Workflows for future observations

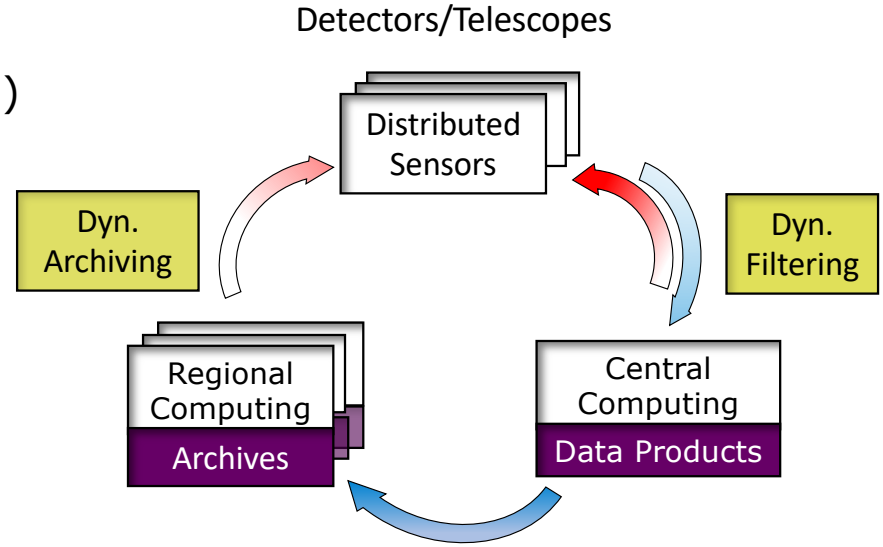
Astronomy / particle physics

Volker Büscher, Christof Buchbender, Hermann Heßling,
Ramesh Karuppusamy, Cristina Manzano, Jacob Nordin,
Andreas Redelbach, Stephan Schlemmer,
Christian Schmidt, Arno Straessner

March 18, 2025

Workflows for future observations

1. Which elements do they involve? Connection to TA / pillars and requirements on them.
   - **Continuation of TA5**
   - Realtime computing
     - Specialized hardware (GPUs, FPGAs, future HW)
   - Offline Computing
     - Memory-based computing
   - ML (⇔ Toolbox)
   - Software-to-the-data
     - Containerization
   - Connection to further TAs/pillars
     - Federated Infrastructures (⇐ AAI)
     - Data management (⇔ Metadata)

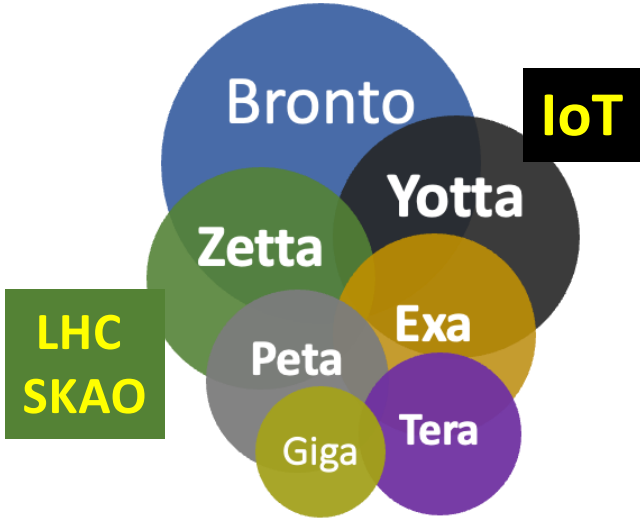


2. Which problems do they solve?
   - The selection of “interesting information” in real time from large data streams is complex (requires expertise knowledge in hardware, stream processing, physics, software engineering, HPC, …). PUNCH 2.0 could contribute to the further development of selected topics in this area.
   - Towards **Smart Green Computing**: AI-based effective reduction of data volumes already during data acquisition

Workflows for future observations

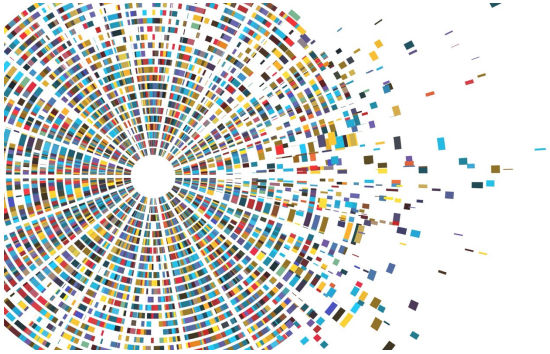
3. Which gaps do they fill?

