

# Machine learning projects at DESY

Peek at some recent AI/ML activities

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Hamburg, 23. January 2025

# Overview

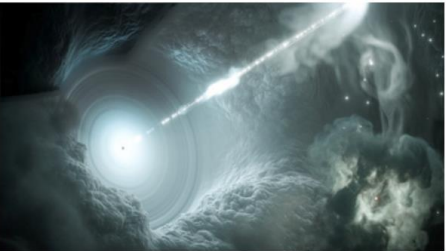
Many areas where AI/ML is used – will concentrate on accelerator division

## Accelerators



Machine Learning for  
optimization of design  
automated system co  
particle accelerators

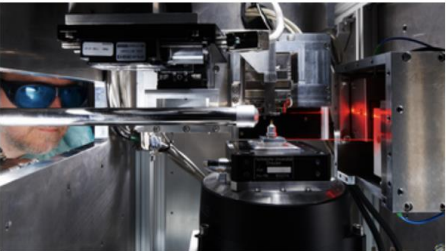
## Astroparticles



## Particles



## Photon Science



Machine Learning in various  
fields of physics, chemistry, biology, and nano science

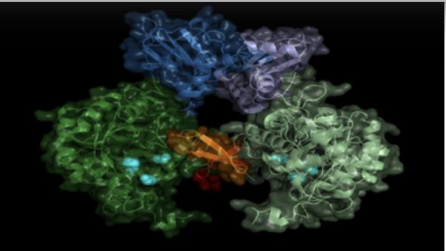
# 7th Round Table on Deep Learning@DESY

7th Round Table on Deep Learning at DESY: Friday 22 Nov 2024

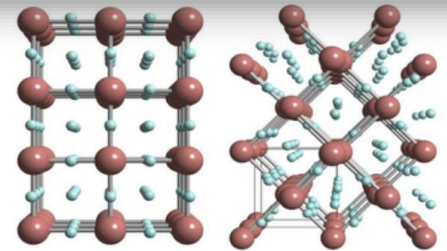
## European XFEL



Machine Learning in data  
handling and analysis at the X-ray  
Free Electron Laser



Machine Learning applied to  
investigations in structural  
biology



Machine Learning driven  
investigation and design of  
materials



Research and service in AI and  
HPC

## High Performance Computing Technology

# Overview

## Very good computing infrastructure at DESY

Compute	specs		Infiniband	specs		Storage	specs
CPU+GPU nodes	798		root switches	6		GPFS exfel	~40 PB
Total number of cores with hyperthreading	61696		top switches	12		GPFS petra3	20 PB
Total number of PHYSICAL cores	30898		leaf switches	42		GPFS cfel	1.6 PB
Theoretical CPU peak performance	1074 TFlops		IB cables (#)	~1500		GPFS cssb	11 PB
Total RAM	420 TB		IB cables (length)	~10km		DUST	3 PB

GPU nodes	180	Total number of GPUs	379	Theoretical GPU peak performance	2330 TFlops	Total peak performance	3404 TFlops
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# Remarkable AI/ML projects in the accelerator division

For sure not complete!

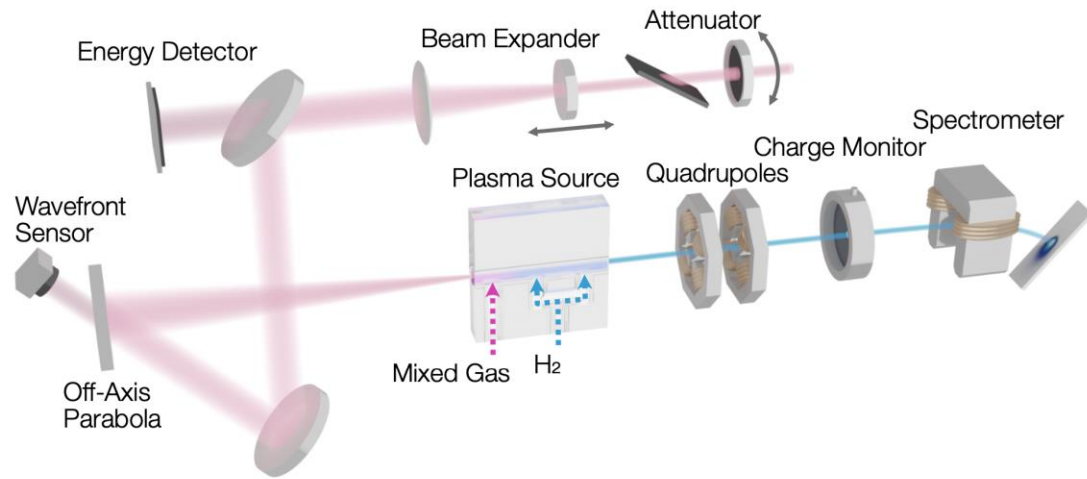
- Basics or mathematical optimization
  - Xopt, Badger, generic optimizer, ...
  - Bayesian optimization → [Example](#)
- Reinforcement learning
  - Developed from scratch at ARES → [Example](#)
  - To be ported to EuXFEL (dump line optimization)
- LLMs
  - Many activities at DESY
  - Chat bots for: data analysis, laser on-call support, EuXFEL operation assistant → [Example](#)
- Robotics
  - MARVIN, radiation measurements (with Technical University Hamburg)
  - augmented/mixed/extended reality for robot tele operation (with University of Hamburg) → [Example](#)

