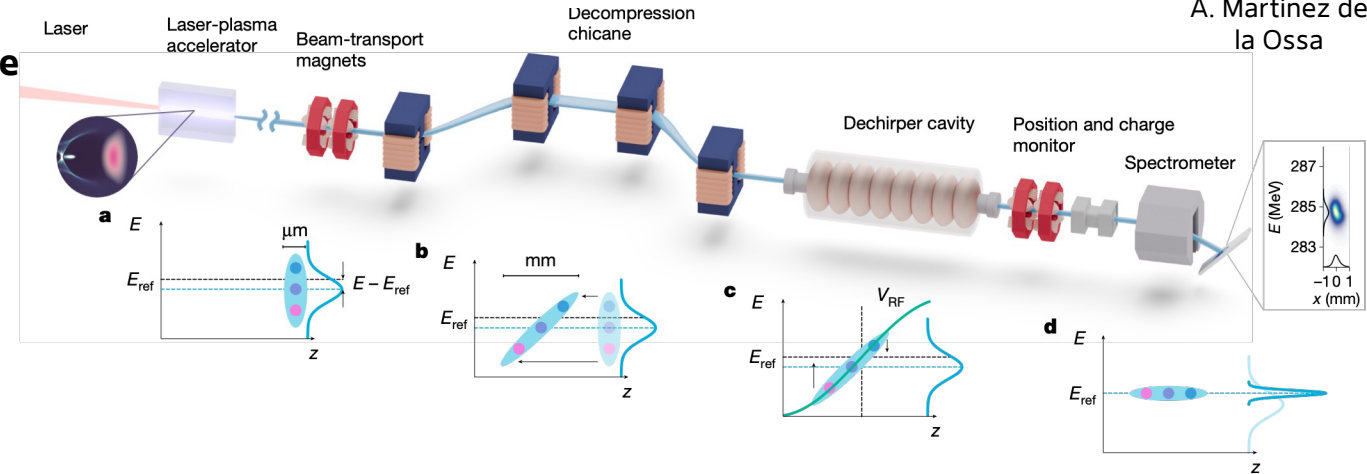
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LUX design + energy compression beamline



A. Martinez de la Ossa

- Challenges: 6 GeV beams, few nC/s, **1% energy acceptance**
- LPA built on LUX design for reliability
- HOPI channel for energy efficiency
- Energy Compression Beamline
- 30 Hz with filling pattern



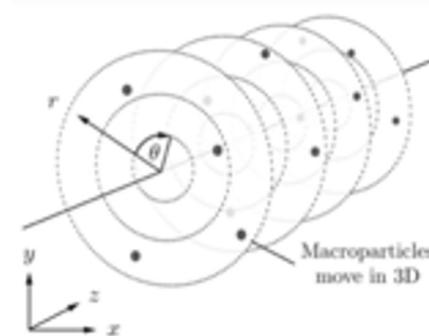
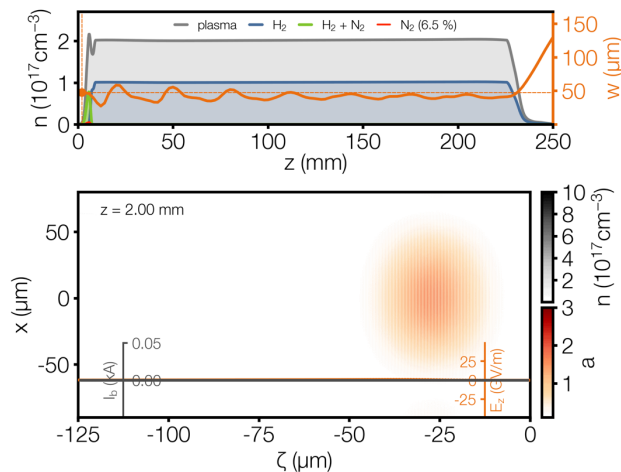
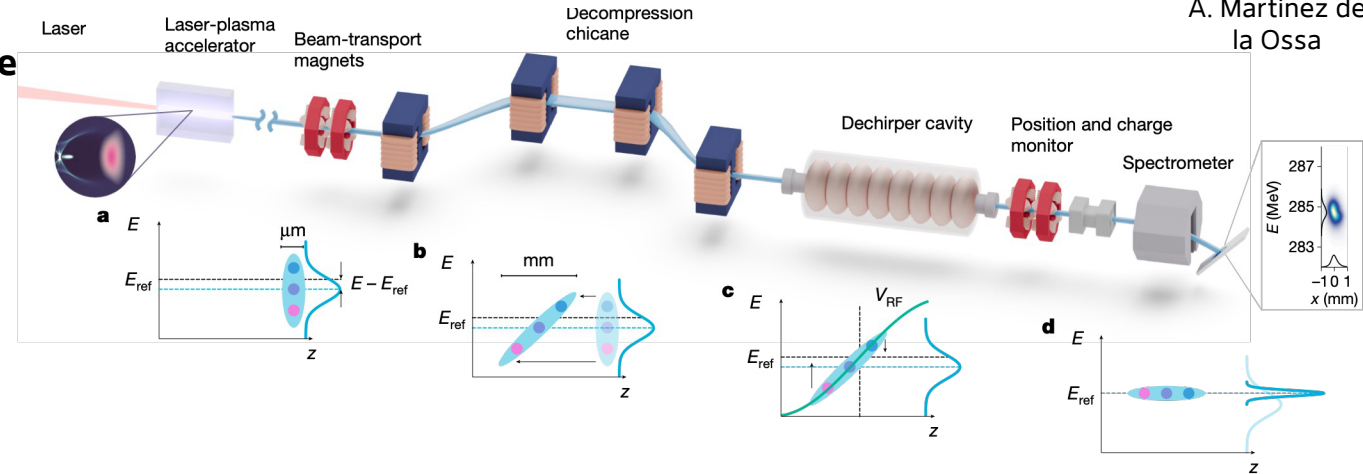
M. Kirchen *et al.* *PRL* 126.17 (2021)
 S. Antipov *et al.*, 24, *PRAB* 111301 (2021)
 A. Ferran Pousa *et al.* *PRL* 129, 094801 (2021)
<https://github.com/fbpic/fbpic>
 R. Lehe *et al.*, *Comput. Phys. Commun.* 203 (2016)
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LUX design + energy compression beamline



A. Martinez de la Ossa

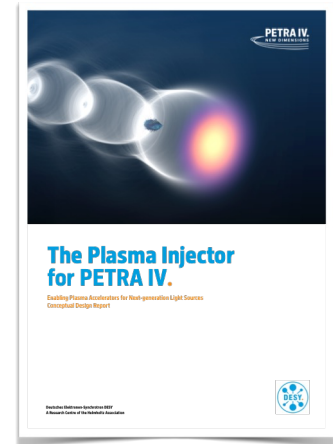
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Simulations with



2D cylindrical (quasi-3D) PIC



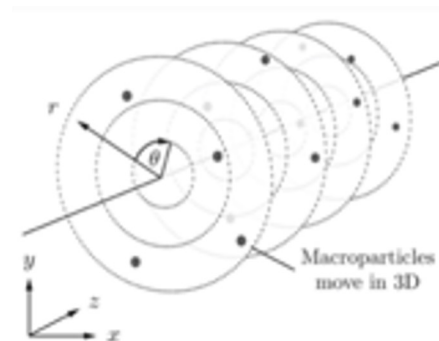
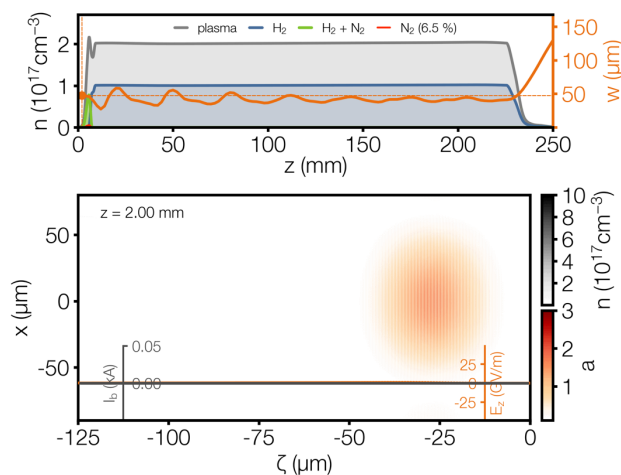
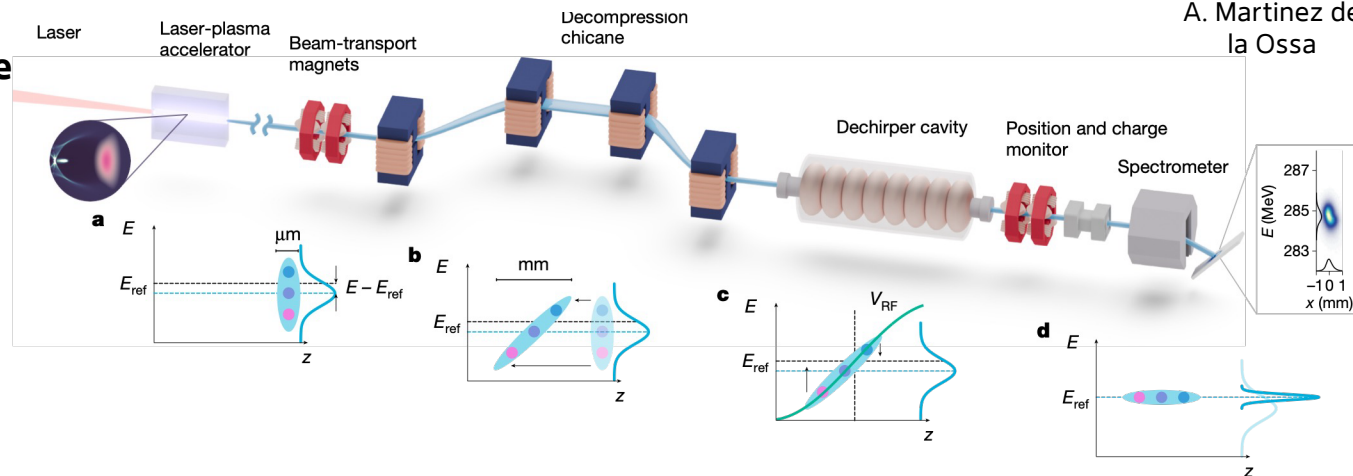
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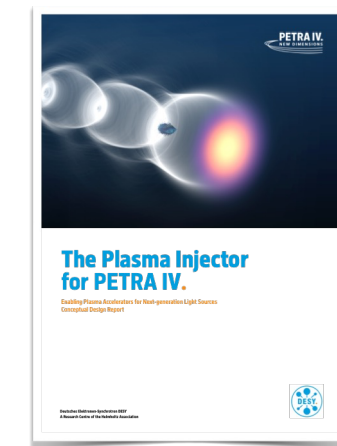


2D cylindrical (quasi-3D) PIC

Open questions

- What misalignment can we tolerate between HOFI and LPA laser?
- Can the injection method be combined with HOFI?

M. Kirchen *et al.* *PRL* 126.17 (2021)
 S. Antipov *et al.*, 24, *PRAB* 111301 (2021)
 A. Ferran Pousa *et al.* *PRL* 129, 094801 (2021)
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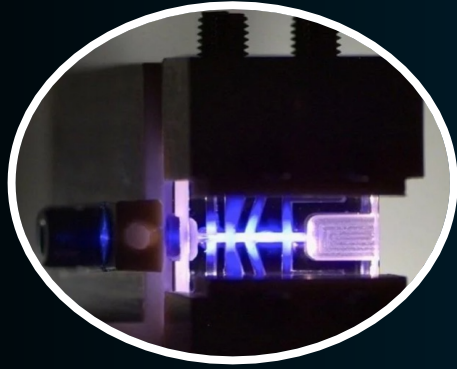


<https://doi.org/10.3204/PUBDB-2024-06078>

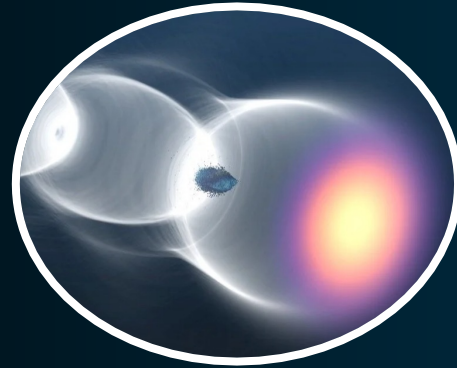


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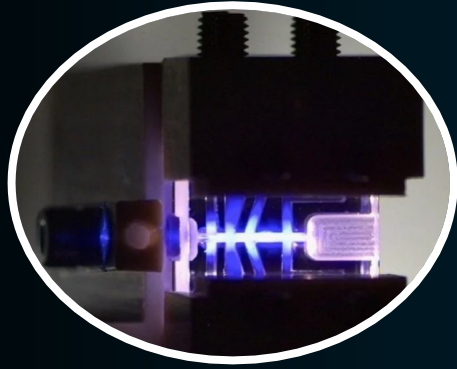
Shape the source



