Sirepo: an open-source cloud-based software interface for X-ray source and optics simulations

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Abstract

Sirepo — an open source cloud-computing framework, which includes a sophisticated browser-based GUI for X-ray source and optics simulations [1]. Currently, Sirepo is interfaced with popular codes in the fields of synchrotron radiation source and optics simulations, such as SRW and SHADOW3, particle accelerators (Elegant, Hellweg and Warp), and a few others. Sirepo is a flexible framework that can be relatively easily integrated with scientific codes to provide a convenient GUI for simulations in the cloud.

SRW (Synchrotron Radiation Workshop) is a physical optics computer code, allowing simulation of entire experimental beamlines using the concept of a 'virtual beamline' with accurate treatment of synchrotron radiation generation and propagation through the X-ray optical system [2, 3, 4]. SRW is interfaced with Sirepo by means of a Python API.

Sirepo utilizes interactive widgets and dynamically accessed data from community databases for X-ray optics [5, 6]. These computational tools are extensively used for the development and commissioning of new X-ray beamlines and for testing feasibility and optimization of experiments.

Features

- **Sirepo** for SRW contains a number of predefined textbook examples as well as simulations of the wavefront propagation through existing beamlines at NSLS-II and LCLS.
- **Source** simulation page allows users can simulate and optimize the source of the synchrotron radiation (e.g. undulator, dipole, etc.) Contains predefined electron beam and undulator parameters.
- **Beamline** simulation page allows to construct a 'virtual' beamline emulating the layout of real X-ray or general optical beamlines. Fully- and partially-coherent simulations of wavefront propagation can be performed.
- **Sirepo** supports most of the optical elements currently used at beamlines, including recent developments in SRW. Basic simulation of samples is available via a generic transmission object.
- Rich interactive visualization and reporting capabilities available in Sirepo.
- Publicly available community databases (CXRO, X-ray server) can be dynamically queried for error-free access to material characteristics.
- **Sirepo** works on a local computer, a remote server or a high-performance cluster. Sirepo is available online and also within the NSLS-II firewall.

Server-side implementation

- **Python** — widely used high-level programming language for general-purpose programming
- **Flask** — lightweight framework for web development with Python based on Werkzeug WSGI toolkit
- **Nginx** — industry standard HTTP server and a reverse proxy
- **JSON (JavaScript Object Notation)** — a lightweight data-interchange format
- **Celery and RabbitMQ** — asynchronous job queue and cluster management (to be replaced by the Docker-based queue)
- **Open MPI/mpi4py** — technology used to run scientific codes in parallel across a cluster of computational nodes on a network

Client-side implementation

- **HTML5** — markup language used for structuring and presenting web content
- **CSS3** — style sheet language used for describing the presentation of a document written in a markup language
- **Bootstrap** — HTML, CSS and JavaScript framework for developing cross-platform web applications
- **AngularJS** — structural framework for dynamic web apps
- **D3.js** — JavaScript graphics library which is used to generate interactive plots in the browser. D3 supports large datasets and dynamic behaviors for interaction and animation.

Links

- https://sirepo.com (publicly available)
- https://expdev.nsls2.bnl.gov (behind NSLS-II firewall)
- https://github.com/radiasoft/sirepo
- https://github.com/ochubar/SRW
- https://hub.docker.com/r/radiasoft
- https://github.com/radiasoft/sirepo/wiki/Development

