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# Simulation Framework SYRIS tested for Microtomography Applications at the Imaging Beamline P05 / PETRA III

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**Abstract.** The Helmholtz-Zentrum Geesthacht, Germany, is operating the user experiments for microtomography at the beamlines P05 and P07 using synchrotron radiation produced in the storage ring PETRA III at DESY, Hamburg, Germany. In recent years the software pipeline and sample changing hardware for performing high throughput experiments were developed. To test and optimize the different measurement techniques together with quantification of the quality of different reconstruction algorithms a software framework to simulate experiments was implemented. Results from simulated microtomography experiments using the photon source characteristics of P05 will be shown.

## INTRODUCTION

X-ray based tomography (CT) is a highly versatile non-destructive imaging tool, which offers cross-sectional and fully three-dimensional structural information of scanned samples via reconstruction from projection images. The use of synchrotron radiation (SR) opens up the possibility to scan samples with micrometer resolution (SRμCT) while achieving high throughput at synchrotron radiation beamlines. The quality of μCT-data taken during synchrotron radiation experiments however, is heavily influenced by the optimal choice of numerous experimental parameters, including X-ray energy, number of recorded projections and exposure time. Being able to simulate critical parameters and study their influence on the reconstructed results beforehand can save valuable time during the experiment and might lead to overall improved results.

For the reconstruction of SRμCT-data, several image processing steps are crucial. With increasing complexity of μCT-experiments, treatment of artifacts induced during the measurement process, data processing or reconstruction phase becomes difficult. Since the original sample structure is usually not known (only projections are recorded), benchmarking of different reconstruction algorithms is tedious. At this point, virtual experiments might be beneficial, as in the virtual case the original sample object is exactly know (*ground truth*). Furthermore, there is a need of simulated data including different systematic and non systematic measuring artifacts to test and optimize different reconstruction methods for the different tomography techniques. This data should then become public, so external groups can optimize their code.

With SYRIS (Synchrotron Radiation Imaging Simulation), a software tool is at hand to calculate the experimental results and the corresponding *ground truth* while taking all critical experimental parameters into account. SYRIS is being developed by Faragó *et al.* at Karlsruhe Institute of Technology (KIT) [1]. As part of a joint master's thesis project between TU Dortmund and Helmholtz-Zentrum Geesthacht (HZG), the SYRIS framework was tested and implemented at the imaging beamline P05 at PETRA III, DESY. The produced simulation results will be presented.

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# MICROTOMOGRAPHY SETUP AT P05, PETRA III, DESY

At the imaging beamline P05 (IBL) at PETRA III, DESY two experimental hutches with dedicated focus on microtomography [2] and nanotomography [3] are operated. An overview of the P05 experimental site is presented in Fig. 1, showing the two experimental hutches, optics and control hutch. A 2 m-undulator source provides synchrotron radiation, which is being monochromatized with either a Double-Multilayer-Monochromator (DMM) or by use of a Double-Crystal-Monochromator (DCM). The monochromatized X-rays are collimated by a system of slits and propagated onto the sample. In the case of microtomography, the X-rays are detected after penetration of the sample by a detector system in experimental hutch 2. Either a CCD or a CMOS camera is used inside the detector in combination with scintillators and microscope optics. Remote sample exchange is possible via a robot arm in experimental hutch 2, which can load the rotation stage with samples from a pre-equipped magazine.

Figure 2 shows the schematic beamline layout. Due to the propagation distance of X-rays between source and sample position (about 85 m), synchrotron radiation is partly coherent when interacting with the sample. This opens up different possibilities for phase contrast imaging. A selection of beamline operational parameters is collected in Tab. 1.

