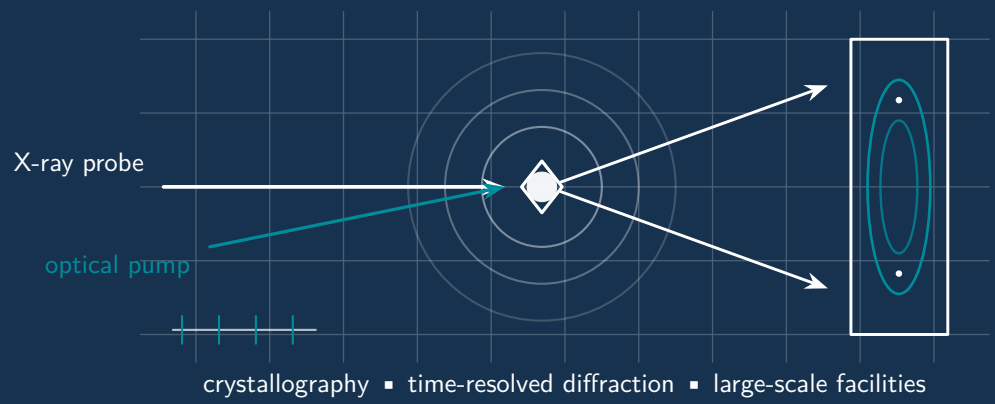
XRDpy

User Manual

Simulation and Analysis



Python toolkit for X-ray diffraction simulation and analysis

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About this edition

This manual documents the two major XRDpy branches in a single PDF: Simulation and Analysis. The branches share the same distribution and installation but remain computationally independent. Simulation output is not required as input to the Analysis workflows, and experimental Analysis workflows do not depend on running the Simulation branch first.

This edition documents the 5.1.0 source release. The project is named XRDpy on GitHub and Zenodo, distributed on PyPI as `trxrdpy`, and imported in Python as `trxrdpy`. The Simulation chapters cover orientation fitting from measured single-crystal Bragg pixels, independent 2D/3D detector scan sliders, optional intensity displays, and detector-limited powder patterns. The Analysis branch retains representative-image and resumable single-shot one-dimensional final-pattern routes for FemtoMAX and SACLA; both converge on standardized `xy_files` products.

Scientific conventions

Instrument-specific geometry, detector orientation, azimuthal convention, and reference choices should always be checked against the user's experiment. The examples in this manual show the package interface and the expected reproducibility record; they do not replace beamline- or sample-specific validation.

Project identifiers

Repository	https://github.com/julioguzmanb/XRDpy
Concept DOI	https://doi.org/10.5281/zenodo.18634909
PyPI distribution	`trxrdpy`
Python import	`import trxrdpy`
License	Creative Commons Attribution 4.0 International (CC BY 4.0)

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How to read this manual

Chapter 1 defines the package scope. Chapter 2 covers installation and a minimal verification. Part I is self-contained: it introduces the simulation model, explains its inputs and conventions, develops powder and single-crystal workflows, describes the GUI, and ends with reference and troubleshooting material.

Readers interested only in powder diffraction can proceed from Chapters 3–4 directly to Chapter 6. Readers interested in oriented crystals should also read Chapters 7 and 8. The API reference in Chapter 12 is selective: it documents the stable, user-facing surface rather than every internal helper.

Readers using the Analysis branch should begin with Chapters 14 and 15, then follow the facility-specific data-reduction chapter and complete calibration before choosing a final-pattern source in Chapter 18. The representative-image route is available to all supported facilities. FemtoMAX and SACLA additionally support progressive single-shot one-dimensional production and aggregation; ID09 remains image-based. The viewer, differential-analysis, and fitting chapters apply after either supported route has written the standard final patterns.

Manual organization

The manual is organized into three parts.

Front matter and general introduction

- Title, package version, author, repository, DOI, citation, and license
- Purpose, intended readership, scope, and limitations
- Installation from PyPI or source and first verification
- Package naming, imports, optional dependencies, and GUI launch commands
- Complete table of contents

Part I: Simulation

Simulation model and conventions
: Beam, lattice, reflections, detector, units, coordinate systems, rotations, transforms, and coordinate-system diagnostics.

Crystallographic input and lattice construction
: Explicit cell parameters, CIF parsing, reciprocal lattice, allowed reflections, Bragg-condition testing, and sample orientation.

Detector definition and calibration
: Manual detectors, binning, pyFAI registry detectors, PONI import/export, Fit2D conversion, orientation changes, laboratory grids, and validation checks.

Polycrystalline diffraction
: One-dimensional CIF-based patterns, two-dimensional detector rings, three-dimensional diffraction cones, PONI input, interpretation, and reproducible figure generation.

Diffractometers and motor-chain geometry
: Motors, local and laboratory frames, Euler and kappa geometries, custom instruments, serialization, and geometry inspection.

Single-crystal diffraction
: Legacy and geometry-aware 2D/3D simulation; explicit reflections; parameter and named-motor scans with optional mapping slices; detector scans; fixed-energy inverse targeting; reciprocal-space and Ewald views; result objects; and generated figures.

Plotting, GUI, and examples
: Plot families, saving outputs, Simulation GUI operation, screenshots, complete programmatic examples, and reproducibility records.

Reference and validation
: Public Simulation API, return-object behavior, validation hierarchy, troubleshooting, performance, and reproducibility.

Part II: Analysis

Analysis branch overview and data organization
Independent Analysis scope, supported facilities, shared and facility-specific layers, path conventions, standardized outputs, and overall data flow.

Facility-specific data reduction
ESRF ID09, Max IV FemtoMAX, and SPring-8 SACLA data structures; metadata selection; representative images; supported single-shot one-dimensional caches; ID09-specific processing; external software; legacy environments; and HPC submission.

Calibration, diagnostics, and azimuthal integration
Detector calibration, masks, polarization, detector/cake diagnostics, q-band azimuthal-distribution analysis, representative-image integration, supported single-shot aggregation, ID09 integration, and generation of standardized one-dimensional `xy` patterns.

Shared downstream analysis
Pattern visualization, differential analysis, peak fitting, absolute/normalized/relative evolution displays, per-experiment azimuthal selection, export, uncertainty and quality checks, and reproducibility.

Analysis GUI and reference
Session preparation, facility selection, Data Reduction, calibration, Azimuthal Integration, viewer, differential, fitting tabs, API reference, and troubleshooting.

