TOWARDS MILESTONE ARD.01

POV IV: 2021 – 2023 – 2027

From usage of machine learning to possible impact in the ARD research program

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Pierre Schnizer, HZB
Nico Hoffmann, HZDR
Andrea Santamaria Garcia, KIT

https://indico.desy.de/event/33132/contributions/127211/
Sep 27, 2022, 15:40-16:00
8th Annual MT Meeting

ARD.01 – FROM USAGE OF MACHINE LEARNING TO POSSIBLE IMPACT IN THE ARD RESEARCH PROGRAM

All of ARD shall contribute to answer ARD.01

Update

- **For comparison see 2021:** A. Jankowiak, J. Osterhoff, ARD, 7th MT Days / Part Two,16.06.2021, pp. 7-8; https://indico.desy.de/event/29414/contributions/100337/

2021

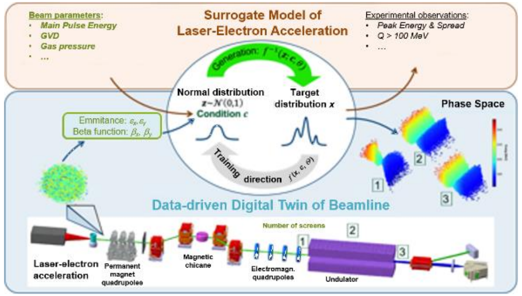
Recap of guiding (teaser) questions

- Where does **ARD profit** from ML and ML-guided research?
- Where are **break-even points** to conventional approaches?
- Can a **common understanding/language/ARD-ML-taxonomy** be found?
- Can ML **improve efficiency** (**incl. energy**) and **replace tedious/cumbersome tasks**?
- Are ML-algorithms **transferable**? Can they be **standardized** and **easy to use**?
- Is ML **fast enough for fast-feedback and control** tasks?
- What about **safety-critical applications**, if the ML-decision-process is complex?

ARD.01 - REVIEW THE USAGE AND IMPACT OF MACHINE LEARNING ON THE ARD RESEARCH PROGRAM - 2023

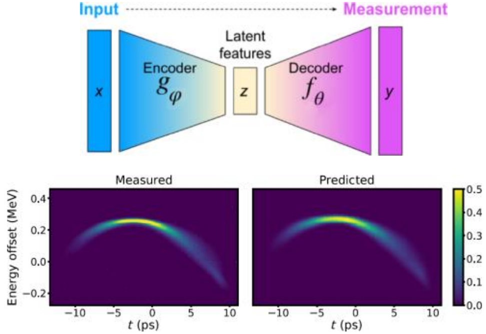
ML is ubiquitous in ARD - Examples

Data-driven digital twin with surrogate model at HZDR



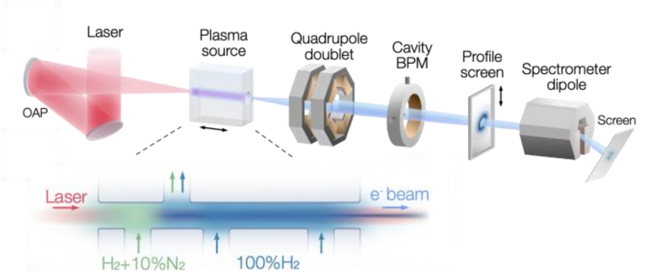
N. Hoffmann, 2022

Mega-pixel image prediction at XFEL



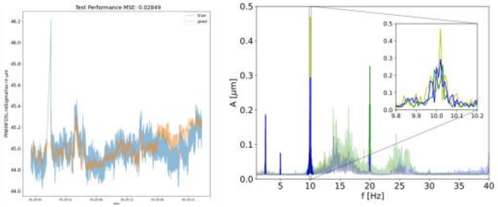
J Zhu *et. al*. arXiv:2201.05769 (2022)

Bayesian optimization at LUX



S. Jalas *et al*., Phys. Rev. Lett. 126, 104801 (2021)

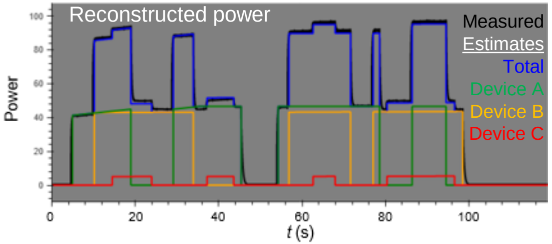
Beam prediction + orbit control at BESSY II



A. Schütt. B.Sc. thesis. 2021.

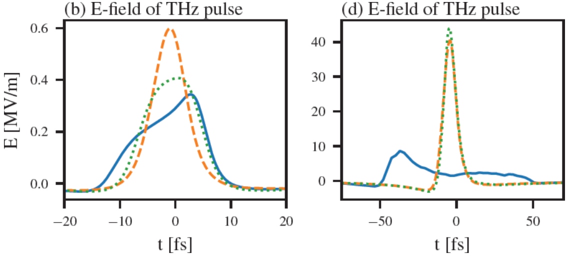
L. Vera Ramirez *et al*., THAL01, ICALEPS 2021

Predictive maintenance at GSI/FAIR Non-intrusive load monitoring (NILM)



