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An easy to use XRD data analysis framework for users and scientists, online and offline

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Motivation

- When doing Xray diffraction experiments it is often necessary to perform several steps of data reduction and analysis in order to evaluate a result.
- In some cases data might even be found to be completely useless upon inspection after the experiment has concluded.
- Online analysis at the beamline can be useful in these cases.

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Motivation contd.

- Users are not necessarily specialists in xray diffraction or scientific computing
- It would be nice to be able to give external users not just their data, but also the tools to process them, wouldn't it?

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Implementation

Started xraylib as intern three months last summer. Continued this year from march as part of master degree “technical physics“ at NTNU, Norway.

Python

- High level $\Rightarrow$ Quick and easy to develop and prototype.
- Yet high performance when using compiled libraries
- Evergrowing library of tools for scientific computing.
- No license necessary (unlike matlab)

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Dependencies

- No dependency on ESRF computing infrastructure
- Python libraries
  - pyFAI Fast azimuthal integration on GPU / CPU
  - scipy / numpy Almost all you need for arrays/images/matrices
  - scikits-image Branch of scipy. More filters, including tomographic reconstruction (FBP, SART)

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Installation

- Scripts for setting up xraylib for use *and* development are provided.
- In theory this is all you should need if you have system-wide access

```
git clone https://github.com/amundhov/xraylib.git
cd xraylib
./install.sh or ./develop.shp
```

- Python library dependencies maintained in **requirements.txt** and can be parsed by standard python package tools such as **pip** and **distutils**.

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Installation cntd.

- In practice it is best to have your system administrator install the required python libraries. On debian based systems these are all available through APT.
- For development or local installation make use of python's virtual environments:

```
virtualenv –system-site-packages venv
source venv/bin/activate
[ perform steps from previous slide ]
```

- Whenever venv/bin/activate is sourced xraylib will be available on your path along with the scripts in scripts/

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What's in it (for me)?

Some examples

- Calculation of sample properties such as xray absorption at given energy.
- Simplified file access (EDF, multiframe EDF, hdf5, anything fabio supports)
- Utility functions and examples for making small scripts and workflows.

We'll have a look at applications shortly.

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xraylib + DAWN

- Data exploration. Rich support for slicing and visualising data in HDF5 format.
- Peak fitting and export.
- Integration with python scripts possible in their workflow tool. Lots of functionality coming, but currently not used.

In summary: process data with xraylib, visualise with DAWN.

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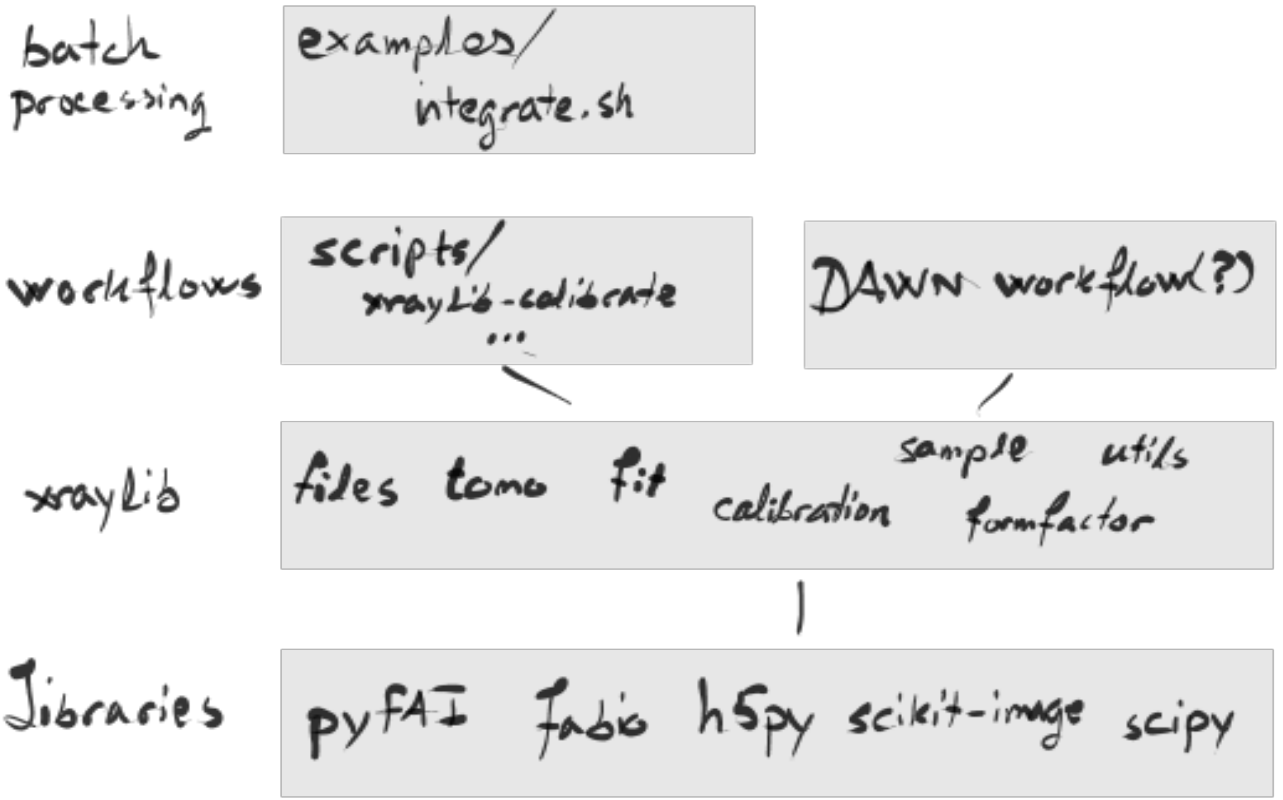
Structure



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Current applications of the framework

1. Detector calibration. Detector tilt and beam origin.
2. Azimuthal integration.
3. Sinogram assembly of specific phases in diffraction tomography experiments [DSCT]
4. Sinogram correction and reconstruction