Part III: Shared reference and appendices

- Project versioning, compatibility, contributions, issues, citation, license, and acknowledgments
- Glossary of diffraction and package terminology
- Simulation and Analysis package/module map
- Figure manifest and revision record

Contents

About this edition i

How to read this manual ii

Manual organization iii

1 Introduction 1

1.1 What XRDpy is . . . 1

1.2 Purpose of the Simulation branch . . . 1

1.3 Intended readership . . . 1

1.4 Scope and limitations . . . 2

2 Installation and first verification 3

2.1 Requirements . . . 3

2.2 Install from PyPI . . . 3

2.3 Verify the installation . . . 3

2.4 Launch the Simulation GUI . . . 4

2.5 Imports used in this manual . . . 4

I Simulation 5

3 Simulation model and conventions 6

3.1 Conceptual model . . . 6

3.2 Quantities and units . . . 6

3.3 Laboratory and detector axes . . . 7

3.4 Rotations and transforms . . . 7

4 Crystallographic input and lattice construction 8

4.1 Explicit lattice parameters . . . 8

4.2 CIF input . . . 8

4.3 Generating reflections . . . 9

4.4 Testing the Bragg condition . . . 9
4.5 Orienting the crystal . . . 9

5 Detector definition and calibration 11
5.1 Manual detector . . . 11
5.2 Binning . . . 12
5.3 pyFAI detector registry . . . 12
5.4 PONI calibration files . . . 12
5.5 Exporting PONI geometry and converting Fit2D values . . . 13
5.6 Changing orientation . . . 14
5.7 Detector validation checklist . . . 14

6 Polycrystalline diffraction 15
6.1 Available workflows . . . 15
6.2 One-dimensional pattern from CIF . . . 15
6.3 Detector-limited one-dimensional patterns . . . 17
6.4 Relative-intensity detector views . . . 18
6.5 Three-dimensional powder cones . . . 19
6.6 Two-dimensional detector projection . . . 20
6.7 Manual detector from experimental geometry . . . 21
6.8 Using a PONI detector . . . 23
6.9 Interpreting powder output . . . 23

7 Diffractometers and motor-chain geometry 24
7.1 Why use motor chains . . . 24
7.2 Lab-fixed and local axes . . . 24
7.3 Predefined Euler geometry . . . 24
7.4 Predefined kappa geometry . . . 25
7.5 Custom geometry . . . 25
7.6 Inspecting and serializing geometry . . . 26

8 Single-crystal diffraction 27
8.1 High-level simulation . . . 27
8.2 Detector-view scans and intensities . . . 28
8.3 Orientation matrices from measured Bragg pixels . . . 30
8.4 Geometry-aware simulation . . . 31
8.5 Explicit additional reflections . . . 32
8.6 Searching sample orientations . . . 32

8.6.1 Legacy two-angle convenience workflow . . . 33
8.6.2 Named-motor two-dimensional scan . . . 34
8.7 Scanning two parameters . . . 35
8.8 Mapping display, filtering, and extra slices . . . 36
8.9 Collecting Bragg reflections with detector rotations . . . 40
8.9.1 Legacy detector Euler scan . . . 40
8.9.2 Detector motor-chain and geometry scans . . . 40
8.10 Fixed-energy inverse targeting . . . 41
8.11 Reciprocal space and Ewald construction . . . 44

9 Plotting and result inspection 48
9.1 Plot families . . . 48
9.2 Separating calculation from presentation . . . 48
9.3 Plot interpretation . . . 48
9.4 Saving figures . . . 49

10 Simulation graphical interface 50
10.1 Purpose and architecture . . . 50
10.2 Launching the interface . . . 50
10.3 Polycrystalline tab . . . 50
10.4 Single-crystal tab . . . 53
10.4.1 Functions and scan controls . . . 54
10.5 Find Orientation Matrix . . . 55
10.6 Extra Functions . . . 57
10.6.1 Matrix Rotation . . . 57
10.6.2 Equivalent Reflections . . . 58
10.6.3 q / d / Angle Conversion . . . 59
10.6.4 pyFAI / Fit2D geometry . . . 60
10.6.5 Photon Attenuation Length . . . 61
10.7 Sessions and logs . . . 63
10.8 Background tasks and reusable simulation results . . . 63
10.9 GUI operating sequence . . . 64

11 Complete simulation examples 65
11.1 Example data files . . . 65
11.2 Example A: lattice and detector inspection . . . 65
11.3 Example B: powder detector prediction . . . 66

11.4 Example C: manual detector from calibration values 67
11.5 Example D: geometry-aware single crystal 69
11.6 Example E: reproducible parameter record 71

12 Simulation API reference **73**
12.1 High-level modules 73
12.2 Core classes 74
12.3 Geometry factories 74
12.4 Common utility functions 74
12.5 Return objects and cached state 75

13 Validation, reproducibility, and troubleshooting **76**
13.1 Validation hierarchy 76
13.2 Common problems 76
13.2.1 Import fails 76
13.2.2 CIF cannot be read 76
13.2.3 No reflections satisfy Bragg condition 76
13.2.4 No reflections appear on the detector 76
13.2.5 Powder rings are displaced or mirrored 77
13.2.6 Geometry scan is unexpectedly slow 77
13.2.7 Changing angles has no effect 77
13.2.8 Unexpected lattice state after repeated rotations 77
13.3 Reproducibility record 77
13.4 Known interface cautions 77

II Analysis **78**

14 Analysis branch overview **79**
14.1 Scope of the Analysis branch 79
14.2 Supported facilities 79
14.3 Analysis data flow 80
14.4 Programmatic and GUI routes 81

15 Data organization and file conventions **82**
15.1 Experiment root and analysis root 82
15.2 Scan specifications and tags 84
15.3 Standardized intermediate products 84
15.4 Reproducibility records 84

16 Facility-specific data reduction **86**
16.1 Max IV FemtoMAX . . . 86
16.1.1 Optional scan-delay assignments . . . 87
16.1.2 FemtoMAX delay-scan 2D image production . . . 88
16.2 ESRF ID09 . . . 93
16.2.1 ID09 2D image production example . . . 94
16.3 SPring-8 / SACLA . . . 95
16.3.1 SACLA 2D image production example . . . 95
16.4 Facility comparison . . . 96

17 Calibration, masks, and detector diagnostics **97**
17.1 Calibration inputs . . . 97
17.2 Detector and cake diagnostics . . . 97
17.3 Azimuthal windows . . . 99
17.4 Calibration peak fitting . . . 100
17.5 Cake azimuthal-distribution analysis . . . 101

18 Azimuthal integration and standardized 1D patterns **104**
18.1 Shared 2D integration workflow . . . 104
18.2 Single-shot 1D integration . . . 105
18.3 Delay-scan patterns . . . 110
18.4 Fluence-scan patterns . . . 111
18.5 Quality checks before fitting . . . 112

19 Differential analysis **113**
19.1 Peak and background specifications . . . 113
19.2 Delay differential traces . . . 113
19.3 Fluence differential traces . . . 116
19.4 Multi-experiment comparison . . . 117

20 Peak fitting **118**
20.1 Fitting philosophy . . . 118
20.2 Delay peak fitting . . . 118
20.3 Fluence peak fitting . . . 122
20.4 Fit outputs and diagnostics . . . 123
20.5 Displaying fitted-property changes . . . 123