R. J. Steinhagen: Detailed project report by the end of 2022

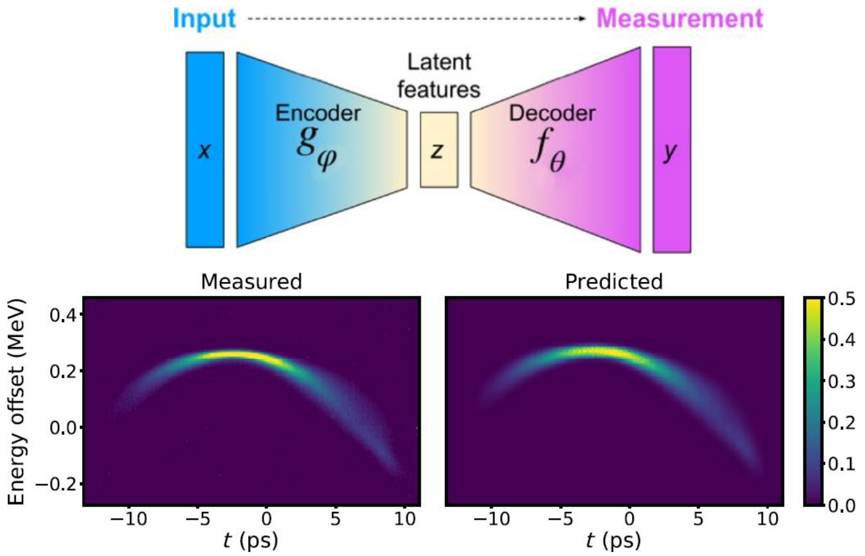
Parallel Bayesian optimization at FLUTE



C. Xu *et al*., WEPOMS023, IPAC22 (2022)

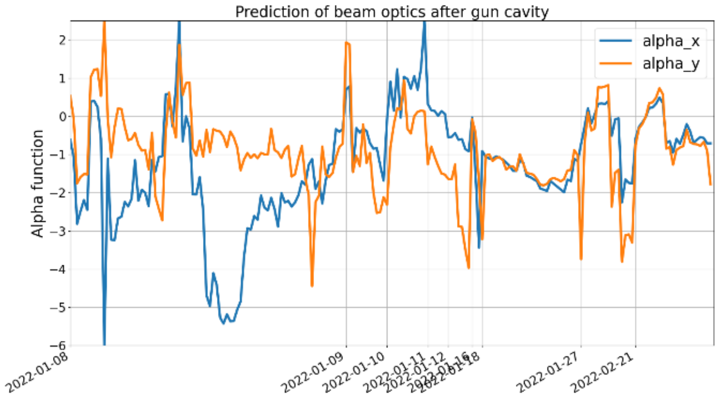
ARD.01 – VIRTUAL DIAGNOSTICS: HIGH-QUALITY MEGA-PIXEL IMAGE PREDICTION

Demonstrated usage of machine learning…



Using an auto-encoder, XFEL and DESY scientists improved **virtual diagnostics** methods to provide insights on the longitudinal beam properties

... and impact in the ARD program



- **Non-destructive diagnostics increase availability**
- Community is motivated
- Robustness is key

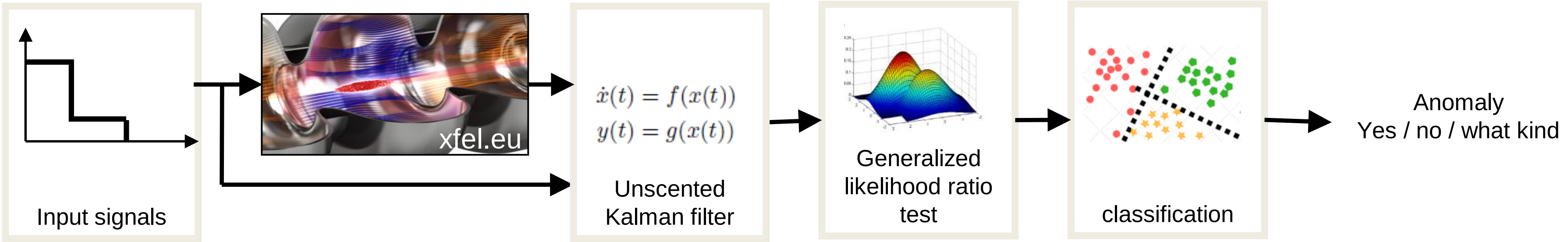
J. Zhu *et. al.*, Mixed Diagnostics for Longitudinal Properties of Electron Bunches in a Free-Electron Laser, *arXiv preprint arXiv:2201.05769*. doi: 10.48550/arXiv.2201.05769
J. Zhu *et. al.*, High-Fidelity Prediction of Megapixel Longitudinal Phase-Space Images of Electron Beams Using Encoder-Decoder Neural Networks, *Physical Review Applied* 16 (2), 024005. doi: 10.1103/PhysRevApplied.16.024005

Courtesy: M. Thévenet (DESY)

ARD.01 – ANOMALY DETECTION FOR SRF CAVITIES AT XFEL

Demonstrated usage of machine learning…

… and impact in the ARD program



Model-free, semi-supervised learning method with recurrent neural networks (RNN) for **online detection** and classification of anomalies

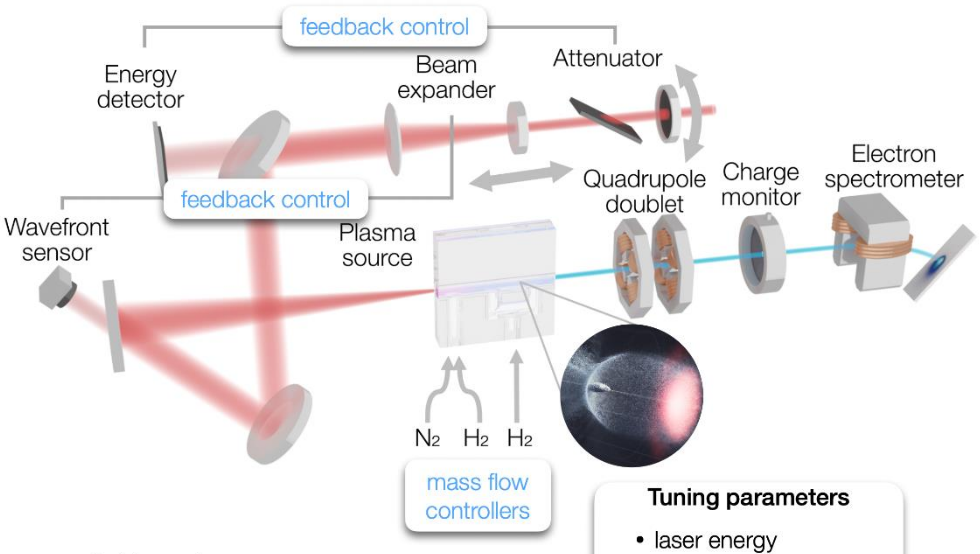
- Fine-grained **anomaly detection** and **classification**
- Next steps: in-situ testing and ML-based support

