

# Toward a Digital Twin at the NeXus File Level.

Gerrit Günther // Simone Vadilonga // Peter Baumgärtel // Oonagh Mannix

Helmholtz-Zentrum Berlin für Materialien und  
Energie, Hahn-Meitner-Platz 1, 14109 Germany

gerrit.guenther@helmholtz-berlin.de

## 1. Real Instrument Output

(Meta)data of real world comes from various sources:

- Detectors deliver the primary data of interest
- Experiment control collects various metadata such as temperature from a sensor or the position of a motor
- ELN contains notes or manual setup changes

## 2. Simulation Input

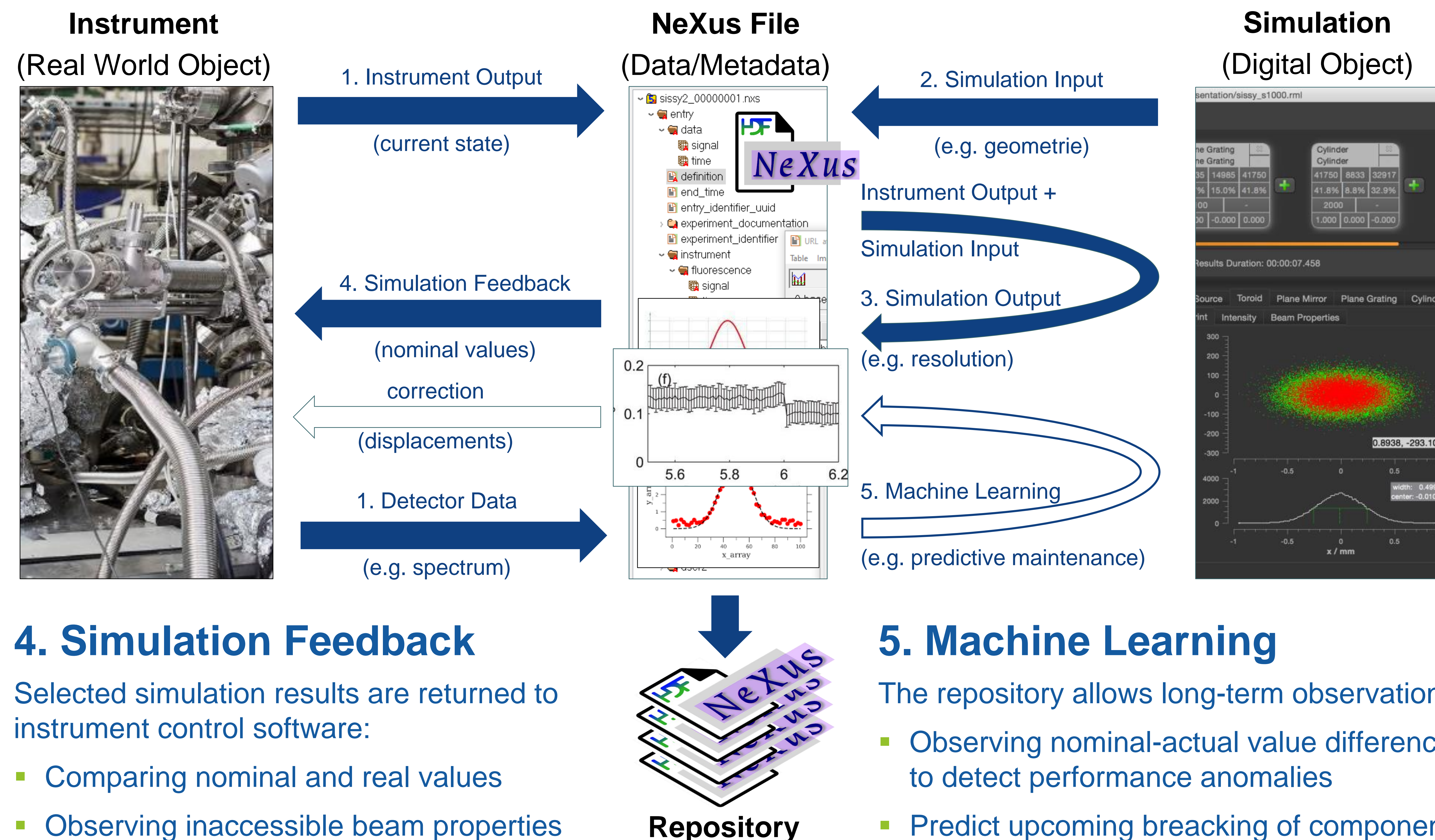
Simulation input meets the real world object in sense of performance (verified during commissioning):

- Complete list of performance-relevant components
- Global geometry and arrangement of components
- Key parameters of individual components

## 3. Simulation Output

Combining metadata from real instrument and digital counterpart allows simulation of the current state which yields:

- Inaccessible beam properties along the stream such as the beam shape at the sample position
- (Meta)data that is comparable to the real world object such as detector data of background measurements (without sample)
- Would allow subsequent simulation of the sample (e.g. position and intensity of peaks at the detector)



## 4. Simulation Feedback

Selected simulation results are returned to instrument control software:

- Comparing nominal and real values
- Observing inaccessible beam properties

## 5. Machine Learning

The repository allows long-term observations:

- Observing nominal-actual value difference to detect performance anomalies
- Predict upcoming breacking of components

## 6. Both Worlds in Single File

Both worlds in a NeXus file is advantageous due to:

- **(Meta)data enrichment:** detailed instrument section by simulation parameters
- **Context:** classify (meta)data – where to put it?
- **Semantics:** relation and nomenclature of terms – where does both worlds match?
- **Interoperability:** same tools to access data
- **AI-Ready:** (meta)data is exploitable by AI/ML techniques; extended simulations can be performed from file  
-> repository becomes training classroom for machines
- **Whole picture:** inaccessible real-world (meta)data, e.g. beam profile at sample position