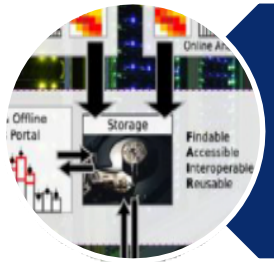
# DMA – Sub-topic Structure

DMA creates new synergies between centers, facilities & communities & leverages them

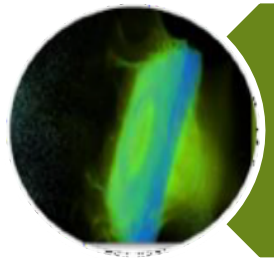



**ST1 – The Matter Information Fabric**

- Exa-scale data management
- F.A.I.R. data & Meta-data
- Long-term preservation

**ST2 – The Digital Scientific Method**

- Artificial intelligence
- Exa-scale computing
- Quantum computing



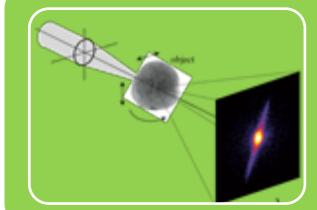
**ST3 – The Digital Experiment and Machine**

- Exa-scale simulations
- In-situ data analytics
- Near-real-time feedback and machine optimization

regular exchange & common projects

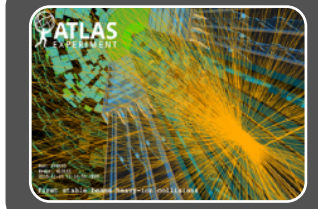
# DMA — ST3 „THE DIGITAL EXPERIMENT AND MACHINE”

## Subtopics projects and milestones within POF IV period 2021-2027:



**2024**
- Prototypes for near real time analysis with feedback

**2025**
- Operation-critical intelligence on machine & experiment status



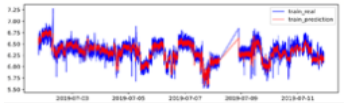

**2027**
- Complete simulations of systems, experiments & machines

- Helmholtz centres involved in DMA ST3: DESY, FZJ, Hereon, HZB, HZDR, KIT
- Working on “pilot projects”: produce first results in the near future
- Further collaborators and resources / funding on DMA / centre / (inter)national level

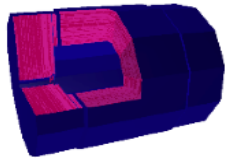
HELMHOLTZ AI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

ErUM-Data

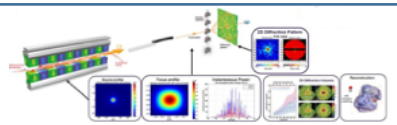
LEAPS League of European Accelerator-based Photon Sources



A.I.-optimized injection



Full, generic detector descriptions



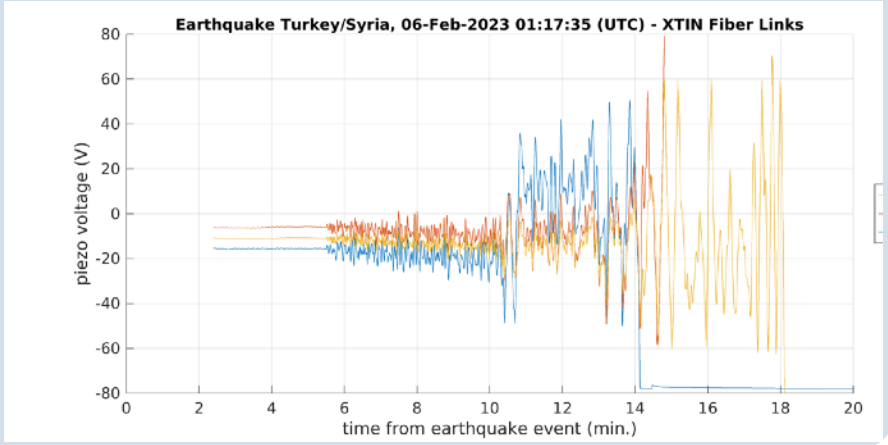
Start-to-end workflows

Accelerator optimization

# DATA DRIVEN ML @ DESY

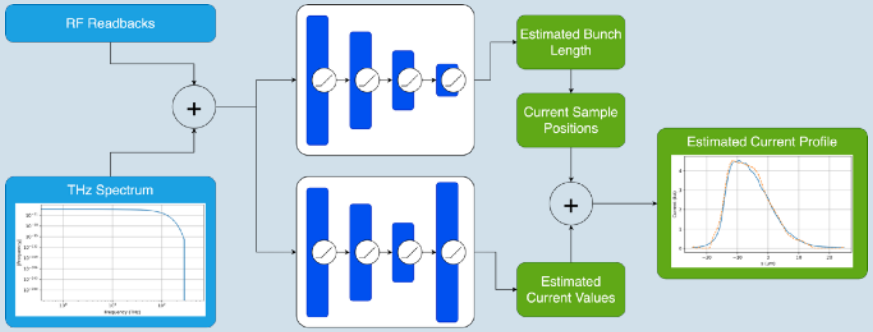
## Identifying environmental influences at stability