A. Sulc *et al*., A data-driven anomaly detection on SRF cavities at the European XFEL., *13th IPAC*, PUBDB-2022-02580 (2022)
A. Eichler *et al*., Anomaly Detection at the European XFEL using a Parity Space based Method, *arXiv:2202.02051* (2022)
A. Grünhagen *et. al*., Fault Analysis of the Beam Acceleration Control System at the European XFEL using Data Mining, *Proc. Asian Test Symposium (ATS)*, 61-66 (2021). doi
G. Martino *et. al*., Comparative evaluation of semi-supervised anomaly detection algorithms on high-integrity digital systems, *Proc. Euromicro Conf. on Digital System Design*, 123-130 (2021). doi

Courtesy: M. Thévenet (DESY)

ARD.01 – OPTIMIZATION: BAYESIAN OPTIMIZATION OF A PLASMA ACCELERATOR

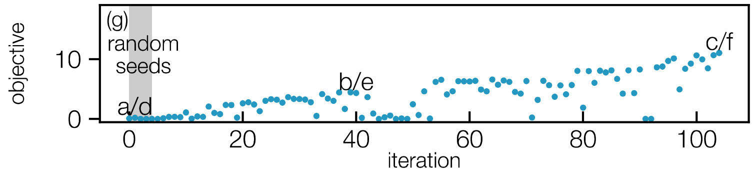
Demonstrated usage of machine learning…



S. Jalas et al.
Bayesian optimization of a laser-plasma accelerator
PRL 126, 104801 (2021)

Autonomous tuning of laser plasma accelerators (LPAs) using **Bayesian optimization** at LUX

... and impact in the ARD program



The objective is a measure of the beam quality (combining charge and energy spread)

- Used in production for
  - better and faster operator-agnostic tuning
- Greatly **reduces cost** of LPA design studies
- **Next steps**: multi-objective, higher repetition rate, standardized interface shared in the community

J. Kaiser *et al.,* Learning-based Optimisation of Particle Accelerators Under Partial Observability Without Real-World Training, PMLR 162:10575 - 10585, 2022. https://proceedings.mlr.press/v162/kaiser22a/kaiser22a.pdf
A. Ferran Pousa *et al*., Multitask Optimization of laser-plasma accelerators using simulation codes with different fidelities, IPAC2022, WEPOST030, (2022) https://doi.org/10.18429/JACoW-IPAC2022-WEPOST030

Courtesy: M. Thévenet (DESY)

ARD.01 – SUSTAINABLE & TRANSFERABLE AI ECO- SYSTEM I/II

Core/meta-goals – **developing**, **investing**, and **fostering** …

… **standardized** digitization, tooling & related SW infrastructure

- pre-requisite for any machine-learning system
- still a lot of heterogeneity across labs and industry
- ➢ emphasis on free & open-source tooling & infrastructure

(N.B. strong prerequisite for any scientific reproducibility, verifiability or peer review)

… **sustainability of AI eco-system**

- op. integrated, exchangeable & transferable across different labs and applications

(N.B. still most one-of' proof-of-concept ML-projects do not survive the test of time! ↔ reproducibility)

… **public-private partnerships** with other institutes and industry

- ➢ "building people & systems"

Public Money
Public Code
publiccode.eu

Courtesy: R. J. Steinhagen (GSI)

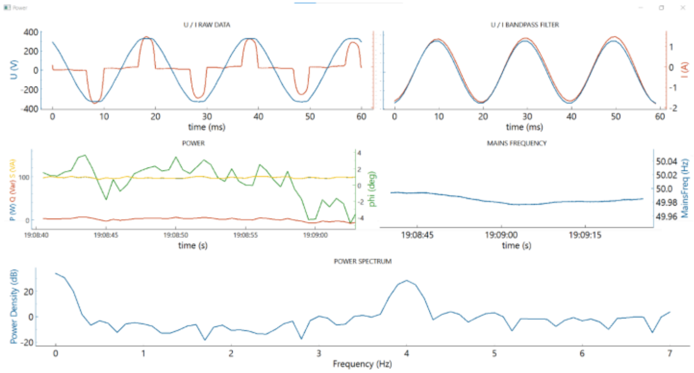
ARD.01 – SUSTAINABLE & TRANSFERABLE AI ECO-SYSTEM II/II

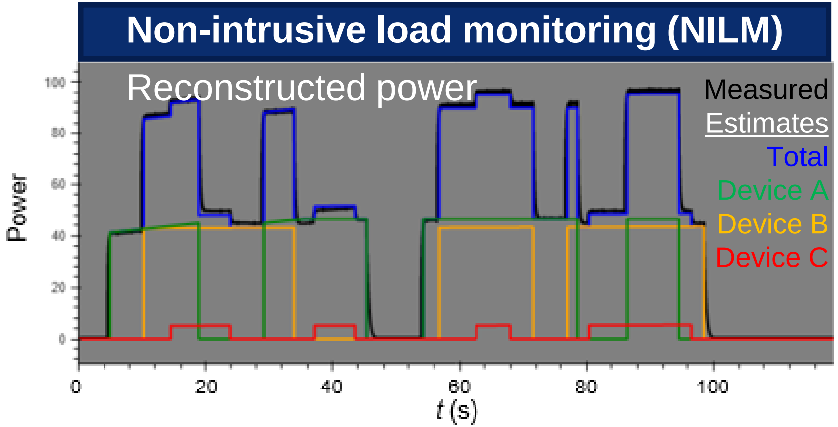
Specific ARD demonstrator applications/incubator projects in 2021/22

- **Pulsed-power monitoring system**
  - **Facility compliance with energy supplier constraints on reactive load**
  - Non-intrusive load monitoring (NILM) aka. ‘load disaggregation’
  - Cost-effective device-level energy-meter & break-down of energy consumption w/o per-device-DAQ
  - Anomalous power consumption and failing devices detection → enhances **predictive maintenance**
  - Test-bed and benchmark for interchangeable ML modelling and integration

