Sirepo: a web-based interface for physical optics simulations – its deployment and use at NSLS-II

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ABSTRACT

"Sirepo" is an open source cloud-based software framework which provides a convenient and user-friendly web-interface for scientific codes such as Synchrotron Radiation Workshop (SRW) running on a local machine or a remote server side. SRW is a physical optics code allowing to simulate the synchrotron radiation from various insertion devices (undulators and wigglers) and bending magnets. Another feature of SRW is a support of high-accuracy simulation of fully- and partially-coherent radiation propagation through X-ray optical beamlines, facilitated by so-called "Virtual Beamline" module. In the present work, we will discuss the most important features of Sirepo/SRW interface with emphasis on their use for commissioning of beamlines and simulation of experiments at National Synchrotron Light Source II. In particular, "Flux through Finite Aperture" and "Intensity" reports, visualizing results of the corresponding SRW calculations, are being routinely used for commissioning of undulators and X-ray optical elements. Material properties of crystals, compound refractive lenses, and some other optical elements can be dynamically obtained for the desired photon energy from the databases publicly available at Argonne National Lab and at Lawrence Berkeley Lab. In collaboration with the Center for Functional Nanomaterials (CFN) of BNL, a library of samples for coherent scattering experiments has been implemented in SRW and the corresponding Sample optical element was added to Sirepo. Electron microscope images of artificially created nanoscale samples can be uploaded to Sirepo to simulate scattering patterns created by synchrotron radiation in different experimental schemes that can be realized at beamlines.

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1. INTRODUCTION

We present a portable and user-friendly tool for scientific simulations named Sirepo. Our interface provides a convenient way to perform such portable simulations. Sirepo consists of a graphical web interface based on JavaScript with a backend server (either on local machine or a remote server) able to serve many different software packages, including already implemented interfaces with Synchrotron Radiation Workshop (SRW) for accurate X-ray source and optics simulations[1,2,3], Shadow3 – a ray optics code with many sophisticated features for X-ray beamlines[4,5], and a number of codes for particle accelerators simulations. The source code of Sirepo could be quickly extended[6] to support the codes from different scientific domains such as condensed matter physics, material science, chemistry, biology and other areas utilizing codes which require complex and at the same time flexible input and comprehensive output in the form of interactive visualization, data files and unified exchange format.

In the present work, we will focus on SRW, which is used at light source facilities for design and optimization of X-ray sources and beamlines by means of simulation of wavefront propagation through optical system of the X-ray beamlines. It is written in C++ with Python bindings. A "Virtual Beamline" module is used for convenient way to execute simulations in console. SRW is also interfaced with WaveMetrics' Igor Pro for advanced simulations, data analysis and visualization of the results. Sirepo is a complementary interface build on top of SRW-Python interface, allowing to perform comparable advanced simulations and data visualization in a browser. Below we will explain the implementation and main features of Sirepo and the details of the Source and Beamline pages. Finally, we will discuss basic examples and advanced simulations, including virtual beamlines implemented for NSLS-II.

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2. IMPLEMENTATION OF SIREPO

2.1 Server-side implementation

The Sirepo server consists of the following components. It is based on *Python* – an interpreted general-purpose programming language widely used nowadays for scientific software development. It features many libraries and is suitable for software development of various purposes. Web applications can be conveniently implemented in Python using *Flask* – a lightweight framework for web development. Flask applications are efficiently served by *Nginx* – a reliable HTTP server and a reverse proxy used in production environments. Besides, *Celery* and *RabbitMQ* are used for scheduling jobs (sequential and parallel) and managing a cluster of computing nodes. *OpenMPI* is a technology used to run scientific codes in parallel across a cluster of computing nodes on a network. In Python, the *mpi4py* library is used to provide high-level access to MPI, and SRW utilizes this package to perform multi-electron and partially-coherent (and usually long-running) simulations. All these components work seamlessly to provide a reliable and productive backend by means of mutual exchange of the data with the simulation codes.

2.2 Client-side implementation

The Sirepo client is written in *JavaScript* (an interpreted client-side programming language) and *AngularJS* (a structural framework for dynamic web application), and therefore can run natively in virtually any modern browser. *HTML5* and *CSS3* are used for presenting web-pages. On top of HTML, CSS and JavaScript, the *Bootstrap* framework is used for developing cross-platform web applications. For advanced interactive graphics, such as 1D plots and 2D plots (heatmaps), the *D3.js* library is used to visualize simulation results, typically, large datasets. The Sirepo client interacts with the server using the *JSON* (JavaScript Object Notation) language-independent unified exchange format.

2.3 Distribution of Sirepo

Sirepo is distributed in several formats. It can be downloaded as a source code from *GitHub*[7], a web-based version control repository, which offers all of the distributed version control and source code management functionality of Git as well as adding its own features. As an out-of-the-box solution, Sirepo could be obtained within a container, either Docker[8] or Vagrant[9]. *Docker* is an open platform for distributed applications. It enables rapid deployment of applications to the cloud. Using Docker on Linux, it is possible to create a file that contains a scientific code(s), plus all required tools and dependencies, which can then be copied to any Linux server or cluster and rapidly activated. A user can connect to the container via console interface, if necessary, or the software can be accessed remotely through a web-based UI. This removes the pain of software installation on Linux, and it enables cloud-based scientific computing by providing on-demand access via a local cluster, supercomputer or commercial service. *Vagrant* enables cross-platform containerization of applications. Just like Docker, it is used to create and configure lightweight, reproducible, and portable Linux development environments. This is essential for developing and testing Linux applications on non-Linux computers. Since our source code resides on GitHub, it provides a way to efficiently test the code and perform its distribution via the *Python Package Index* (PyPI) and the Docker and Vagrant repositories by means of *Travis CI*, the continuous integration and continuous delivery platform. After each commit to the GitHub repository, a new version of the Python-installable package is uploaded to the PyPI server and a new container is placed automatically to the Docker repository.