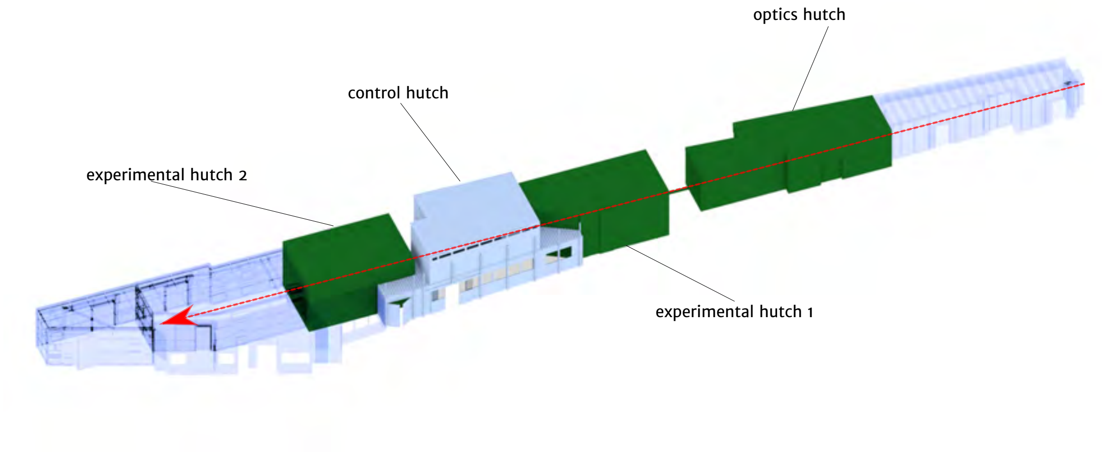


**FIGURE 1.** Overview rendering of the imaging beamline P05 at Petra III, DESY. Path of synchrotron radiation is marked by dashed arrow. Transparent areas belong to the neighboring beamline (P06).

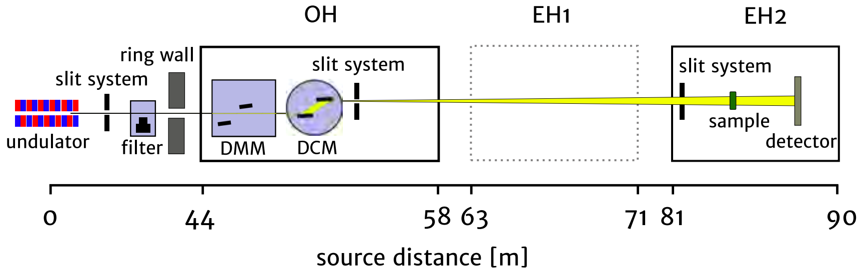


**FIGURE 2.** Schematic layout for the imaging beamline P05 at Petra III, DESY. The microtomography setup is installed in experimental hutch *EH2*.

**TABLE 1.** Design parameters of beamline P05 at PETRA III, DESY.

| **Parameter** | Value |
|---|---|
| **Energy range** | (5–50) keV |
| **Insertion device** | U29 undulator in low-$\beta$ section |
| **Source size** | 36.0 µm × 6.1 µm (at 10 keV) |
| **Source divergence** | 28.0 µrad × 4.0 µrad (at 10 keV) |
| **Filters** | 4 mm glassy carbon and 300 µm CVD with 50 µm Cu |
| **Monochromators** | Double Crystal Monochromator, Si[111]/Si[311] in Bragg geometry ($\Delta E/E \approx 10^{-4}$)<br>Double Multilayer Monochromator with three different ML pairs ($\Delta E/E \approx 10^{-2}$) |
| **Spatial resolution** | 0.7 µm |
| **Field of view** | up to 7.4 mm × 2.0 mm (at 87.5 m, low-$\beta$) |
| **Coherence** | Various phase contrast imaging techniques possible [4] |

## The SYRIS framework

The open-source project SYRIS enables users to simulate synchrotron radiation experiments, while specifying experimental parameters such as X-ray source type, sample shape and material, detector statistics, frame rate and exposure time. Special care is taken to let users define the movement of sample and source elements, which allows for studies on detector image blurring or intensity fluctuations due to beam drift. The ability to account for sample movement (e.g. rotation) also opens up potential applications for the simulation of tomography experiments. Besides virtual detector data, SYRIS also offers the possibility to produce the *ground truth* (information about true sample structure and movement), to use as reference. This might be used for e.g. benchmarking a image processing pipeline.

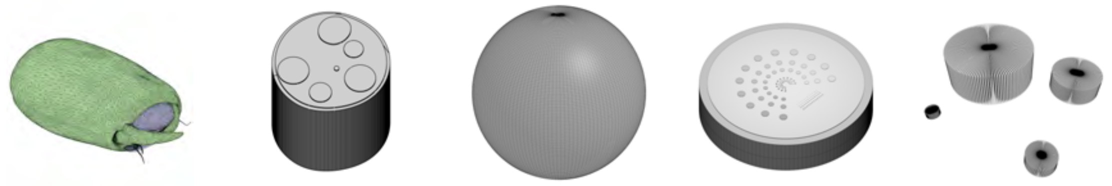
SYRIS offers a Python 2 user interface (https://www.python.org/) and is implemented using the OpenCL framework, which allows for efficient computation on various platforms including large speedups when using systems accelerated by graphics processing units (GPUs) due to parallel computation. The source code and documentation are freely available on the web[1].