Detailed project report by the end of 2022

Pulsed-power energy feed monitoring





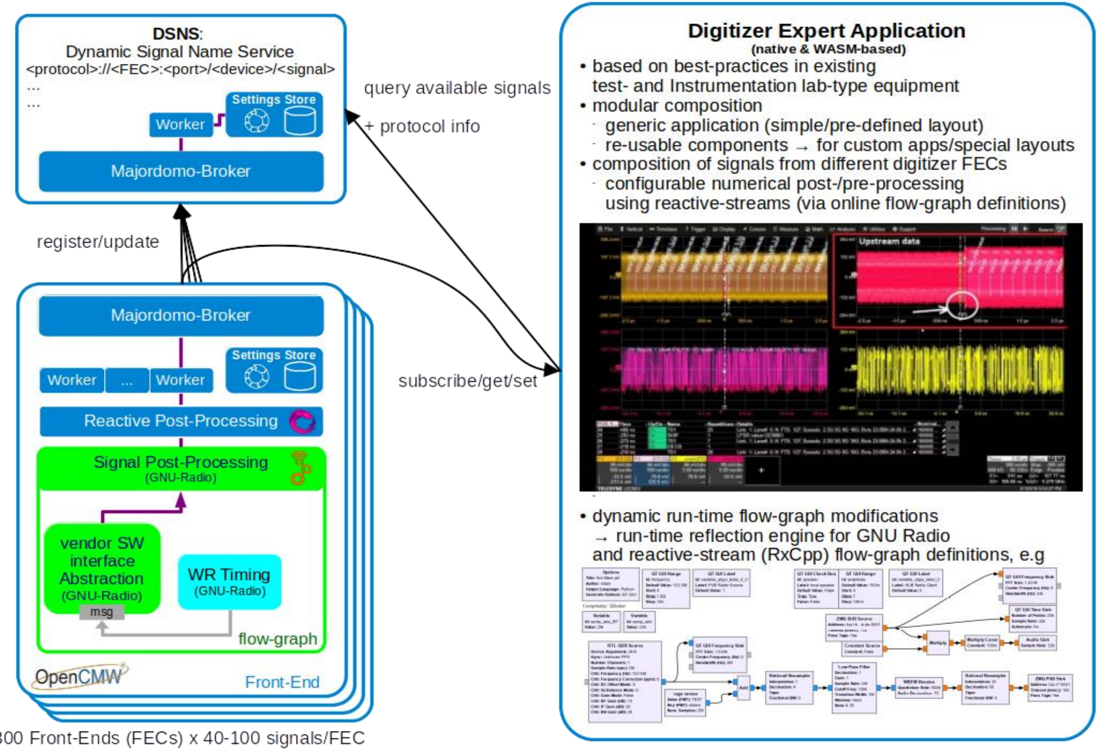
Courtesy: R. J. Steinhagen (GSI)

ARD.01 – USER INTERFACE TECHNOLOGIES

- **Generic digitizer FECs**
  - Actual-vs-reference monitoring
  - SDR- & flow-graph integration
- **Digitizer expert application**
  - Full control over all FEC parameter
  - Prototyping/debugging by devices
- **Operational digitizer application**
  - Reduced functionality ↔ OP focus
  - Specialized UI layouts
- **Machine-experiment interfaces**
  - CIT/SDE, Hades, (m)CBM
  - (Super-)FRS, …
- **Dynamic (signal) name service**
  - Registry (where to find which signal)
  - Site-wide & redundant

UI technologies: native, web browser, mobile/tablets, …

… in the FCC, tunnel, or anywhere else @GSI/FAIR

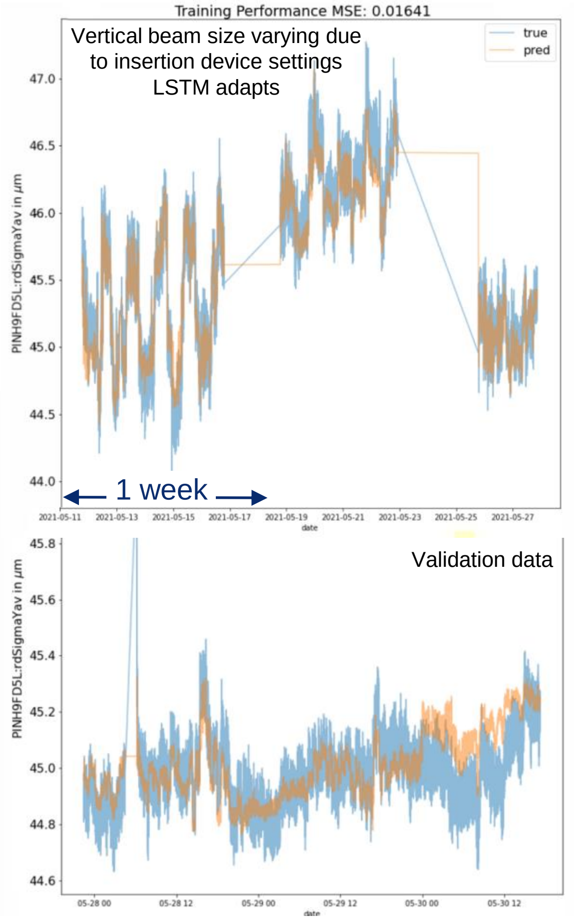


ARD.01 – BEAM SIZE PREDICTION AT BESSY II

- **Beam size**: **user influence each other**
- Trained LSTM network ← thermal effects
  - LSTM: long short-term memory
- **Can predict on the short term**: training on larger data sets

- **Impact**
  - BESSY II: nice to have
  - BESSY III / 4th generation light sources → **necessity**

- **Testing**
  - Other operation modes
  - Transfer tests on MLS



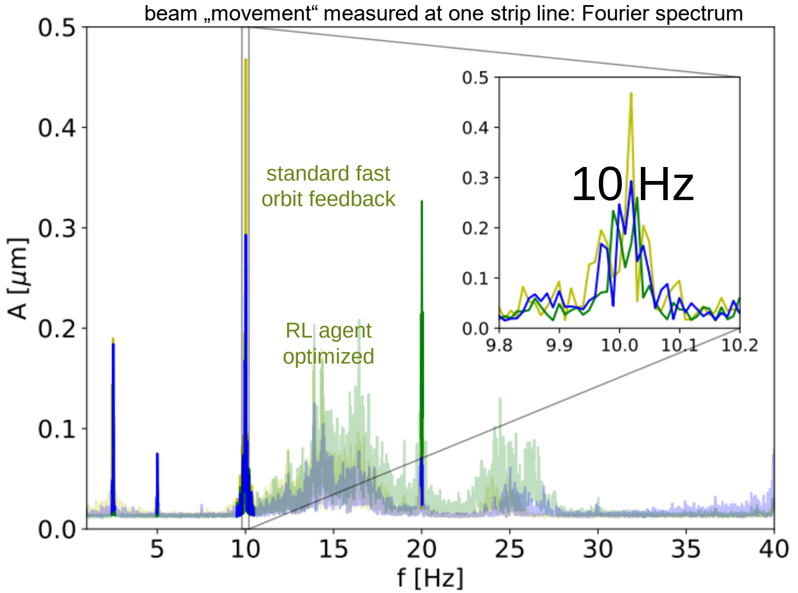
A. Schütt. Bachelorthesis. 2021.
https://tubcloud.tu-berlin.de/s/k4s33NQGxA6ad7X