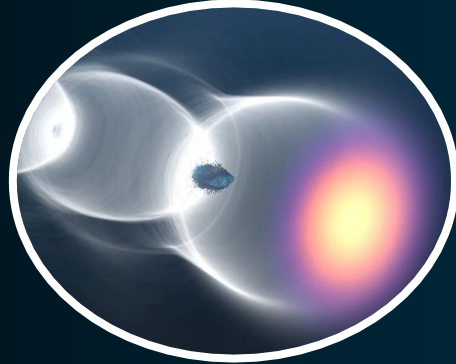
Do the wakefield



Use the beam



Shape the source



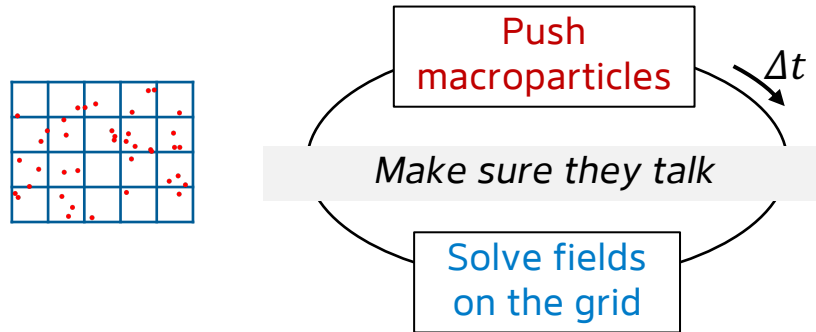
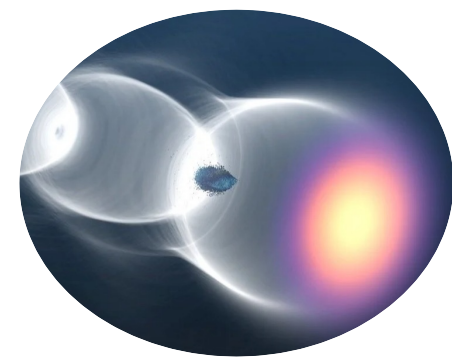
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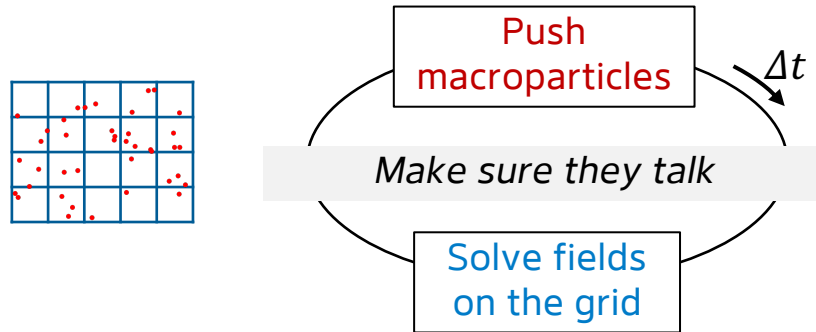
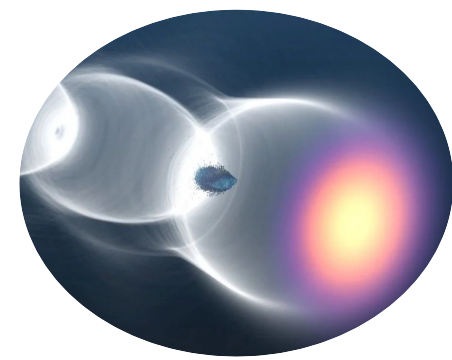
*From the market
Cheetah, Ocelot, Elegant, Genesis, ..*

Do the wakefield: 2 flavors of PIC available



- ❖ **Particle-In-Cell is expensive**
1000 compute units for hours is common
- ❖ **plasma acceleration requires many (millions) timesteps**
CFL with small timesteps vs. long accelerating distance
- ❖ **Solution 1: the boosted frame** J.-L. Vay PRL **98**, 130405 (2007)
Reduce scale discrepancy with a Lorentz transform
- ❖ **Solution 2: the quasistatic approximation** P. Mora and T. M. Antonsen PRE **53** (1996)
Calculate the plasma response assuming the laser is frozen: $z_R \gg \lambda_p$
Fast and accurate but cannot capture injection

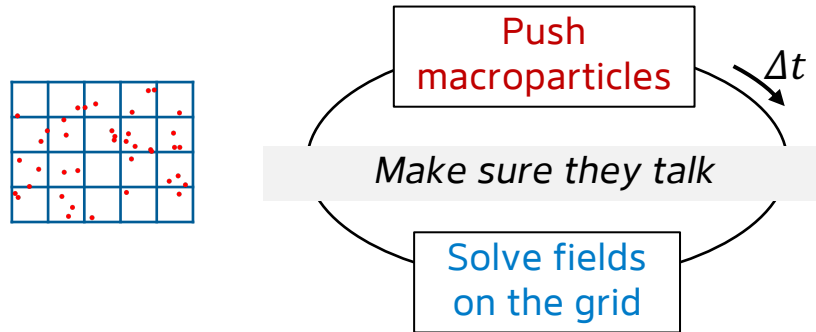
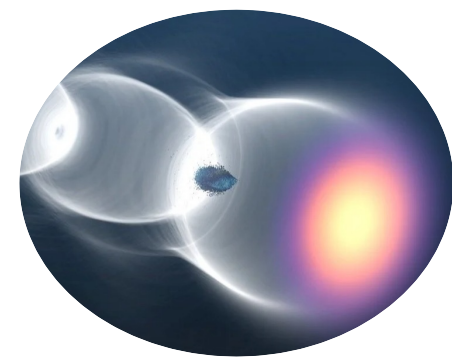
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Courtesy of J.-L. Vay

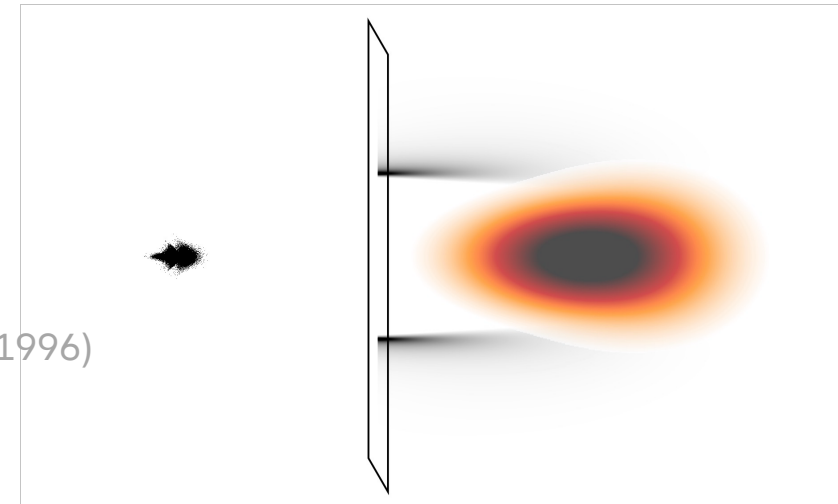
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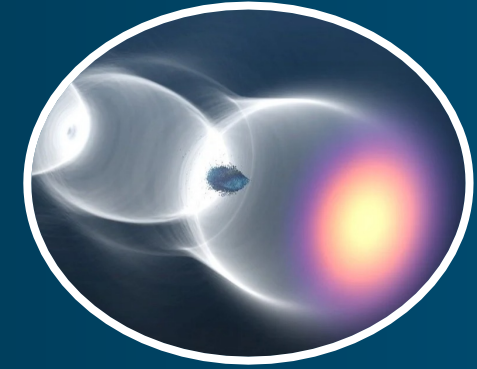


Courtesy of J.-L. Vay

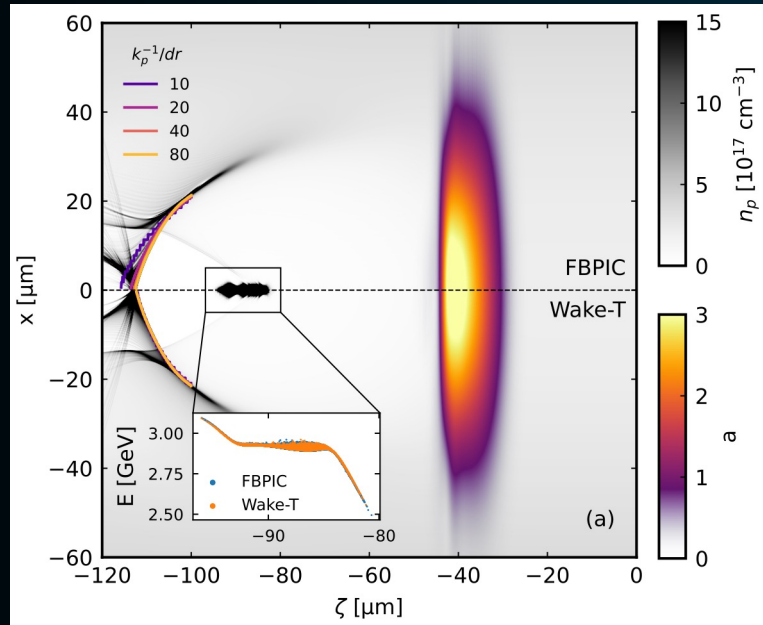
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Wake-T: cylindrical + quasistatic for fast runs



Hours on A100



Minutes on laptop



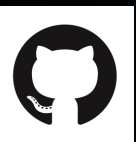
Ángel Ferran Pousa



I-Lin Yeh

Accurate simulations within minutes on a laptop

- 2D RZ + quasistatic
- Laser-driven or beam-driven
- Adaptive grid & ion motion



<https://github.com/Wake-T/Wake-T>

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

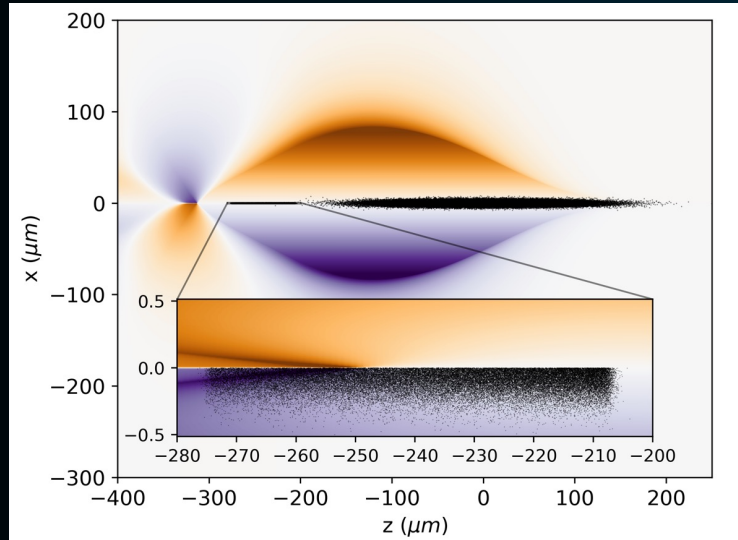
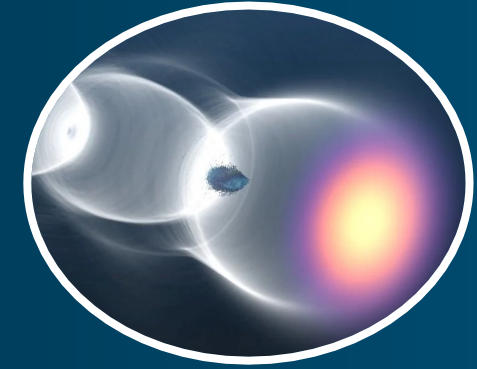
C. Benedetti et al., PPCF 60 014002 (2018)

P. Baxevanis and G. Stupakov, PRAB 21 (2018)

A. Ferran Pousa et al., *accepted in CPC*

DESY

HiPACE++: 3D quasistatic PIC at scale



Affordable 3D simulations on top supercomputers

- Optimized for GPU computing
- Little sister of WarpX, C++, built on AMReX
- Beam-driven & laser-driven
- Multiphysics (collisions, ionization, ...)



Alexander Sinn

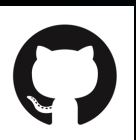


Xingjian Hui



Emanuele Marchetti

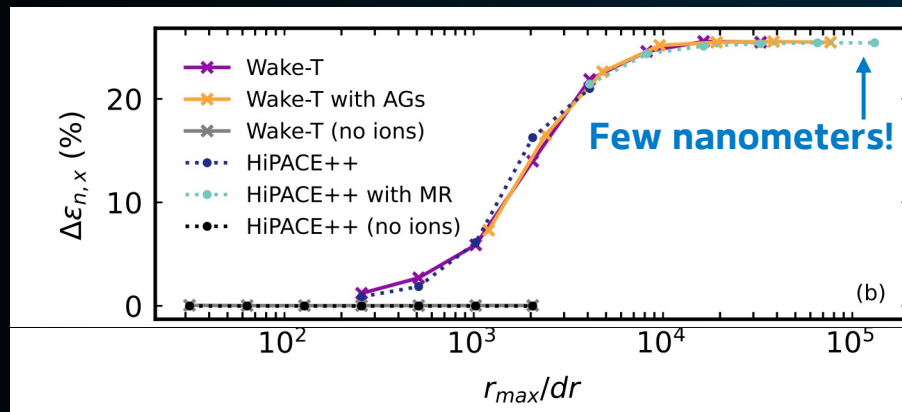
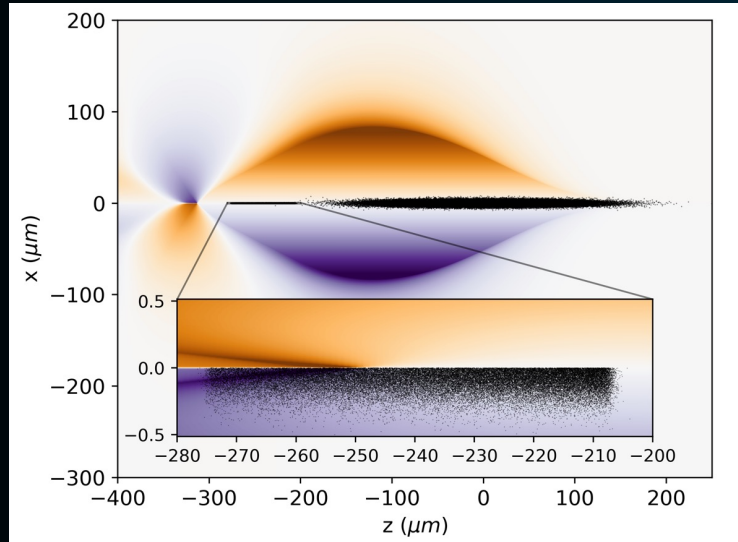
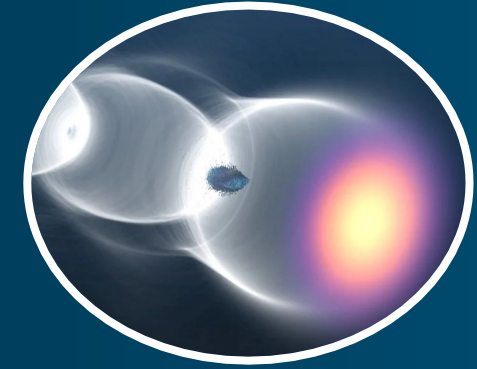
LBL AMP + BELLA
CEA