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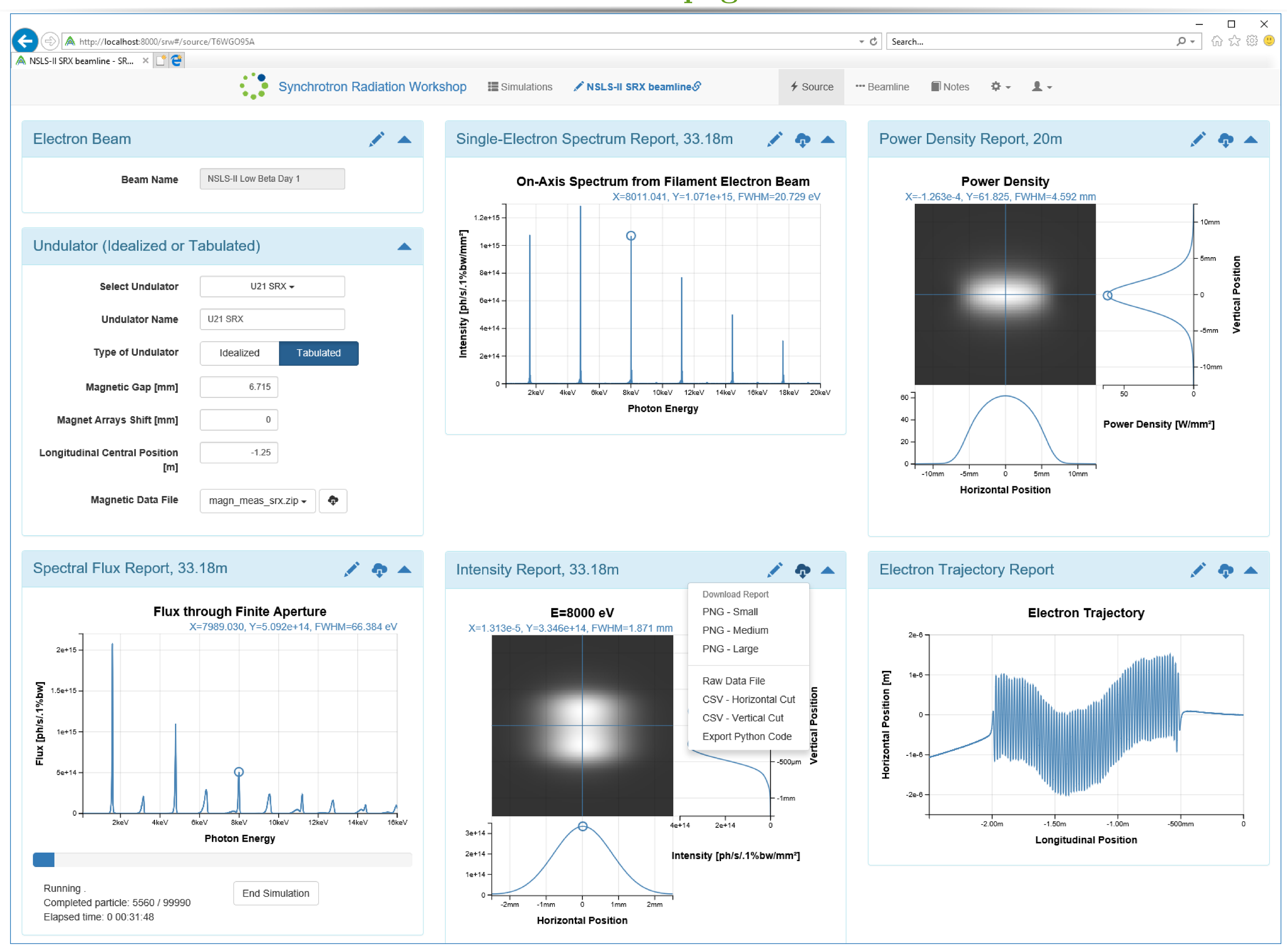