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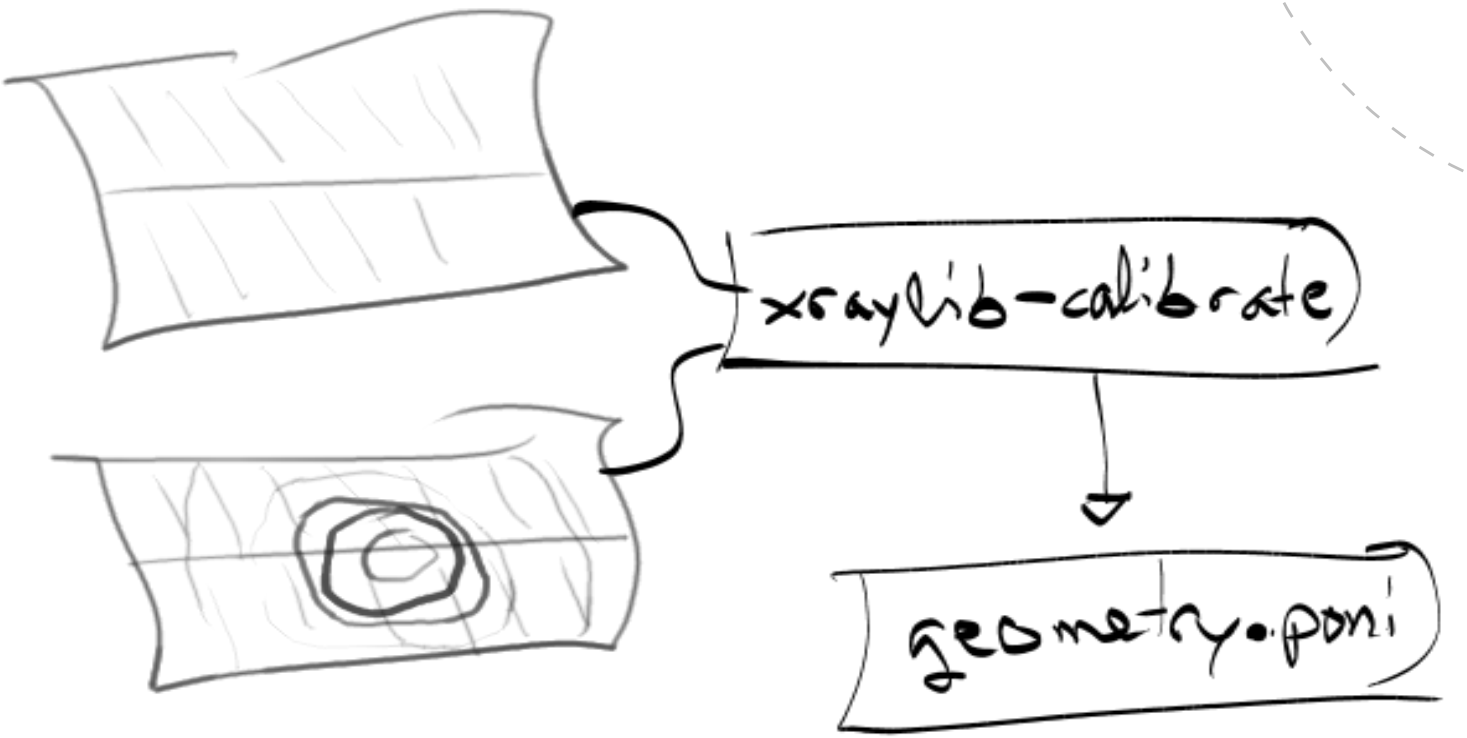
scripts/xraylib-calibrate



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scripts/xraylib-calibrate

```
Usage: xraylib-calibrate <options> CALIBRATION_IMAGE [DARK_CURRENT1,DARK_CURRENT2,...]

         XRD calibration routine based on ring shape.

Options:
  -s, --silent          supress output to terminal.
  -t, --timings         Report execution times.
  --pixels              Origin and calibration limits in pixels instead of mm.

  File options:
    --out=FILE          Save calibration image after subtracting darkcurrent.
    --data-set=STRING   Location to save data set.
    -p=FILE, --poni=FILE
                        File to save detector geometry.

  Detector options:
    -D DETECTOR_NAME, --detector=DETECTOR_NAME
                        Detector name
    --distance=distance [mm]
                        Detector distance from sample
    --binning=x y       Number of pixels that detector is set to group.
    --tilt=a b [degrees]
    --origin=x y [mm]   Initial detector origin wrt beam

  Calibration options:
    --limits=lower upper
                        Radial distance [mm] to use for calibration.
```

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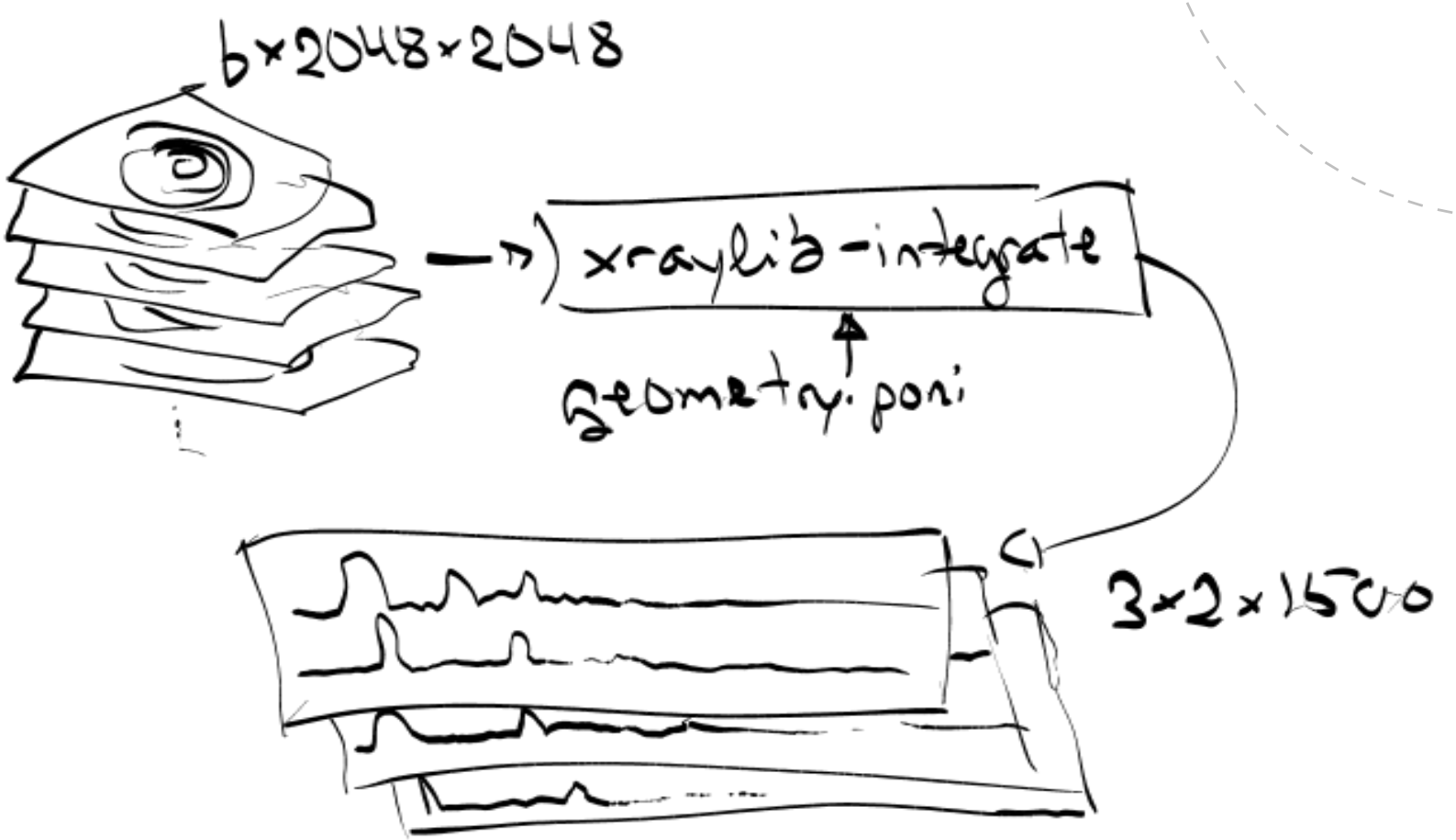
scripts/xraylib-integrate



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scripts/xraylib-integrate

```
Usage: <options> --data-prefix=/mnt/data/../EXPERIMENT_...

         Integrate diffraction images and assemble into dataset.
Experiment parameters are assumed to be separated by underscore
NAME_xxx_yyy_zzz.edf will produce a data set with powder profiles in
dimensions x,y,z.

Options:
  -s, --silent          supress output to terminal.
  -t, --timings         Report execution times.
  --nbuffer=NBUFFERS    Number of files to buffer when loading files
  --points=POINTS       Number of points to keep radially.

  Input options:
    --data-path=/path/IMAGE_xyz_
                        Integrate files starting with this path.
    --dark-path=/path/DARK_xyz_
                        Average darkcurrent files starting with this path.
    --dark=DARK         Use single darkcurrent image.
    -p PONI_FILE, --ponit=PONI_FILE
                        Name of poni file with detector geometry.

  Output options:
    -o FILE, --out=FILE
                        File to save integrated dataset.
    --data-set=STRING   Location to save data set.
```