*Xopt*

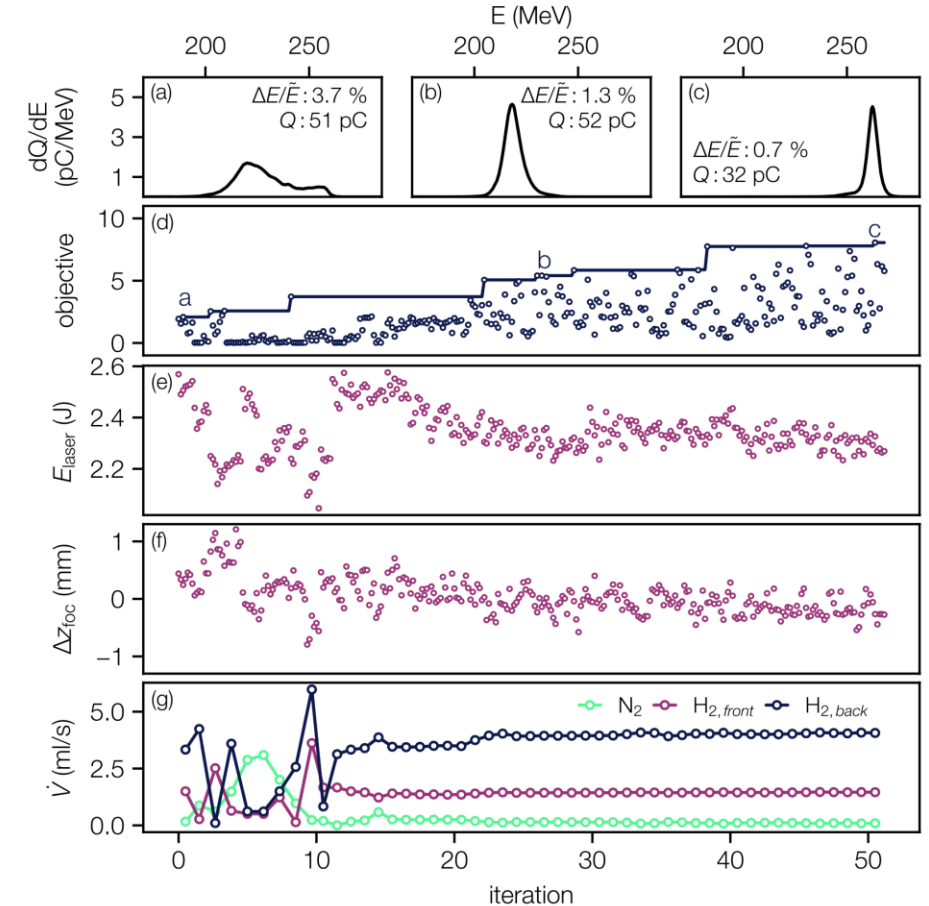
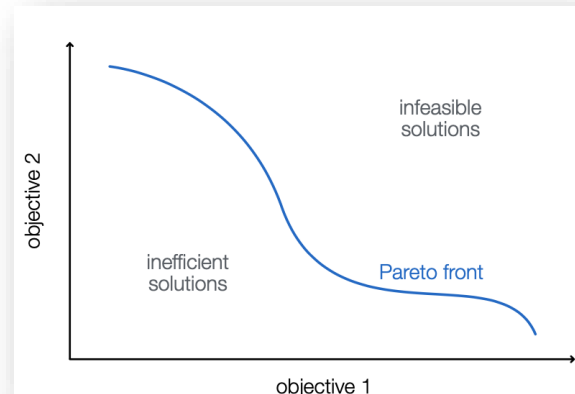


# Example: Optimization

## Bayesian Optimization of a Laser-Plasma Accelerator



- Goal: multi-parameter optimization LPA
- Using multi-objective Bayesian Optimization