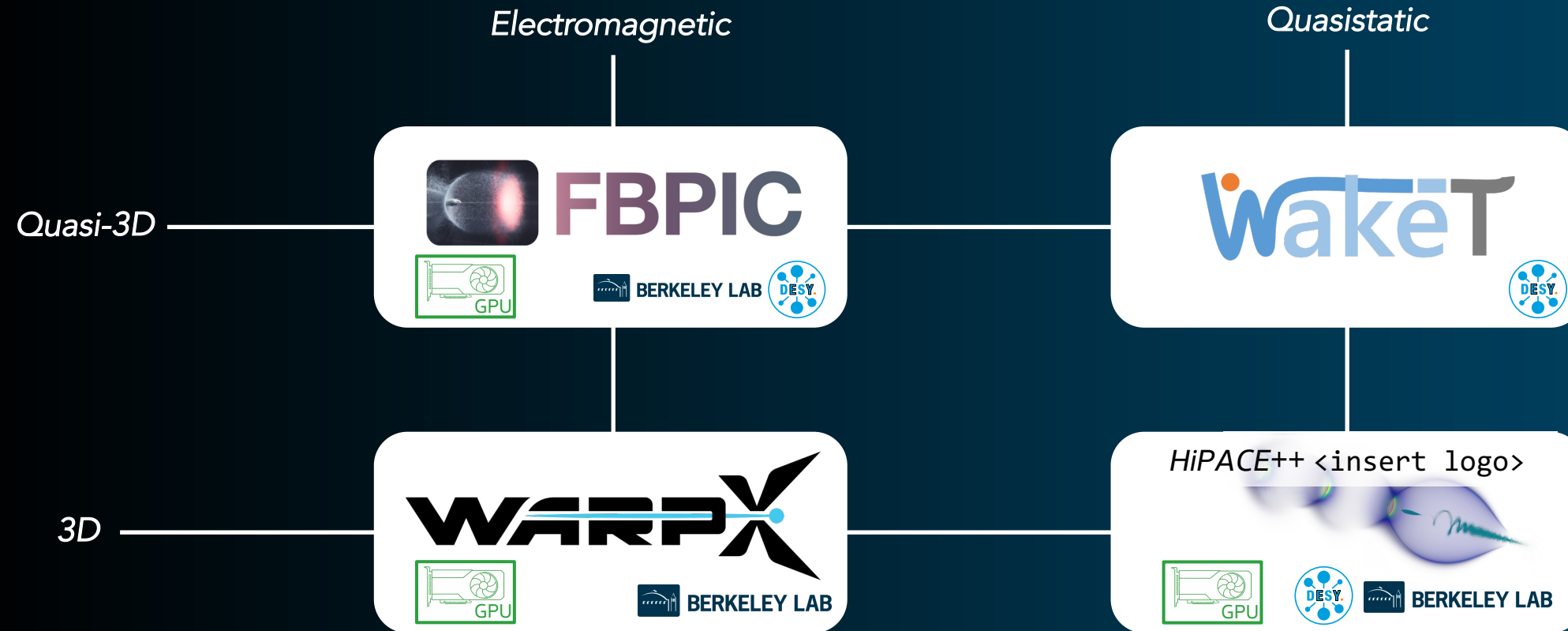
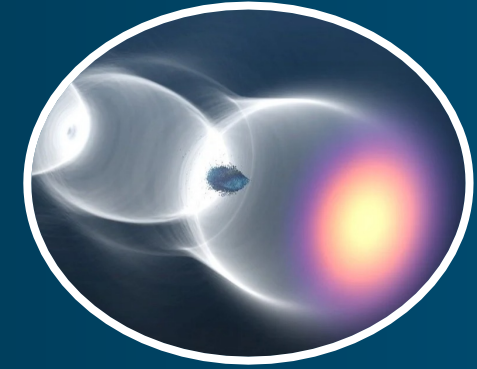
<https://github.com/Hi-PACE/hipace>

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

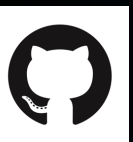
Both codes agree on challenging simulations



An array of open-source GPU-capable codes



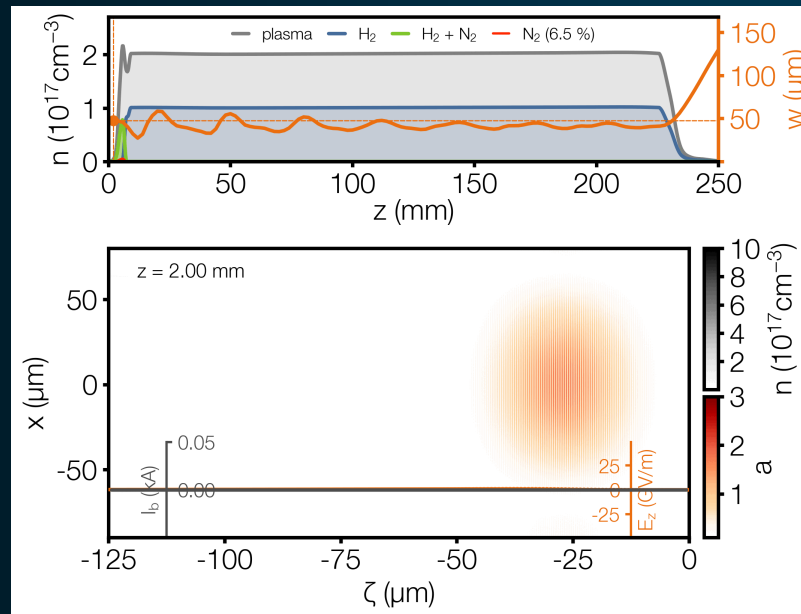
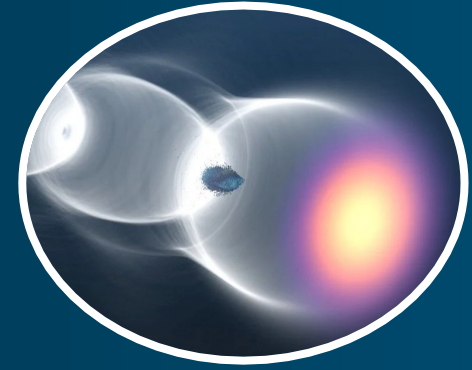
Other codes are available: OSIRIS4.0, PIconGPU, SMILEI, VSIM, QPAD, QuickPIC, WAND-PIC, ...



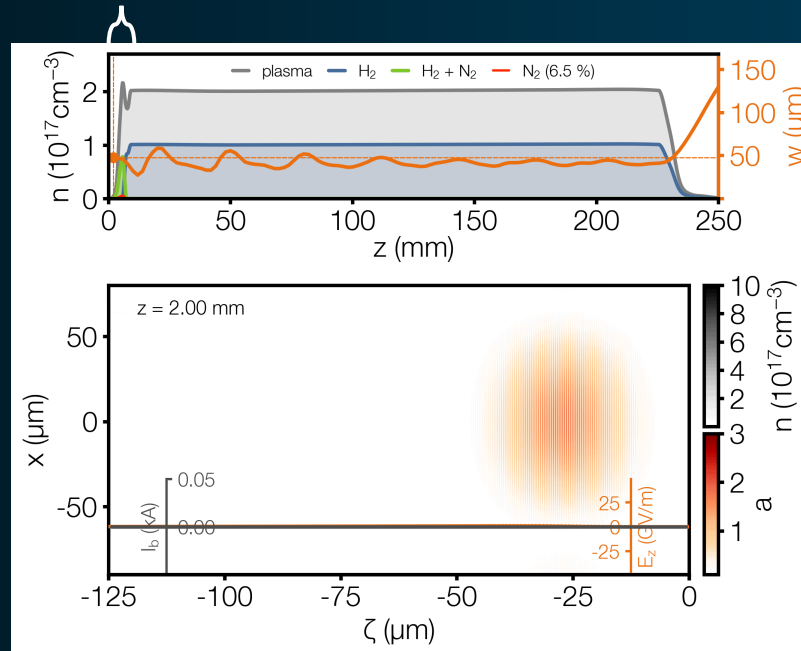
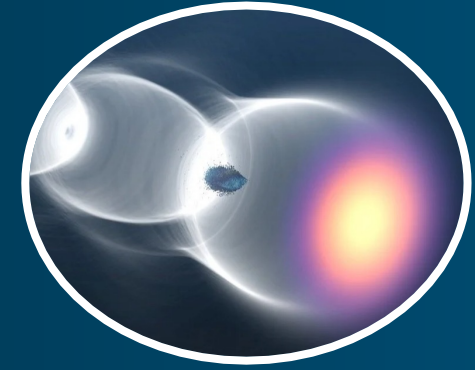
DESY.

<https://github.com/Wake-T/Wake-T>
<https://github.com/fbpic/fbpic>
<https://github.com/Hi-PACE/hipace>
<https://github.com/ECP-WarpX/WarpX>

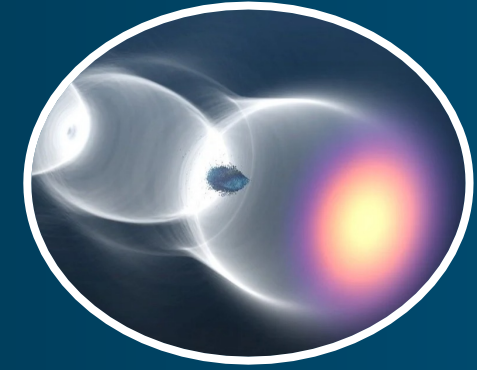
Can we plug codes together?



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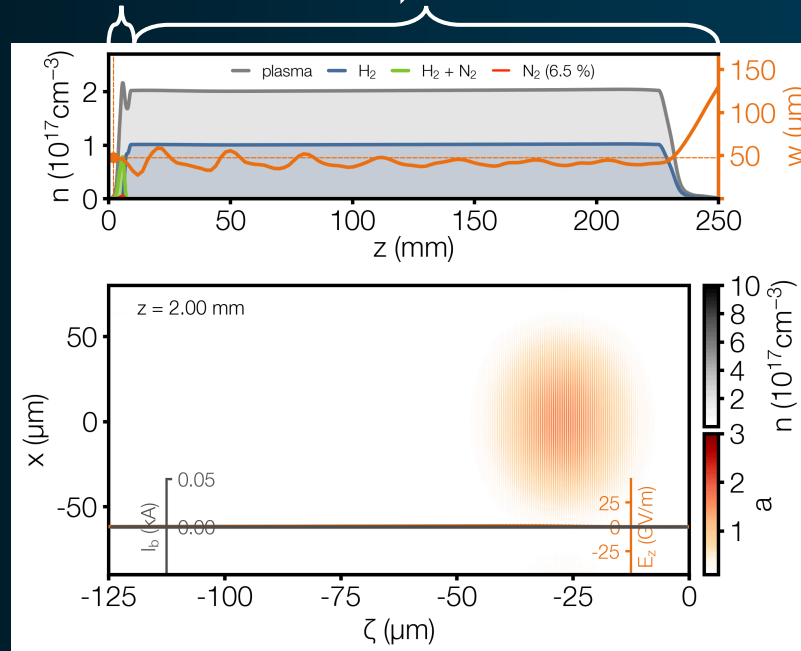


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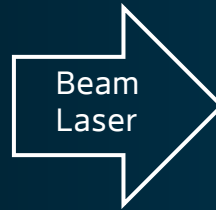
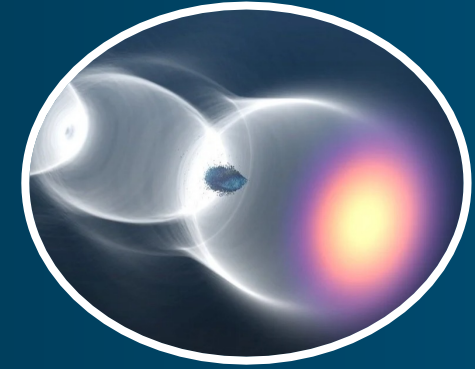


Beam
Laser

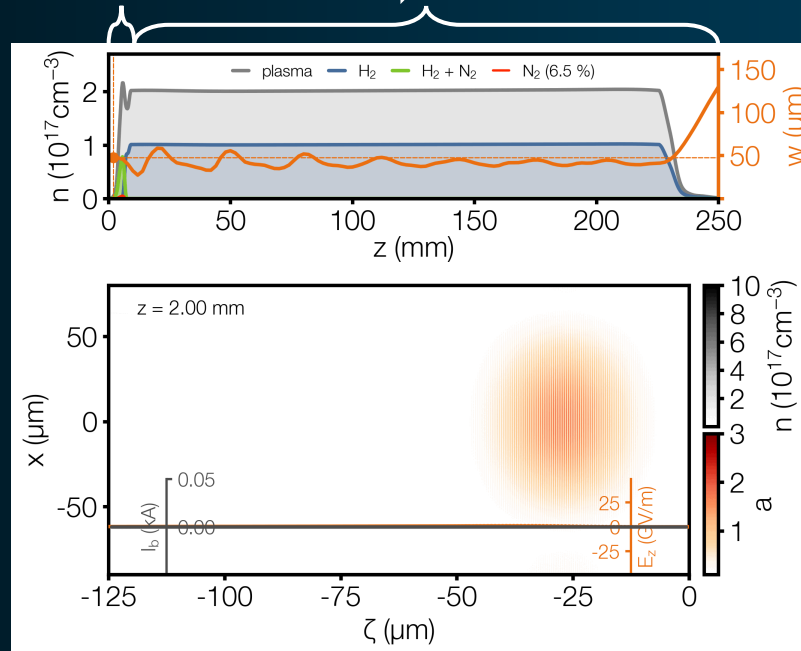
WakēT



Can we plug codes together?