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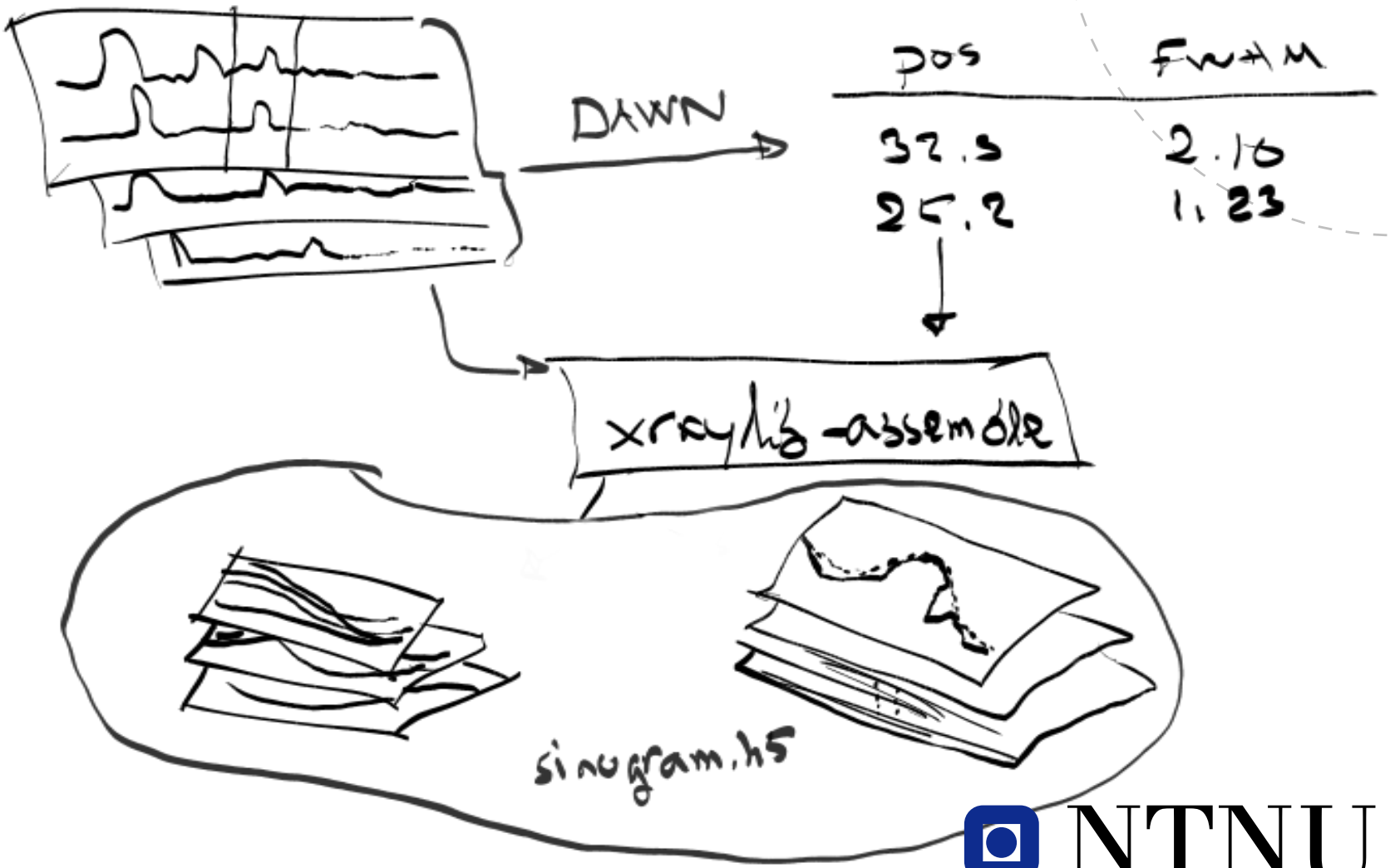
scripts/xraylib-assemble



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scripts/xraylib-assemble

```
Usage: xraylib-assemble <options> diffractogram.h5

Options:
  -s, --silent          supress output to terminal.
  -t, --timings         Report execution times.
  --flip                Flip every other scan line.

  Input options:
    --position=PEAK_POSITION
                        Peak channel position
    --fwhm=PEAK_FWHM    Peak FWHM full width at half maximum
    --shape=PEAK_SHAPE  Peak shape. [gaussian|delta]
    --peak-file=FILE    Exported peaks from DAWN.
    --input-set=STRING  Override data set [default /xraylib/diffractogram].

  Output options:
    -o FILE, --out=FILE
                        Output file.
```

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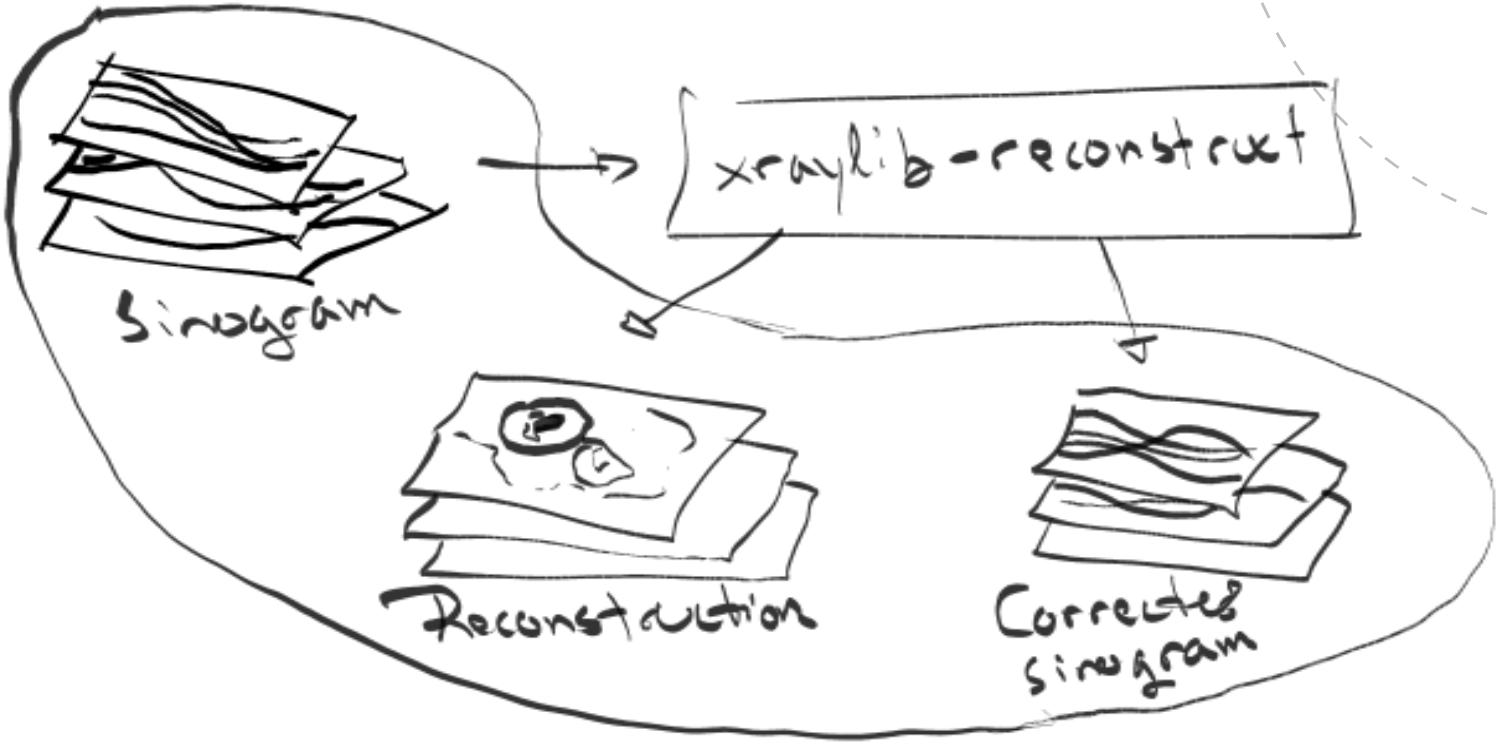
scripts/xraylib-reconstruct