How do earthquakes influence the optical synchronization system and thus the stability of the European XFEL



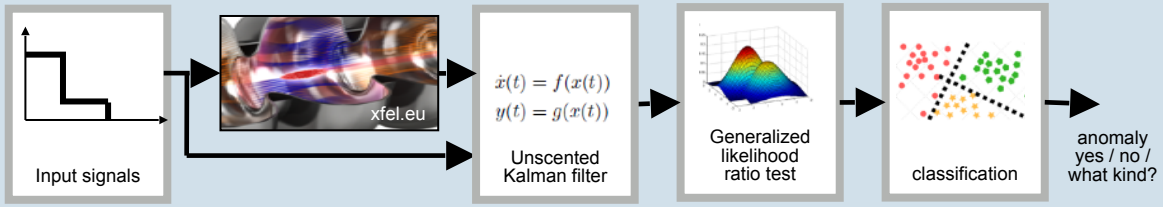

## Virtual diagnostics for electron current profile

Neural networks for combined scalar- and spectral longitudinal phase space reconstruction



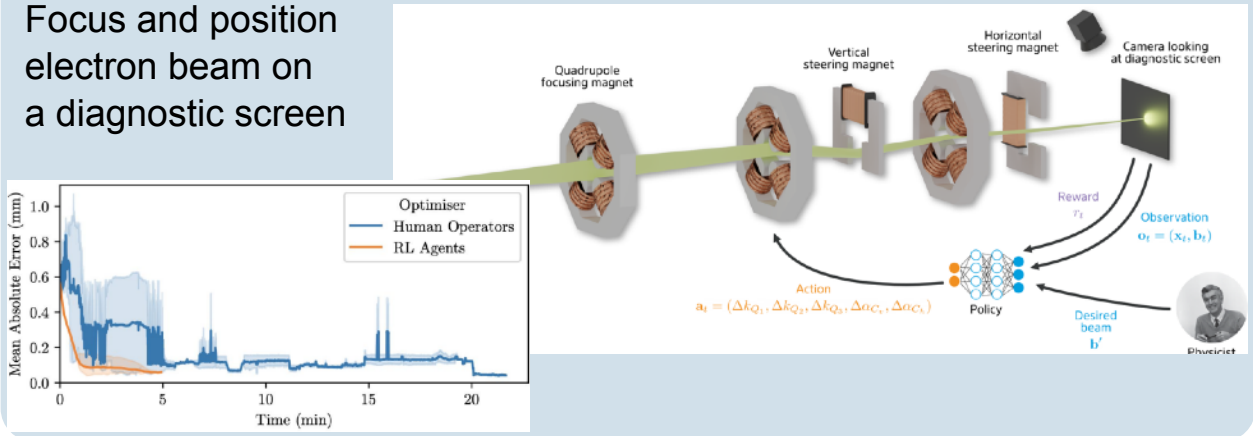

## Quench detection for the LLRF system

Hybrid fault diagnosis: Model-based feature extraction and AI-based classification (with unsupervised clustering)




## Reinforcement Learning at ARES

Focus and position electron beam on a diagnostic screen



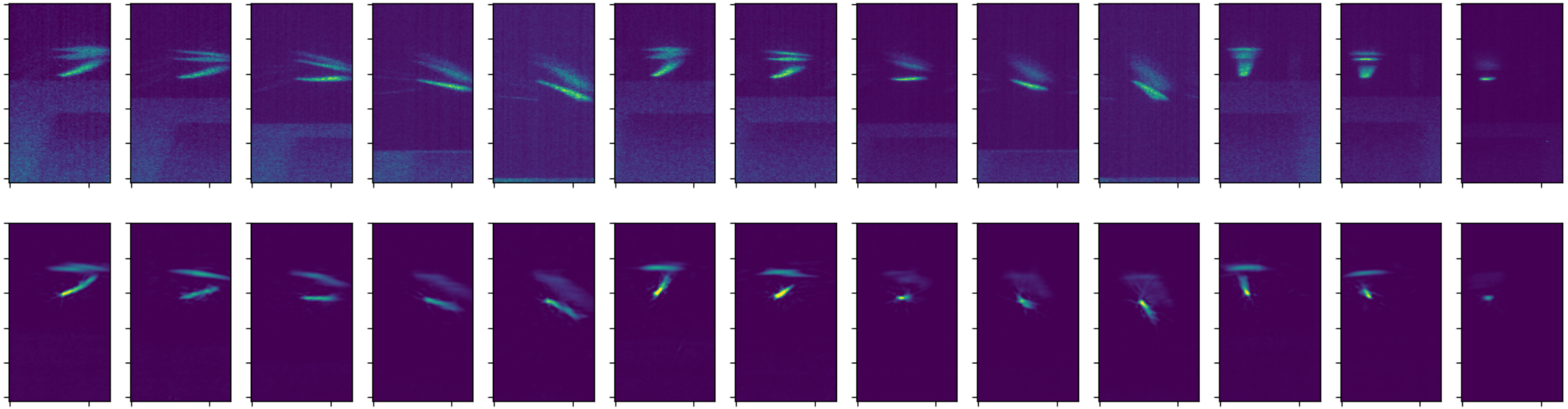

Real-world application!