Waket



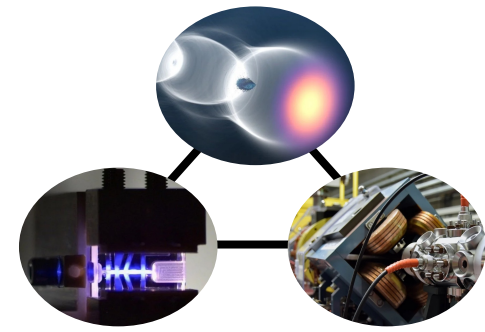
Beam ✓

Laser ✗

Electric field vs. vector potential
Full field vs. envelope

...yes with a bit of help

LASY LAser manipulations made eaSY



- 3D Cartesian or cylindrical
- Envelope representation
- Readers from measurement (INSIGHT, etc.)
- Python, open-source
- Converters (field/envelope, E/A)

imports

physical
description
of laser

simulation
parameters +
create object

propagate
+ plot / save

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

wavelength = 800e-9 # Laser wavelength in meters
polarization = (1, 0) # Linearly polarized in the x direction
energy = 1.5 # Energy of the laser pulse in joules
spot_size = 25e-6 # Waist of the laser pulse in meters
pulse_duration = 30e-15 # Pulse duration of the laser in seconds
t_peak = 0.0 # Location of the peak of the laser pulse in time

laser_profile = GaussianProfile(wavelength, polarization, energy, spot_size, pulse_duration, t_peak)

dimensions = "rt" # Use cylindrical geometry
lo = (0, -2.5 * pulse_duration) # Lower bounds of the simulation box
hi = (5 * spot_size, 2.5 * pulse_duration) # Upper bounds of the simulation box
num_points = (300, 500) # Number of points in each dimension

laser = Laser(dimensions, lo, hi, num_points, laser_profile)

laser.propagate(-2e-6) # Propagate the pulse upstream of the focal plane

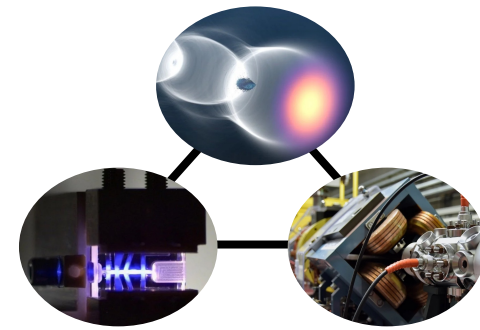
laser.show(envelope_type='intensity') # Plot the intensity profile of the laser pulse
laser.write_to_file('test_laser', 'h5') # Save the laser to file for use in a simulation
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Rob Shalloo

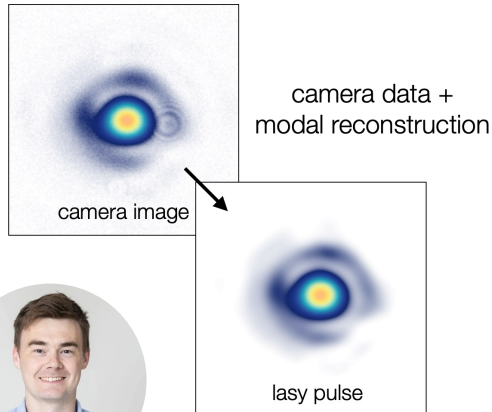


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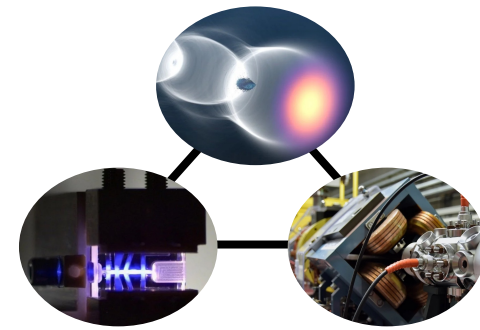
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BERKELEY LAB

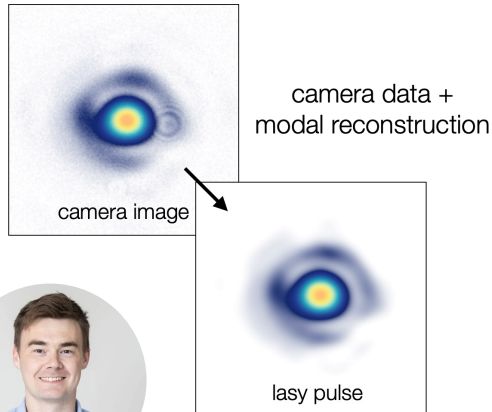


LASY LAser manipulations made eaSY



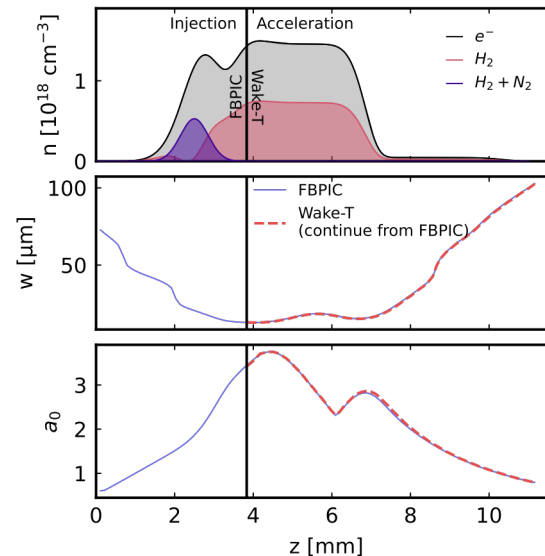
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```
from lasy.laser import Laser
from lasy.profiles.gaussian_profile import GaussianProfile

wavelength = 800e-9 # Laser wavelength in meters
polarization = (1, 0) # Linearly polarized in the x direction
energy = 1.5 # Energy of the laser pulse in joules
spot_size = 25e-6 # Waist of the laser pulse in meters
pulse_duration = 30e-15 # Pulse duration of the laser in seconds
t_peak = 0.0 # Location of the peak of the laser pulse in time

laser_profile = GaussianProfile(wavelength, polarization, energy, spot_size, pulse_duration, t_peak)

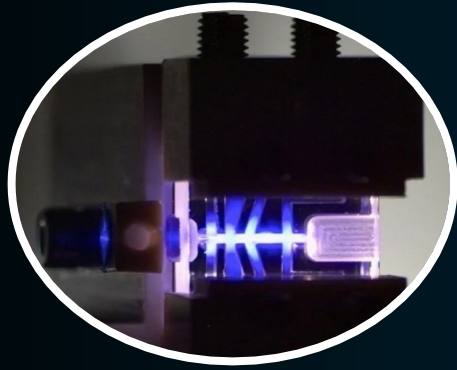
dimensions = "rt" # Use cylindrical geometry
lo = (0, -2.5 * pulse_duration) # Lower bounds of the simulation box
hi = (5 * spot_size, 2.5 * pulse_duration) # Upper bounds of the simulation box
num_points = (300, 500) # Number of points in each dimension

laser = Laser(dimensions, lo, hi, num_points, laser_profile)

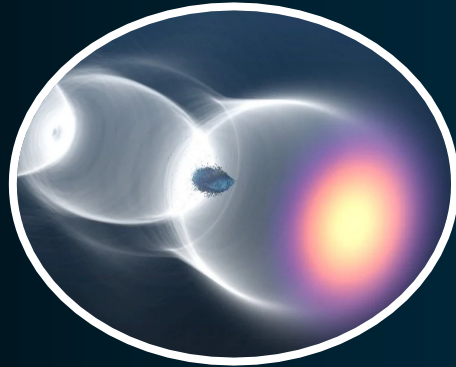
laser.propagate(-2e-6) # Propagate the pulse upstream of the focal plane