2.4 Authentication

By default, Sirepo identifies users by the cookies saved in a browser, and therefore it is possible that users may lose all their calculations if the browser's cache/cookies were cleaned, or if they use another browser to access the Sirepo server. It is highly recommended for users to log in the Sirepo server and to back up the simulations data. A user can use the GitHub credentials to authenticate at a Sirepo server if the authentication feature is enabled and configured on that server. The user will benefit from accessing all his/her simulations from any browser – the simulation will never be lost if the browser's cache is cleaned, or if the user switches to another browser. The steps to authenticate can be found at our Wiki-page[10].

2.5 Sharing simulations

Users can exchange SRW/Sirepo simulations in several formats:

Python script – we have found that users want the ability to download valid Python scripts, which can then be specialized to implement more sophisticated simulations – for example, capabilities that the GUI does not yet support.

The “Export Python File” menu item provides a way to export a Python script used for execution of the report. This allows the end user to run an SRW simulation from the command line.

JSON file – as an accompanying tool, we have implemented exporting of the JSON files, which fully describe the simulation, via the “Export JSON Data File” menu item. This assures portability of Sirepo simulations.

Zip-archive – in many cases SRW simulations involve additional files, e.g. mirror height profiles and magnetic measurements data for the tabulated undulator, which cannot be exported as a single Python file. For that purpose, we implemented exporting of a zip-archive with Python, JSON and all related data files via the “Export as Zip” menu item.

Self-extracting simulation – an advanced exporting feature of a self-extracting simulation in HTML format was implemented – “Self-Extracting Simulation” menu item to allow a one-click importing to a remote server.

To provide a robust mechanism for sharing the simulations across multiple installations of Sirepo and/or SRW, we complemented the exporting capabilities by the advanced importing features. Currently, Sirepo accepts importing of the standardly formatted “Virtual Beamline” Python scripts as well as previously exported JSON files and zip-archives. When the user attempts to import a Python script, optional command-line arguments could be provided (for instance, to select the desired beamline layout to import). More details about sharing the simulations can be found at our Wiki-page[11].

3. FEATURES OF SIREPO

In SRW users typically start from setting up the parameters of the source of the synchrotron radiation which involves the parameters of the electron beam and the source (“idealized” or “tabulated” undulator, dipole, or Gaussian beam). The next step is to check the trajectory of the relativistic electrons traveling through the magnetic system of an undulator or a damping wiggler. Particular characteristics of interest after the check often include the resulted spectrum for the specified parameters, the single-electron spectrum, the flux through finite aperture and intensity and power density distributions at some distance from the source. The next step towards simulation of a beamline is wavefront propagation through an optical system of the beamline. This involves single-electron and partially-coherent simulations with use of different X-ray optical elements like mirrors, CRLs, Double Crystal Monochromators, etc. The treatment of the height profile imperfections is also implemented in SRW and available in Sirepo interface. Finally, X-ray beamline scientists may be interested in the X-ray scattering patterns of samples, which now could be simulated in SRW. All these stages of the simulations can now be conveniently performed in the web interface of Sirepo. Below we provide more detailed insight into each feature.

3.1 Source page

The source page of Sirepo consists of the following widgets (see Figure 1).

Electron Beam – used for setting up the parameters of the electron beam. There are a number of predefined “electron beams” with nominal parameters from existing light source facilities (such as the electron beam current, vertical and horizontal emittance, etc.). Those parameters are dynamically obtained from SRW source code to ensure the parameters correspond to the base code. One can either use the predefined parameters (indicated by the inactive input fields), or can click “Edit Beam” and tune the parameters as necessary – in this case the input fields will become active and a user-defined copy of the beam will be created, which is shared across all user’s simulations. The electron beam is defined by the Twiss parameters by default, but can be defined by the second order statistical moments (RMS size, RMS divergence, etc.) by clicking the Moments button. The Position tab allows one to specify the position of the beam, its angle and the electron beam longitudinal drift to be performed before a required calculation, which is calculated automatically for the idealized undulator. For the tabulated undulator it is set to zero by default, but can be changed to an arbitrary value as needed.

Idealized or ***Tabulated Undulator*** – after the parameters of the electron beam are set up, one needs to define the parameters of an undulator. SRW supports the definition of the source of the synchrotron radiation by either the magnetic field peak value or detailed magnetic measurements data. The second method provides a more accurate method to simulate undulator radiation spectra and predict their realistic performances at different magnetic gap values. This method is now routinely used for commissioning of the NSLS-II beamlines. In Sirepo an undulator source can now be specified by either an “idealized undulator” or an undulator characterized by the data from the measured magnetic field (a so-called “tabulated undulator”). In the case of the idealized undulator, users tune the spectrum by changing either the deflecting parameter *K* or the components of the magnetic field (the parameters are mutually dependent and are recalculated interactively if one of the parameters changes). In the case of the tabulated undulator, users tune the spectrum by the undulator gap, but still could switch between the idealized and tabulated representations for faster comparison of the results. It is possible to either use the predefined set of the archives with the magnetic measurement data in a special ASCII format or to upload a new archive.