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scripts/xraylib-reconstruct

```
Usage: xraylib-reconstruct <options>

         Correct sinograms and perform reconstruction.
By default the sinogram is split into odd and even rows
which are correlated to correct for offset in interleaved
scans, followed by a search for the center of rotation.

Options:
  -s, --silent          supress output to terminal.
  -t, --timings         Report execution times.

  Input options:
    --sinogram-group=SINOGRAM_GROUP
    --iterations=SART_ITERATIONS
                        Number of iterations to perform SART reconstruction.
                        [default=1]
  Output options:
    --output-sinogram
    --output-reconstruction
    -o FILE, --out=FILE
                        Write reconstruction slices to file.
```

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Experimental application

Just two weeks ago diffraction tomography data was collected to test the diffraction tomography workflow.
Dummy sample consisting of small ($\approx 150 \mu m$) glass spheres suspended from a needle using wax.

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[unintentionally blank]

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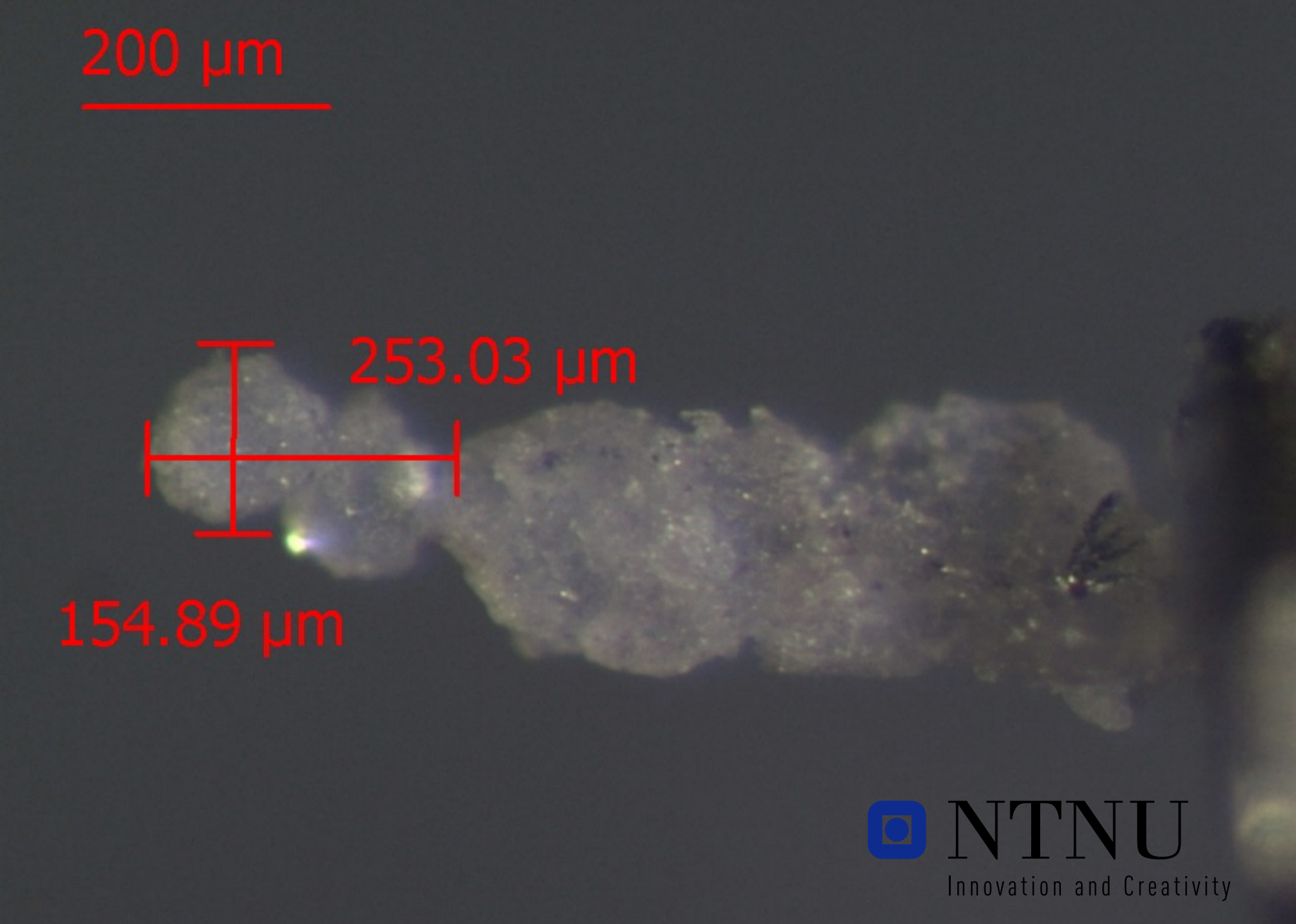

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Results

We will see the sinograms, corrected sinograms and their respective reconstructions using filtered back projection.