21 Facility-specific worked analysis examples **125**

21.1 Max IV FemtoMAX . . . 125
21.1.1 FemtoMAX single-delay-scan example . . . 125
21.2 SPring-8 / SACLA . . . 131
21.2.1 SACLA delay-scan examples from cached one-dimensional data . . . 131
21.2.2 SACLA fluence-scan examples from cached one-dimensional data . . . 138

22 Analysis GUI workflows **146**
22.1 GUI workflow map . . . 146
22.2 Session and facility setup . . . 147
22.3 Data Reduction tab . . . 147
22.4 Calibration and Azimuthal Integration tabs . . . 150
22.5 Differential and fitting tabs . . . 153

23 Analysis API reference and troubleshooting **155**
23.1 User-facing API map . . . 155
23.2 Common analysis failures . . . 155
23.3 Publication checklist . . . 156

III Shared reference and appendices **157**

24 Project and contribution information **158**
24.1 Versioning and compatibility . . . 158
24.2 Reporting issues . . . 158
24.3 Citation, license, and acknowledgments . . . 158

Bibliography **159**

A Glossary **161**

B Package map **162**

C Citation and license **164**

Chapter 1

Introduction

1.1 What XRDpy is

XRDpy is a Python toolkit for X-ray diffraction (XRD) simulation and beamline-dependent analysis, with particular attention to time-resolved and pump–probe experiments. It combines two broad capabilities in one distribution:

- **Simulation**: crystal and detector geometry, powder rings and patterns, single-crystal reflections, orientation searches, diffractometer motor chains, and graphical workflows.
- **Analysis**: facility-specific data preparation, azimuthal integration, calibration, differential analysis, and fitting.

These branches share a project and installation but are computationally independent. A user may employ the Simulation branch without adopting the Analysis branch, or use the Analysis branch on experimental data without first running a simulation.

1.2 Purpose of the Simulation branch

The Simulation branch connects crystallographic descriptions, an incident X-ray beam, and detector geometry. Its main tasks are to:

- construct a lattice from explicit cell parameters or a CIF file;
- generate space-group-allowed reflections and reciprocal-space vectors;
- test reflections against a finite incident-energy bandwidth;
- represent manually specified, pyFAI-registered, or PONI-calibrated area detectors;
- visualize polycrystalline cones and detector rings;
- visualize single-crystal diffraction in three dimensions and on the detector plane;
- scan sample or detector rotations for Bragg conditions; and
- describe Euler, kappa, and custom motor-chain geometries.

The package offers both high-level functions for common tasks and lower-level objects for workflows that require explicit control.

1.3 Intended readership

This manual assumes familiarity with Python and the basic language of diffraction: Miller indices, reciprocal space, Bragg's law, detector distance, and beam center. It does not assume familiarity with the internal structure of XRDpy. The geometry chapters are also intended for beamline scientists or advanced users who need to encode real motor axes.

1.4 Scope and limitations

The Simulation branch is a geometrical and crystallographic toolkit. Results depend on the supplied lattice, detector calibration, coordinate conventions, energy, bandwidth, and orientation. A simulated detector hit is not by itself a prediction of experimentally observable intensity. Sample texture, absorption, extinction, instrument resolution, background, polarization, and other effects require explicit treatment where relevant.

The one-dimensional powder workflow can calculate crystallographic intensities from a CIF and supports selected corrections and peak convolution. The two- and three-dimensional powder workflows primarily position labeled reflections geometrically. Single-crystal routines identify reciprocal-lattice directions compatible with the specified beam and detector geometry.

Chapter 2

Installation and first verification

2.1 Requirements

XRDpy 5.1.0 requires Python 3.10 or newer. Its core dependencies include NumPy, SciPy, Matplotlib, pandas, h5py, lmfit [16], pyFAI [9, 10], fabio [11, 12], PyCifRW [13], and xrayutilities [14, 15]. The graphical interfaces additionally require PyQt5 and mplcursors.

2.2 Install from PyPI

Install the base distribution with:

```
python -m pip install trxrdpy
```

Install the GUI dependencies when graphical use is required:

```
python -m pip install "trxrdpy[gui]"
```

The optional `analysis` extra is not required for the Simulation branch. A complete development installation from a source checkout is:

```
git clone https://github.com/julioguzmanb/XRDpy.git
cd XRDpy
python -m pip install -e ".[analysis,gui]"
```

2.3 Verify the installation

Run a small import and unit-conversion check:

```
import trxrdpy
from trxrdpy.simulation import utils

energy_ev = 10000.0
wavelength_m = utils.energy_to_wavelength(energy_ev)

print(trxrdpy.__name__)
print(f"{wavelength_m * 1e10:.4f} angstrom")
```

A 10 keV photon has a wavelength of approximately 1.2398 Å. The exact printed value follows the physical constants used by the installed package.

2.4 Launch the Simulation GUI

The installed console entry point is:

```
trxrdpy-sim-gui
```

The equivalent module invocation is:

```
python -m trxrdpy.simulation.gui.main_window
```

On a remote system, a graphical display or an appropriate forwarding mechanism is required.

2.5 Imports used in this manual

```
from trxrdpy.simulation import (
    cif,
    detector,
    diffractometers,
    geometry,
    polycrystalline,
    sample,
    single_crystal,
    utils,
)
```

Importing individual modules makes examples explicit and avoids relying on internal names that are not part of the public interface.

Part I

Simulation

Chapter 3

Simulation model and conventions

3.1 Conceptual model

A simulation combines four descriptions:

1. a beam, defined by photon energy and a relative energy bandwidth;
2. a sample lattice, defined by cell parameters, symmetry, and orientation;
3. reciprocal-lattice reflections, derived from the lattice or provided explicitly; and
4. a detector plane, defined by pixel geometry, position, and orientation.

The high-level functions assemble these descriptions into an `Experiment`. Lower-level use constructs a `LatticeStructure` and `Detector` directly, then supplies them to `Experiment` or calls their methods.

3.2 Quantities and units

Quantity	Unit	Notes
Photon energy	eV	High-level defaults are typically `10e3`.
Wavelength	m	Utility and geometry functions use SI meters. Convert to Å for display if desired.
Cell lengths	Å	Values `a`, `b`, and `c`.
Reciprocal magnitude q	$Å^{-1}$	Reflection range and powder input.
d **spacing**	Å	Related by $q = 2\pi/d$.
Angles	degrees	Public rotation arguments and motor-angle maps use degrees.
PONI rotations	radians in file	Converted to degrees by the PONI reader when building a detector.
Detector distance	m	Sample-to-detector distance.
Pixel size	m	Unbinned size on construction; effective size is stored after binning.
PONI coordinates	m	Axis 1 is slow/vertical; axis 2 is fast/horizontal.
Energy bandwidth	percent	Full relative bandwidth $\Delta E/E$, not a fractional value.

For elastic scattering,

$$q = \frac{4\pi \sin\theta}{\lambda}, \qquad d = \frac{2\pi}{q}, \qquad 2\theta = 2\arcsin\left(\frac{q\lambda}{4\pi}\right). \tag{3.1}$$

The user-facing utilities `energy_to_wavelength` and `wavelength_to_energy` convert the beam quantity. The functions `q_to_two_theta` and `d_to_two_theta` convert diffraction coordinates.