To obtain virtual detector images, SYRIS handles the whole image formation process from source to detector by following a propagation-based approach. In this approach a wavefield is being propagated from the source point towards the imaging plane, and modulated upon interaction with objects along the beam path. A benefit of this approach is the possibility to simulate phase effects such as edge-enhancement due to the coherent nature of the incoming SR-radiation. In this way specialized techniques such as phase contrast imaging can be accessed. For extensive information about the framework the reader may refer to [1] and the SYRIS documentation.

## MICROTOMOGRAPHY SIMULATION RESULTS

To explore SYRIS capabilities for simulation of microtomography experiments at beamline P05, a set of virtual samples was chosen to represent different applications of microtomography (Tab. 2). Samples objects *b – e* were modeled and sample *a* was edited using the open-source modeling software Blender (https://www.blender.org) and imported into SYRIS using the onboard functionality. Table 3 lists simulation parameters for all samples.

**TABLE 2.** Set of virtual test samples. Illustrations show renderings of the simulated sample objects *a – e*.



*(a) Larval head* *(b) Cylinder phantom* *(c) Double sphere* *(d) Contrast phantom* *(e) Star phantom*

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[1] Source code and many examples are available on Github (https://github.com/ufo-kit/syris). The documentation is maintained via Read the Docs (https://syris.readthedocs.io/en/latest/).

**TABLE 3.** Simulation parameters for sample objects *a* – *e*. Each simulation was done for the P05 undulator source and monochromated X-ray radiation ($\Delta E/E = 10^{-4}$). The simulated camera model was EHD SC900 in all cases. For conversion of X-rays to visible light a scintillator (100 µm $CdWO_4$) was simulated. Tomographic reconstructions were carried out using an IDL implementation of the gridrec algorithm by Marc Rivers [5].

| **Category** | Parameter | *a* | *b* | *c* | *d* | *e* |
|---|---|---|---|---|---|---|
| **X-ray** | Photon energy E | 8 keV | 20 keV | 20 keV | 12 keV | 20 keV |
| **Detector** | Exposure time | 100 ms | 100 ms | 100 ms | 100 ms | 100 ms |
| | Magnification | 5x | 10x | 5x | 5x | 5x |
| | Numerical aperture | 0.2 | 0.5 | 0.5 | 0.2 | 0.2 |
| **Sample** | Detector distance* | 0 m | 0 m | (0.15–3.08) m | 0 m | 0 m |
| **Dataset** | Experiment type | Tomography | Tomography | Radiography | Tomography | Tomography |
| | Projections | 360 | 2400 | 1 | 360 | 360 |

* As seen from the sample position.

### *Sample (a): Complex biological sample*

To study the simulation workflow for complex sample objects, reconstructed and segmented tomography data of a larval head (*Rhyacophila*, see Friedrich *et al.* [6]) were used as virtual sample for simulations with SYRIS. As starting point for all simulations with this sample, a readily reconstructed and segmented three-dimensional surface model of the larval head was available. As first order approximation, material properties of chitin were assigned to the model. Raw calculated projection images and thereof reconstructed slices are shown in Fig. 3. Simulated projections prove SYRIS capability to handle complex and highly space-resolved models as samples. Since the volumes described by the surface model are interpreted as areas of constant density, reconstructed slices contain two density levels (sample and environmental density). Bright spots in the reconstructed slices appear where two sample volumes intersect each other. This artifact is introduced during model preparation and can be avoided by adaptions during the segmentation process.