- ML/algorithms for realtime analysis of huge data streams
- Training the users/scientists and developing the workflows and environments for fast data processing, in particular for non-standard data processing hardware like FPGAs



4. How could they be generalized?

- Taming data floods important in more and more areas (IoT, Smart Cities, Photon Science, Genomics, …)



Workflows for future observations

5. End-to-end FAIR use case?

   - Repositories of workflows ⇒ open software
   - Enabling close-to FAIR access to portions of raw data, e.g. at the level of
     - (calibrated) hits in particle/nuclear physics
     - (calibrated) voltages in radio astronomy

6. Connection to DRP? – a digital output of a research process
   (which category: publication, data set, software, …)

   - ML models and training data can be published both as software or as articles outlining the technique

7. How is the use case viewed from outside of PUNCH?
   (which category: publication, data set, software, …)

   - Blueprint for real-time analysis workflow based on fast hardware/algorithms plus (F.A.I.R.) metadata
   - ML models may find applications in other areas of astrophysics (eg. GW astronomy), or extracting patterns from Smart City's network of sensors

Workflows for future observations

9. Operation model? - what is required for the use case, and how to organize that?

- Postdocs and PhD students
- 1/2 research, 1/2 supporting “services” of TAs
  - Mainly related to Toolbox, but also to (Meta)Data Management and Federated Infrastructures
- Storage (meta-/data from experiments, Digital Twins) + compute resources ⇐ DZA

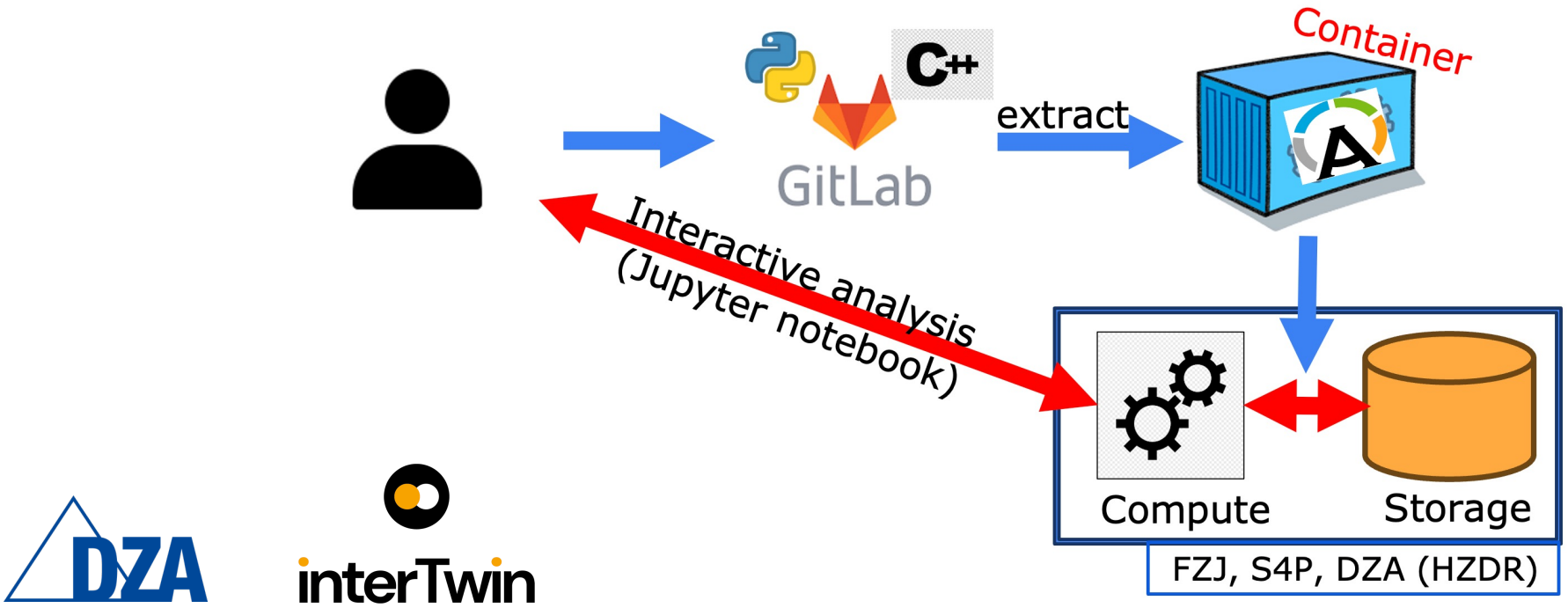
10. Sustainability?