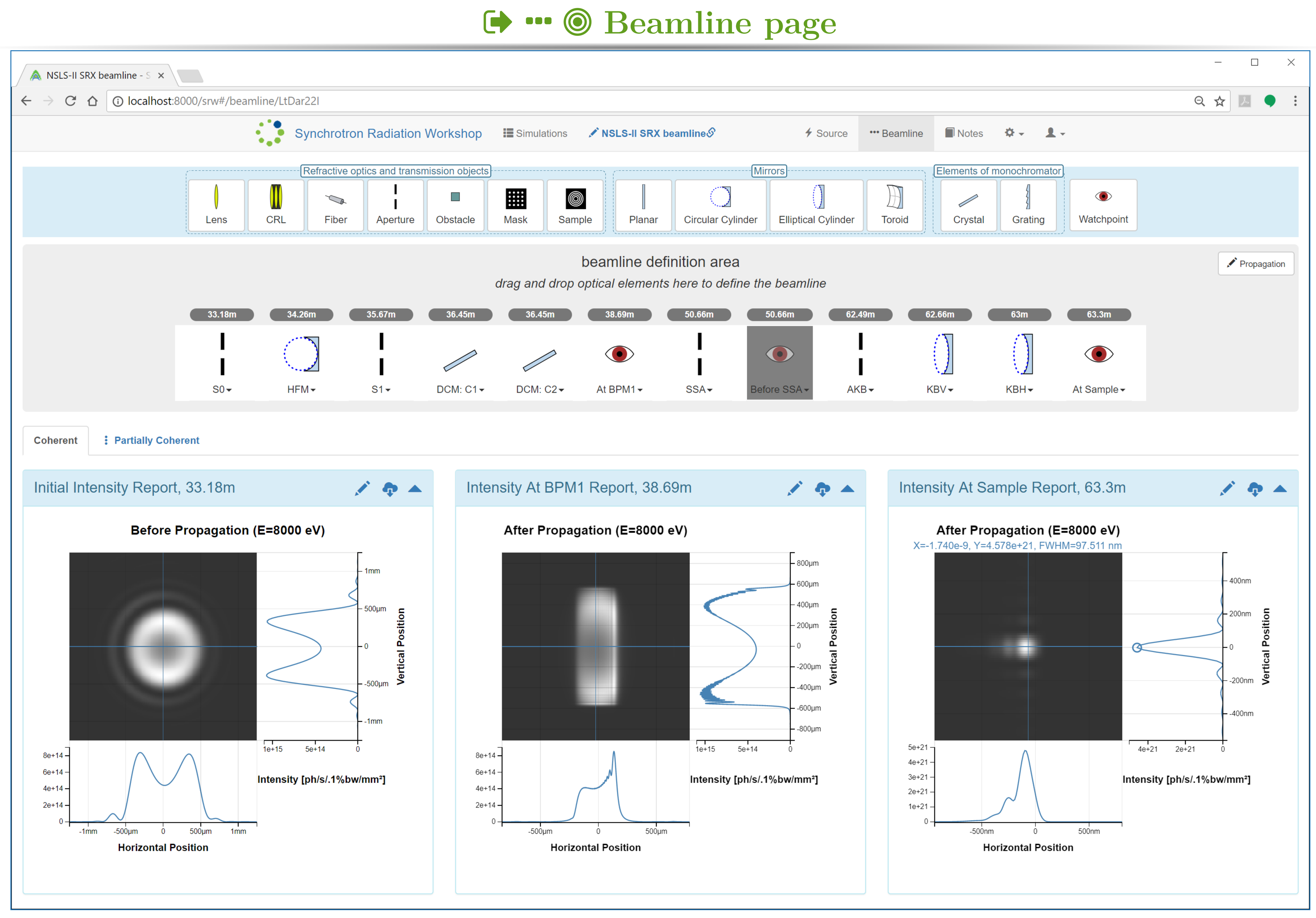
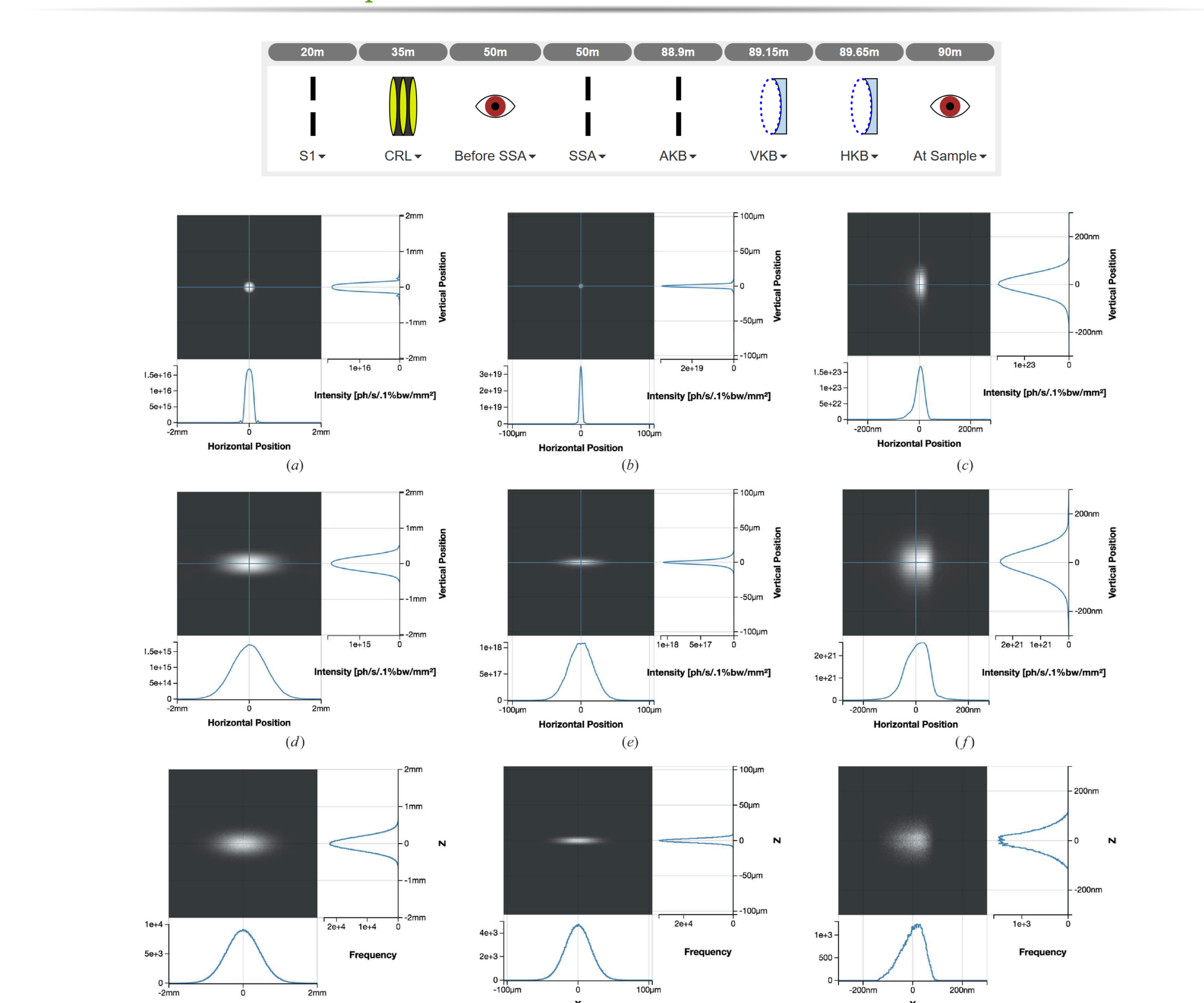
Source page