# 10 PARAMETER OPTIMIZATION

HZB Helmholtz Zentrum Berlin

**Experiment**

**Precision: ~0.01mm**



**Prediction**

**Optimizer($X_0$)**

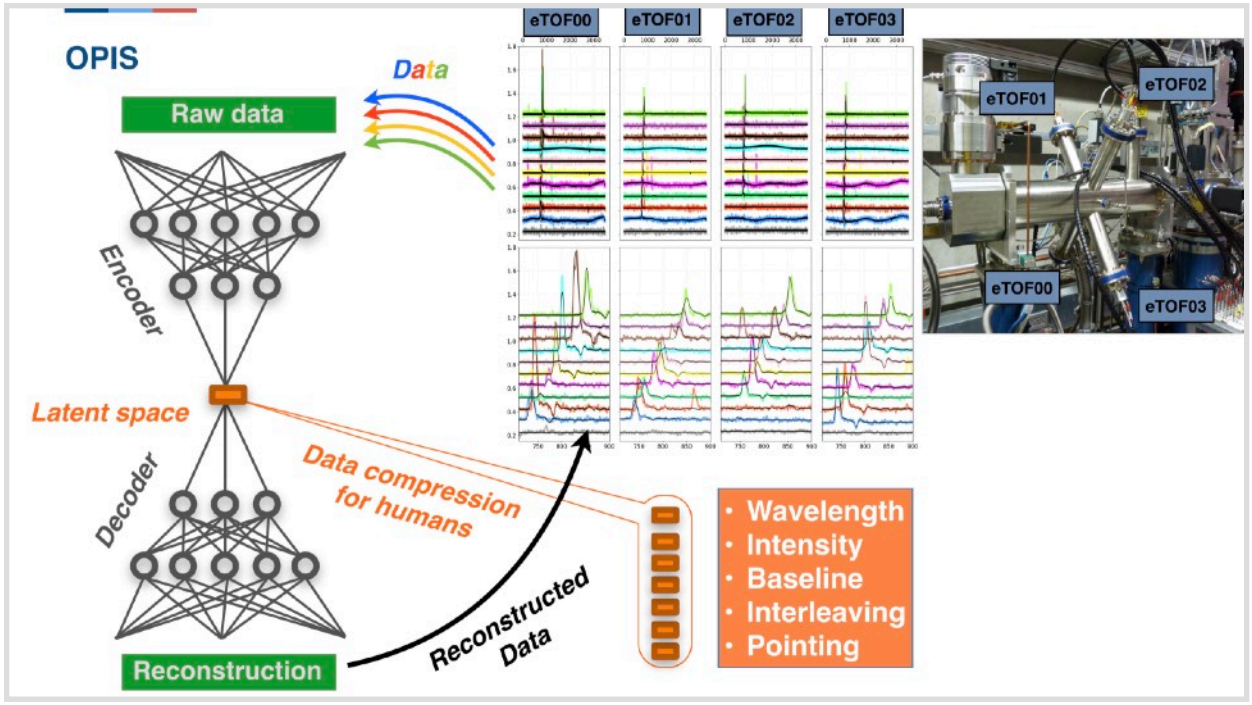
*Peter Feuer-Forson*

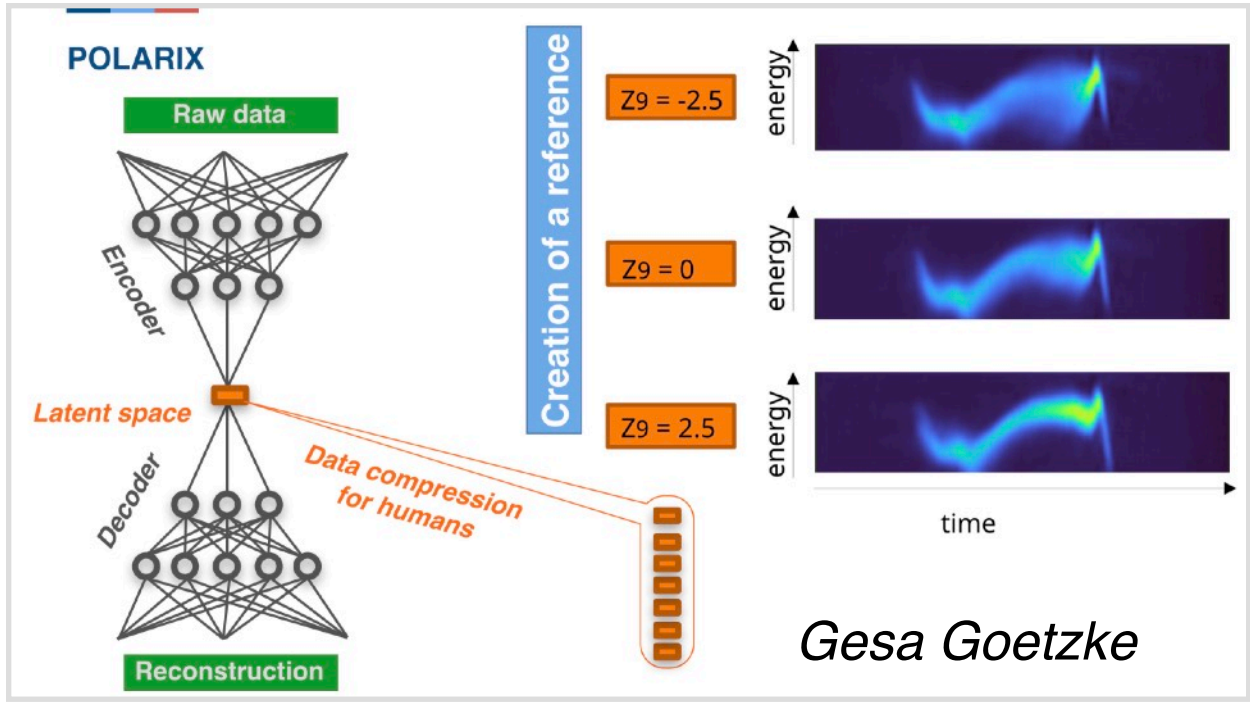
# PHOTON DIAGNOSTICS

HZB Helmholtz Zentrum Berlin

DESY.






*Gesa Goetzke*

# DATA HANDLING

## Helmholtz Laser-Plasma Metadata Initiative

- HELPMI: within HMC (Helmholtz Metadata Collaboration)
  - GSI, HI Jena and HZDR
  - April 2023-'25
- Initiative: **start** the development of a data standard for LPA experiments
- Adopt NeXus standard from Photon and Neutron community
  - Use existing base classes, possibly define new ones
  - Propose application definition
- Extend the openPMD standard and API for arbitrary hierarchies
  - Currently established for simulations in LPA community
  - Fileformat-agnostic
- Definition and development in close contact to the LPA community

This project (ZT-I-PF-3-066) was funded by the Initiative and Networking Fund of the Helmholtz Association in the framework of the HMC project call.

GSI

HI JENA HELMHOLTZ Helmholtz-Institut Jena

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Findable Accessible Interoperable Reusable