- Creation of well documented and maintained software libraries
- Long-term support of archives + (selected) pipelines (beyond PUNCH 2.0) ⇐ DZA

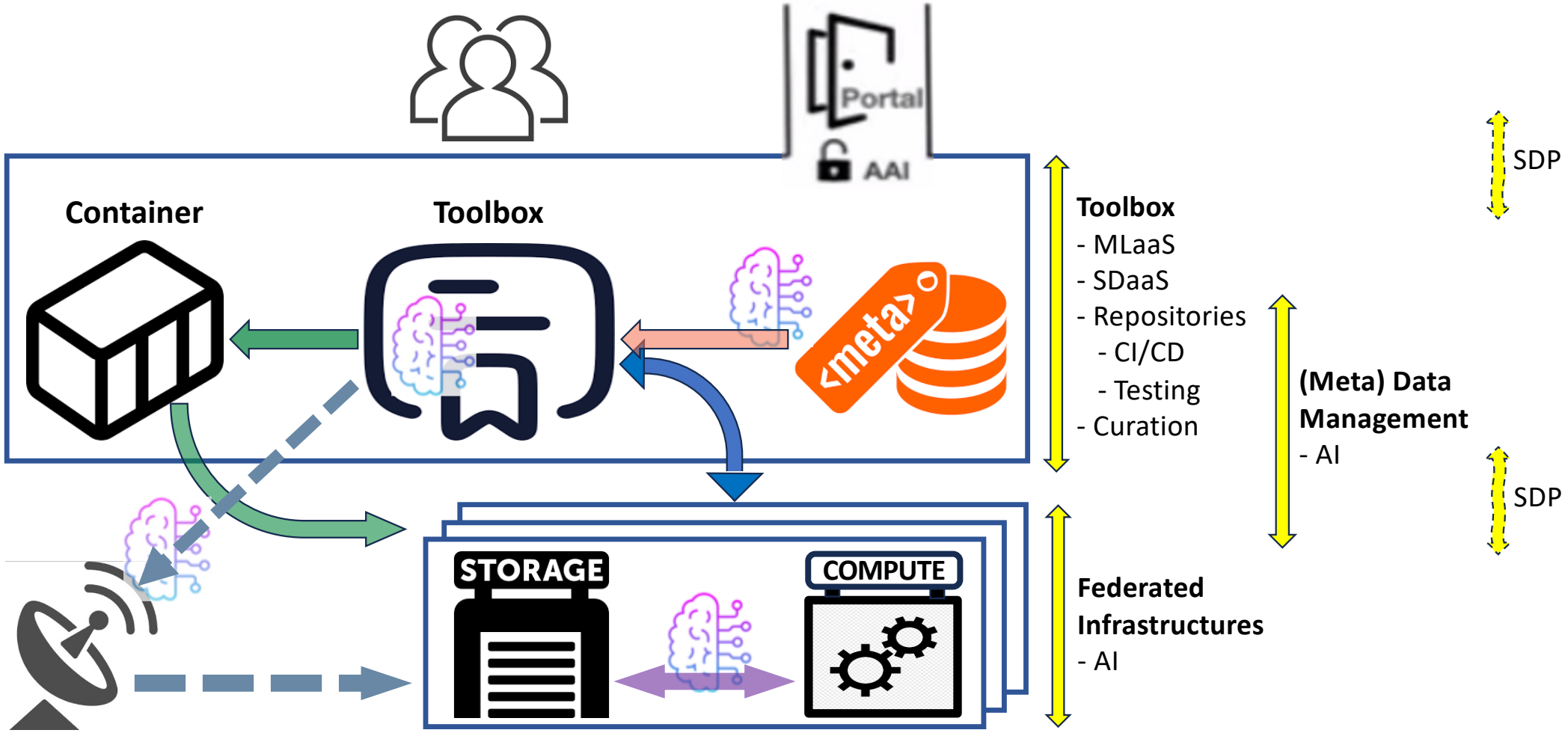
Workflows for future observations

8. Define input – procedure – output? Specify workflow.

- TA5: Machine Learning-based Pipeline for Pulsar Analysis (ML-PPA)



Workflows for future observations



Toolbox: working groups (WG)

WG 1: Software Development as a Service (SDaaS)

- Continuous Integration / Continuous Development (CI/CD)
- Automated testing
- Container generation (in cooperation with “federated infrastructures”, important: security)
- PUNCH Quality (PunQ) Award: gold, silver, bronze
  - Criteria: status of repository, containerization, use of infrastructures, documentation, …

WG 2: ML as a Service (MLaaS)

- Optimization of existing AI-based workflows for use in HPC
  - GPU cluster, parallelization of training
- ML in real-time computing (FPGAs, re-training in real-time, …)
- Analysis of huge data objects (memory-based computing)

WG 3: Curation

- Long-term support of workflows astro/particle physics
  - In cooperation with long-term support of archives (and experiments)
  - Container registry (in cooperation with “(meta) data management”)

WG 4: Tools for metadata handling

- Searching
- Accessing
  - Large language models
- Easy generation of new metadata tags
- In cooperation with “(meta) data management”

WG 5: Training & Teaching

- Summer schools (on selected topics from WG 1-3)
- Support for applying ML in astro/particle physics