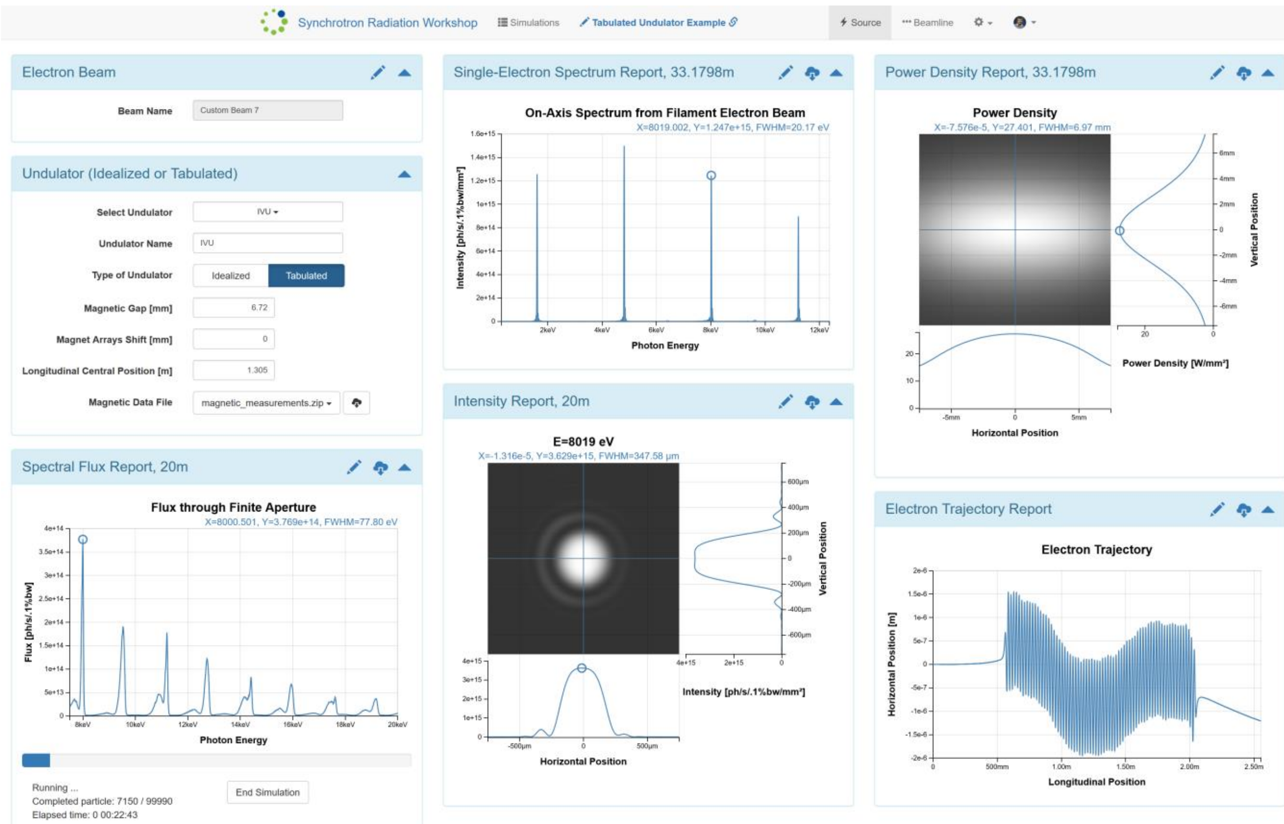

Figure 1. The source page of an example with the “tabulated” undulator in Sirepo.

Electron Trajectory Report – the report provides a convenient and a straightforward way to observe the trajectory of the electrons traveling through the magnetic field of the undulator, which helps to characterize quality of its shimming. The reports show the spectrum of the synchrotron radiation produced by the undulator.

Single-Electron Spectrum Report and ***Spectral Flux Report*** – the first report displays the spectrum of a single electron radiation while the second report shows the spectrum of the electron flux, which simulates synchrotron radiation on the light source facilities more realistically. The latter report in the case of the tabulated undulator is designed to perform long-running parallel simulations involving a large number of macro-electrons, traveling in a (possibly imperfect) magnetic field of an undulator, and to accurately predict the spectral performance. The interactive report is updated periodically to visualize the most recent data from the iterative process performed by SRW and the progress bar shows the current progress of the calculation.

Intensity Report and ***Power Density Report*** – the reports show the intensity and power density distributions correspondingly at a distance from the source in a form of a 2D heatmap. Users can see the 1D cuts of the plots. The coordinates of the focus point on the 1D cut at the bottom of the 2D heatmap are shown right above the plot along with the corresponding value of the FWHM: X corresponds to the horizontal position of the point at the fixed vertical position of the cut and Y corresponds to the intensity value at that particular point. The plot could be zoomed by mouse scroll for better detailing. For users’ convenience, the photon energy is displayed in the title of the plot and the distance where the intensity is observed is shown next to the name of the report.