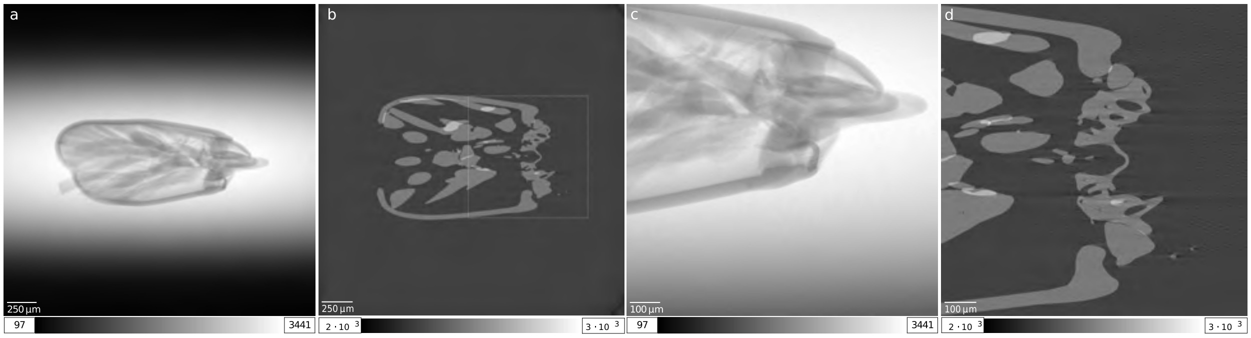

**FIGURE 3.** Calculated projections and reconstructed slices for a complex sample object (*Rhyacophilia* larval head). Panels *a* and *b* show full view images of one projection and a reconstructed slice, respectively. The detail views *c* and *d* show the mouth region. Bright spots and streaks in the reconstructed slices are artifacts due to intersection of surfaces in the sample model (see text).

### *Sample (b): Cylinder phantom with inclusions of varying absorbance*

On basis of an already existing X-ray phantom at P05, a cylinder phantom is modeled in Blender and simulated to compare between actual measured data and calculated images. The phantom consists of 6 rods with different diameter and material, enclosed inside a 5 mm thick cylinder segment. Figure 4 shows simulated and measured projections, with good agreement between the measured and calculated gray values for reconstructed slices. For this simulation, a new X-ray source type was implemented into SYRIS, which allows to import photon flux distributions from third party code[7]. For this result, the P05 undulator source was simulated using SPECTRA, a synchrotron radiation calculation code [8], and then imported into SYRIS. For the enclosed rods, the following material properties were assigned (starting from top, clockwise): Magnesium, PTFE, Aluminum, Nylon, PMMA, PCTFE.

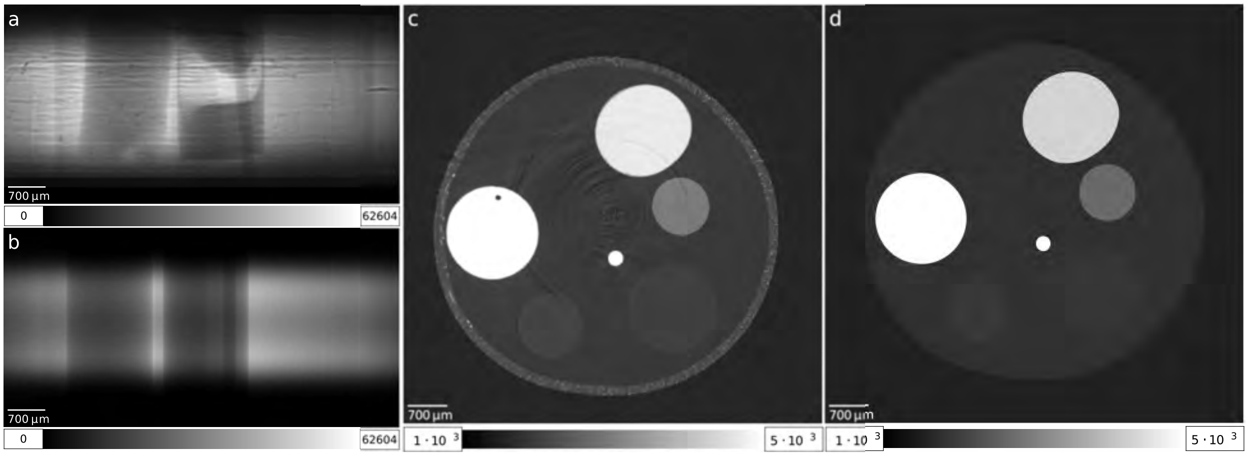

**FIGURE 4.** Comparison between measured and calculated data. Panels *a* and *c* show data recorded at P05, DESY and a reconstructed slice. Panel *b* shows a calculated projection, with the reconstructed slice in panel *d*.

### *Sample (c): Sphere phantom with propagation enhanced contrast*

The sample object is inspired by a double wall sphere phantom described in [9]. Figure 5 displays calculated radiograms of the sample for two different sample-detector distances (0.15 m and 3.08 m). The outer sphere wall has a thickness of 15 µm and consists from parylene, for the inner core material properties of polystyrene are assigned. The calculated radiograms reveal good resolution and rendering of the edge regions between the two spheres as well as edge-enhancement due to the propagation of the wavefield.