Courtesy: P. Schnizer (HZB)

ARD.01 – REINFORCEMENT LEARNING USED IN BESSY II OPERATION

- **Reinforcement learning**
  - Reduction of harmonic excitation of beam motion
  - Model free approach
  - Trained on machine
- **Demonstrated to surpass classical approaches**
  - Fast orbit feedback control
- **Current limitations**
  - Real-time action (set-value) delivery
- **Requires hardware upgrade**
  - ML-grade machine with reflective memory

Reducing random beam motion
Roughly ~2 of peak performance



L. Vera Ramirez *et al.* „Machine learning tools improve BESSY II operation”
THAL01, ICALEPS 2021

Courtesy: P. Schnizer (HZB)

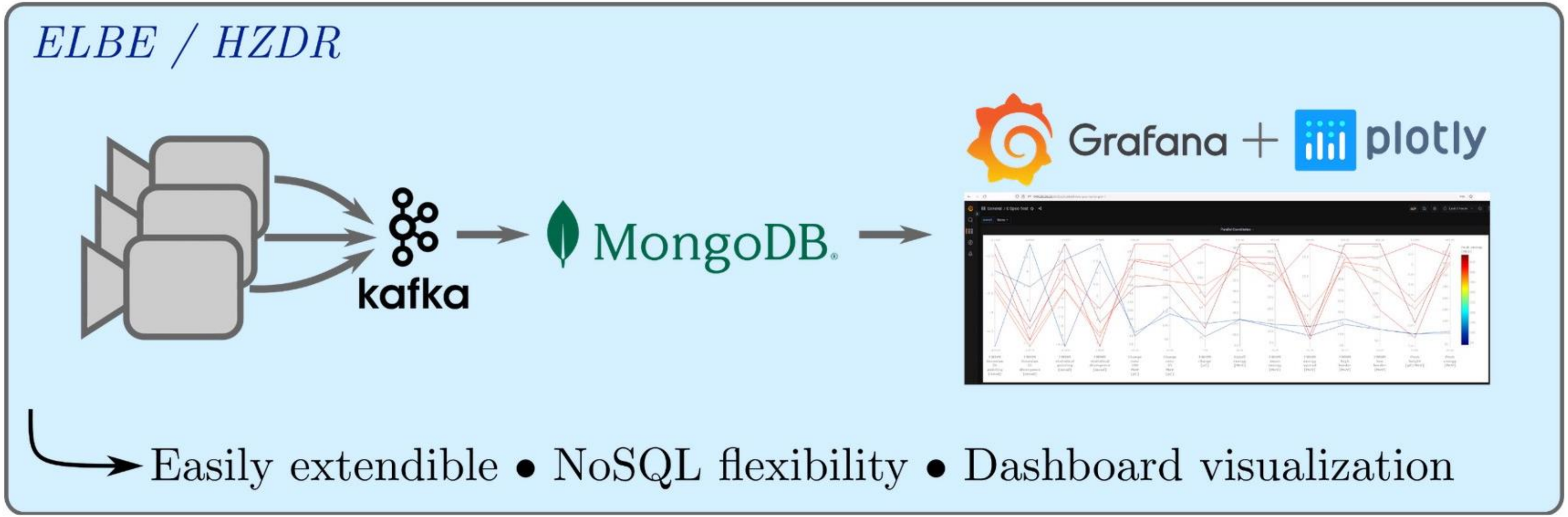
ARD.01 – VIEWS FOR BESSY II, MLS AND BESSY III

- **Supervised learning long short-term memory** (LSTM): towards beam size **forecast**
  - BESSY II **nice to have**
  - MLS transfer target → **improve user operation**
  - BESSY III considered **a necessity**
- **Reinforcement learning**: beam vibration **control**
  - Model pre-trained with archiver data
  - Further training on machine
  - **Demonstrated**: can surpass classical algorithms
  - **Hardware upgrade required** for next steps
- **Gaussian processes for optimization tasks**
  - Different optimizations of the BESSY II machine
  - Using Gaussian processes for reducing required time towards minimum
  - Experience being built up

Courtesy: P. Schnizer (HZB)