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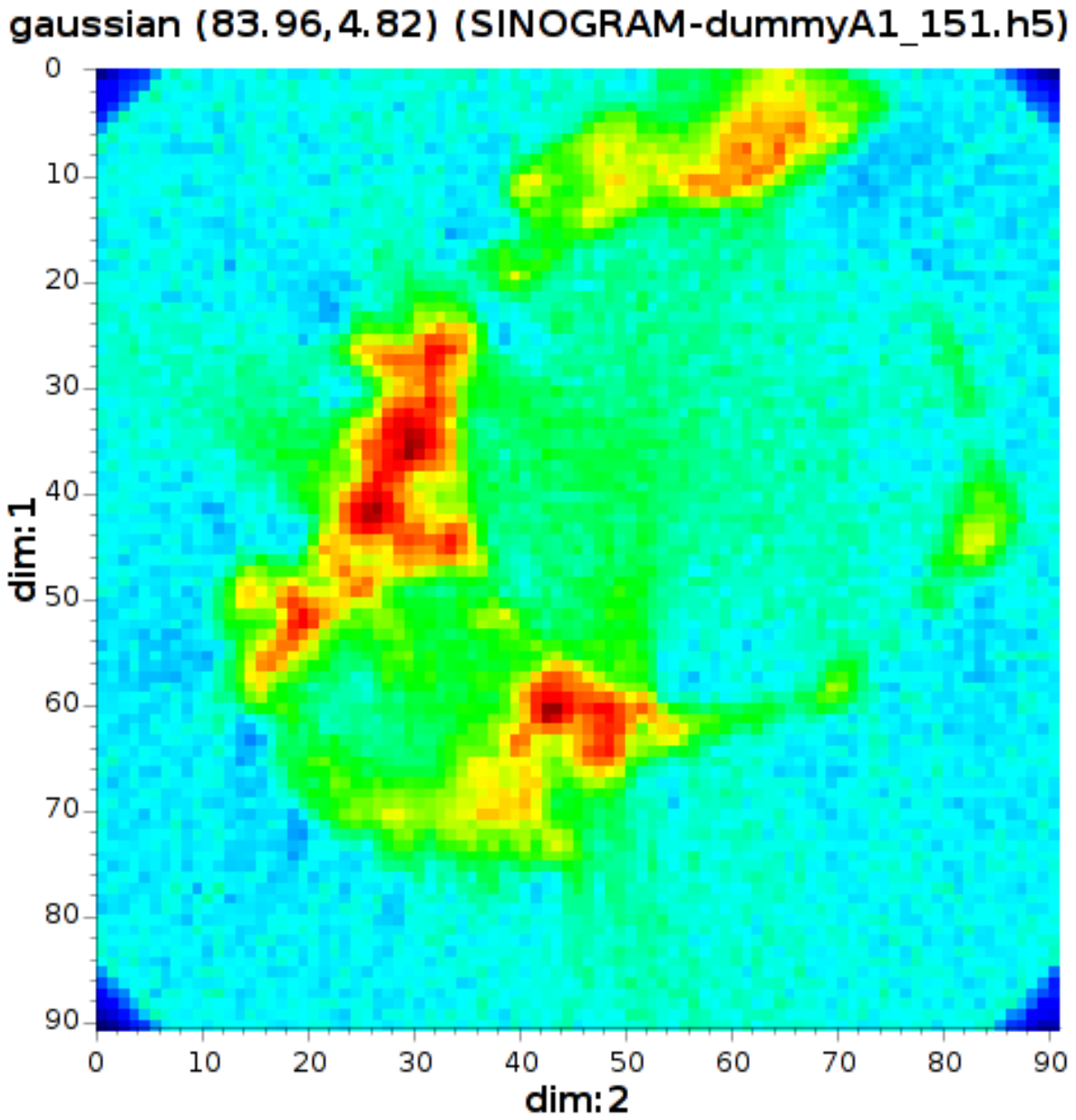
gaussian (83.96,4.82) (SINOGRAM-dummyA1_151.h5)
dim:1
dim:2
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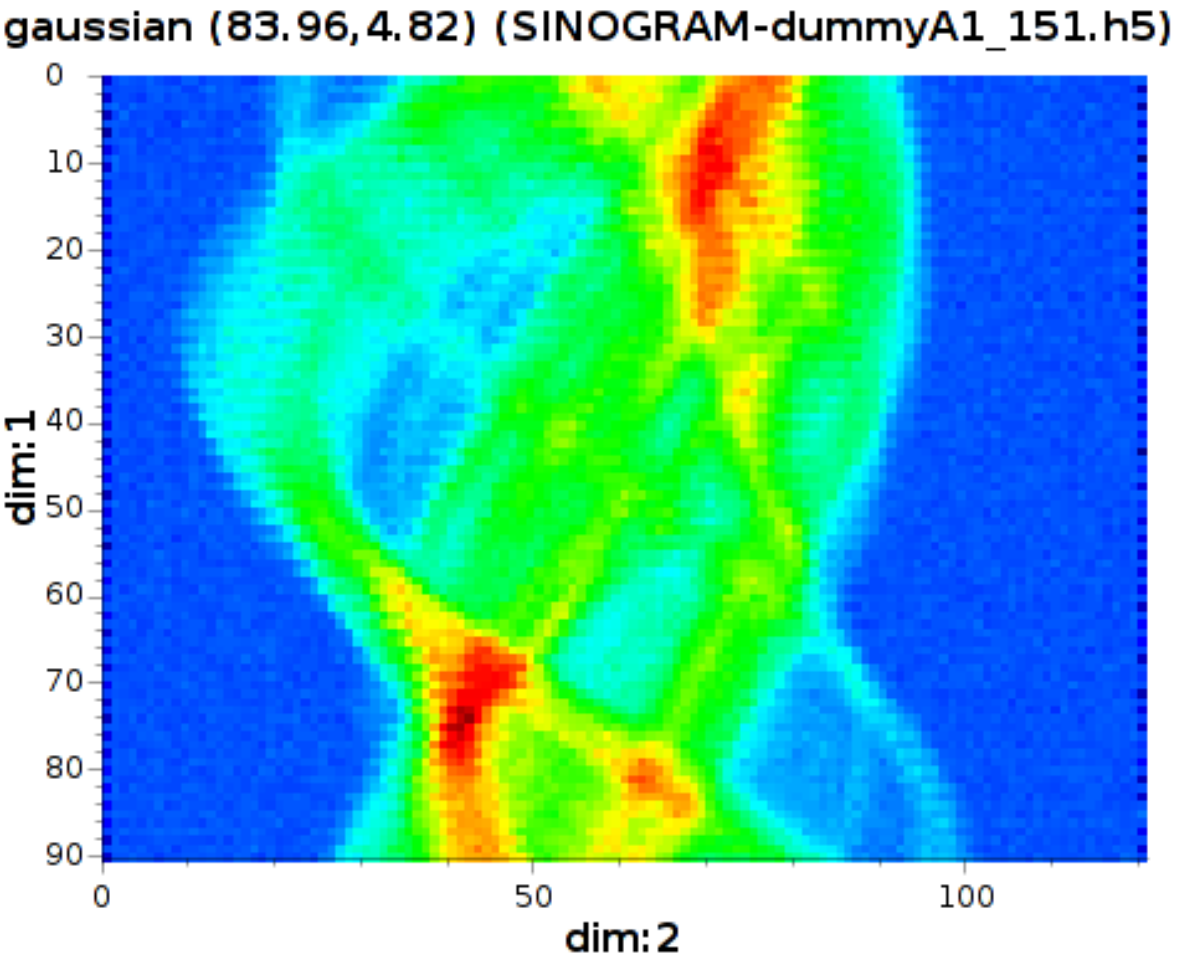
gaussian (83.96,4.82) (SINOGRAM-dummyA1_151.h5)
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dim:1
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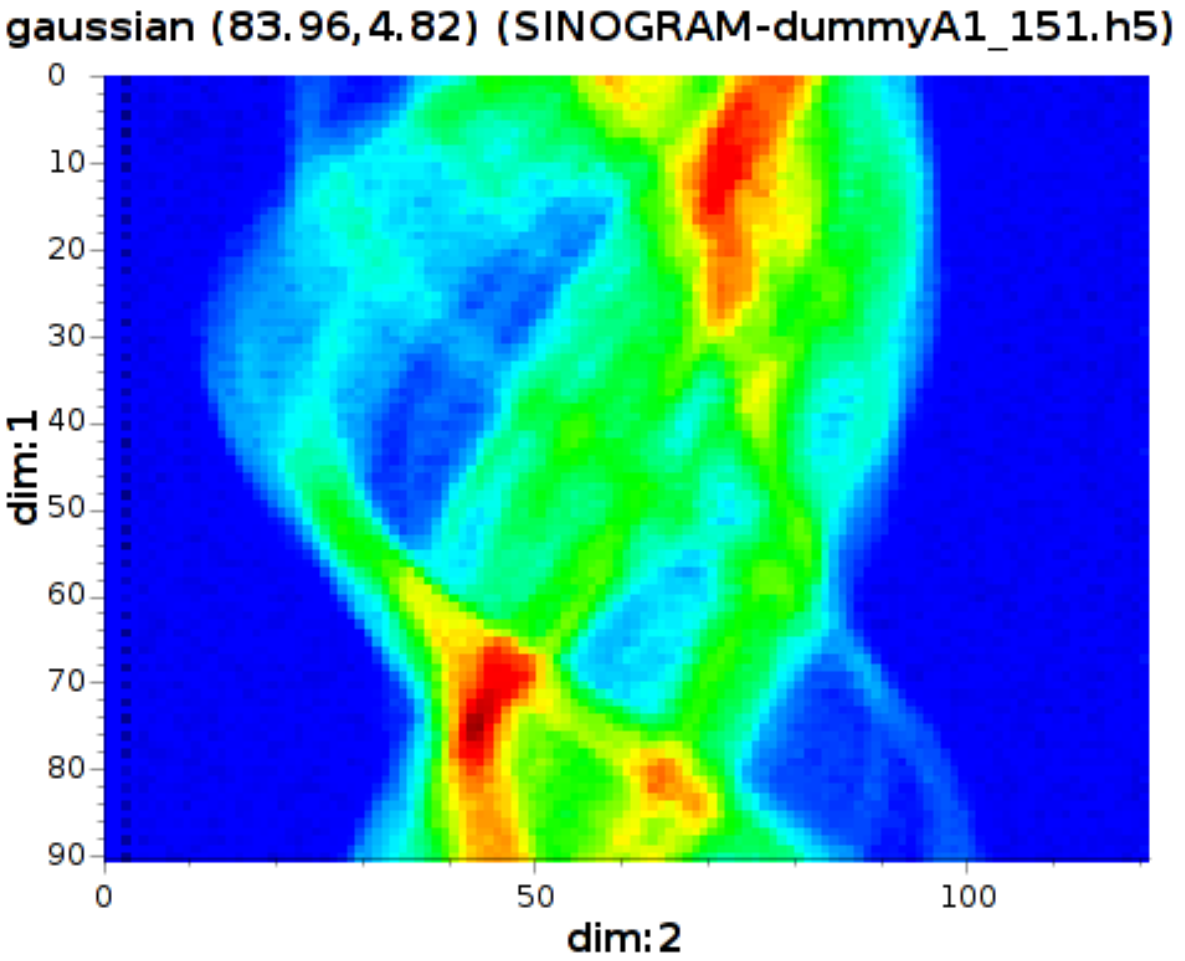
dim:2