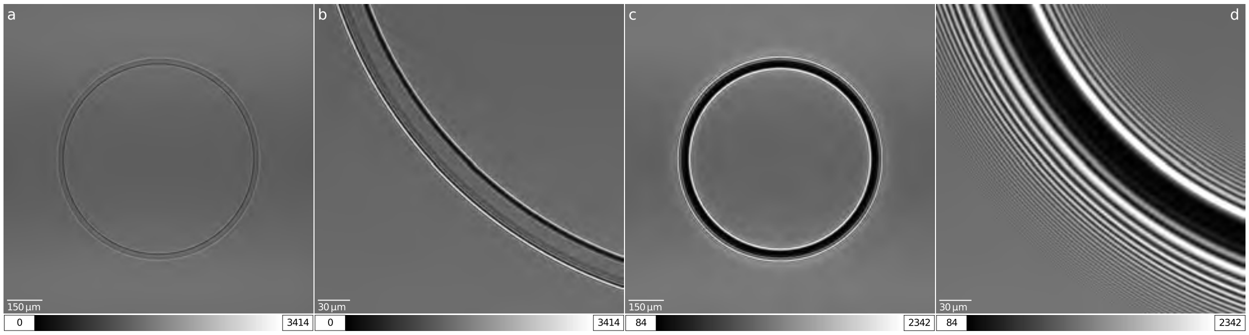

**FIGURE 5.** Calculated radiograms showing edge enhancement with different propagation distances for a sphere phantom. Panels *a* and *b* are calculated at a propagation distance of 0.15 m. For Panels *c* and *d* the propagation distance was set to 3.08 m.

### *Samples (d,e): Cylinder phantoms with different absorbance levels and Siemens star*

Two X-ray phantoms, one for contrast studies, the other a Siemens star for spatial resolution studies, are being simulated. The contrast phantom consists of urethane, with inclusions of different concentrations of iodine. The Siemens star phantom consists of 128 sectors, with aluminum assigned as material. Reconstructed slices based on simulated results are displayed in Fig. 6 and demonstrate the spatial resolution and the density resolution of the method. The reconstructed slices of the Siemens star phantom exhibit good reproduction of the original star structure, and can be used to benchmark the in-slice resolution of the virtual imaging process [1, 7].

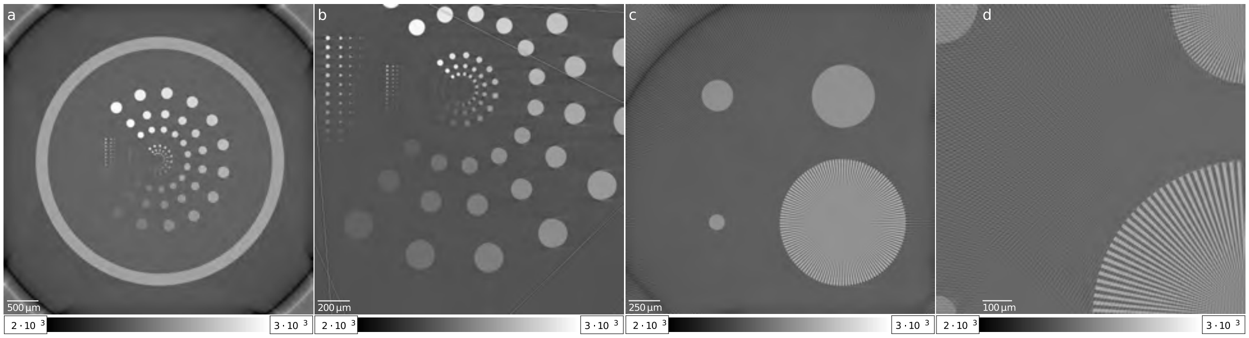

**FIGURE 6.** Tomography slices reconstructed from simulated projection data. Panels *a* and *b* show a contrast phantom with different density levels. A star phantom for investigation of spatial resolution is shown in panels *c* and *d*. Artifacts (streaks and rings) are introduced due to simulated beam movement. Bright lines are due to simulated missing values in six of the projections.

## SUMMARY & OUTLOOK

Different virtual samples were simulated for parameters of beamline P05, PETRA III, DESY. First results indicate a broad range of possible applications for the SYRIS framework including experiment preparation, instrument operation and analysis benchmarks. SYRIS Python interface enables easy and powerful expansion for custom needs, as was successfully demonstrated by implementation of a new source type and expanded import functionality during tests at P05. Those expansions allowed the investigation of various experimental parameters, including source characteristics, samples, detector statistics and artifacts such as beam movement. By implementing SYRIS at the P05 beamline, first steps towards comparison and studies on different reconstruction algorithms were also archived. The creation of systematic benchmarking datasets together with further benchmarking remains to be done in the future.

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