FAIR Data of Physical and Digital Beamlines

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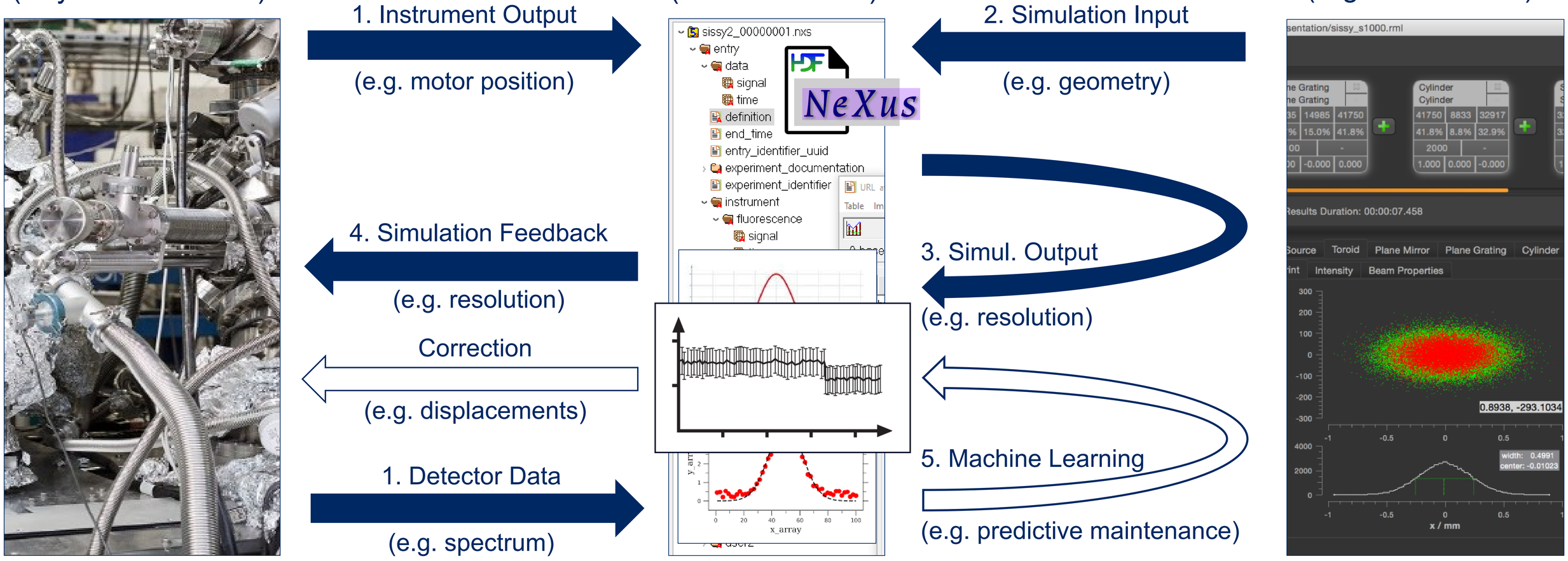
Combining Experimental and Simulation (Meta)data

- We use the instrument control system to connect the physical and digital beamline.
- Using NeXus to store beamline data in a meaningful way so the connection between experimental and simulation data is visible to human and machine agents.
- (Meta)data is considered AI/ML ready; beamline simulation can be performed from NeXus file.
- Implemented at Aquarius at BESSY II which is testing the next-generation experiment control system, based on BlueSky, and (meta)data software at HZB.



1. Instrument Control

(Meta)data originates from various sources:

- detectors deliver the primary data of interest,
- motors provide positions of devices.

2. Simulation Input

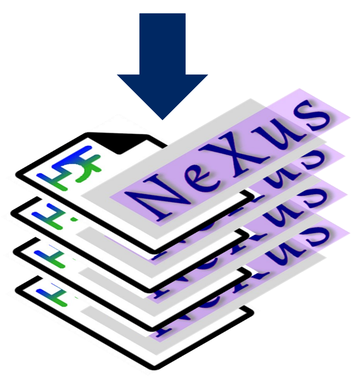
Simulation input is verified during commissioning:

- list of performance-relevant components,
- global geometry and facing of components,
- key parameters of individual components.

3. Simulation Output

Combine 1. + 2. to simulate current beamline state:

- inaccessible beam properties complement instrument description to improve reusability,
- (meta)data comparable to the physical beamline such as detector signal (without sample).



Repository

4. Simulation Feedback

Selected simulation results are returned to instrument control software:

- comparing nominal and real values such as measured resolution vs. instrument resolution could reveal broadening of signal,
- observing inaccessible beam properties such as beam dimensions at sample position,
- helps instrument team to make decisions.

5. Machine Learning

The repository would allow long-term observation:

- observing nominal-actual value difference to detect performance anomalies,
- identify upcoming breaking of components (predictive maintenance).

(Meta)data of both worlds in single NeXus file

- (Meta)data enrichment: detailed instrument section improves reusability
- Creating context by placing experimental and simulation data next to each other
- Semantics: matching simulated and real-world nomenclature
- Interoperability: same tools to access data
- AI-ready: (meta)data exploitable by AI/ML techniques; extended simulations can be performed from file
- Whole picture: simulated observations of inaccessible real-world (meta)data

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