gaussian (83.96,4.82) (SINOGRAM-dummyA1_151.h5)
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dim:1
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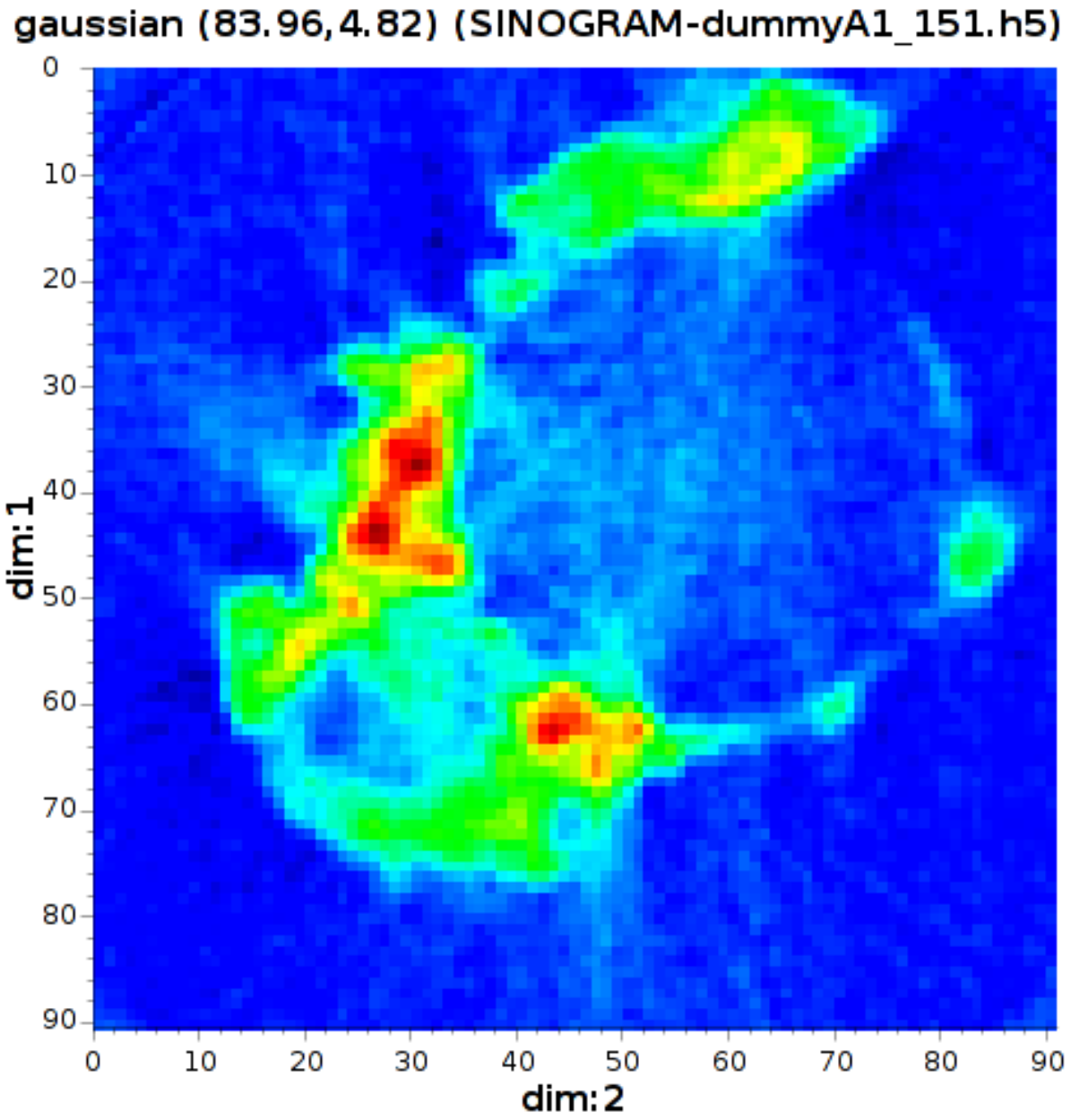
dim:2