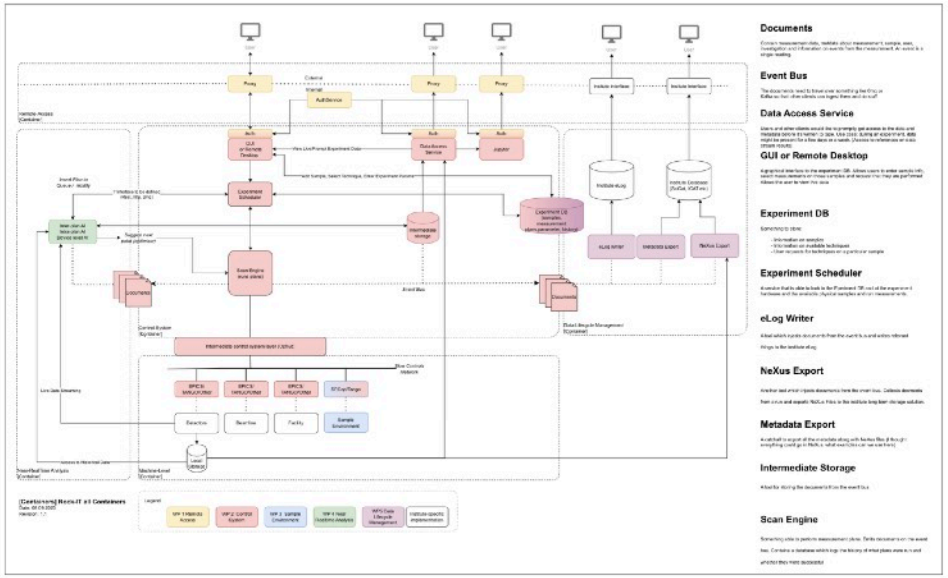
NX

openPMD

Helmholtz Laser Plasma Metadata Initiative

Contact: helpmi@hzdr.de

## Rock-IT



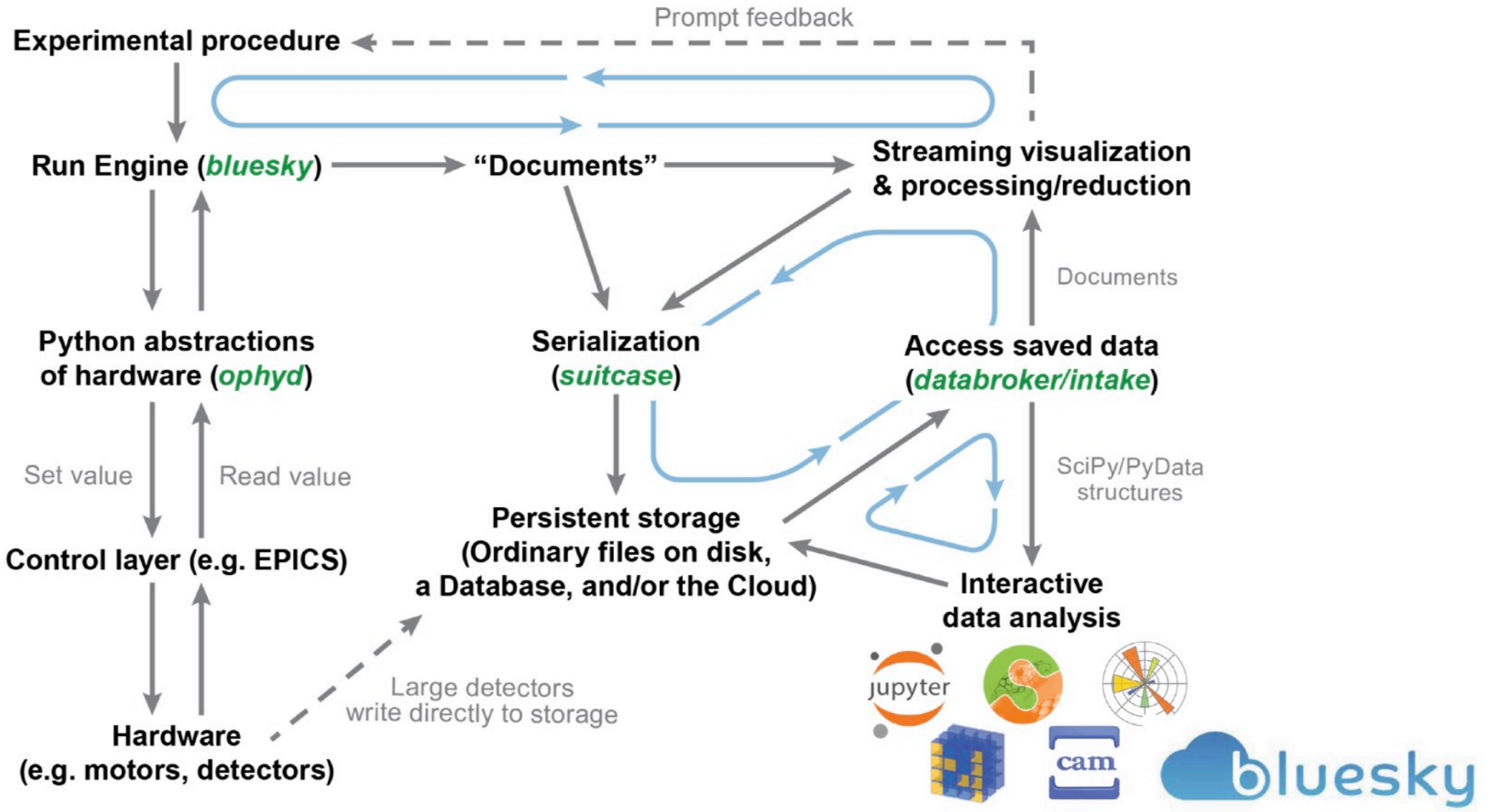