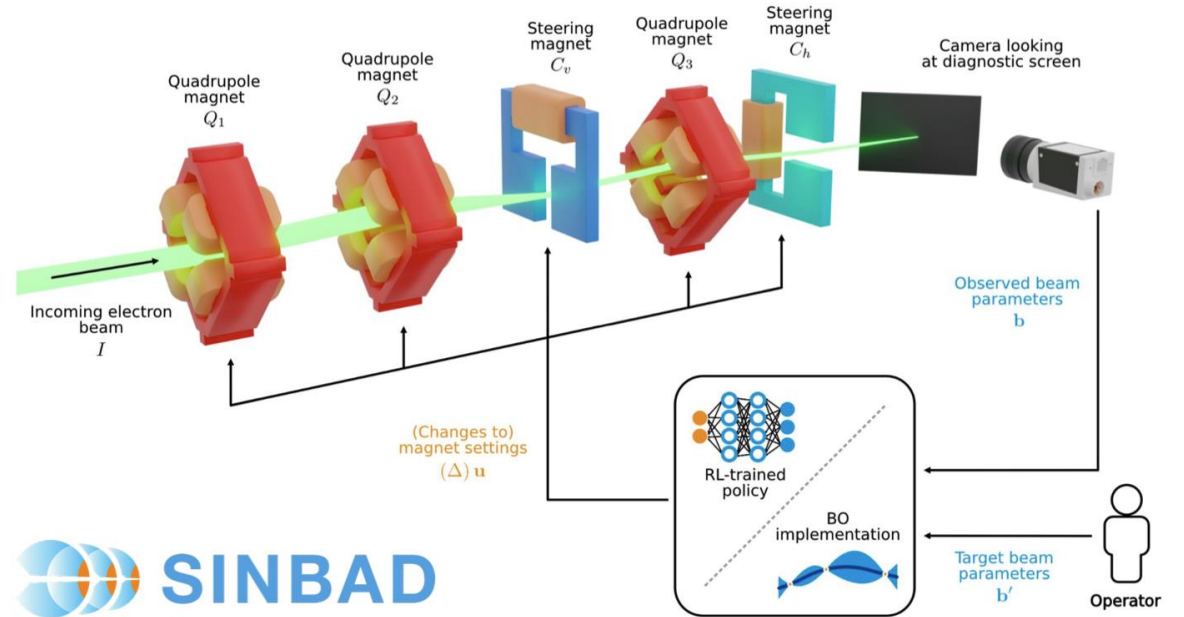
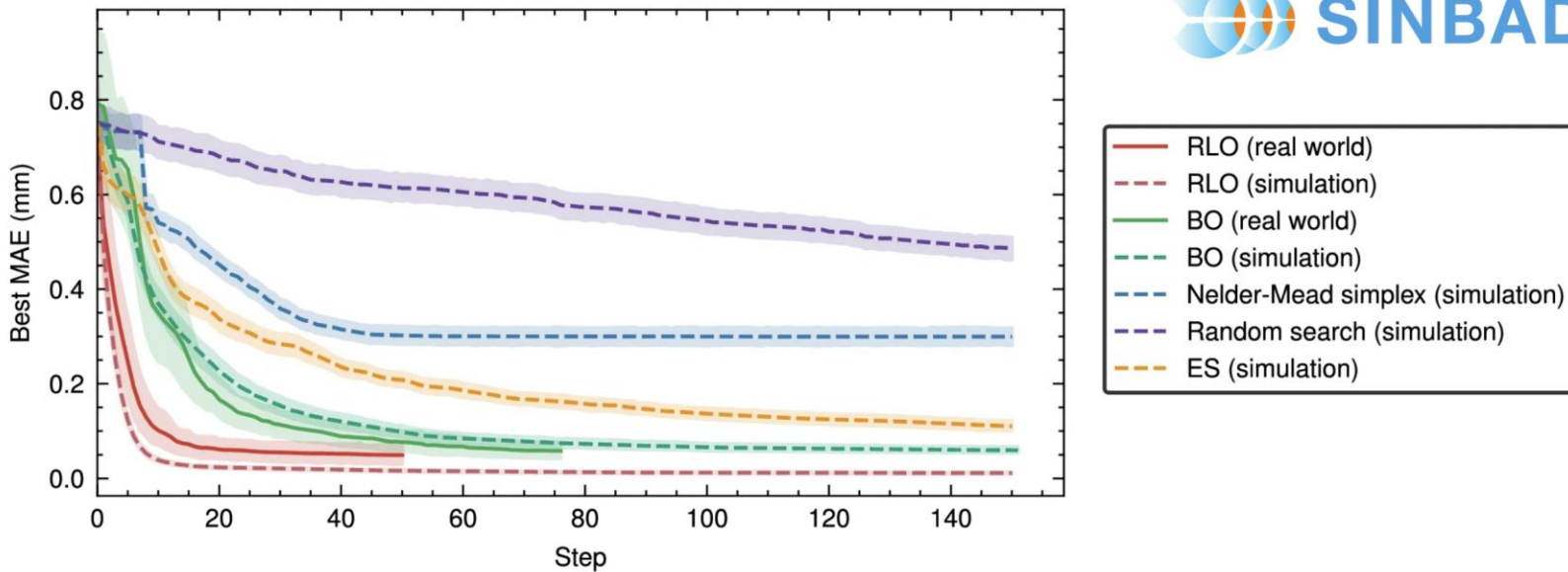
Courtesy S. Jalas