3.3 Laboratory and detector axes

The unrotated detector plane is placed at positive laboratory x, with the incident beam directed along the detector-distance axis. Within the detector representation:

- PONI axis 1 is the slow image dimension and vertical direction;
- PONI axis 2 is the fast image dimension and horizontal direction;
- `pxsize_v` and `num_pixels_v` refer to axis 1;
- `pxsize_h` and `num_pixels_h` refer to axis 2; and
- binning is ordered `(horizontal, vertical)`.

In the detector grid, the horizontal coordinate includes a sign reversal relative to increasing axis-2 pixel index. This is a plotting and laboratory-frame convention, not a statement about every detector file format.

Coordinate-system check

Before comparing a simulated detector image with experimental data, confirm the beam direction, image origin, axis order, handedness, and any display flips. A correct PONI calibration cannot compensate for a mismatched image convention.

3.4 Rotations and transforms

Legacy interfaces describe sample and detector orientation with three Euler angles and a rotation-order string. The accepted order is a permutation of `xyz`; detector defaults commonly use `zyx`, while sample defaults commonly use `xyz`.

Modern interfaces also accept:

- a 3×3 rotation matrix;
- a 4×4 homogeneous transform;
- an `AxisRotation` or `RotationChain`;
- a named `MotorChain`; or
- a `DiffractometerGeometry` with independent sample and detector chains.

A custom detector transform takes precedence over legacy Euler values until `clear_transform()` is called. For a sample, `mode="absolute"` applies the requested orientation to the initial lattice, while `mode="relative"` starts from the current orientation.

Chapter 4

Crystallographic input and lattice construction

4.1 Explicit lattice parameters

`LatticeStructure` infers symmetry-constrained parameters from the International Tables space-group number. For example, a cubic cell needs only `a`; a hexagonal cell needs `a` and `c`; a triclinic cell needs all three lengths and all three angles.

```
from trxrdpy.simulation.sample import LatticeStructure

silicon = LatticeStructure(space_group=227, a=5.431)
print(silicon.phase)              # cubic
print(silicon.crystal_orientation)
```

The initial orientation matrix contains the direct-lattice vectors as rows. It is derived from the supplied cell unless `initial_crystal_orientation` is supplied explicitly as a 3×3 array.

4.2 CIF input

A CIF file can supply the unit cell, International Tables space-group number, and fractional atom positions:

```
from trxrdpy.simulation.cif import Cif
from trxrdpy.simulation.sample import LatticeStructure

cif_data = Cif("sample.cif")
print(cif_data.get_lattice_parameters())
print(cif_data.get_space_group())
print(cif_data.get_atom_positions())

lattice = LatticeStructure(cif_file_path="sample.cif")
```

The reader uses PyCifRW for CIF parsing [13] and selects the first CIF data block containing six present, non-zero cell parameters. Parenthesized uncertainty suffixes such as `5.431(2)` are removed during numeric parsing. Fractional coordinates must lie in the inclusive interval $[0, 1]$.

CIF requirements

The current reader expects `_space_group_IT_number` and the atom-site label and fractional-coordinate columns. A syntactically valid CIF that omits these fields may still be unsuitable for this workflow. Inspect imported values before simulation.

4.3 Generating reflections

Reflection generation is deliberately explicit in the lower-level API:

```
lattice = LatticeStructure(space_group=227, a=5.431)
lattice.calculate_reciprocal_lattice()
lattice.create_possible_reflections(qmax=6.0)
lattice.calculate_q_hkls()
lattice.calculate_d_hkls()

print(lattice.allowed_hkls[:5])
print(lattice.q_hkls[:5])
print(lattice.d_hkls[:5])
```

`create_possible_reflections(qmax)` uses the xrayutilities space-group lattice [14, 15] to retain allowed Miller indices up to a positive reciprocal-space limit in Å^{-1}. The derived arrays are cached on the object. Recalculate them after changing any lattice property outside the provided rotation methods.

4.4 Testing the Bragg condition

```
from trxrdpy.simulation.utils import energy_to_wavelength

wavelength = energy_to_wavelength(15000.0)
lattice.check_Bragg_condition(
    wavelength=wavelength,
    e_bandwidth=1.5,
)

print(lattice.hkls_in_Bragg_condition)
```

The bandwidth is the full relative energy spread in percent. A larger value broadens the accepted Ewald-shell region and can admit more reflections. It should represent the intended source or effective simulation tolerance rather than being increased merely to force a desired reflection.

4.5 Orienting the crystal

Legacy Euler orientation is concise:

```
lattice.apply_rotation(
    rotx=5.0,
    roty=-2.0,
    rotz=12.0,
    mode="absolute",
)
```

For a direct rotation matrix or homogeneous transform:

```
import numpy as np
from trxrdpy.simulation import utils

rotation = utils.axis_angle_to_matrix(
    axis=[0, 0, 1],
    angle=30.0,
```

```
)
lattice.apply_transform(rotation, mode="absolute")
```

The rotation helpers validate matrix shape and, where applicable, rotation-matrix properties. Prefer a named motor chain when angles correspond to real instrument motors; this preserves their meaning and application order.

Chapter 5

Detector definition and calibration

5.1 Manual detector

The manual route requires pixel sizes, pixel counts, distance, and PONI coordinates:

```
from trxrdpy.simulation.detector import Detector

det = Detector(
    detector_type="manual",
    pxsize_h=75e-6,
    pxsize_v=75e-6,
    num_pixels_h=1024,
    num_pixels_v=1024,
    dist=0.30,
    poni1=0.0384,
    poni2=0.0384,
    rotx=0.0,
    roty=0.0,
    rotz=0.0,
    rotation_order="zyx",
    binning=(1, 1),
)
det.calculate_lab_grid()
print(det.lab_grid.shape)
```

The grid shape is `(num_pixels_h, num_pixels_v, 3)`. Large detectors therefore allocate substantial memory; use realistic binning or smaller dimensions while developing a workflow.

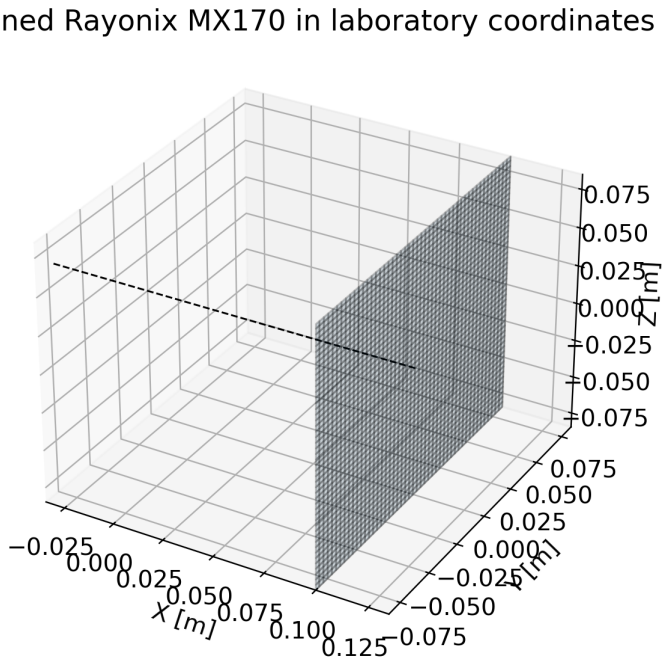

Figure 5.1: Three-dimensional laboratory-coordinate grid for a 16 × 16 binned Rayonix MX170 detector at 0.10 m sample distance.