laser.show(envelope_type='intensity') # Plot the intensity profile of the laser pulse
laser.write_to_file('test_laser', 'h5') # Save the laser to file for use in a simulation
```





Shape the source

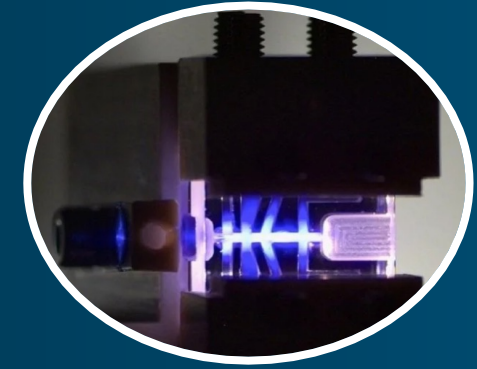


Do the wakefield



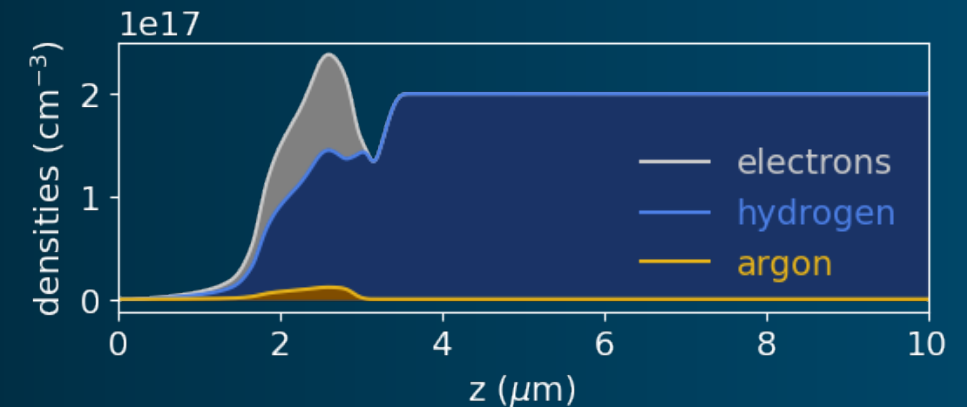
Use the beam

Shaping the source: hydrodynamics



Transverse tailoring for laser waveguide

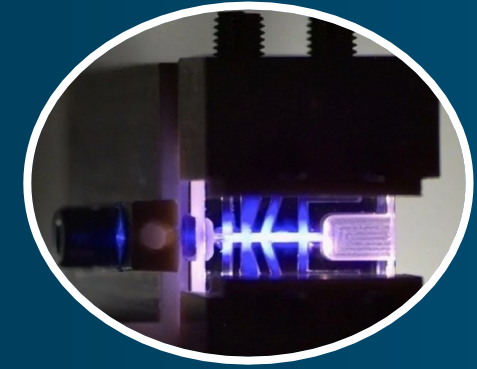
Longitudinal tailoring for injection & matching



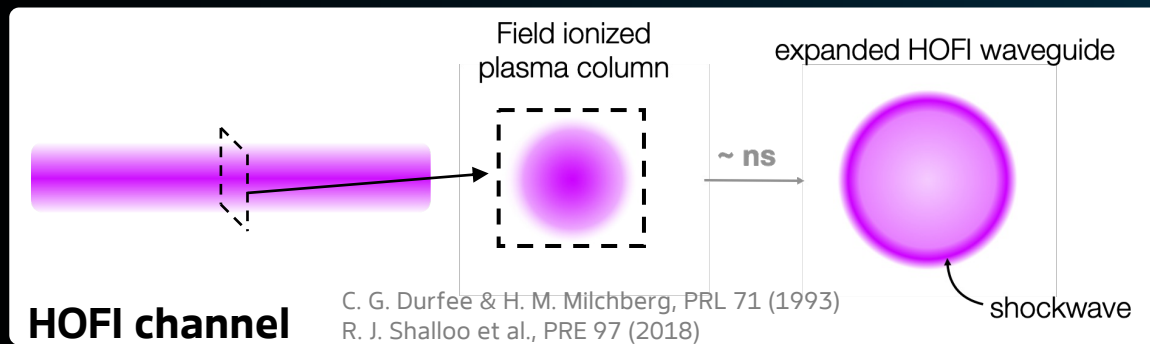
Simulation methods

- Gas flow: existing solutions (ANSYS, COMSOL)
- Plasma shaping: hydrodynamics

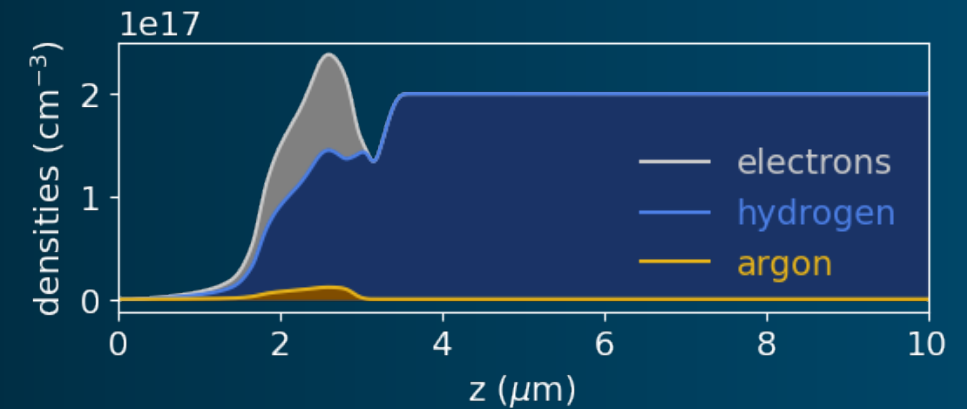
Shaping the source: hydrodynamics



Transverse tailoring for laser waveguide



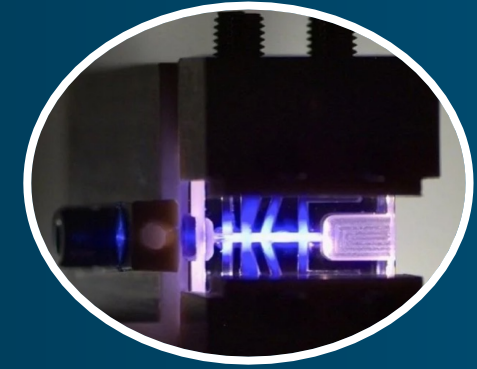
Longitudinal tailoring for injection & matching



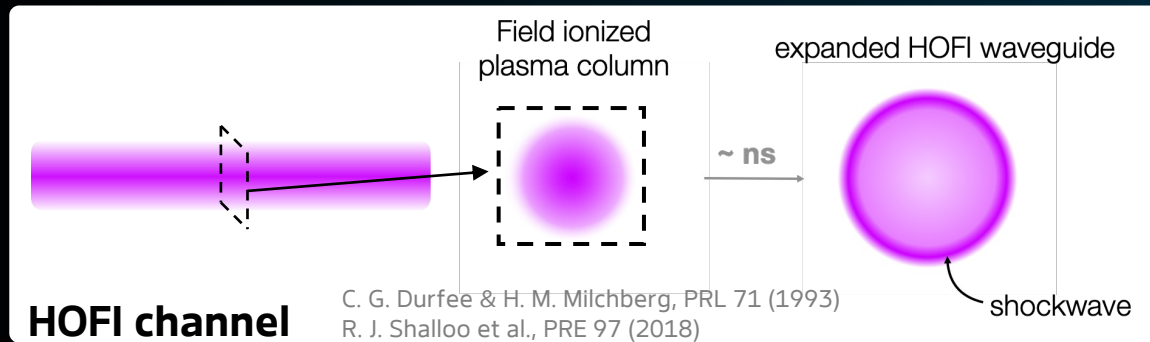
Simulation methods

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- Plasma shaping: hydrodynamics

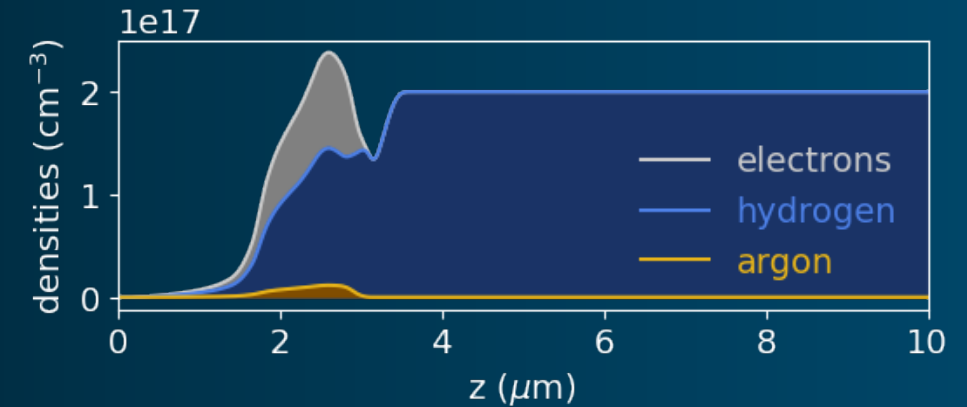
Shaping the source: hydrodynamics



Transverse tailoring for laser waveguide



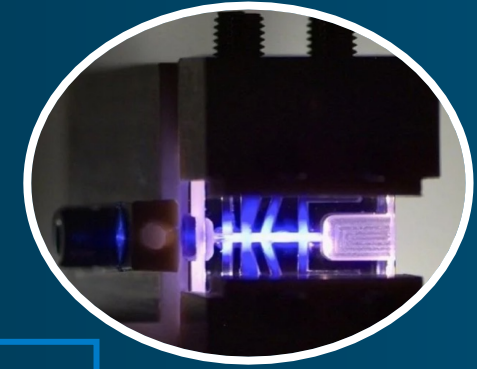
Longitudinal tailoring for injection & matching



Simulation methods

- Gas flow: existing solutions (ANSYS, COMSOL)
- Plasma shaping: hydrodynamics

HYQUP: HYdrodynamic QUasineutral Plasma



Assumes **single, quasi-neutral** fluid

Two temperatures (2T), separate for electrons and heavy particles (ions, atoms, molecules)

Ionization state tracked via collisional **reaction rates**

No explicit EM fields required

Implemented in COMSOL Multiphysics, 1D/2D/3D

Flow

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0$$

$$\frac{\partial \rho \vec{v}}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v} \vec{v}) = -\vec{\nabla} p - \vec{\nabla} \cdot (\eta \vec{\nabla} \vec{v})$$

Key

ρ : mass density
 v : flow velocity
 p : pressure
 B : magnetic field
 τ : viscous stress tensor
 n : number density
 c : stoichiometric const.
 r : reaction rate
 C : heat capacity
 T : temperature
 λ : thermal conductivity
 k_{e-h} : collisional energy transfer
 ΔE : reaction energy
 E : electric field

Electron energy

