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A beamline digital twin

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Abstract. In recent years, the concept of digital twins has become pervasive, yet it carries a degree of ambiguity due to its wide applicability across different domains. Within this framework, our project aims to construct a digital twin of a beamline, leveraging the capabilities of the simulation programs RAY-UI, our X-ray tracer employed for beamline design and commissioning. This work is part of a comprehensive digitalization initiative at the facility, and it aims to provide easy access to beamline simulations, abstracting the complexity that derives from correctly using these programs. The feasibility of this project is significantly enhanced by the adoption of Bluesky, a framework for experiment orchestration and data collection. Chosen as the backbone for experiment orchestration, Bluesky is supported at the facility and has been implemented at an increasing number of beamlines. Written in Python, this modern software facilitates an accessible and flexible approach to experiment management, making it an ideal platform for this digitalization initiative. RayPyNG is a Python API made to RAY-UI. We exploit its ability to read the RAY-UI beamline configuration file and modify it, and to communicate with the RAY-UI program. Through the RayPyNG-bluesky package, we achieve integration of all optical elements into the Bluesky device abstraction framework. This integration allows beamline operators to simultaneously run simulations and manage actual systems via a unified interface, enhancing operational efficiency, and giving them the ability to directly compare theoretical predictions with real-time outcomes, without the need to learn an additional interface or program.

1 Introduction

BESSY II is currently undergoing a comprehensive upgrade process known as BESSY II+, aimed at ensuring the sustained operation and modernization of the center in anticipation of our next-generation source, BESSY III. As we prepare for BESSY III, our efforts are focused not only on developing new beamline concepts but also on the comprehensive digitalization of the center. The term digitalization encompasses a range of initiatives. These include leveraging advanced control systems for *Intelligent Experimental Control* to enhance the precision and adaptability of experimental procedures; implementing automated systems and robotics for *Automation and Robotics* to improve efficiency and accuracy in experimental setups; utilizing artificial intelligence in *AI Methods* to optimize operations and data analysis, fostering smarter, faster scientific discoveries; ensuring that all data generated is findable, accessible, interoperable, and reusable through *High-Quality FAIR Data Archival*, thereby maximizing its scientific value; and creating virtual replicas of physical systems in *Digital Twins and Efficient Simulation* to predict the behavior of beamlines under various conditions and to streamline operations.

Within this framework of digitalization, a key component is the development of what we refer to as a beamline digital twin. A beamline digital twin is a simulation model that mirrors the real physical beamline and it is embedded in the beamline control system. It is designed to simulate and predict the behavior of the beamline in real-time, enabling operators to make informed decisions quickly and accurately.

The integration of these digital twins into our experimental control software is crucial for several reasons:

- **Easy Access for Non-Expert Users**: Simplifying the interface allows users who may not be experts in simulation software to effectively operate and benefit from the digital twin technology.
- **Offline Training for Beamline Staff and Users**: Providing a simulation environment for training purposes, thereby reducing the learning curve and risk during actual operations.
- **Real-Time Comparison with Experimental Results**: Enabling immediate comparison between simulated predictions and actual experimental outcomes, which is vital for on-the-fly adjustments and optimizations.

These advancements are not just enhancements to our technological infrastructure; they are transformative changes that will redefine how beamlines are operated at BESSY II and pave the way for BESSY III.

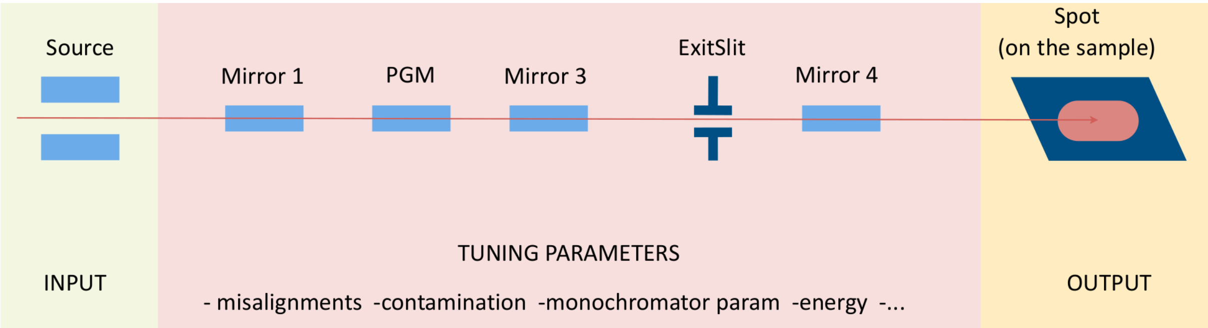

Figure 1: Digital Twin of a Beamline

2 A Beamline Digital Twin for BESSY II

To construct a comprehensive digital twin for BESSY II, three fundamental building blocks are required, alongside appropriate hardware and a robust network infrastructure. These building blocks include an advanced simulation engine, a modern software interface for design and manipulation, and a flexible system for experiment orchestration. Together with the necessary physical infrastructure, these components enable the creation of a dynamic and responsive digital twin that mirrors and predicts the behavior of the actual beamline in real-time.