5.2 Binning

Constructor pixel sizes are unbinned. With `binning=(H,V)`, stored horizontal and vertical pixel sizes are multiplied by their respective factors, while stored pixel counts are divided by them. The overall detector extent is preserved subject to integer truncation.

5.3 pyFAI detector registry

A detector name accepted by `pyFAI.detectors.detector_factory` can replace manual pixel geometry. XRDpy uses pyFAI for detector models, PONI geometry, masking, and azimuthal regrouping in the simulation and analysis workflows [9, 10]:

```
det = Detector(
    detector_type="rayonixmx170",
    dist=0.10,
    poni1=0.085,
    poni2=0.085,
    binning=(16, 16),
)
```

The registry supplies pixel sizes and maximum shape. Distance, PONI coordinates, rotations, and binning remain experiment-specific. The Rayonix MX170 example is binned for a fast diagnostic plot while preserving the physical detector size.

5.4 PONI calibration files

The PONI route loads detector geometry from a pyFAI calibration file:

```
det = Detector(
    detector_type="poni",
    poni_file="calibration.poni",
)
det.calculate_lab_grid()
```

The reader extracts distance, PONI coordinates, rotations, wavelength metadata, detector information, pixel sizes, and detector shape when available. Both JSON and Python-literal forms of `Detector_config` are accepted. Values supplied by the PONI file override explicit detector geometry arguments.

PONI axis mapping is:

PONI field	XRDpy name	Meaning
`PixelSize1` / `pixel1`	`pxsize_v`	slow, vertical
`PixelSize2` / `pixel2`	`pxsize_h`	fast, horizontal
shape index 0	`num_pixels_v`	vertical pixels
shape index 1	`num_pixels_h`	horizontal pixels
`Poni1`	`poni1`	vertical coordinate
`Poni2`	`poni2`	horizontal coordinate

5.5 Exporting PONI geometry and converting Fit2D values

Both simulation tabs have *Save PONI...* at the end of Common Detector Parameters. The export uses the current pixel counts, editable pixel sizes, binning, detector pose, and beam energy. Predefined detectors populate those visible dimensions; editing them creates an explicit flat-detector template for subsequent simulations. The export converts the actual detector transform, including motor-chain translations, into pyFAI coordinates. Existing files require overwrite confirmation. A flat PONI file cannot carry detector-specific distortion maps, masks, or the full instrument motor chain; retain those separately. Saved GUI states include the edited detector values, and older states recover their predefined detector sizes.

For a script, `poni.write_poni_file` writes PONI 2.1. Distances and pixel sizes are in metres, `max_shape` is `(vertical, horizontal)`, and `rot1/rot2/rot3` are pyFAI angles in radians. Supply exactly one of energy in eV or wavelength in metres:

```
from trxrdpy.simulation.poni import write_poni_file

write_poni_file(
    "detector.poni", dist=0.1, poni1=0.05, poni2=0.05,
    pixel1=75e-6, pixel2=75e-6, max_shape=(1024, 1024),
    rot1=0.0, rot2=0.0, rot3=0.0, energy_ev=15000,
)
```

The Extra Functions *pyFAI / Fit2D* window loads a PONI file or accepts either set of values and converts in both directions through pyFAI. Its fields show the units of each convention. The conversion leaves the active simulation detector unchanged. Fit2D cannot encode an independent pyFAI `rot3`; converting back yields the canonical pyFAI orientation. The complete utility workflow and screenshot are in Section 10.6. Check the resulting detector grid and beam position before using an exported calibration.

5.6 Changing orientation

Euler angles can be updated after construction:

```
det.set_rotation_angles(roty=3.0, rotation_order="zyx")
det.calculate_lab_grid()
```

A custom transform can instead be attached:

```
rotation = utils.axis_angle_to_matrix([0, 1, 0], 3.0)
det.set_transform(rotation)
det.calculate_lab_grid()

# Restore the legacy Euler path later.
det.clear_transform()
```

Changing an angle or transform does not automatically recalculate the detector grid. Call `calculate_lab_grid()` before plotting or using the updated geometry.

5.7 Detector validation checklist

Before interpreting simulated hits, verify:

- pixel sizes and counts correspond to the unbinned detector input;
- binning order is horizontal then vertical;
- distance and PONI values are in meters;
- PONI axes match the image storage order;
- rotations use the intended order and sign convention;
- the calibration belongs to the relevant detector configuration; and
- the resulting lab grid and beam-center position are physically plausible.

Chapter 6

Polycrystalline diffraction

6.1 Available workflows

The high-level powder interface exposes three complementary views:

`simulate_1d` Build a powder pattern from a CIF, calculate discrete peaks, and optionally convolve them into a continuous profile.

`simulate_2d` Draw continuous, detector-clipped powder rings at the cone intersections with an area detector.

`simulate_3d` Plot diffraction-cone surfaces and their detector-intersection curves in laboratory coordinates.

The 1D workflow derives reflections and intensities from a CIF. For 2D and 3D, the GUI defaults to generating reflection families from a CIF or entered lattice up to `qmax`; manual q or d positions with matching Miller-index labels remain available. The direct `simulate_2d` and `simulate_3d` functions take reflection positions explicitly, while `powder_preparation.run_powder` performs the same automatic preparation used by the GUI.

6.2 One-dimensional pattern from CIF

The distributable manual example uses the room-temperature corundum phase of V_2O_3 supplied in `cif_files/V2O3_R-3c_room_T.cif`. Keeping crystallographic inputs beside the manual makes examples executable and records the exact structure used to generate each result. For publication or redistribution, retain the CIF citation metadata and confirm that the source permits redistribution.

```
from trxrdpy.simulation import polycrystalline

result = polycrystalline.simulate_1d(
    cif_file_path="cif_files/V2O3_R-3c_room_T.cif",
    qmax=6.0,
    energy=15000.0,
    x_axis="q",
    include_lorentz_polarization=True,
    include_multiplicity=False,
    atom_positions=True,
    step=0.002,
    fwhm=0.04,
    convolve=True,
    normalize=True,
    plot_result=True,
)
```

```
q = result["x"]
intensity = result["I"]
peaks = result["peaks"]
```

Set `x_axis="two_theta"` for 2θ in degrees or `x_axis="d"` for spacing in Å. The GUI offers the same three choices alongside `q`. A positive `fwhm` applies Gaussian broadening in the selected axis units, and `step` sets its sampling interval. A zero or omitted FWHM in the GUI gives a stick pattern. The d plot runs from larger to smaller spacing left to right, matching the order of increasing q and 2θ. Returned `x` values remain sorted in ascending order. If `convolve=False`, consult the returned discrete peak table rather than assuming the continuous arrays are populated in the same way.