$$\frac{\partial C_e T_e}{\partial t} + \vec{\nabla} \cdot [(C_e T_e + p_e) \vec{v}] - \vec{v} \cdot \vec{\nabla} p_e - \vec{\nabla} \cdot (\lambda_e \vec{\nabla} T_e)$$

$$= -k_{e-h}(T_e - T_a) - \sum_{j, \alpha} \Delta E_j r_j$$

Similar for atoms

Transport Coefficients

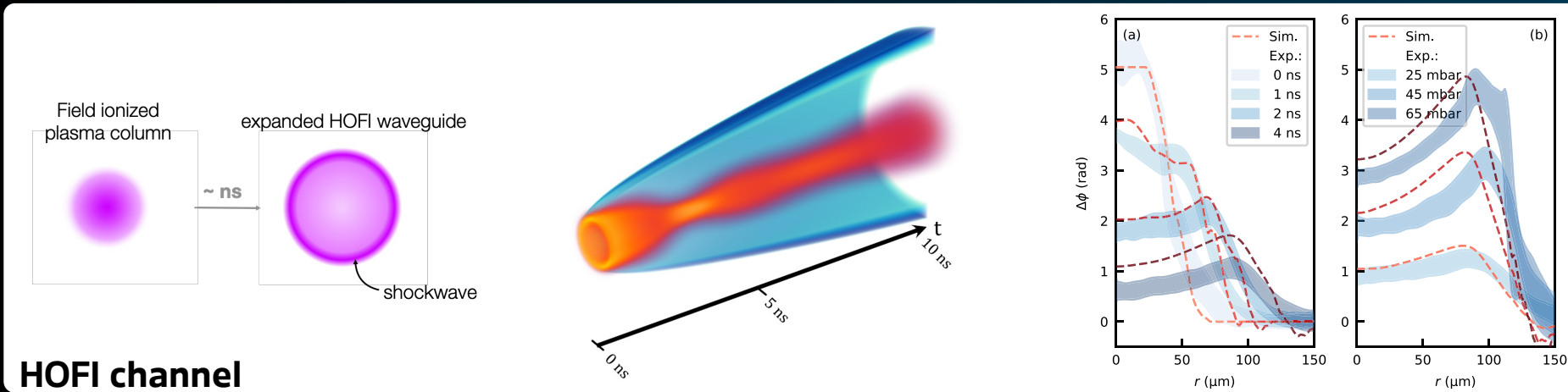
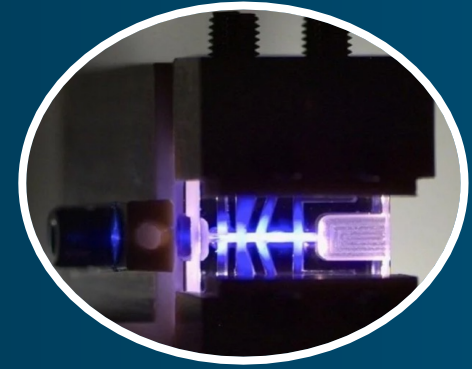
Species α

$$\frac{\partial n_\alpha}{\partial t} + \vec{\nabla} \cdot (n_\alpha \vec{v}) = \sum_j c_{j\alpha} r_j$$



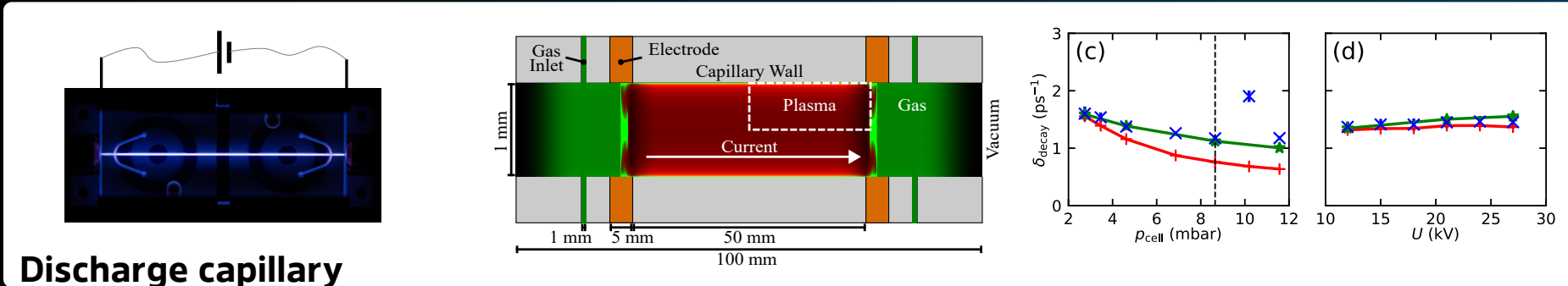
Mathis Mewes

HYQUP was benchmarked against experiments



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

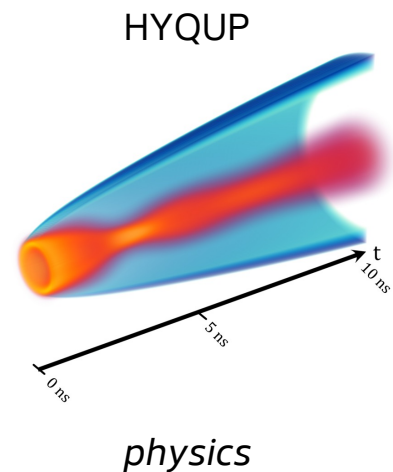
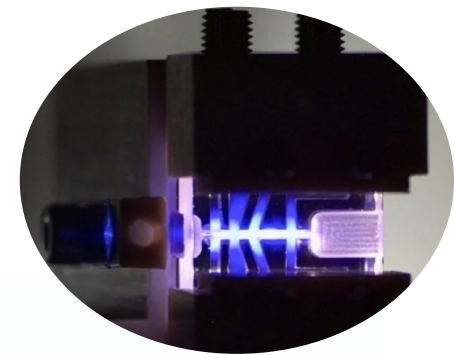
Experiments at Oxford University (S. Hooker)



M. Mewes et al. PRR 7, 043193 (2025)

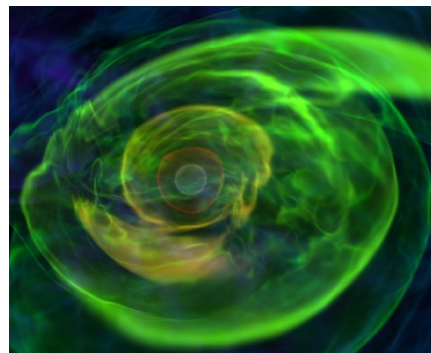
Experiments in the ADVANCE lab at DESY (J. Wood)

CHEQUP: open-source HOFI simulations



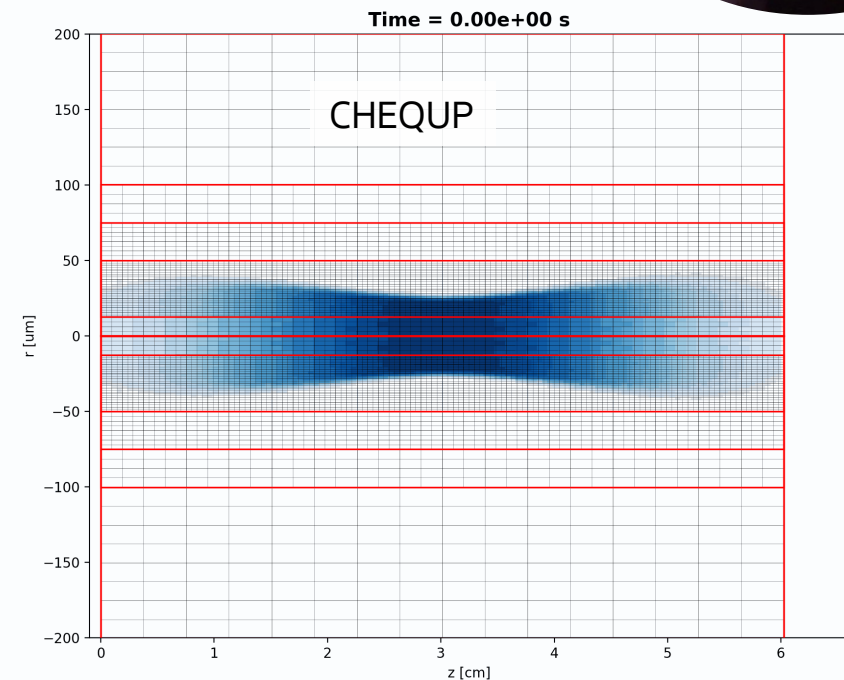
+

CASTRO (Stony Brook Uni + LBNL)



C++, GPU, MR

=



Remi Lehe



Christian McCombs



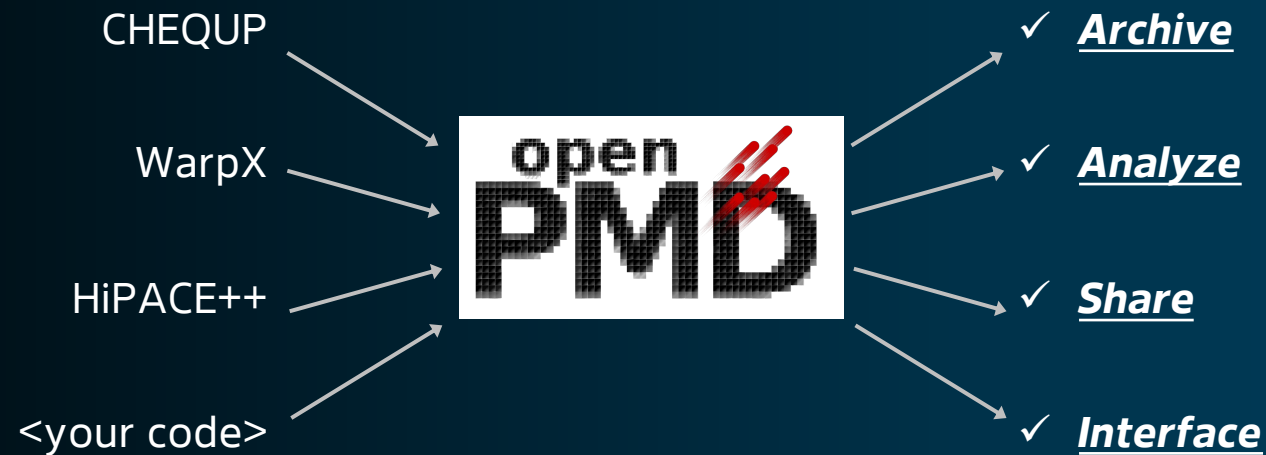
Alexander Sinn



Thibault Benahmed

- Project initiated by R. Lehe (LBNL), DESY joined merrily
- Open-source since June 24
- Go check talk by Christian McCombs (LBNL)

Start-to-end supported by openPMD standard



BERKELEY LAB

HZDR

HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

- Open standard for Particle Mesh Data
- Comes with C++ & Python implementations
- Largely simplifies start-to-end simulations

<https://github.com/openPMD>
<https://github.com/openPMD/openPMD-api>
<https://github.com/openPMD/openPMD-viewer>

An international suite of open-source tools for S2E

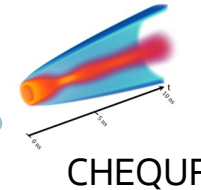
Simulate wakefield acceleration and more...



❖ Plasma source tailoring



❖ Realistic experimental profiles

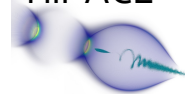


❖ Plasma recovery for repetition rate

❖ Parallel Bayesian optimization



HiPACE++



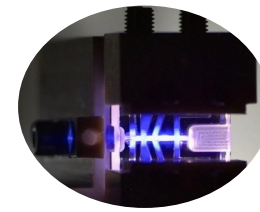
... harnessing the fastest supercomputers

- All open-source
- All **openPMD**

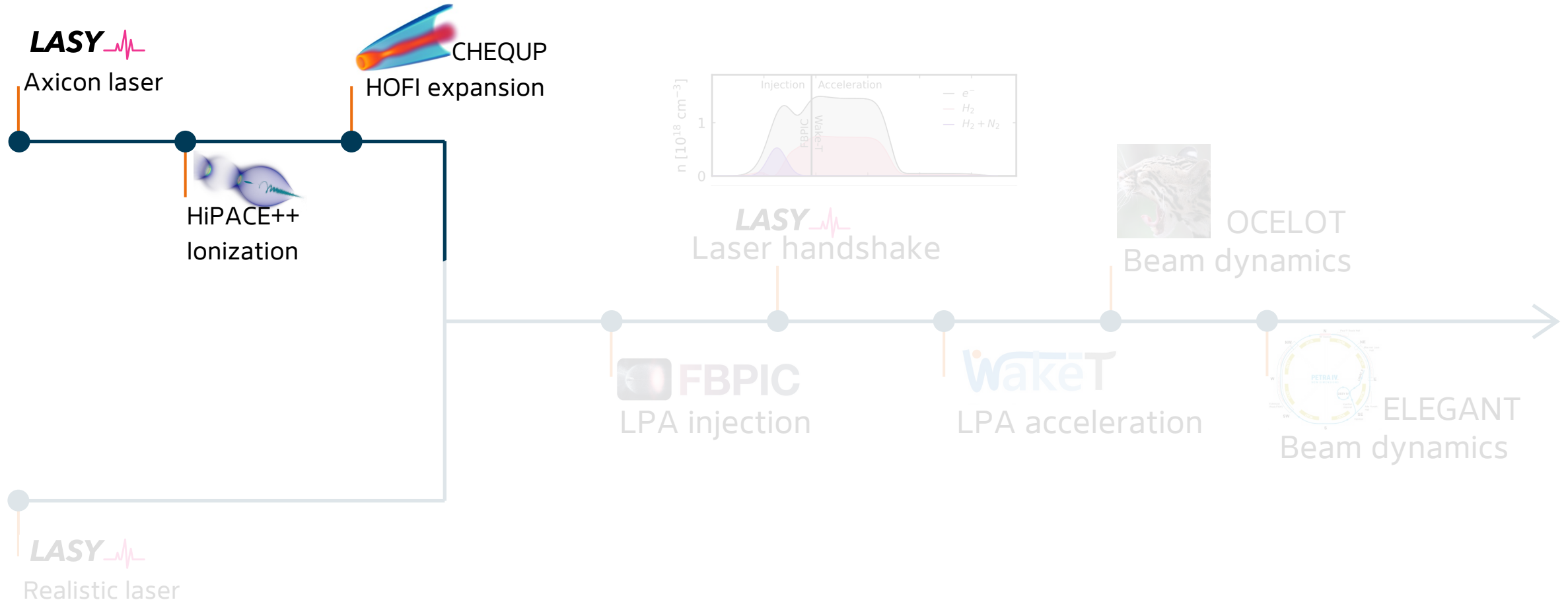
Highlights