Beamline page



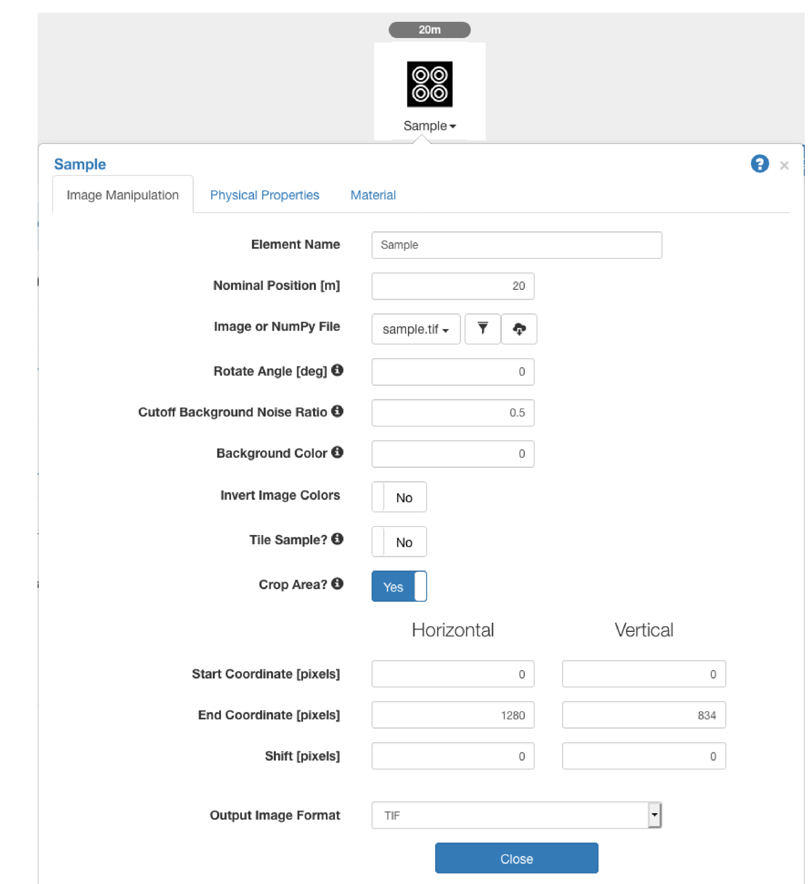
Comparison of SRW and SHADOW3 simulations