3.2 Beamline page

The beamline page is designed to simplify the process of generation of the "Virtual Beamline" replicating an experimental beamline, so that SRW could perform the wavefront propagation through the constructed optical system. All SRW propagator options were made available in the Sirepo JavaScript GUI via dedicated menus, dialogs, widgets, and Wiki-pages of documentation. Figure 2 displays the Beamline page of the NSLS-II CHX beamline simulation in partially-coherent mode. The figure shows a toolbar with all available optical elements implemented in Sirepo. Users can edit the beamline with a drag-and-drop editor. To add a new element in the expert mode, the user can drag it from the toolbar menu and drop it anywhere in the beamline. The program then pops up a parameters screen to specify details about the optical element. Depending on the type of the element, the parameters dialog may have several tabs with basic and advanced parameters. When the user drags and drops a watchpoint in between the existing elements, after clicking the "Save Changes" button a new Intensity Report for the added watchpoint will appear. Users could visualize intensities in multiple locations after any desired optical element. Below we will briefly explain the optical elements.

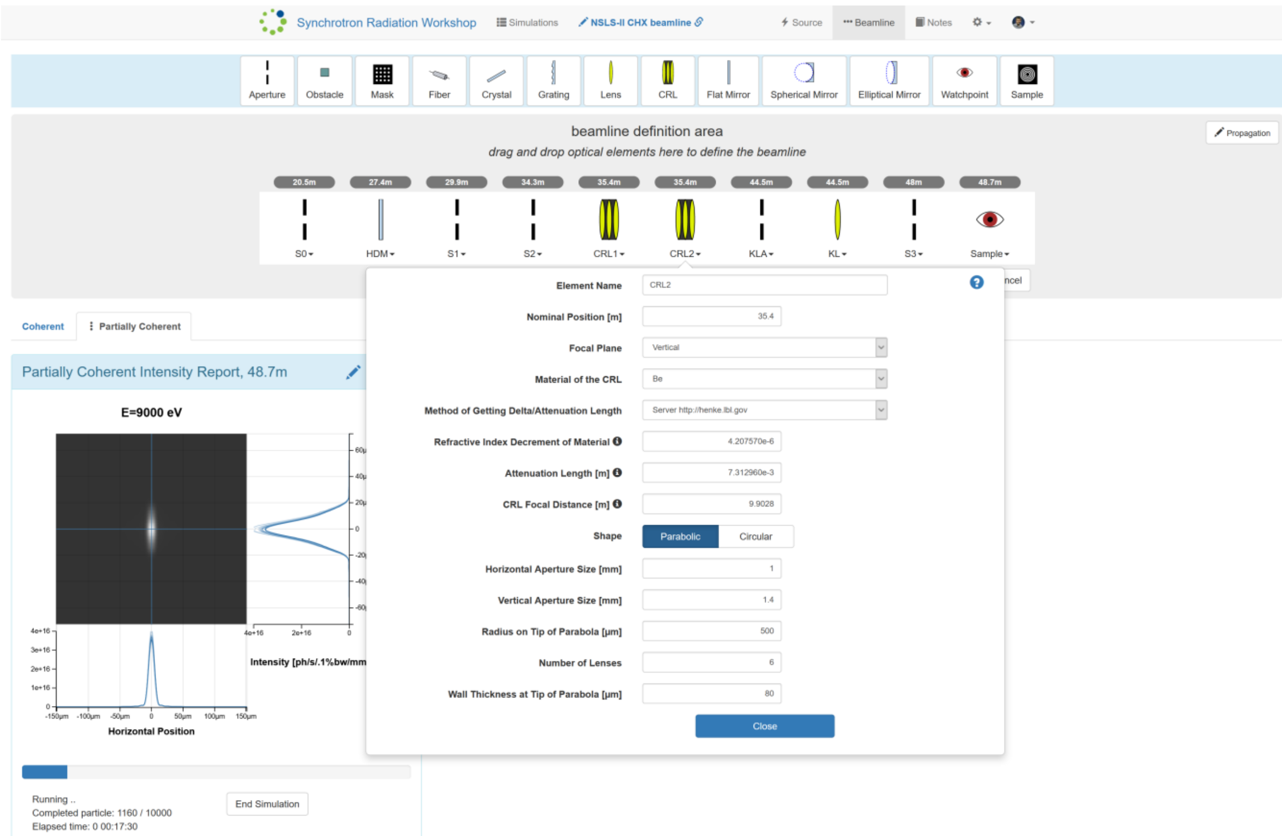

Figure 2. The Beamline page of the NSLS-II CHX beamline example.

Mirrors – users can use 1D and 2D height profiles describing imperfections of the mirror surfaces. The optical path difference can be visualized to better understand the surface quality of a mirror. The normal and tangential vector components describing the orientation of the Grating, Spherical Mirror and Elliptical Mirror optical elements in the beamline are calculated automatically from the grazing angle provided by the user.

Lenses – the compound refractive lens (CRL) element allows focusing of X-rays (see the pop-up menu in Figure 2). The values of the refractive index decrement and the attenuation length of the material are dynamically accessible from the CXRO website[12] at Lawrence Berkeley National Laboratory – a widely used online database with the comprehensive information about X-ray interactions with matter. The refractive index decrement and the attenuation length strongly depend on the material and the photon energy of interest, and so its inclusion benefits users. The detailed description of the feature is available at our Wiki-page[13].

Crystal – a perfect crystal is available in Sirepo. Individual crystals are used as constituent parts of Dual Crystal Monochromators – obligatory optical devices for X-ray beamlines, in which dynamical diffraction on high-quality single crystals is used to cut a narrow bandwidth from a wide spectrum of synchrotron radiation. Based on the specified photon energy, the material and Miller's indices, the crystal reflecting planes' d-spacing, the diffraction plane angle and the real and imaginary parts of the crystal polarizability/susceptibility (chi-zero, chi-h) are automatically obtained by programmatically accessing the API provided by Dr. Stepanov's server[14] at the Argonne National Laboratory. Any change in the photon energy, material or Miller's indices triggers a new request to the server and the corresponding fields are populated by the newly received values. Any change of the angles, the d-spacing or the 0^{th} Fourier components of the crystal polarizability results in a recalculation of the components of the normal and tangential vectors by Sirepo to correctly orient the crystal for the particular energy and material, providing a helpful tool for beamline scientists attempting to simulate beamlines with the crystals. Our Wiki-page demonstrates the usage of this feature[13].