- 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++*.

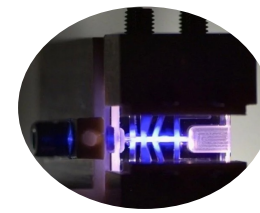
Build your own toolchain



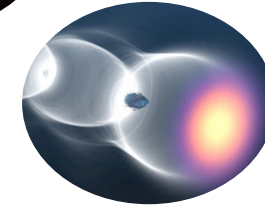
Shape the source



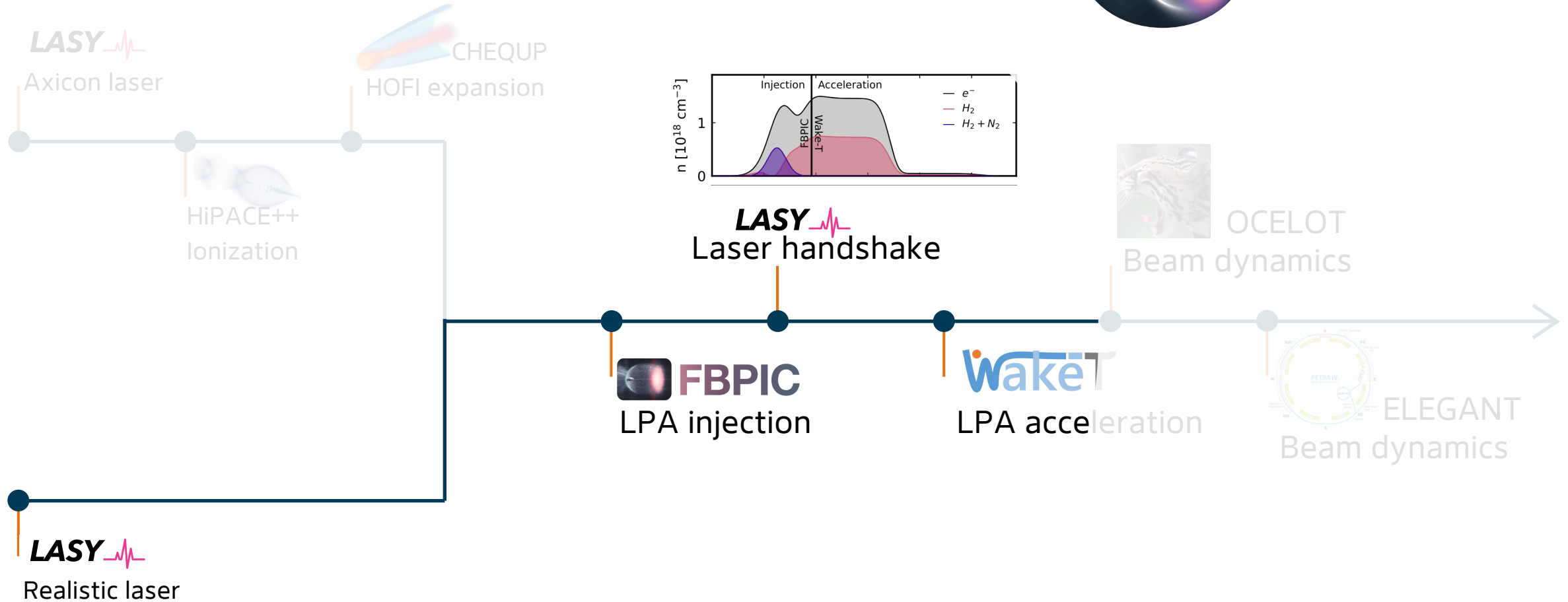
Build your own toolchain



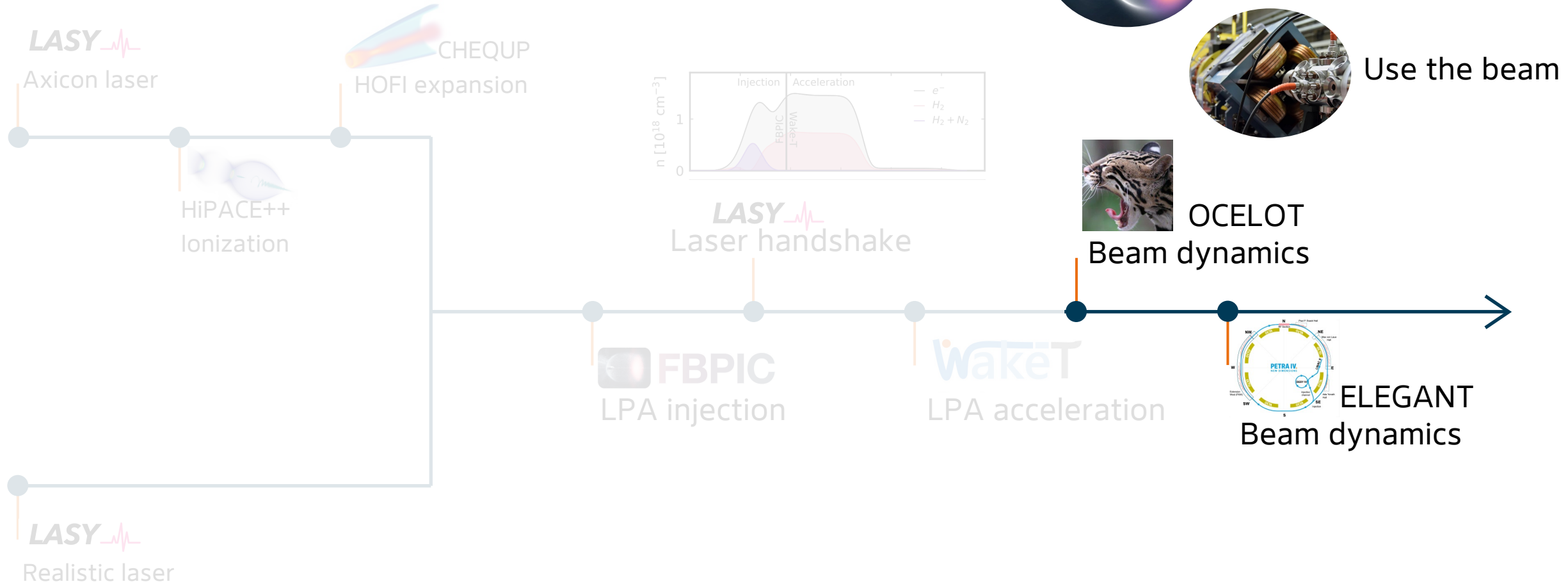
Shape the source



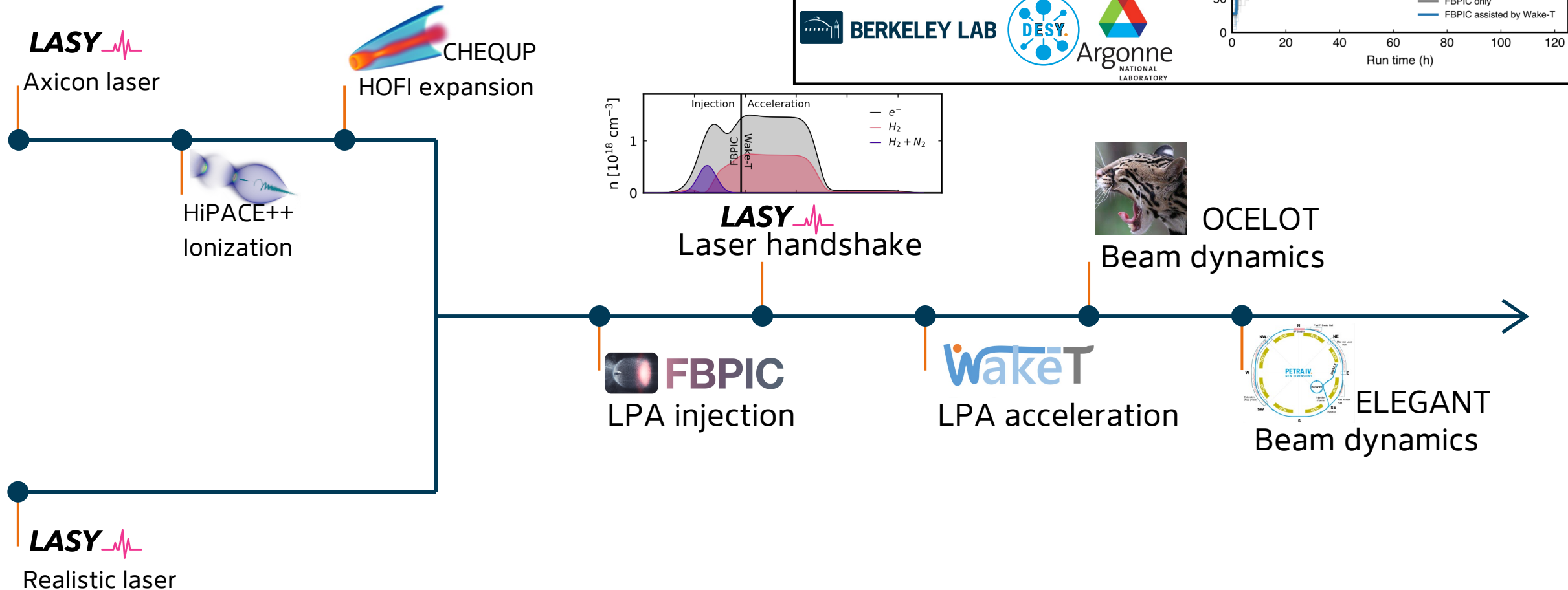
Do the wakefield



Build your own toolchain



Build your own toolchain



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

<https://github.com/Libensemble/libensemble>

Hudson et al. IEEE Trans. Parallel Distrib. Syst. 33 (2021)



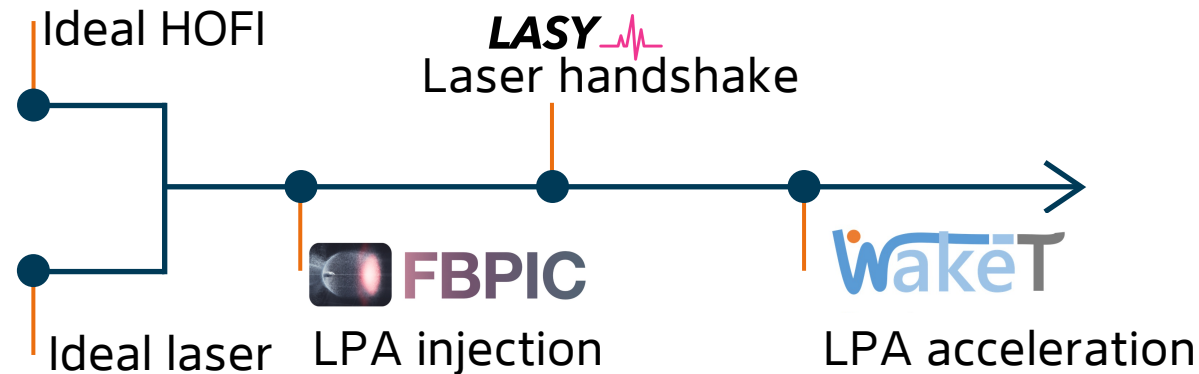
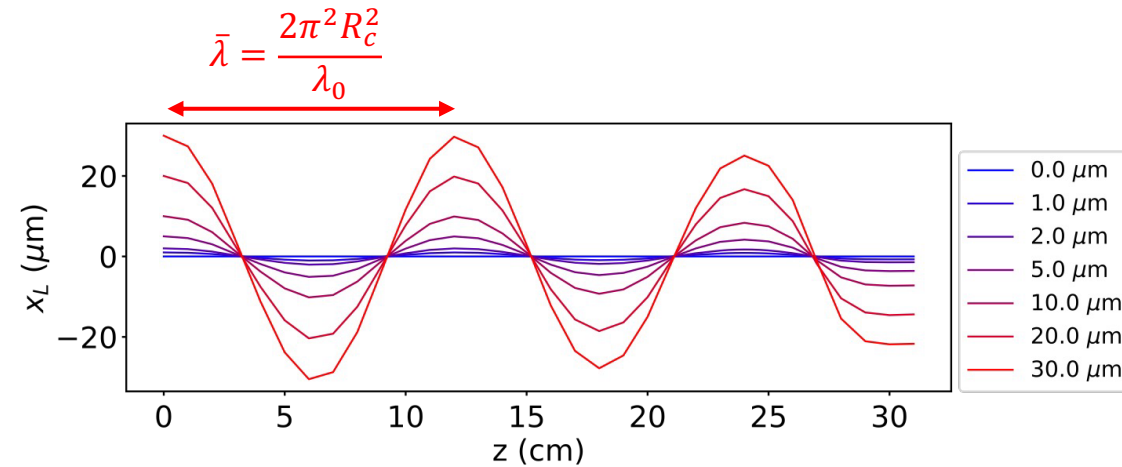
PIP4 simulation

- **The plasma injector for Petra IV**
Science case, Conceptual Design Report, open questions
- **Progress on simulation methods**
Wakefield, hydrodynamics
- **Tolerance to transverse misalignment** Preliminary
3D simulations for misalignment in waveguide
- **How to make the plasma waveguide** Preliminary
Simulating HOFI + LPA

Laser pointing jitter causes beam degradation



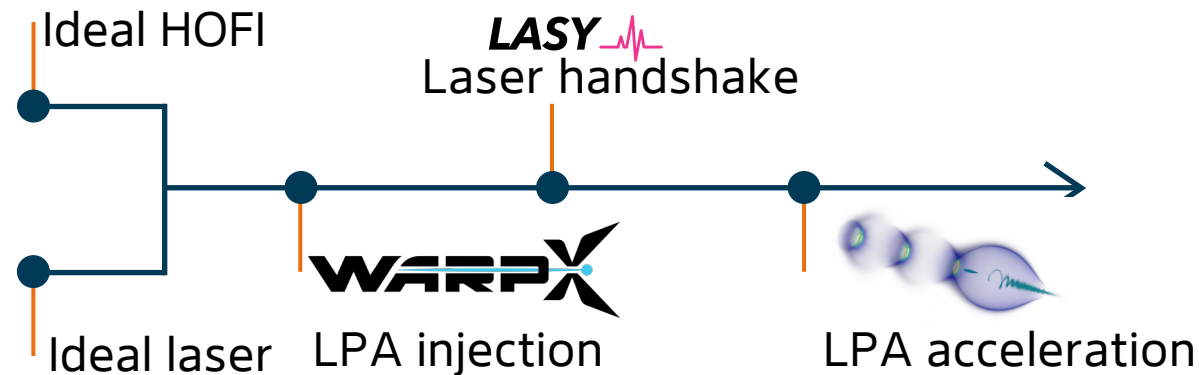
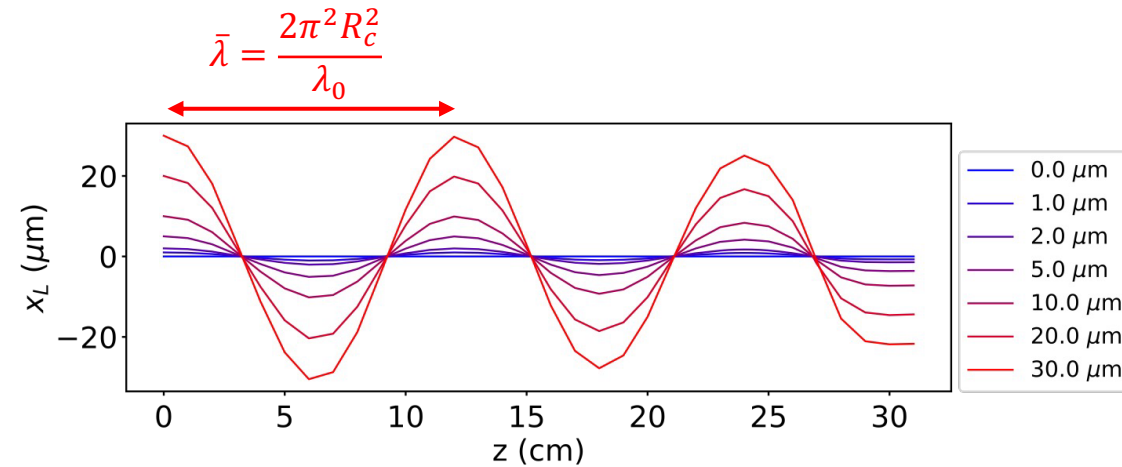
Alexander Sinn



Laser pointing jitter causes beam degradation



Alexander Sinn



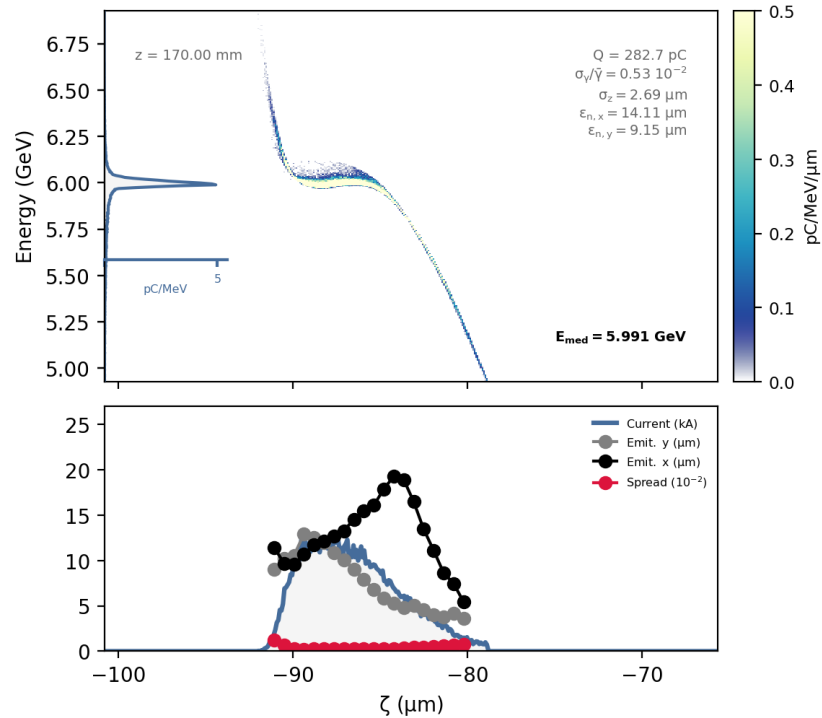
➤ Replace cylindrical codes with 3D codes

We can reproduce initial WP in 3D

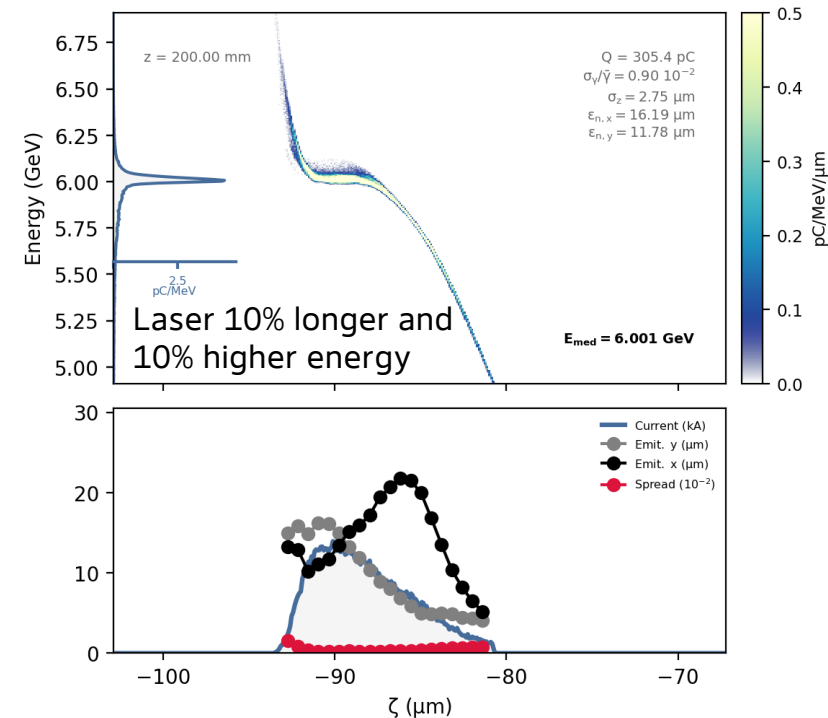


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Cylindrical FBPIC+Wake-T



Full 3D WarpX + HiPACE++



Preliminary

Laser 20 J, 33 fs, 37 μm spot, focus 2.2 mm
Plasma $2 \times 10^{17} \text{cm}^{-3}$, $w_M = 40$ μm , 20 cm

WarpX: 14 node-hours / cm

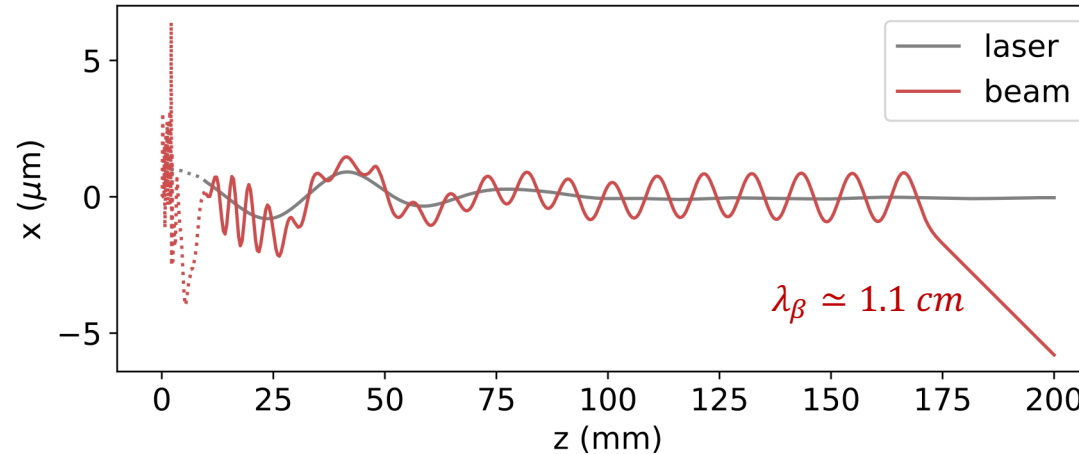
HiPACE++: 0.25 node-hours / cm (but **cannot** model injection)

➤ Connecting electromagnetic and quasistatic model is worth it!

Current setup could tolerate micron-scale offset



Alexander Sinn



Preliminary

Offset (μm)	x amplitude (μm)	θ_x amplitude (mrad)	Emittance (μm)	Charge (pC)
0.0	0.290	0.115	16.1	310
0.1	0.213	0.0881	16.3	308
0.4	0.444	0.246	17.3	309
1.0	0.867	0.494	19.4	306
2.5	1.55	0.875	20.1	286
5.0	3.18	1.78	40.6	257
10	4.94	2.69	45.1	207

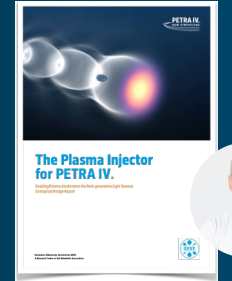