ARD.01 – VIEWS ON ADOPTION OF MACHINE LEARNING

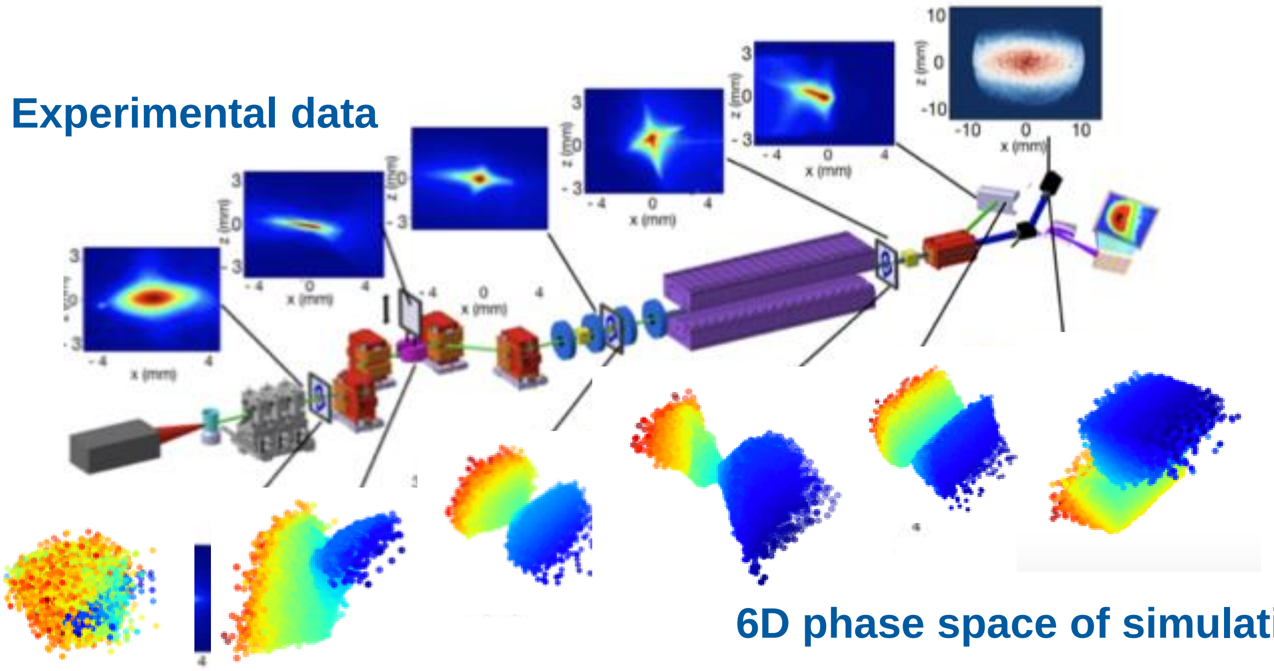
Flexible integration and **visualization** of **experimental (meta-)data** is **key** to **foster** the **adoption rate of ML**



Courtesy: N. Hoffmann (HZDR)

ARD.01 – RESEARCH ON DIGITAL TWINS OF A FEL BEAMLINE

Training on **simulation data** ensures that **inversion** of **experimental data** stays **consistent** to **theory**

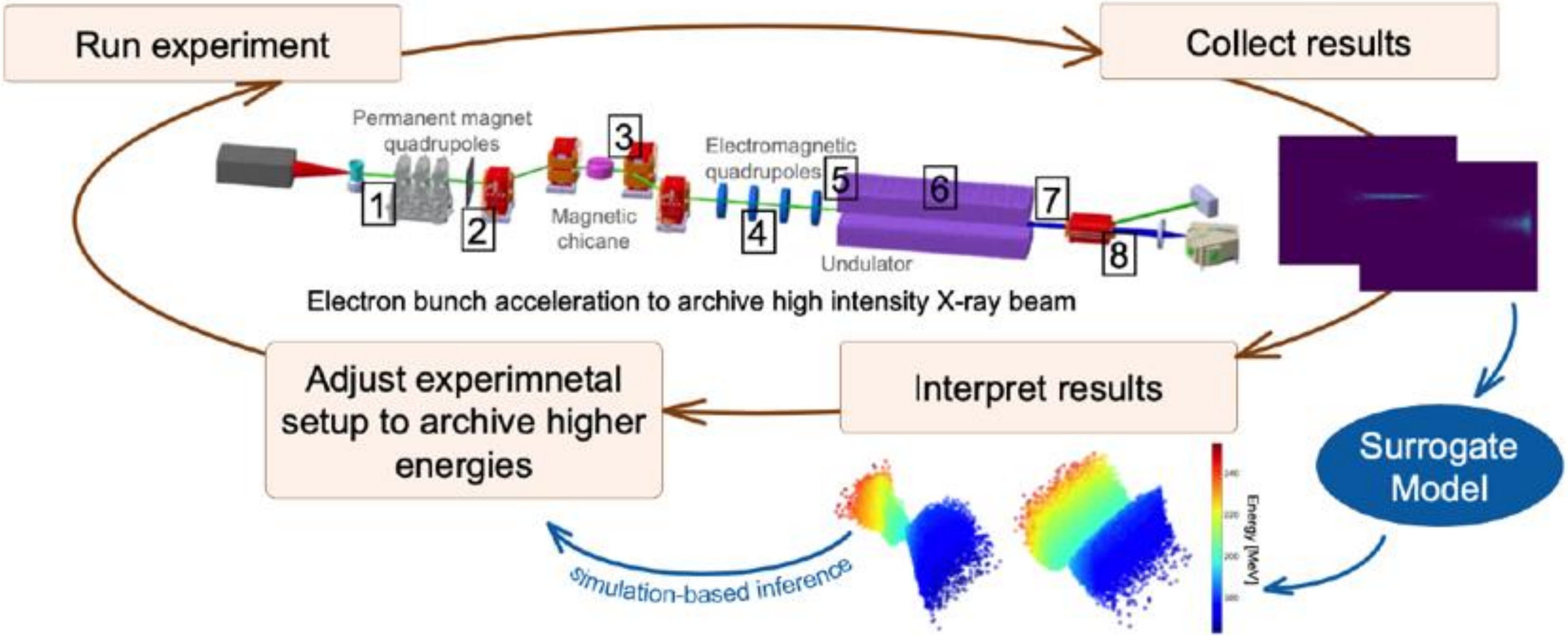


Anna Willmann, Towards a Data-driven Digital Twin of a Free Electron Laser
26.09.2022, https://indico.desy.de/event/33132/contributions/129471/

Courtesy: N. Hoffmann (HZDR)

ARD.01 – PHYSICS-INFORMED DIGITAL TWIN OF THE FEL BEAMLINE AT HZDR

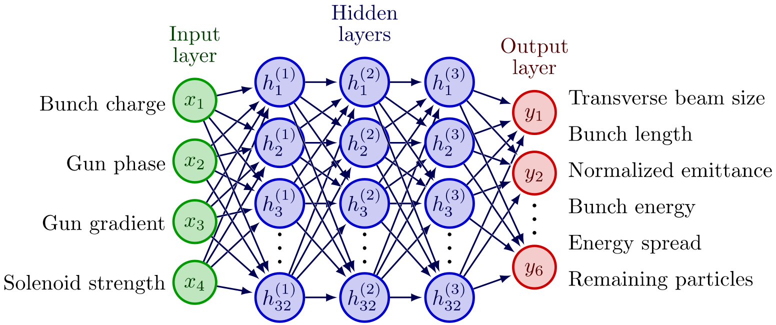
Physics-informed digital twins pave the way for **start-to-end (S2E) model predictive control** & **optimization**