## HMC Proposal

**Logbook 2.0 For Particle Accelerator Research and Development**

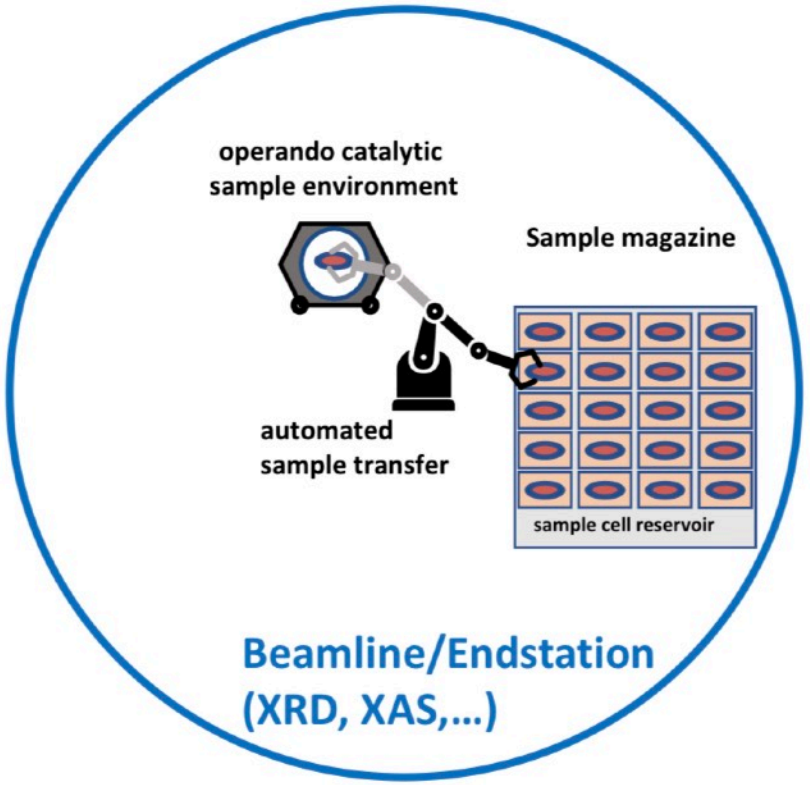
Antonin Sulc (DESY), Gregor Hartmann (HZB)