`atom_positions=True` requests construction of the structure-factor crystal from parsed atomic positions. This requires suitable CIF atom labels and coordinates. Always inspect several peak positions and relative intensities against a trusted reference before using the simulated profile quantitatively.

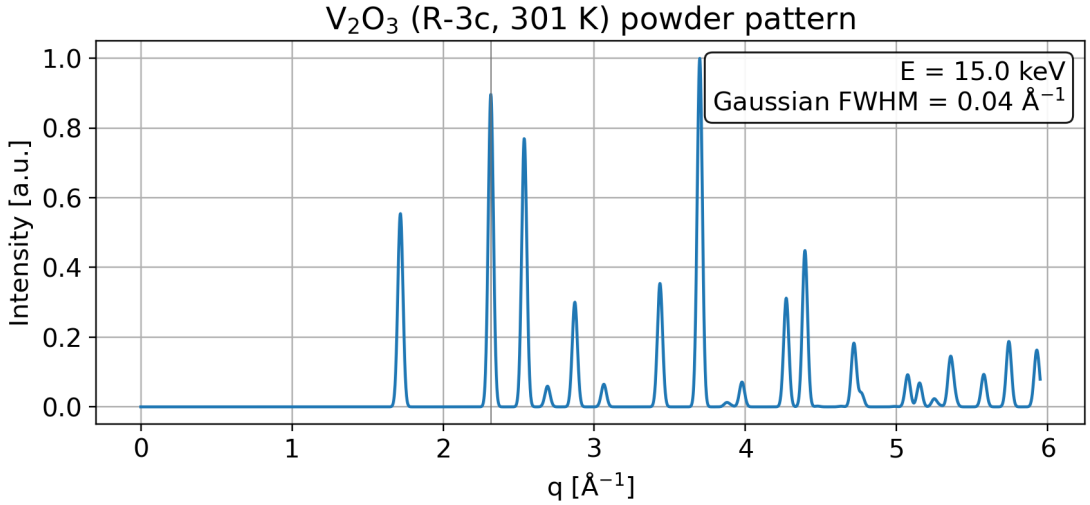

Figure 6.1: Simulated room-temperature R-3c V_2O_3 powder pattern at 15 keV, shown against q with Gaussian FWHM 0.04 $Å^{-1}$.

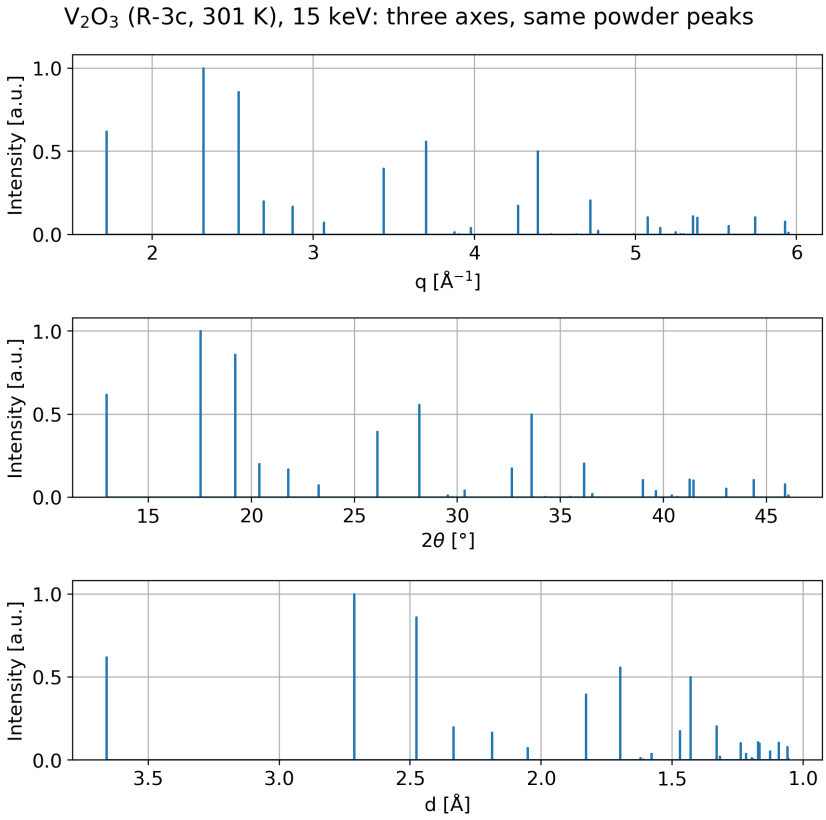

Figure 6.2: The same V_2O_3 powder reflections at 15 keV on q, 2θ, and d axes, plotted as zero-width sticks. The d axis decreases from left to right so corresponding peaks keep the same visual order.

6.3 Detector-limited one-dimensional patterns

Supplying a detector to `simulate_1d` replaces the manual `qmax` cutoff with the largest reachable scattering vector for that detector, beam energy, and selected azimuth. Peaks with no detector intersection are omitted. The returned `coverage_fraction` array corresponds to the retained peak table, while `detector_qmax` records the computed limit. Missing azimuths are absent observations: a partially visible ring is not artificially weakened by averaging over pixels the detector does not contain.

```
from trxrdpy.simulation.detector import Detector
from trxrdpy.simulation.polycrystalline import simulate_1d

detector = Detector(detector_type="rayonixmx170", binning=(4, 4),
                    dist=0.10, poni1=0.085, poni2=0.085)
pattern = simulate_1d(
    "cif_files/V2O3_R-3c_room_T.cif",
    energy=15000, x_axis="two_theta", detector=detector,
    azimuthal_range=(-15, 15), azimuth_offset_deg=0,
    fwhm=0, plot_result=True,
)
print(pattern["detector_qmax"], pattern["coverage_fraction"])
```

The azimuth convention is laboratory-fixed when looking along the beam toward the detector: 0° is up, −90° left, and +90° right. A blank GUI azimuth range or `None` in Python selects the full circle. An offset shifts this reference; it does not rotate with the detector. In the GUI, `(-15, 15)` and `-15,15` both specify a sector. Detector coverage uses the central beam energy and rectangular

detector bounds. It does not account for pixel masks, module gaps, or bandwidth. A sector requires a detector.