gaussian (83.96,4.82) (SINOGRAM-dummyA1_151.h5)
dim:1
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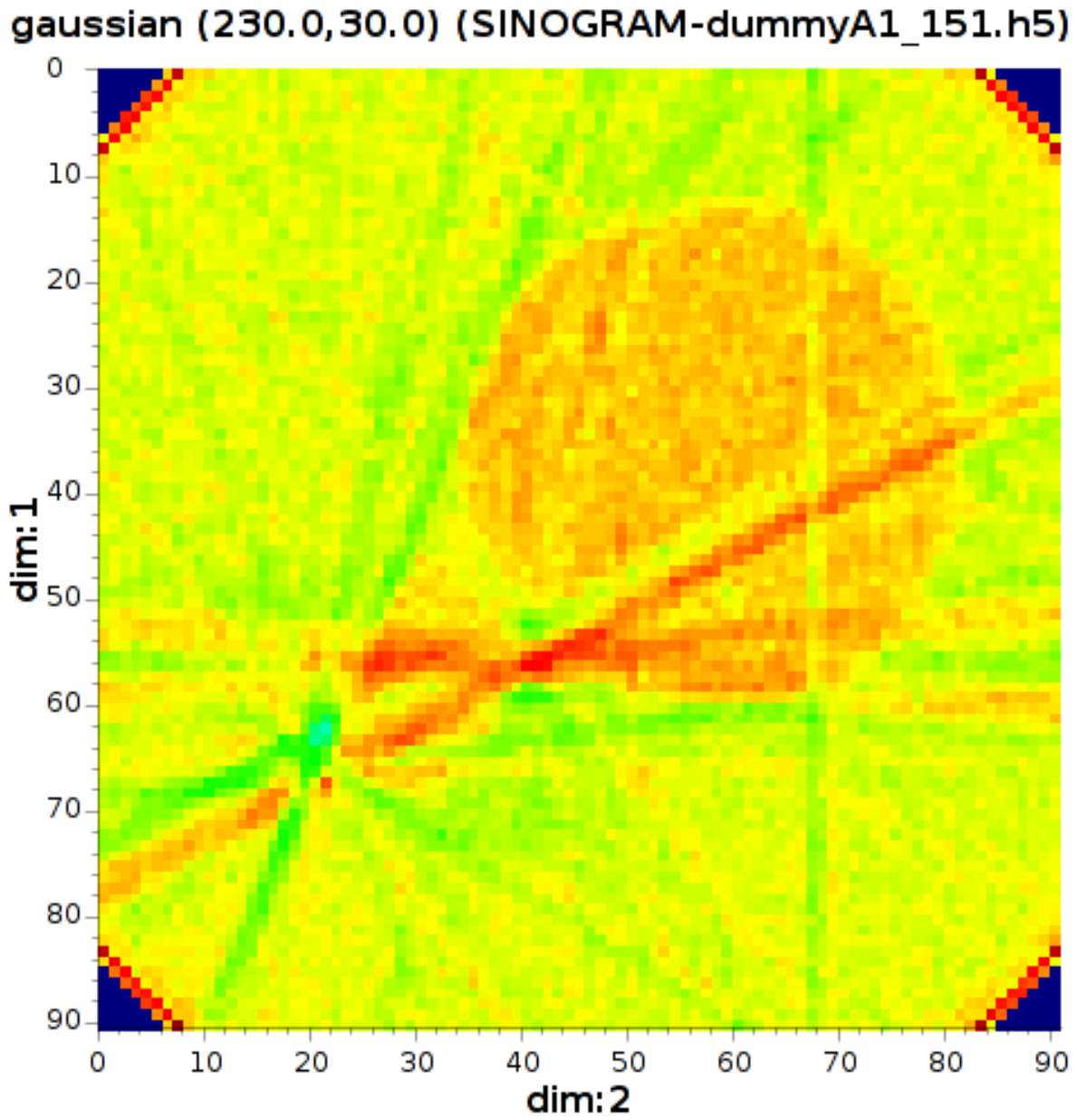
gaussian (230.0,30.0) (SINOGRAM-dummyA1_151.h5)
dim:1
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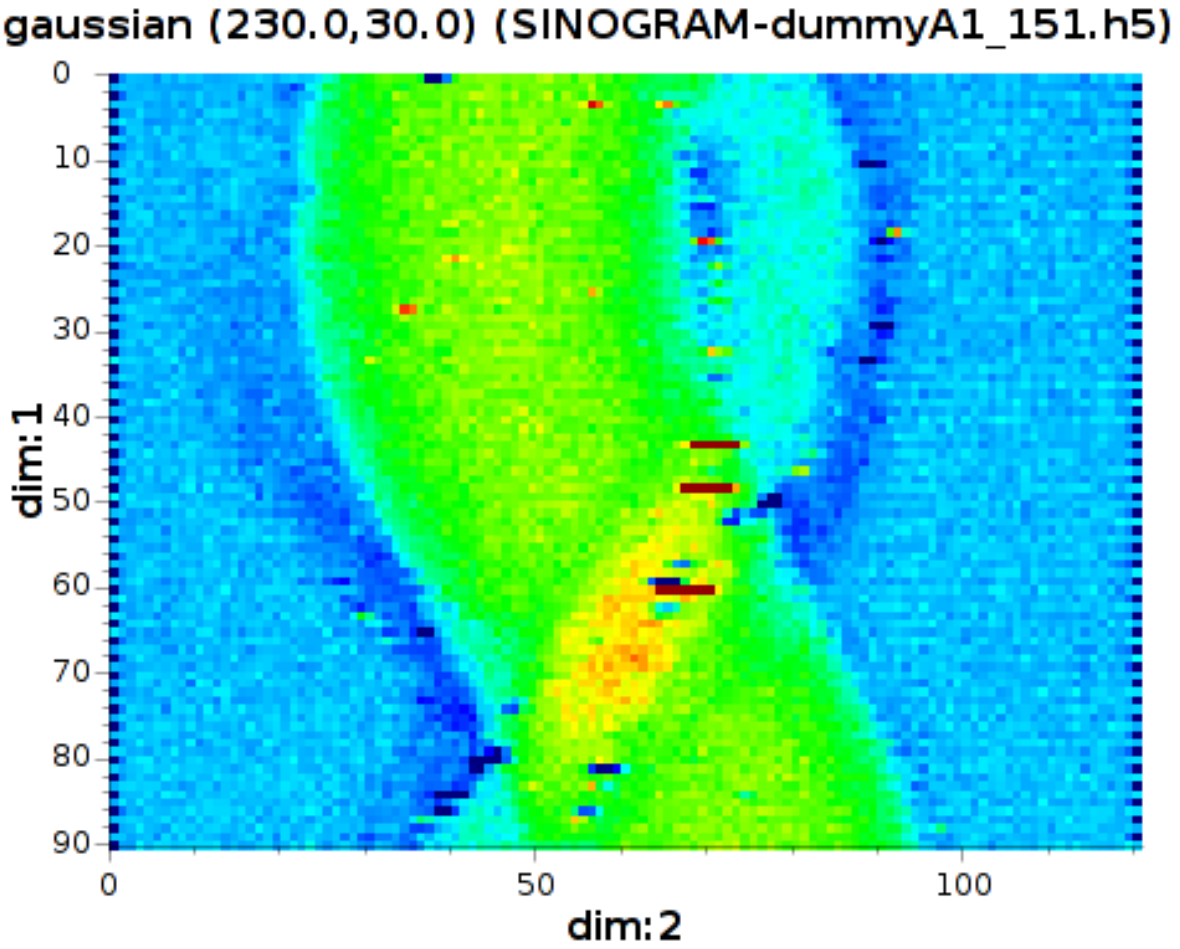
gaussian (230.0,30.0) (SINOGRAM-dummyA1_151.h5)
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dim:1
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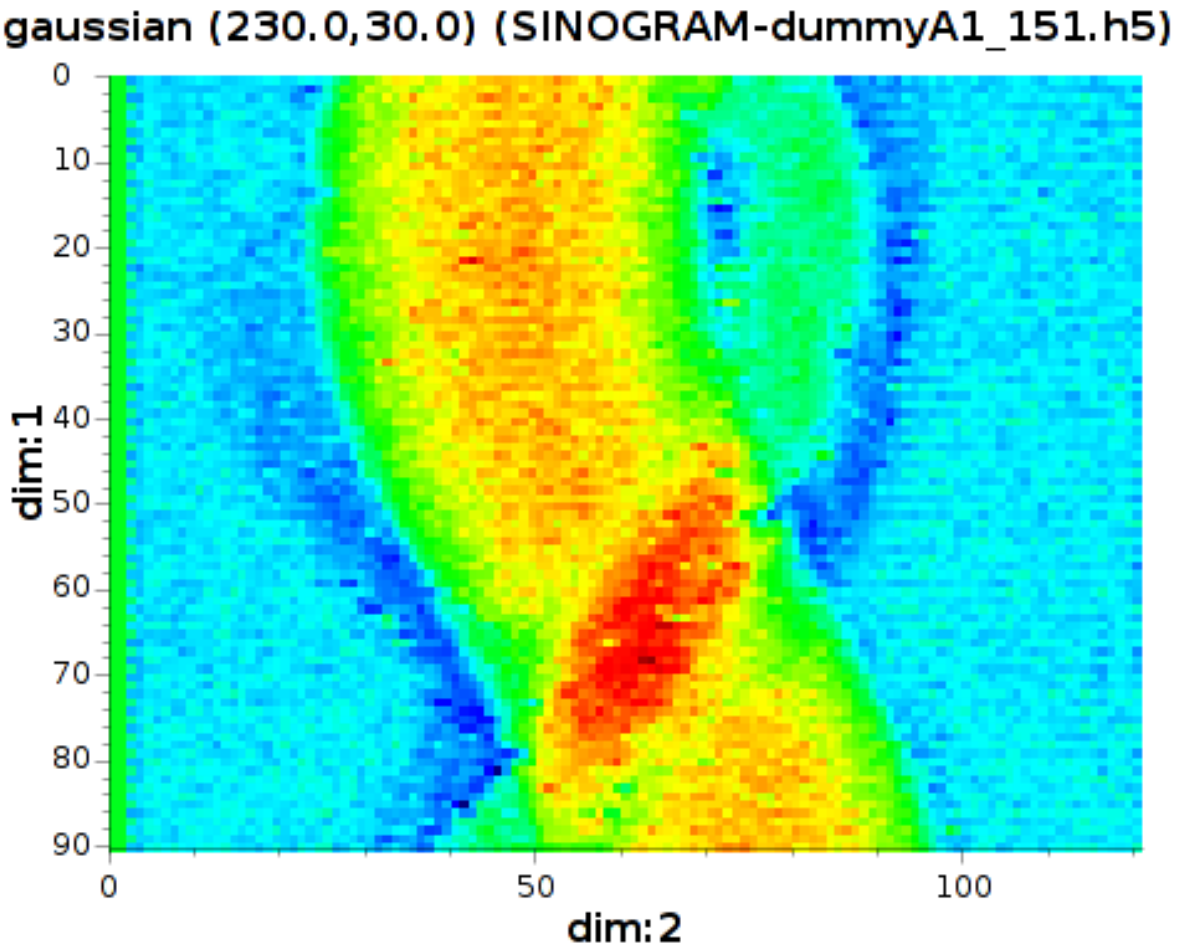
dim:2