Fiber – the Fiber optical element, that can be used for testing X-ray beam coherence, was implemented and used in SRW since some time and its counterpart is available in Sirepo. The refractive index decrement and the attenuation length parameters are obtained automatically by the same method that is used for the CRL.

Mask – the Mask ("pepper-pot") element can be used as a wavefront sensor/analyzer. This project is being performed as part of a collaboration with the Metrology group at BNL (this work is supported by the DOE FWP grant DE-SC0012704; see "Alignment of KB mirrors with at-wavelength metrology tool simulated using SRW" in these proceedings for more information).

Sample – simulation of the radiation propagation through the samples is an important topic and is beneficial for simulation of the whole experiments. In collaboration with the Center for Functional Nanomaterials (CFN) of BNL, we have implemented the samples library in SRW and created the corresponding Sample optical element in Sirepo. The developed Samples Python library performs two steps. For the first step, it reads the image (if it is provided by a user) by means of the Python Image Library (PIL), converts it to a NumPy array, then removes the gray background and the bottom legend part. The algorithm treats all pixels which have less than a half of the maximum intensity (allowed by the bit depth) as the background, and converts all the values to zero (black color). In the second step, the library creates an SRW transmission object treating the thickness of the material at each pixel proportional to the whiteness level of the pixel. The refractive index decrement and the attenuation length parameters are obtained automatically by the same method that is used for the CRL and are used along with the thickness of the material in the amplitude transmission and optical path difference calculations for each pixel. Finally, the resulting transmission object is used by SRW to perform the wavefront propagation through the element and get the speckle pattern images at some distance from the sample. The development is ongoing; however, the library of samples has already been used in the simulations accompanying a few experiments conducted at NSLS-II (see "X-ray optical simulations supporting advanced commissioning of the coherent hard x-ray beamline at NSLS-II" in these proceedings).

4. EXAMPLES

4.1 Landing page: basic examples

When a user accesses a Sirepo server, a landing page with the list of implemented interfaces for software packages appears. When SRW interface is selected, the user is forwarded to the landing page which contains a number of basic examples demonstrating capabilities of SRW, which are explained below. Advanced mode of a simulation is available via accessing "Expert user only" page.

Synchrotron Radiation ("SR Calculator") – this section contains three examples: Undulator Radiation, Bending Magnet Radiation, and Idealized Free Electron Laser Pulse. These examples demonstrate X-ray generation by different X-ray sources.

Wavefront Propagation – this section presents textbook examples of the wavefront propagation through different optical schemes. "Diffraction by an Aperture" example demonstrates a virtual experiment of diffraction of a Gaussian beam (red laser, 635 nm) by a rectangular aperture of 1×1 mm^2. The aperture is located at 0.5 m from the source. Users can observe the resulted intensity in the near and the far fields. The other three examples, named "Young's Double Slit Experiment" show classical Young's interference experiment first performed by Young in 1801. The first example is designed for the X-ray radiation produced by an undulator with the photon energy of 4240 eV, the other two examples are very similar and use Gaussian beam source (green laser, 535 nm), though the last example the optical scheme does not have the focusing lens.

Light Source Facilities – this section contains virtual beamlines for NSLS-II and LCLS facilities. The LCLS beamline example demonstrates the abilities of the new LCLS SXR capabilities. The NSLS-II beamlines (CHX, HXN, SRX, FMX, SMI, and ESM) will be explained in the next subsection.

4.2 NSLS-II beamlines

The results of the above-mentioned developments were extensively used at miscellaneous simulations for X-ray beamlines and various R&D projects at NSLS-II. Also, two high-performance Sirepo servers – **nsls2expdev1.bnl.gov** and **expdev.nsls2.bnl.gov** – were installed and configured at NSLS-II. They are extensively used by beamline scientists, Metrology and ID groups' scientists. Below we provide a brief overview of NSLS-II beamlines implemented in Sirepo.

a. NSLS-II CHX beamline

The Coherent Hard X-ray (CHX) scattering beamline is designed for experimental techniques that rely on the X-ray coherence either for imaging or scattering. The major part of the scientific program of the CHX beamline is dedicated to studies of dynamics on nanometer length scales using X-ray Photon Correlation Spectroscopy (XPCS). XPCS is a photon-starved technique and hence the beamline design targets providing a partially coherent X-ray beam at the sample and offers a possibility of favoring either flux or degree of coherence depending on types of samples and other conditions. The beamline's transport and conditioning optics are required to minimize distortions of the partially coherent radiation wavefront. Distortions that lead to spatial intensity fluctuations at the sample position can cause parasitic correlation signals, as any phase object that is not constant in time, like e.g. a vibrating, imperfect mirror substrate or monochromator crystal, will decrease the coherence.

a)

b)