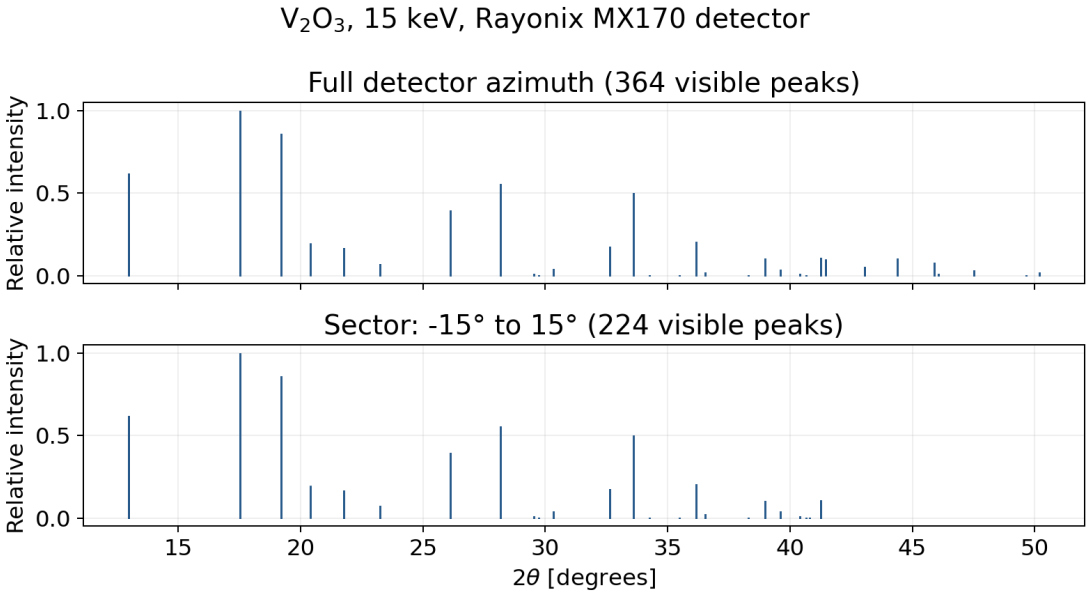

Figure 6.3: Detector-limited V_2O_3 stick patterns at 15 keV in 2θ: full coverage and a laboratory sector from $-15°$ to $15°$. Peaks outside the selected detector acceptance are absent.

6.4 Relative-intensity detector views

The 2D and 3D powder views can color continuous ring intersections by relative structure-factor intensity when *Consider intensities* is enabled and the CIF contains atom sites. Powder strengths include a one-dimensional Lorentz factor; the polarization correction varies with position around the ring. The default beam-polarization factor is $+1$ for horizontal linear polarization; -1 is vertical and 0 is unpolarized. An axis offset rotates the polarization reference. Colormap and color limits change the display, while optional Gaussian noise or Poisson background affects the detector image. Gaussian level is a standard deviation relative to the strongest reflection; Poisson level is a mean relative to it. The returned experiment contains `reflection_intensities` and `detector_intensity_image`. Zero-intensity pixels appear black, and random noise in 3D is confined to the detector face.

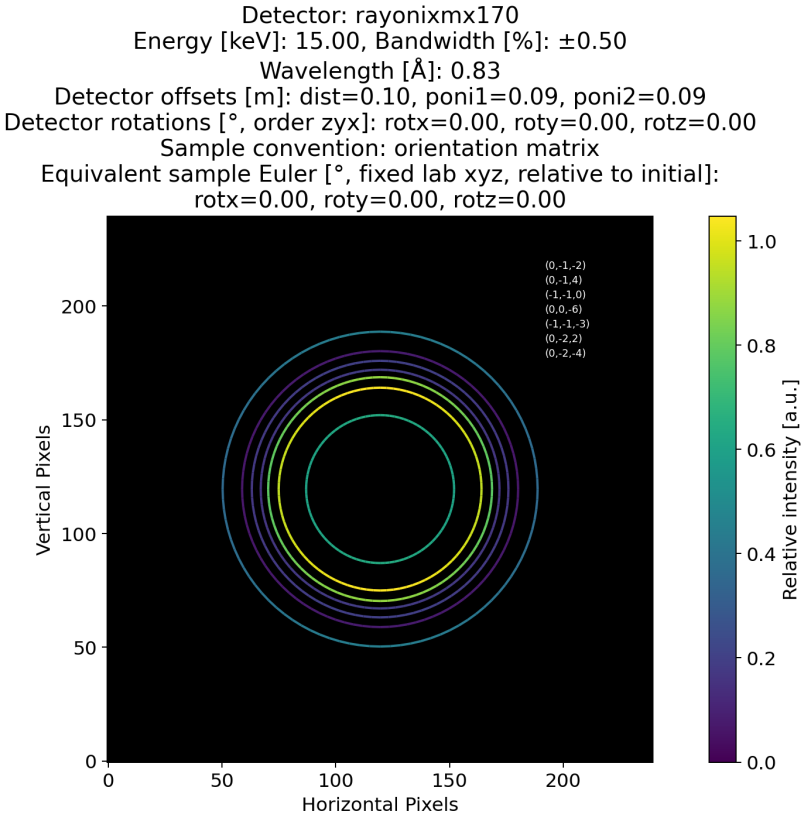

Figure 6.4: Continuous powder-ring intersections colored by relative intensity using the atom-site CIF and a horizontal polarization reference.

6.5 Three-dimensional powder cones

In the GUI, select `simulate_3d`, load the CIF, set `qmax=3.5`, and leave *Use reflections from* at *CIF / lattice (auto from qmax)*. The equivalent Python call uses the shared preparation helper. It generates allowed reflections, removes duplicate powder-family positions, limits them by `qmax` and the incident energy/bandwidth, and passes the resulting q values and representative Miller labels to the simulation.

```
from trxrdpy.simulation import polycrystalline
from trxrdpy.simulation.powder_preparation import run_powder

crystal = {"cif_file_path": "cif_files/V2O3_R-3c_room_T.cif"}
geometry = dict(
    det_type="rayonixmx170",
    det_binning=(4, 4),
    det_dist=0.10,
    det_poni1=0.085,
    det_poni2=0.085,
    energy=15000.0,
    e_bandwidth=1.0,
    qmax=3.5,
)
experiment = run_powder(polycrystalline.simulate_3d, crystal, **geometry)
```

The Rayonix MX170 geometry is supplied by the pyFAI detector registry; the example uses 4×4 binning to keep the calculation responsive while preserving the physical detector size. The PONI

values place the beam center near the detector center. At this cutoff, the CIF produces seven distinct powder-family positions between approximately $q = 1.72$ and 3.43 $Å^{-1}$. Their displayed Miller labels are representative members of symmetry-equivalent families; the choice of signs may differ from a conventional positive-index listing.