gaussian (230.0,30.0) (SINOGRAM-dummyA1_151.h5)
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dim:1
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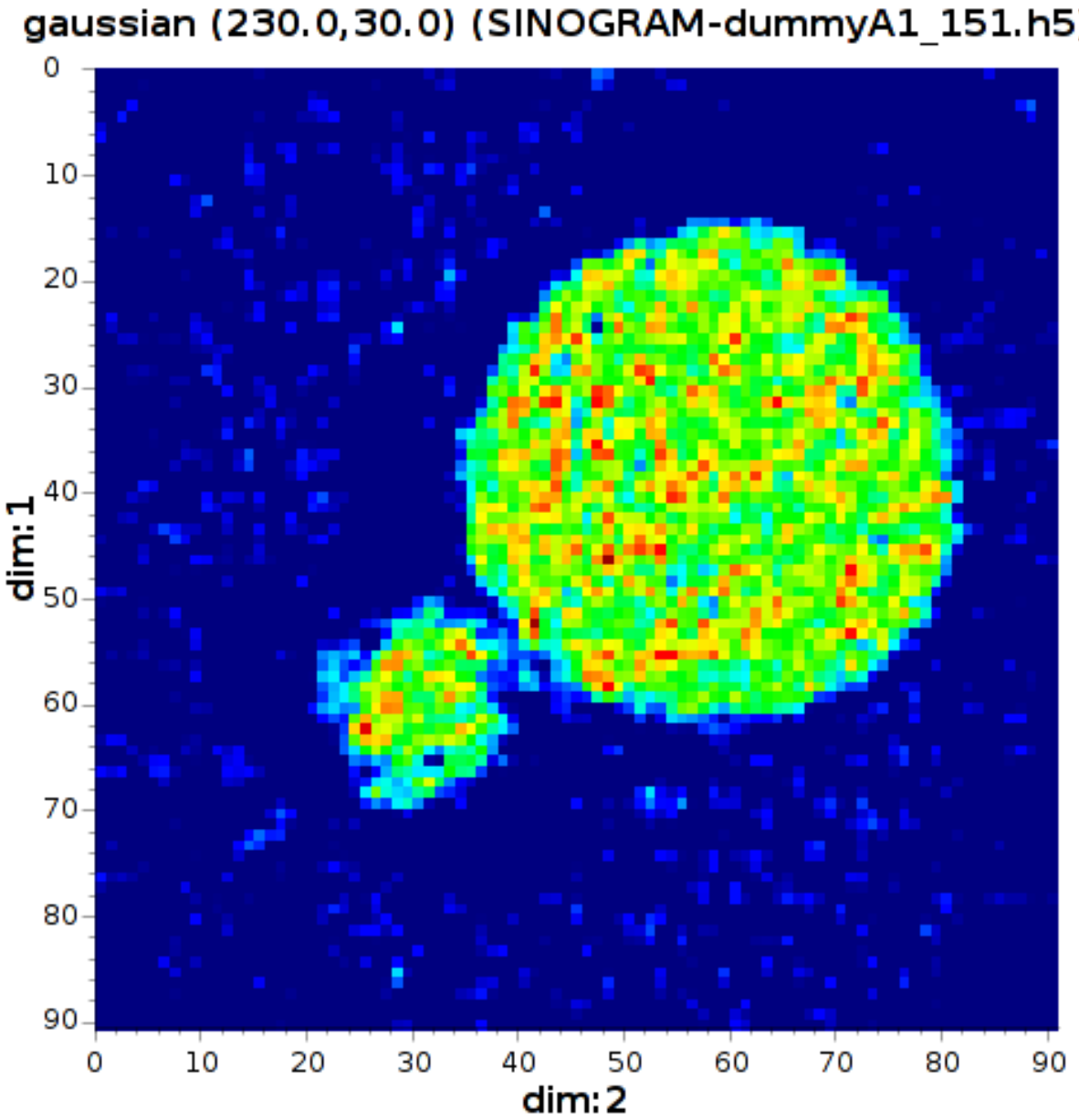
dim:2


gaussian (230.0,30.0) (SINOGRAM-dummyA1_151.h5)
dim:1
dim:2
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80
90

Issues / Further work

- Easy to use?
  - Not everyone comfortable working from the command line.
  - Keep the number of options down, or hidden for power-users
  - Investigate closer integration with DAWN.
  - Beamlines could provide presets for detector calibration and batch scripts.
- More applications. Use beyond basic data reduction and Diffraction Tomography.
- Extend test coverage beyond

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The biggest problem of them all!

We need to call the module something.
Xraylib is already taken.

Suggestions are welcome. . .

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Questions?

Live demonstration of results in DAWN.

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