2.1 The Simulation Engine

RAY-UI [1] serves as the core simulation engine for BESSY II's digital twin initiatives. It is an X-ray tracing program widely used across the facility for the design and commissioning of beamlines. By providing a sophisticated graphical user interface, RAY-UI enables precise simulations of X-ray interactions with various optical elements. The program's ability to model the behavior of X-rays critically aids in optimizing beamline configurations and predicting experimental outcomes.

In addition to RAY-UI, we are also developing RAY-X, its successor, which represents the next generation of simulation tools. RAY-X enhances the simulation capabilities by leveraging modern hardware allowing for significant performance improvements. This new software is designed to meet the evolving needs of both beamline and data scientists, providing a more robust, precise, and accessible toolset for the scientific community.

2.2 RayPyNG: A Modern Approach to Beamline Design

At BESSY II, while RAY-UI serves as our primary X-ray tracing program with an integrated graphical user interface for simulating beamlines, RayPyNG introduces a critical advancement in how we approach beamline simulations [3]. RAY-UI is particularly designed for precise simulations of X-ray beamlines, but

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its GUI-based interaction model inherently limits it.

RayPyNG extends the functionality of RAY-UI by offering a Python API that allows for the scripting and automation of these simulations. This development is crucial for creating reproducible and programmable simulation environments, which are essential for ensuring consistency and reproducibility of the simulations. By moving away from a purely GUI-driven approach, RayPyNG enables to write and execute reproducible scripts that can be shared, version-controlled, and reused across different projects. This not only enhances the efficiency of the simulation process but also significantly improves the reliability of the results.

2.3 Bluesky: The Future Experiment Orchestration Software
Bluesky [2] represents the future of experiment orchestration at BESSY II, providing a robust framework for managing scientific experiments. As an open-source Python library, Bluesky integrates seamlessly with RayPyNG, enabling the orchestration of both real and simulated experimental workflows. The system uses Ophyd to create a uniform interface for all devices, thereby simplifying the experimental process for operators and researchers. The integration of Bluesky into BESSY II's operational framework allows for more efficient data collection and experiment management, fostering a more collaborative and adaptable research environment.

2.4 A Beamline Digital Twin
The concept of a beamline digital twin at BESSY II encapsulates the integration of all these technologies into a cohesive system that mirrors the real beamline operations. This integration is realized with another Python package called bluesky-raypyng [4]. The simplicity of integrating the digital twin using this package is notable; it requires just one line of code alongside a beamline configuration file saved by RAY-UI:

```
RaypyngOphydDevices(rml_path=<path_to_beamline_config_file>)
```

This digital twin enables operators to perform simulations that reflect real-time conditions. The capability to compare theoretical predictions with actual experimental data in real time enhances the ability to fine-tune procedures and compare the beamline performance in different configurations. Ultimately, the digital twin serves as a crucial tool for the ongoing modernization and enhancement of beamline operations at BESSY II.

2.5 Finding the Offset between Real and Simulated Motors
A significant challenge in implementing digital twins at BESSY II involves identifying and rectifying the offsets between real and simulated motors. A rapid machine learning surrogate model has been developed [5] for this purpose and is used within an automated environment to accurately find these offsets. The model employs an approach similar to a random walker to ensure the alignment of the simulation with the actual beamline, adjusting the setup so that rays precisely follow the intended optical paths. This adjustment process considers that certain beamline parameters, such as the shapes of mirrors or the positions of source points, are immutable. The ability to determine and correct discrepancies between the simulated and actual setups is critical, as it allows for the derivation of precise adjustment specifications for the real beamline setup.

3 Current Status
Proof of concept for BESSY II's digital twin technologies has successfully been established with several key developments. RayPyNG, a Python API to RAY-UI, facilitates dynamic and reproducible simulations of beamline operations. Additionally, the Bluesky experiment control software is now actively deployed across multiple beamlines, significantly enhancing the manageability and efficiency of beamline operations and scientific experiments. The integration of bluesky-raypyng ensures the automatic integration of simulated devices, allowing seamless transitions between real and simulated environments.

4 Future Development
Looking ahead, the rollout of Bluesky at additional beamlines and the deployment of a central server for simulations are planned to further enhance the infrastructure for digital twins at BESSY II. The implementation of the client-side of bluesky-raypyng will continue, alongside the further integration of

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simulated devices. Moreover, the introduction of new simulation engines such as RAY-X and machine-learning beamline surrogates will advance the capabilities of these digital twins. A key focus will be on synchronizing the simulated devices with their real-world counterparts to ensure that the digital twins provide an accurate and effective tool for beamline management.

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