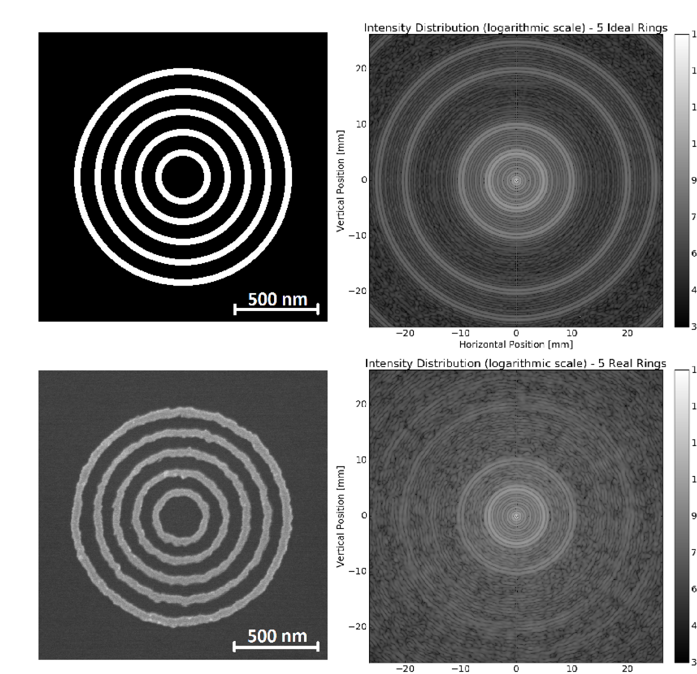


Initial intensity report (at 20 m) and intensity reports for the watchpoints "Before SSA" (at 50 m) and "At Sample" (at 90 m) (left to right) in Sirepo. The first row corresponds to the single-electron (fully coherent) SRW simulation, the second — the multi-electron (partially coherent) SRW simulation, and the third — the fully incoherent SHADOW3 simulation.

https://sirepo.com/srw#/beamline/LA5qG1J1 https://sirepo.com/shadow#/beamline/wsGlwMqv

Simulation of X-ray scattering from experimental samples





Concentric rings sample (left) and simulated diffraction pattern created by it as observed at 4.81 m (right): 'ideal' fabrication error-free case (upper image plots) and the case of a sample object generated for simulations from a real nano-fabricated sample (lower image plots). The outermost diameter/size of both samples is ∼1.35 µm. The simulations were performed with the NSLS-II CHX beamline layout.

The Sample optical element in Sirepo allows such simulations. Users can provide an electron microscope image or a NumPy file describing a real or virtual experimental sample, together with specified spatial resolution of the image and thickness of the sample. The material of the sample can be specified in a drop-down menu, and the refractive index decrement and attenuation length of the material can be obtained automatically from the CXRO online database. Positions of the sample can be specified relative to the source and the origin of the incident beam frame.

Formats: image files (TIFF, PNG, JPEG, BMP, . . .), or a NumPy array file with the data of the sample image.

Sample image → Python Image Library (PIL) → NumPy array → crop ROI from the original image → SRW transmission object (amplitude transmission and optical path difference calculations for each pixel; the thickness of the material is proportional to the grey level of the pixel) → wavefront propagation through the element and drift space → diffraction pattern at the specified distance from the sample.

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[6] http://x-server.gmca.aps.anl.gov/x0h.html.

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