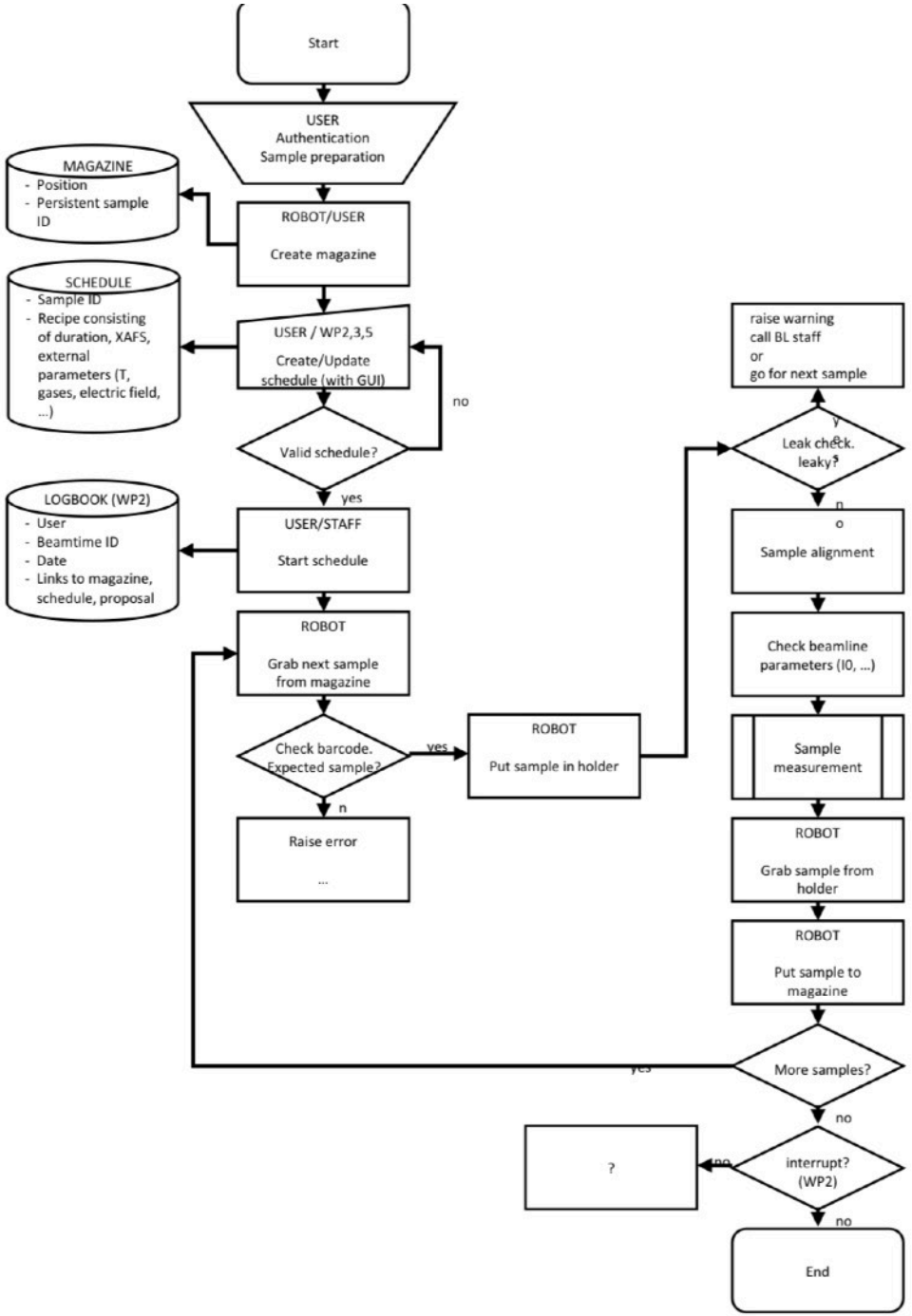
*"ChatGPT + bact"*

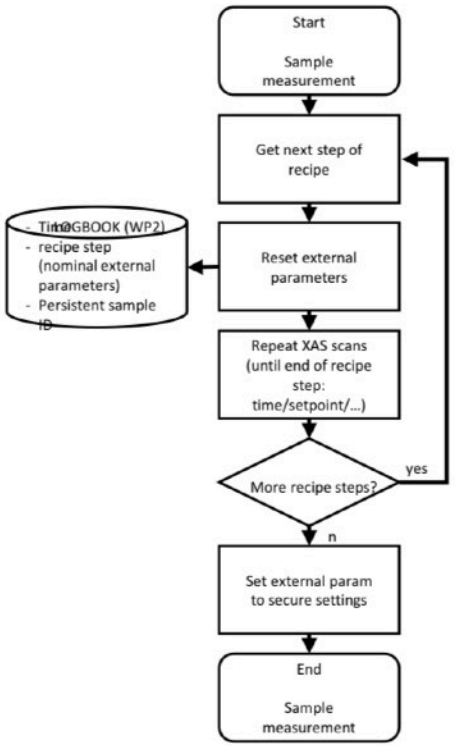
# Proposed control and data scheme using the BLUESKY environment