# Example: Reinforcement Learning

Start simple, ...

- Using small simple test accelerator SINBAD ARES
- Developed RL from scratch in frame of PhD
- Extended to develop fast differentiable linear beam dynamics package (Cheetah)



Courtesy J. Kaiser et al

# Example: LLMs and that stuff

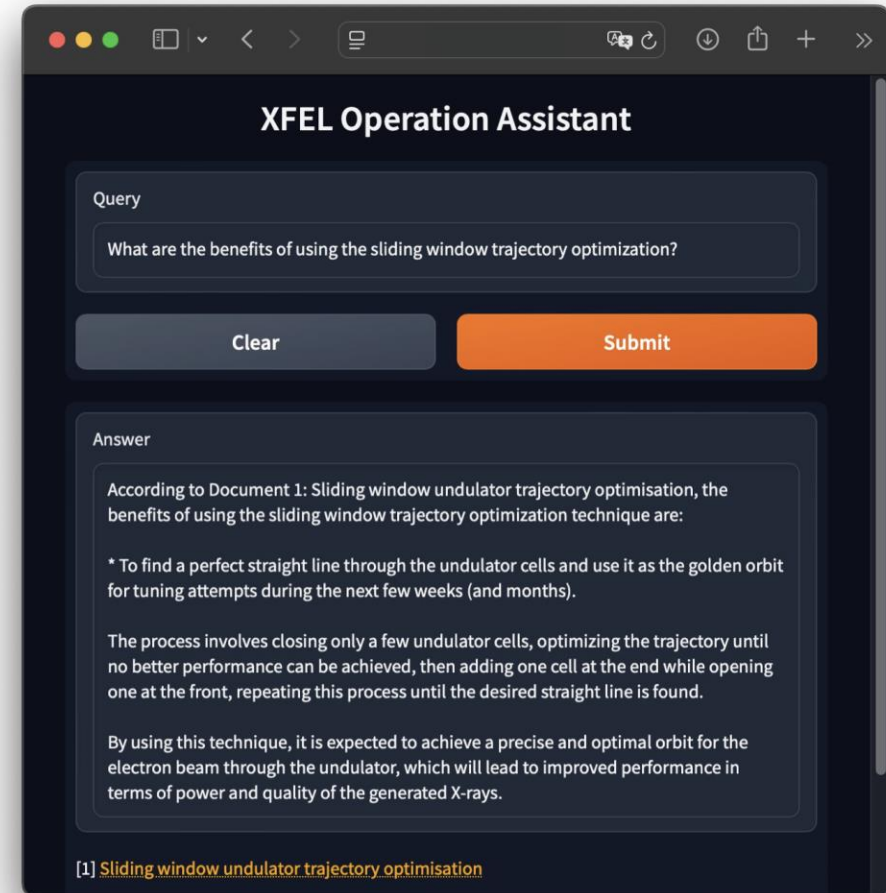
## Present

### Existing projects on campus – a small selection

- **MXL** (Frank Mayet)
  - **Chat bot** with access to operation procedures, blog, and the electronic logbook  
→ Semantic search, summaries, etc.
  - **Advanced reasoning agent** GAIA with access to multiple knowledge retrieval tools, incl. access to the machine control system
  - **Examples**
    - “What are the most recent emittance measurement results?”
    - “Please summarize today’s shift”
    - “What is the current gun amplitude?”
    - “Please summarize the last operation meeting”
    - “How can I cycle magnet XY? Please write a Python script!”
- F. Mayet, *Building an intelligent accelerator operations assistant using advanced prompt engineering techniques and a high-level control system toolkit*, LIPS Symposium, Feb. 2024
- F. Mayet, *GAIA: A general ai assistant for intelligent accelerator operations*, arXiv:2405.01359, May 2024.
- A. Sulc et al., *Towards Agentic AI on Particle Accelerators*, arXiv:2409.06336, September 2024
- A. Sulc, et al., *Towards Unlocking Insights from Logbooks Using AI.*, Proc. IPAC’24, Nashville, USA