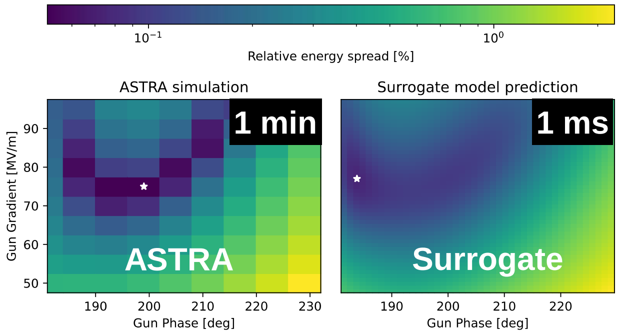


Courtesy: N. Hoffmann (HZDR)

ARD.01 – SURROGATE MODELS AND PARALLEL BAYESIAN OPTIMIZATION

Surrogate model at FLUTE

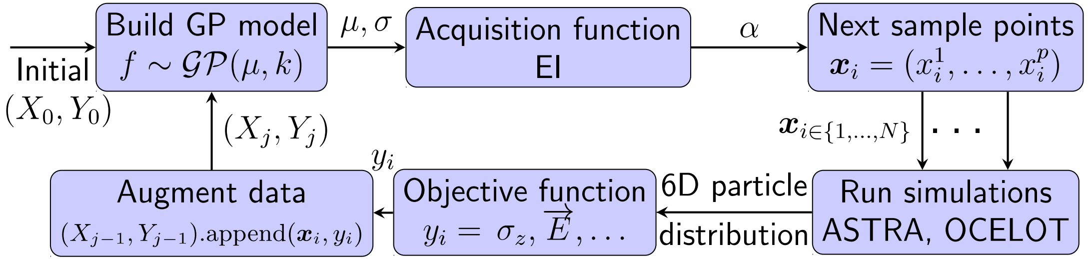




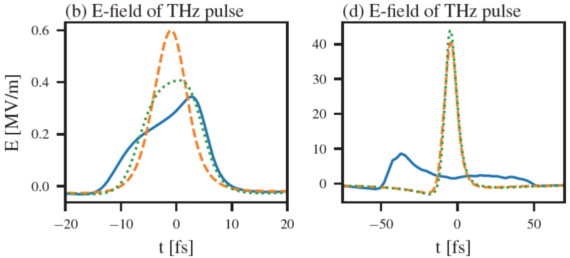
C. Xu *et al*. TUPOPT070, IPAC22

Faster models for **online prediction (virtual diagnostics)** and **reinforcement learning** training

Parallel Bayesian optimization to improve THz pulses



Improvement of conditions at **experiment** and **probabilistic model available**



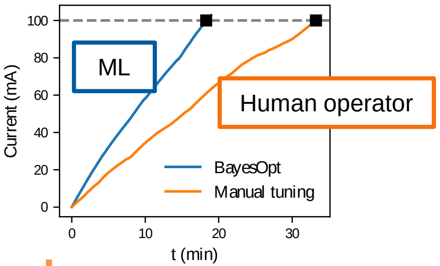
C. Xu *et al*. WEPOMS023, IPAC22

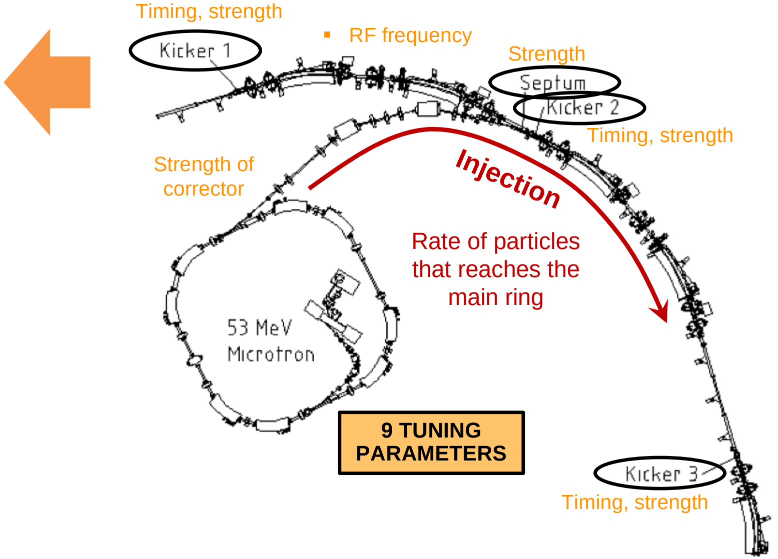
Courtesy: A. Santamaria Garcia (KIT)

ARD.01 – BAYESIAN OPTIMIZATION (BO) AND REINFORCEMENT LEARNING (RL)

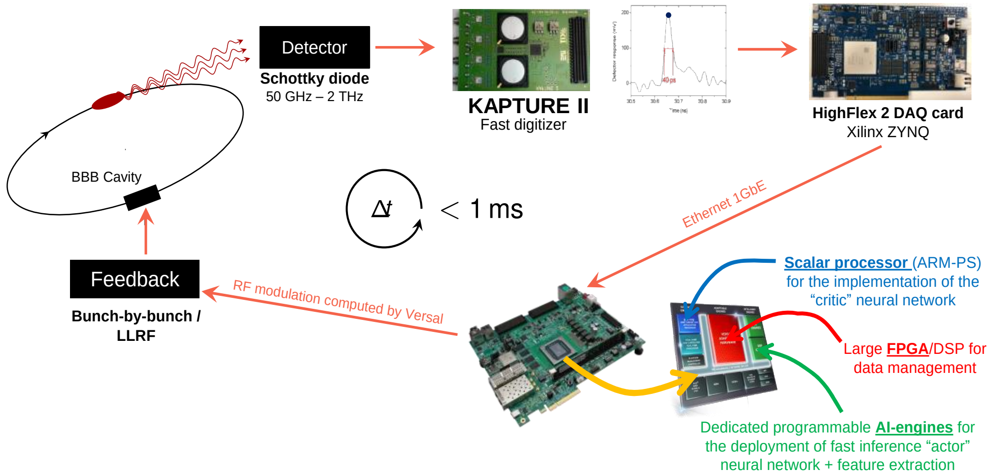
BO for injection efficiency at KARA

Optimization algorithms make the **set-up** and **switch** between **operation modes faster**, as well as **commissioning**