# Proposed flow-chart for typical automated catalytic operando x-ray investigations



# ILL-POSED INVERSION

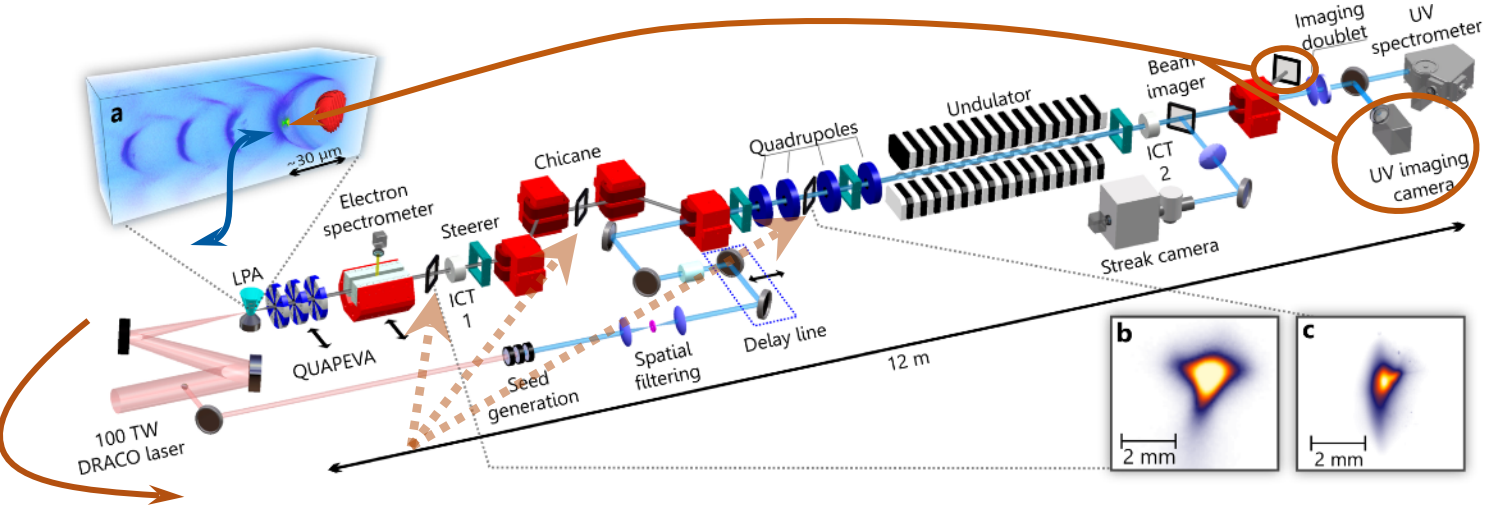
**Anna Willmann et al.**

HZB Helmholtz Zentrum Berlin

**HZB Hackathon**

Ultimate Goal: Control and Optimization of a laser-driven Free Electron Laser

**Automatic inversion** of experimental measurements from the imager and UV imaging camera to beam parameters at the source

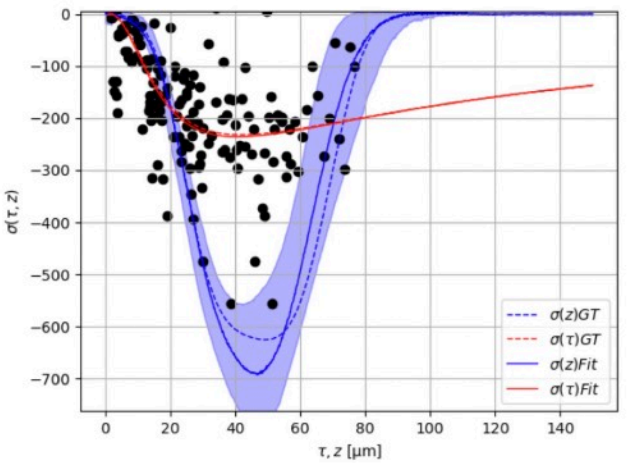



Challenges:

- Large parameter design space
- Destructive diagnostics – lack of empirical data
- Search for consistent parameters with empirical data and prior knowledge

**Virtual diagnostics** provide data from all imagers in digital form with access to phase space of the beam in the beamline

## Improving X-ray analytics: Laplace to real space



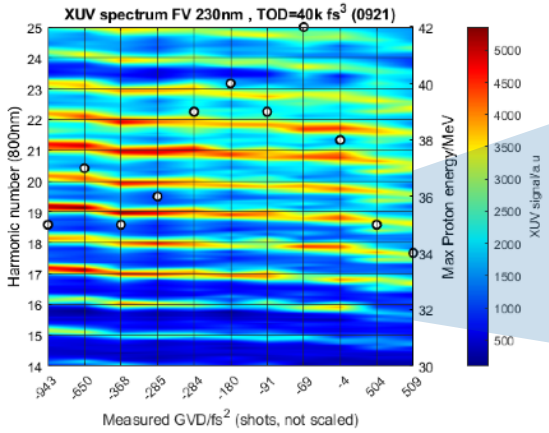
# EXA-SCALE

Alexander Debus et al.