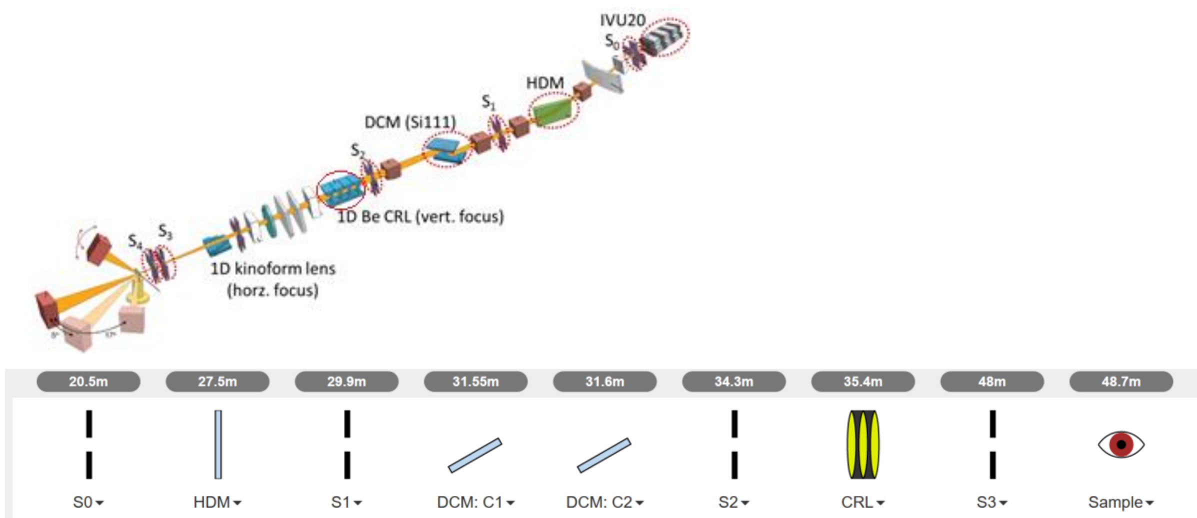

Figure 3. Optical layout of the CHX beamline for an XPCS experiment in Small-Angle X-ray Scattering geometry: a) 3d schematic view with the elements circled were included in the simulations; b) Sirepo-generated sequence of pictograms of these optical elements.

A schematic layout of the CHX beamline is shown in Figure 3. The X-ray source is a 3 m long in-vacuum undulator with 20 mm magnetic period (IVU20), located at the center of a low-beta straight section of the NSLS-II storage ring. The primary slits (S_0) are placed 20.5 m downstream of the straight section center and define the illumination of a Horizontally Deflecting white beam Mirror (HDM) at 27.5 m. Another set of slits (S_1) located at 29.9 m defines the incident beam on a vertically-deflecting pseudo channel-cut Double Crystal Monochromator (DCM) at 31.6 m. The S_2 slits at 34.3 m limit the X-ray beam phase space that is focused, thereby controlling X-ray flux and degree of coherence for different experimental requirements. For a typical small angle scattering experiment with a ~10×10 μm^2 X-ray beam size at the sample position, the remaining optical elements are: slits (S_2) at 34.3 m, 1D parabolic Be CRL at 35.4 m for vertical focusing and 1D Silicon kinoform lenses for horizontal focusing at 44.5 m. The waist of the X-ray beam is located before the sample position (48.7 m) at the location of slit S_3 at 48.0 m. The S_4 slit at 48.4 m serves as a 'guard slit'.

b. NSLS-II HXN beamline

The Hard X-ray Nanoprobe (HXN) ultra-high-resolution microscopy beamline is one of the "flagship" undulator-based beamlines of NSLS-II. A simplified beamline optical scheme of this beamline is presented in Figure 4. The initial part of the scheme includes slits (S_1), Horizontal Collimating Mirror (HCM) and a horizontally-deflecting Si(111) Dual Crystal Monochromator (DCM), followed by Horizontal Focusing Mirror (HFM) and a vertically-focusing Compound Refractive Lens (CRL) capable of creating focus at one of two possible locations of the Secondary Source Aperture (SSA).

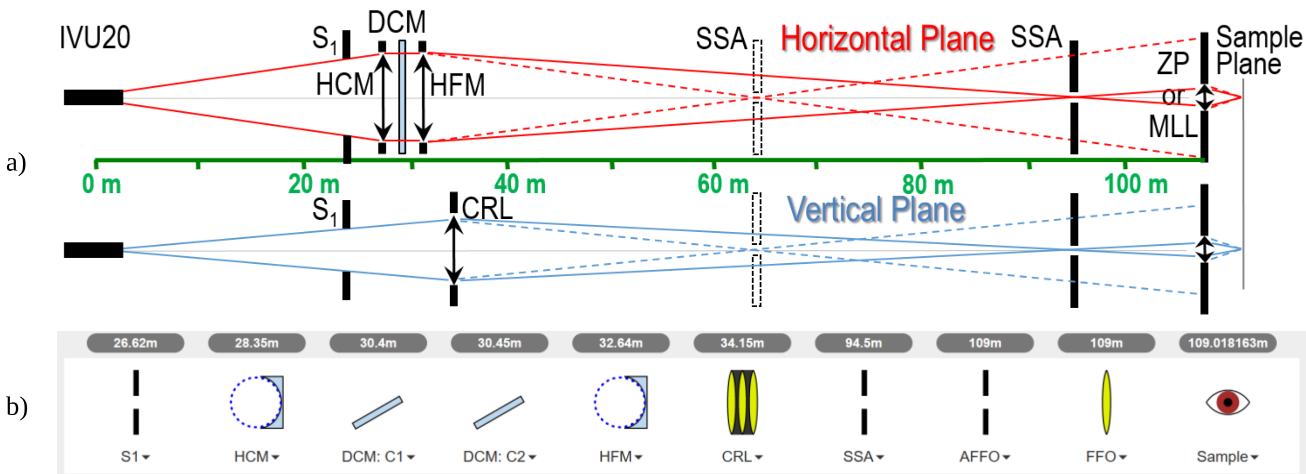

Figure 4. Simplified optical scheme of HXN beamline: a) graphical representation of a complete layout from source to a sample; b) Sirepo-generated sequence of pictograms of optical elements used to simulate intensity distributions at the Sample position at ~109 m from the center of undulator.