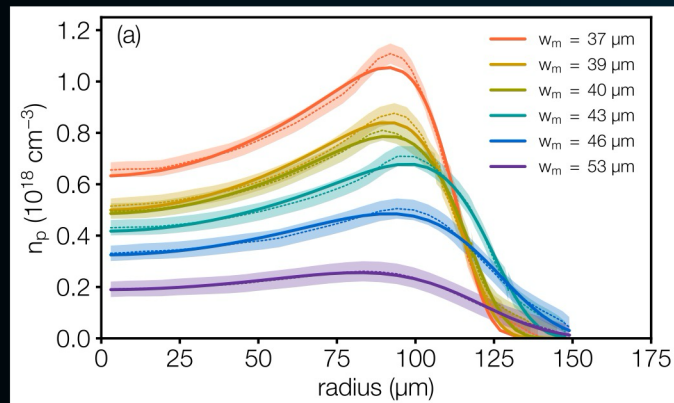
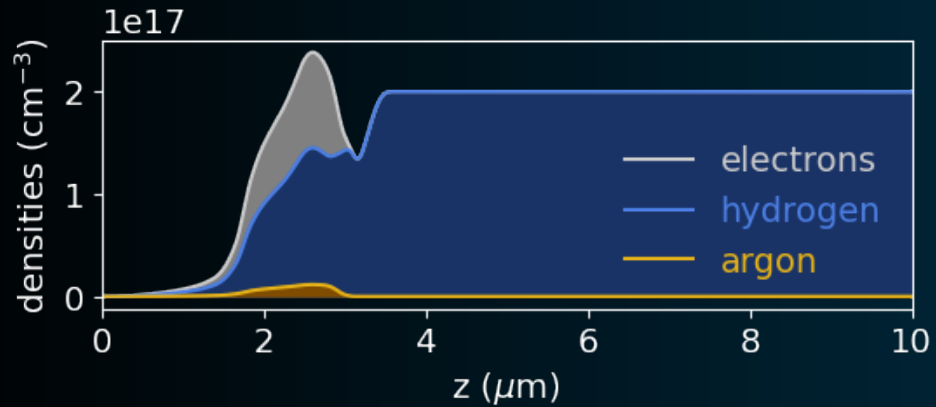
- Laser oscillations damped, coherent betatron oscillations
- No offset: width $\sim \mu m$, divergence $\sim mrad$
- Final betatron phase matters:
 - trade-off final position offset $\sim \Delta x$ vs. pointing $\sim 2\pi\Delta x/\lambda_\beta$
- Few-micron offset comparable to beam width and divergence
- Solutions investigated to reduce offset and mitigate effect



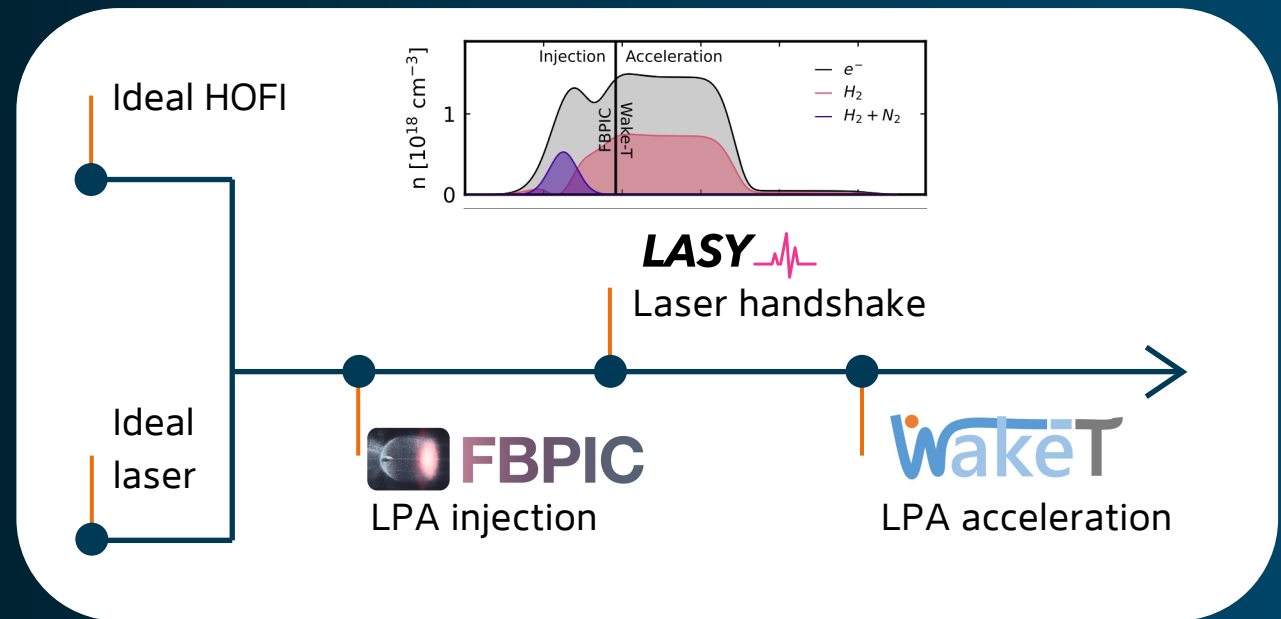
PIP4 simulation

- **The plasma injector for Petra IV**
Science case, Conceptual Design Report, open questions
- **Progress on simulation methods**
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- **Tolerance to transverse misalignment** Preliminary
3D simulations for misalignment in waveguide
- **How to make the plasma waveguide** Preliminary
Simulating HOFI + LPA

Original: simulate LPA from ideal profiles



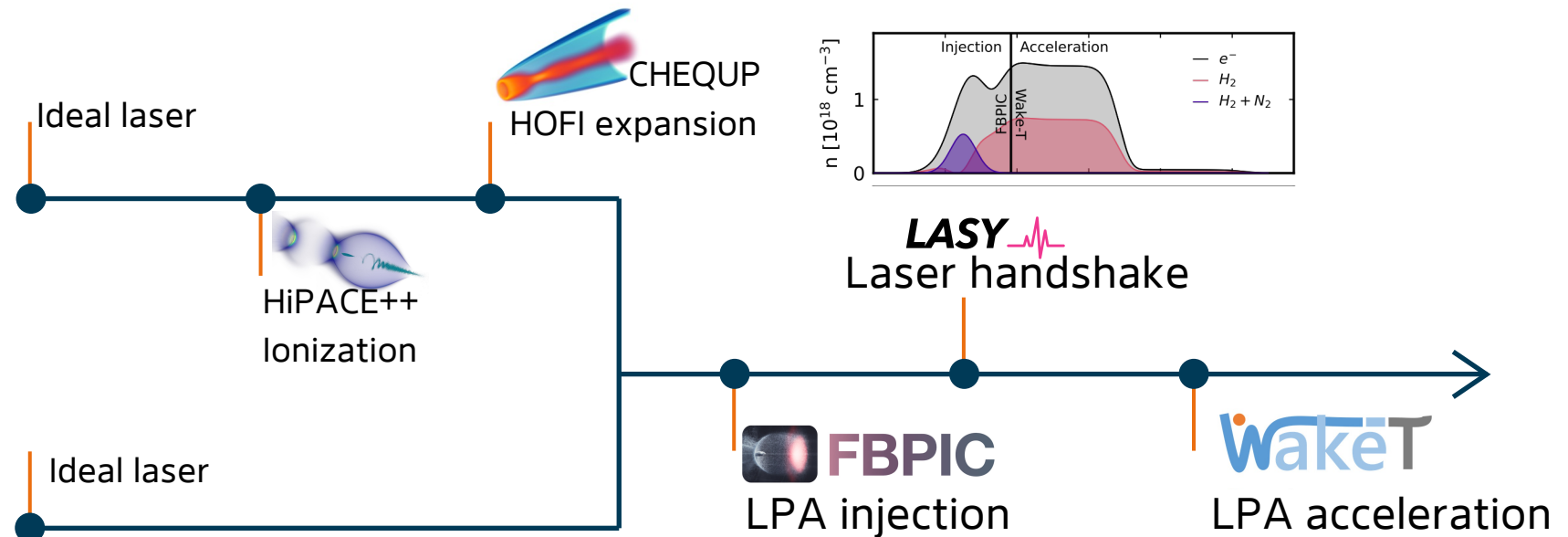
A. Martinez de la Ossa



New: HOFI simulation included in pipeline



Thibault Benahmed

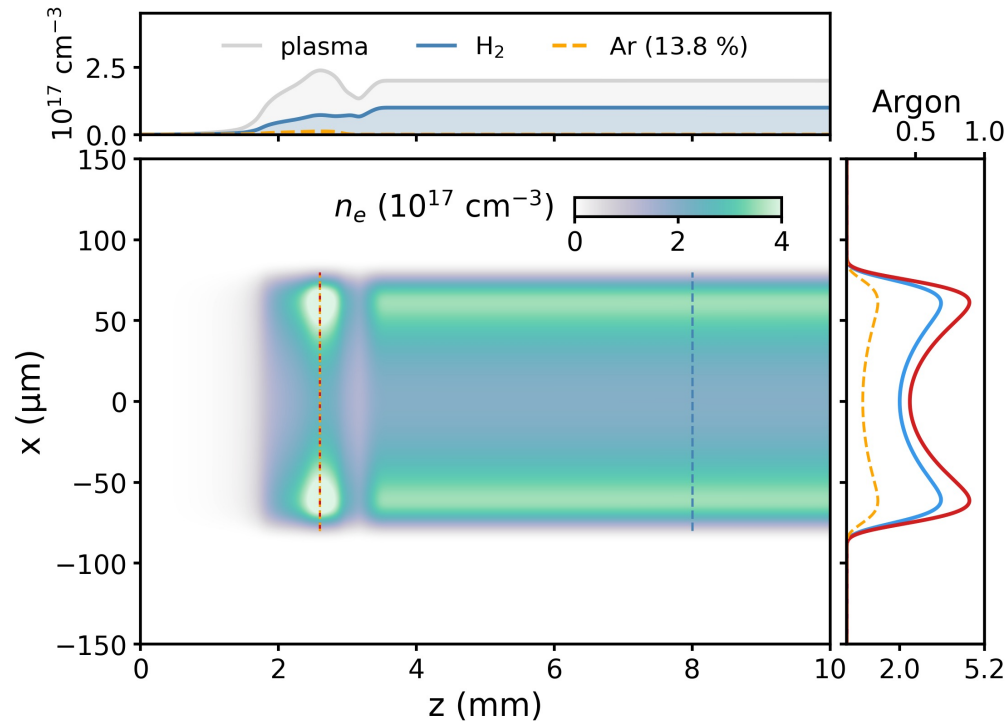


CHEQUP simulations give appropriate profile

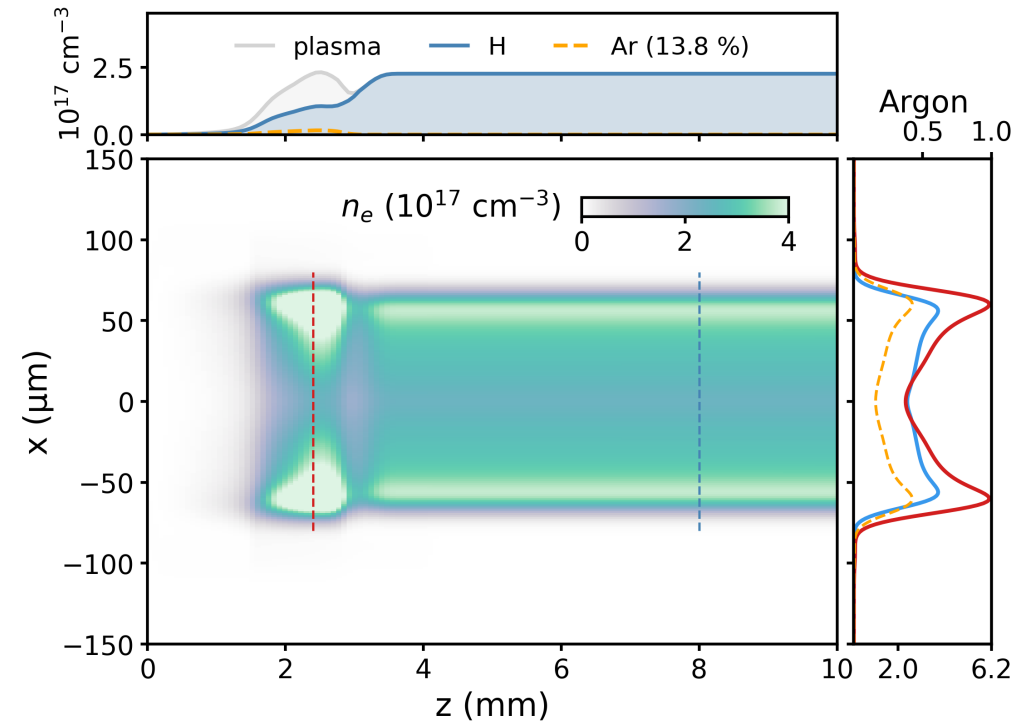


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Ideal plasma profile



Realistic plasma profile

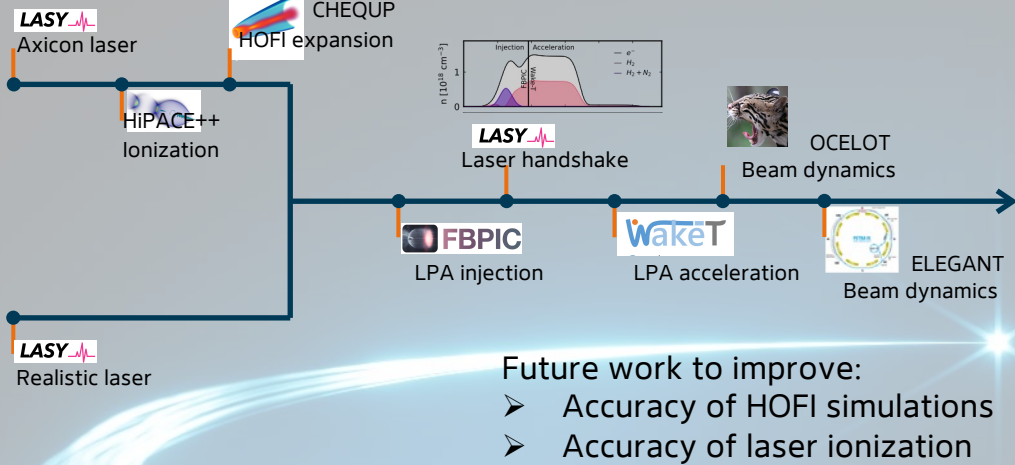


Preliminary

Gas density $2.8 \cdot 10^{18} \text{ cm}^{-3}$
Argon dopant 13.8%
HOPI laser is Gaussian, collimated
 $w_0 = 17 \mu\text{m}$ and $a_0 = 0.04$
Hydro expansion time 3.5 ns
LPA laser: 20 J, focused at 1.93 mm, duration 33 fs

Conclusion & Perspectives

- Plasma injector for Petra IV demands s2e modelling
- Many high-quality open-source tools are available
- standard openPMD + libraries LASY & Optimas
- 3D is affordable e.g. combining EM and QS PIC
- Tight tolerance between waveguide and LPA
- We are working on generating the long HOFI channel
- Happy to share s2e methods, reach out if interested
- More on X-ray generation coming soon



The plasma group



C. McCombs, J. Osterhoff, C. Benedetti, J.-L. Vay, A. Huebl, R. Lehe, A. Myers, W. Zhang, C. B. Schroeder



G. J. Boyle



S. Hooker



L. Fedeli



Thank you for your attention