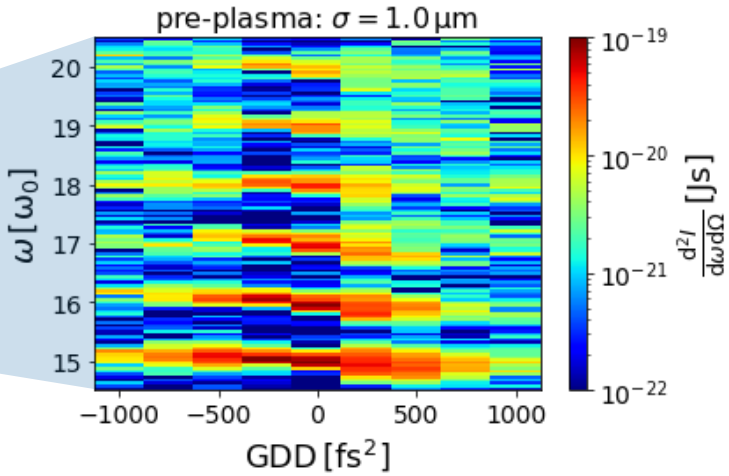
HZDR
HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

## From laser-plasma accelerator experiments to digital twins

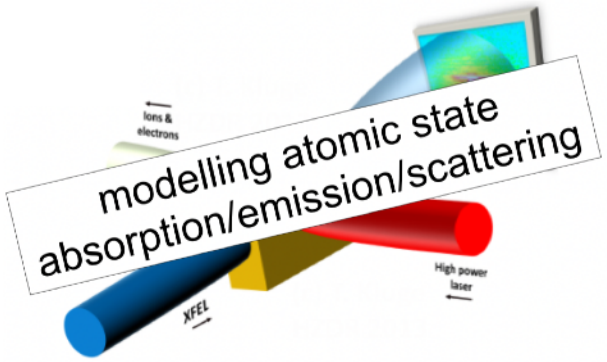
**Experiment**




**Simulation**




Frequency shifts in **experiments and simulations** over GDD **agree with theoretical predictions**:
E. Porat et al. PRR 4 L022036 (2022)




X-ray probing of laser driven for ion acceleration

Experimental data reconstruction

Synthetic diagnostics

PIConGPU


Large-scale start-to-end simulations

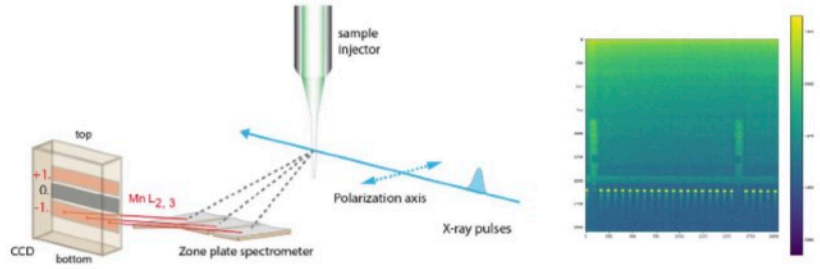
For predictive simulations we also need to care about atomic physics

"Matching" the large parameter space of complex experimental designs to simulations needs to be understood and further constrained.

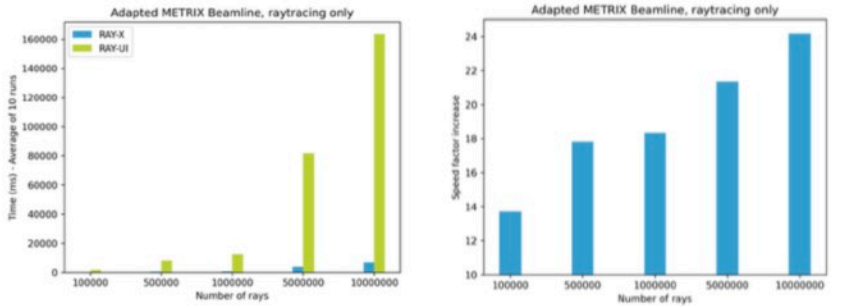
# FAST SIMULATIONS

## RAY-X: EFFICIENT RAY-TRACING

RAY-X is being developed as open source physics based ray tracing software, based on the well known software RAY [1, 2]. The goal is to modernise the code base of RAY as well as to implement new functionality, such as the use of the VULKAN computation API [3], dynamic tracing and grouped objects.




**Grouped objects afford the possibility to simulate complex setups, such as multiple reflection zone plates.**




**Initial Tests demonstrate a 20-factor increase in performance. RAY-X: NVIDIA Corporation TU117GLM [Quadro T2000 Mobile / Max-Q] RAY-UI: intel® Core™ i7-10875H CPU @ 2.30GHz**

# Cheetah - Simulating Faster than Ocelot

**Fast and differentiable beam dynamics simulation for machine learning applications**

Courtesy Jan Kaiser

- Linear beam dynamics simulation Python package based on *PyTorch*.
- Two main features:
  - **High-speed** simulation for fast data generation to generate large datasets needed for **machine learning**, e.g. reinforcement learning.
  - **Differentiable** simulation, enabling **gradient-based optimisation** and **virtual diagnostics**.
- GitHub: https://github.com/desy-ml/cheetah
- Documentation: https://cheetah-accelerator.readthedocs.io