c. NSLS-II SRX beamline

Submicron Resolution X-ray Spectroscopy (SRX) is an undulator beamline at sector 5-ID of NSLS-II providing world-leading, high-throughput spectroscopic imaging capability (2D and 3D) with sub-100 nm spatial resolution and millisecond dwell times/pixel with fly-scan capability. Scientific communities such as environmental sciences, life sciences, and material sciences will take advantage of this beamline to understand complex natural and engineered systems that are heterogeneous on the micron to nanometer scale. The SRX beamline will enable simultaneous X-ray fluorescence and transmission measurements with sub-μm to sub-100 nm spatial resolution with an incident X-ray beam energy of 4.65-25 keV. X-rays are focused onto the sample by a set of Kirkpatrick-Baez mirrors. Sample stages will enable fast 2D scanning and tomography capabilities. X-ray fluorescence imaging and tomography will provide elemental mapping in 2D and 3D, respectively. Spatially resolved X-ray Absorption Near Edge Structure (XANES) spectroscopy can be performed in fluorescence or transmission mode. Full-field imaging and tomography are also possible to provide morphology information. Several different operation modes including high resolution scanning (sub-100 nm focused beam), high flux (sub-μm focused beam) scanning and full-field imaging are available. Figure 5 depicts a simplified beamline optical scheme consisting of Horizontally focusing mirror, Horizontal double crystal monochromator, secondary source slits, Kirkpatrick-Baez mirrors (2 sets – high flux and high-resolution modes, respectively).

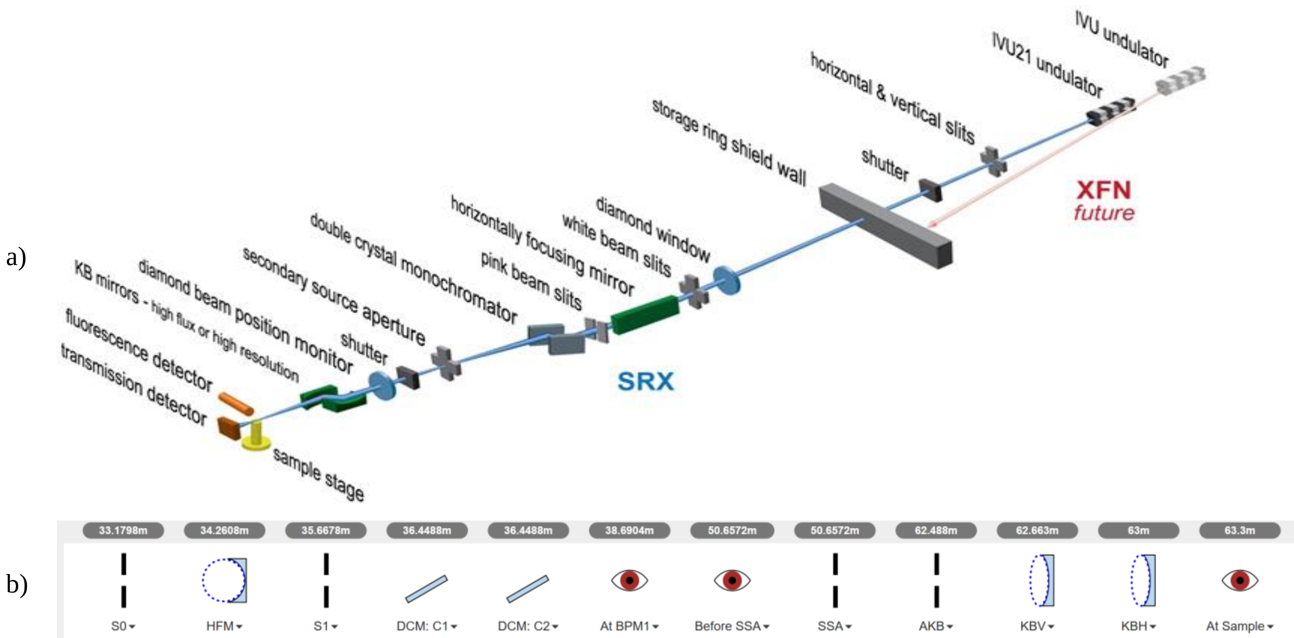

Figure 5. Simplified optical scheme of SRX beamline: a) graphical representation of a complete layout from source to a sample; b) Sirepo-generated sequence of pictograms of optical elements used to simulate intensity distributions after KB-mirror at ~63.3 m from the center of undulator.

d. NSLS-II FMX beamline

Frontier Macromolecular Crystallography (FMX) is an undulator beamline at sector 17-ID for structural biology investigations with micro-focusing macro-molecular crystallography (MX), optimized for challenging bio-crystallographic problems. Its flux density will be unmatched by MX facilities world-wide. The FMX beamline is part of the NIH-funded ABBIX project. It supports single- and multi-axis MX projects, micro-focus crystallography, serial crystallography, and data collection at cryo- and room temperature.