RL for micro-bunching control



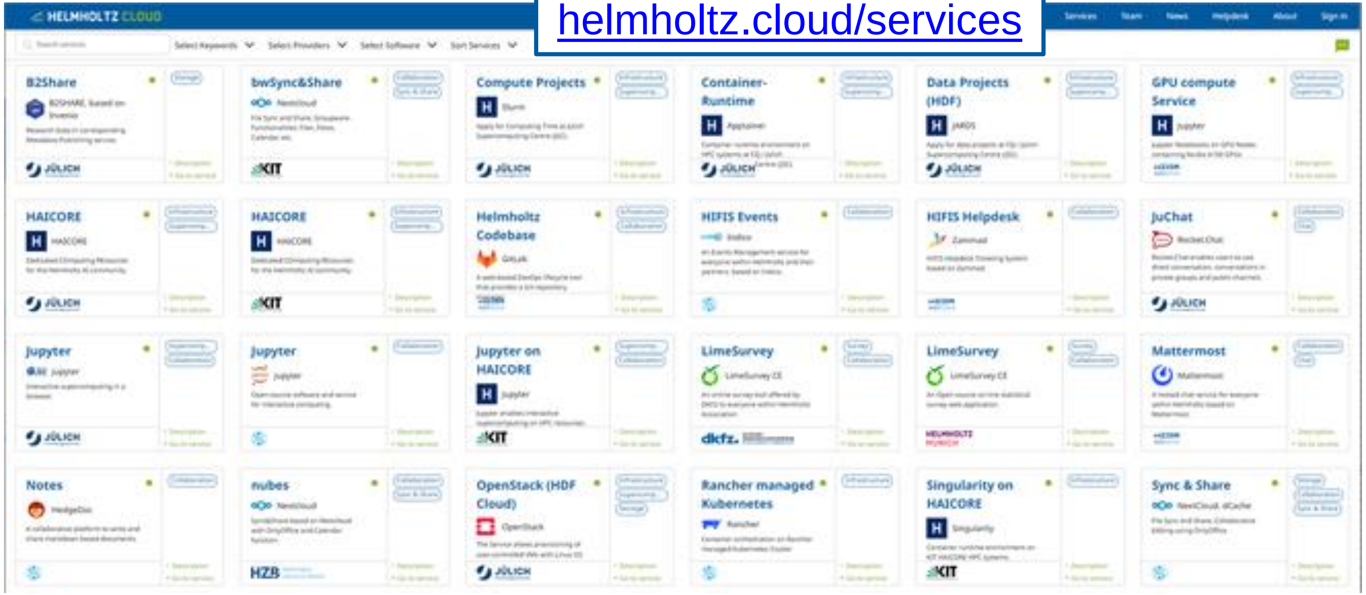
Reinforcement learning and **hardware developments** open the door to **unprecedented control** over unstable beam dynamics

W. Wang *et al.*, doi: 10.1109/TNS.2021.3084515 (2021)

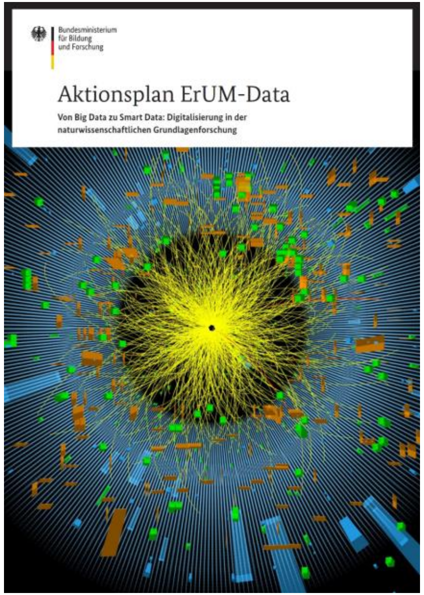
Courtesy: A. Santamaria Garcia (KIT)

ARD.01 – OBSERVE ACTIVITIES AT ALL LEVELS: HELMHOLTZ CLOUD, ERUM-DATA, ...

helmholtz.cloud/services



erumdatahub.de



(2021-2025)

ERUM DATA HUB

ACCLAIM Meeting

Friday Sep 9, 2022, 11:00 AM → 1:00 PM Europe/Berlin

Description Join Zoom Meeting

Link

Helmholtz AI
Autonomous Accelerator

Link

A. Eichler *et al.*, TUPAB298, IPAC2021 (2021)
C. Xu *et al.*, TUPOPT070, IPAC2022 (2022)

Collaboration with applied informatics
(M. Färber, KIT, data and web science)

Other activities?

ARD.01 – REVIEW THE USAGE AND IMPACT OF MACHINE LEARNING ON THE ARD RESEARCH PROGRAM - 2023

Where do we go from here?

- **Next generation light sources** → ML a necessity → AI/ML-grade machines & hardware, fast feedback control (orbit, radiation)
- **Sustainable & transferable AI ecosystem**, standardized digitization, tooling & related SW infrastructure, …
- **Digital twins** (experimental data, simulation, training, inversion, theory, forecast, prediction, …), **surrogate models**
- **…**
- **The human factor**: strategies to foster adoption rate of ML and (meta-)data acquisition

Activities: observe, collect, review & prepare evaluation of impact to complete milestone

- **Exploit synergies** – as much as possible (DMA, DTS, ACCLAIM, Helmholtz AI, HIFIS, …)
- **Plan**: establish collection-site with **one** entry point for **ARD-relevant** ML usage to review
- Organization of & participation in workshops, e.g. **ARD-ST3 pre-meeting ML workshop** https://indico.desy.de/event/35272/
- ***Toward Q4/2023***: ARD workshop "**Impact of ML on the ARD-research program**", communicate results

TOWARDS MILESTONE ARD.01

POV IV: 2021 – 2023 – 2027