Courtesy F. Mayet

MATTER AND TECHNOLOGIES **MT**

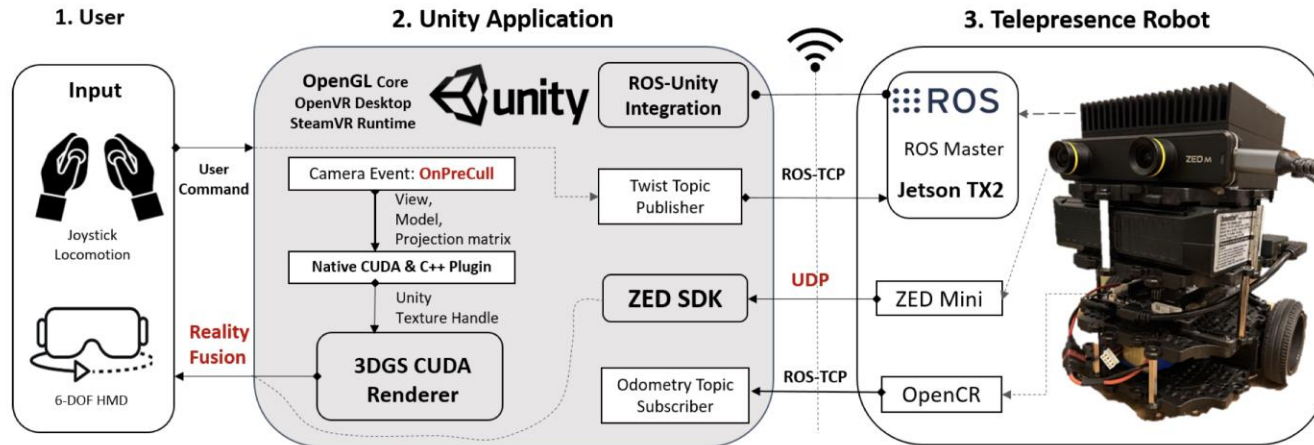


In collaboration with



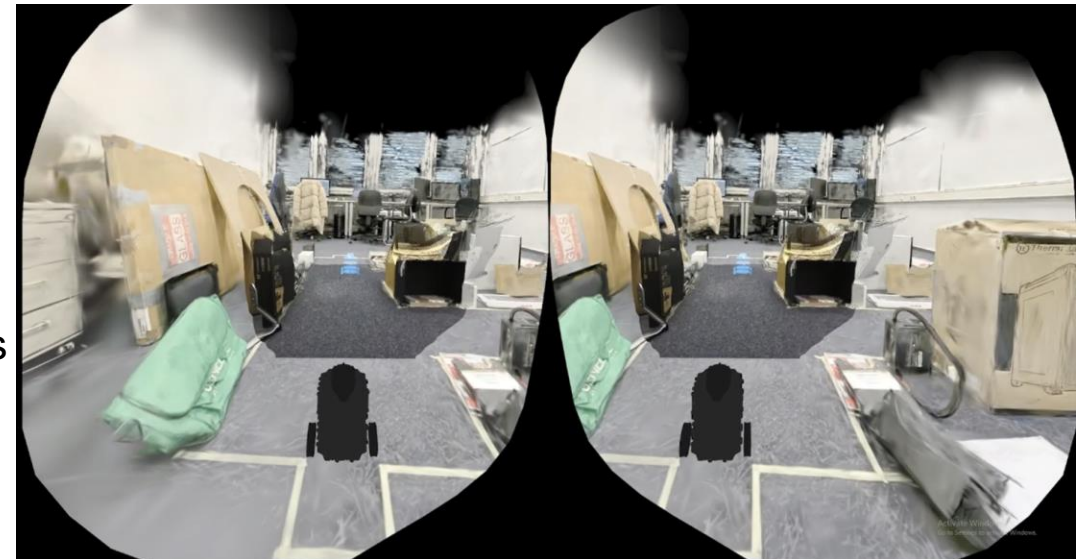
# Example: Robotics

for inspection, maintenance, remote assistance, ...



New PhD to start in March

- Many activities in many labs (CERN, Fermilab, LBNL, ...)
- Heavily building on large frameworks like Unity, CUDA
- Exploring most recent technologies like Apple Vision Pro, gest gloves
- Strong backbone with HCI department University of Hamburg



Courtesy Ke Li