The optical system of the FMX beamline consists of Double crystal monochromator (vertical axis, Si(111)), Horizontally focusing bimorph mirror, Horizontal secondary source aperture, Focusing compound refractive lenses, and KB focusing bimorph mirrors (Figure 6).

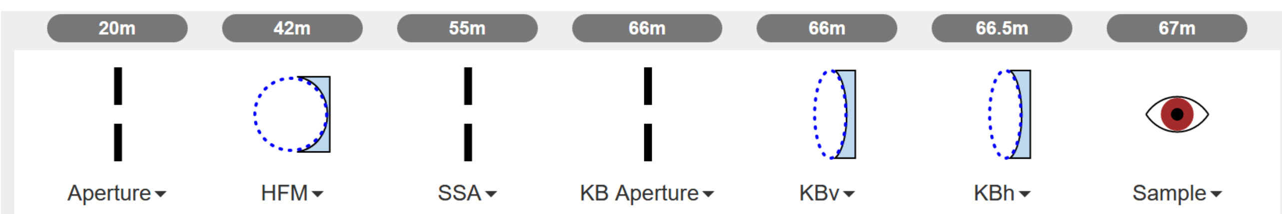

Figure 6. Simplified optical scheme of FMX beamline: Sirepo-generated sequence of pictograms of optical elements used to simulate intensity distributions after KB-mirror at ~67 m from the center of undulator.

e. NSLS-II SMI beamline

The Soft Matter Interfaces beamline will provide Grazing-Incidence SAXS/WAXS and Liquid Interface X-ray scattering capabilities with energy range 2.1-24 keV. SMI is part of the NEXT project. Optical system of the beamline consists of a double crystal monochromator, separate horizontally and vertically focusing mirrors, secondary source aperture and compound refractive lenses (Figure 7). Primary focus is at the Liquid Spectrometer or at GISAXS sample in low divergence mode or microfocus mode with additional optics.

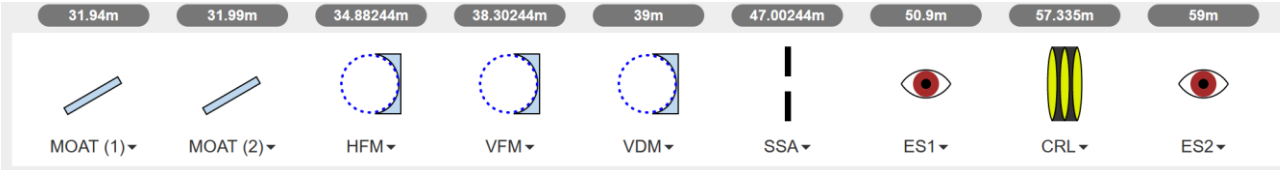

Figure 7. Simplified optical scheme of SMI beamline: Sirepo-generated sequence of pictograms of optical elements used to simulate intensity distributions after CRL at ~59 m from the center of undulator.

f. NSLS-II ESM beamline

The experimental study of the novel materials – often artificially engineered – is the fundamental scientific scope of the ESM beamline. The beamline feeds two photoemission end stations. Branch 1) is a high-resolution SP-ARPES spectrometer and branch 2) is a full-field AC-XPEEM/LEEM instrument (in collaboration with the BNL Center for Functional Nanomaterials).

Optical system of the beamline contains Monochromator (VLS-PGM), Secondary slits, μ-ARPES refocusing: KB pair; XPEEM-refocusing: ellipsoidal (Figure 8).

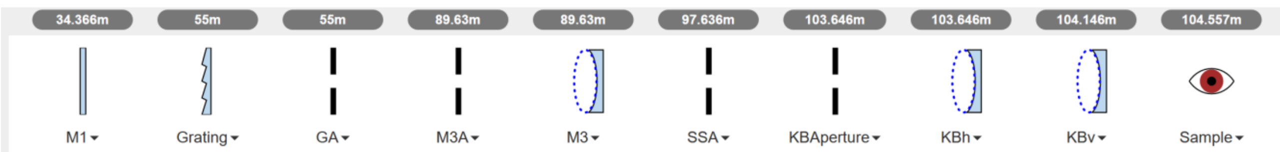

Figure 8. Simplified optical scheme of ESM beamline: Sirepo-generated sequence of pictograms of optical elements used to simulate intensity distributions after KB-mirrors at ~104.6 m from the center of undulator.

5. CONCLUSIONS

We presented Sirepo – a browser-based open-source framework for X-ray optics simulations. Currently, Sirepo is interfaced with a number of leading codes in the fields of X-ray source and optics simulations (SRW and Shadow3) and particle accelerators. Sirepo proved to be a flexible framework which could be relatively easy integrated with the other scientific computer codes requiring convenient GUI to perform simulations in the cloud. In the present paper, we detailed the features of Sirepo interface for Synchrotron Radiation Workshop – a widely used program for physical optics simulations. Sirepo for SRW contains predefined textbook examples as well as simulations of the wavefront propagation through the real beamlines at NSLS-II. Users benefit from both – Source and Beamline pages. On the Source page users can optimize the source or the synchrotron radiation (e.g., undulators, damping wigglers, etc.). On the Beamline page, one can construct a "virtual" beamline emulating layout of a real experimental beamline. Sirepo is empowered with the dynamically changing widgets and dynamically accessed data from the community databases for X-ray optics. Sirepo has being successfully used by many beamline scientists at NSLS-II, APS, LCLS, European X-FEL, etc.

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