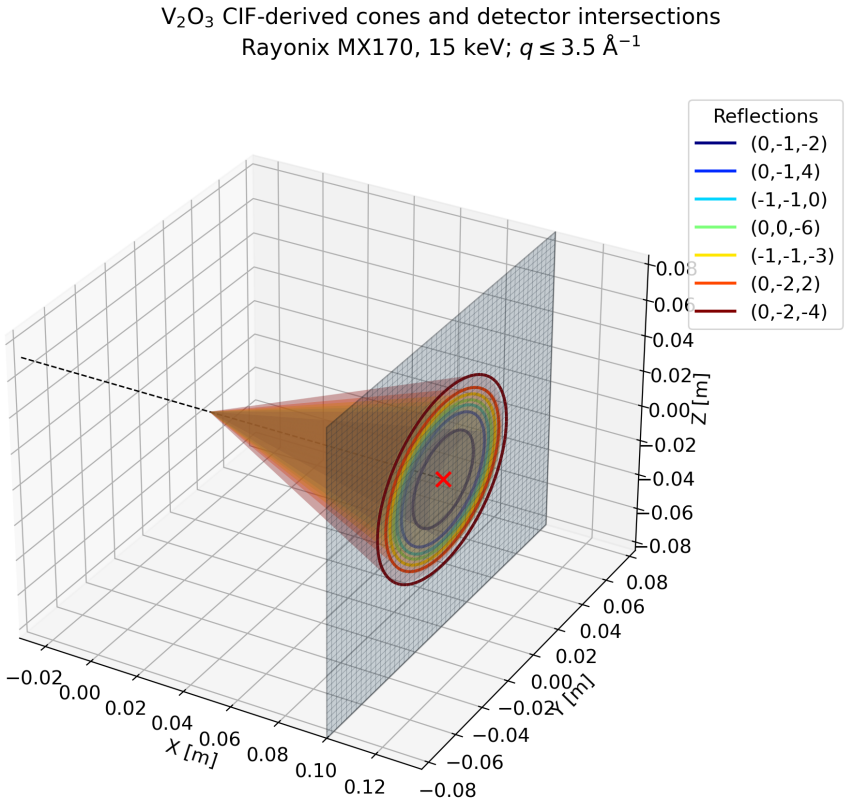

Figure 6.5: CIF-derived R-3c V_2O_3 cone surfaces ($q \leq 3.5$ $Å^{-1}$) and the continuous curves where they intersect the Rayonix MX170 detector plane at 15 keV. The red cross marks the direct beam.

6.6 Two-dimensional detector projection

After checking the cone geometry, switch the GUI function to `simulate_2d` without changing the CIF, cutoff, beam, or detector settings. The same configuration in Python is:

```
experiment = run_powder(polycrystalline.simulate_2d, crystal, **geometry)
```

The 2D routine traces each cone intersection as a continuous ring, clips it to the detector boundary, and samples its curvature adaptively at the detector-pixel scale. The 3D routine shows the same intersections on the detector face together with smooth cone surfaces, so a partial arc in 2D can be checked against its actual geometric intersection in 3D. There is no cone-point-count argument to tune. The returned `Experiment` retains the detector, calculated curves, and Miller labels for further inspection.

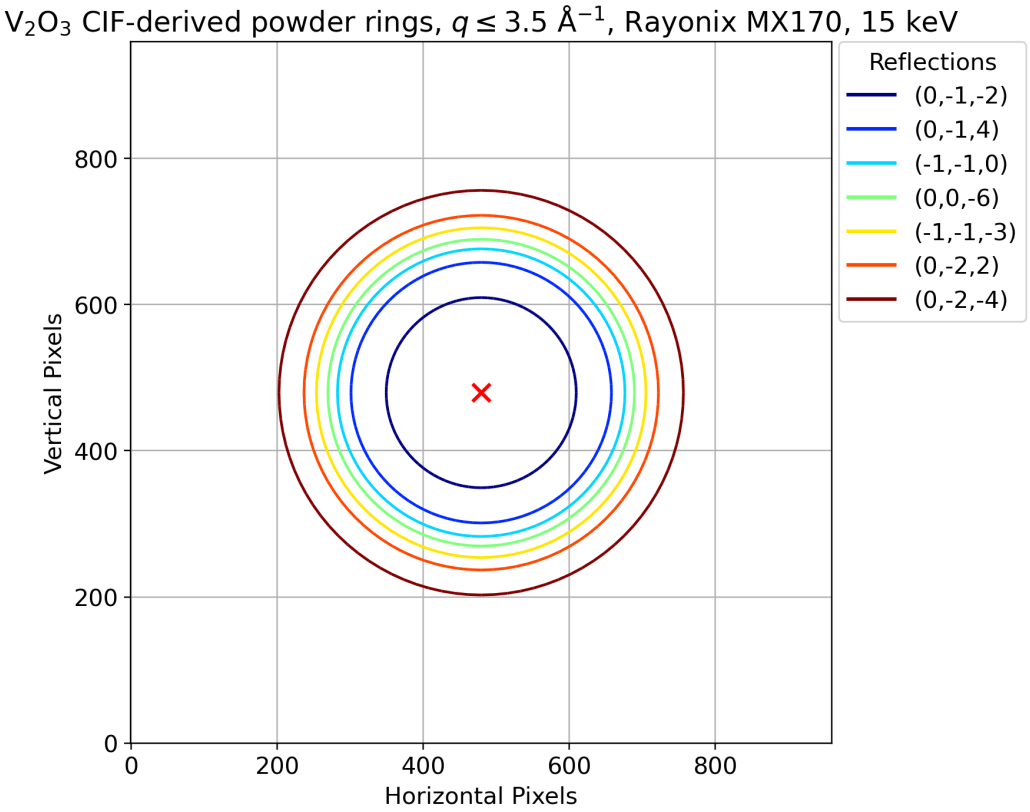

Figure 6.6: Continuous detector-clipped rings from seven CIF-derived R-3c V_2O_3 powder families ($q \leq 3.5$ Å^{-1}) on a 4×4 binned Rayonix MX170 detector at 15 keV and 0.10 m sample distance.

6.7 Manual detector from experimental geometry

For a calibrated experiment, manually supplied reflections can instead be projected onto a detector defined entirely by the experimental geometry. This also demonstrates the GUI's *Manual q/d + hkls_names* reflection source. In the following example, `max_shape=[831,1475]` maps to `num_pixels_v=831` and `num_pixels_h=1475`. The rotation values are written as PONI-style `Rot1`, `Rot2`, and `Rot3` values in radians, then converted to degrees because the XRDpy detector API uses degree-valued Euler angles.

```
import numpy as np

hkls = np.array([[0, 1, 2], [1, 0, 4], [1, 1, 0],
                 [1, 1, 6], [2, 1, 4], [3, 0, 0]])
q_values = np.array([1.7174, 2.3157, 2.5368,
                     3.6979, 4.2700, 4.3938])

wavelength_m = 1.3829804621662048e-10
energy_eV = 12398.419843320026 / (wavelength_m * 1e10)

manual_detector_kwargs = dict(
    det_type="manual",
    det_pxsize_h=0.000172,
    det_pxsize_v=0.000172,
    det_ntum_pixels_h=1475,
    det_num_pixels_v=831,
    det_dist=0.12,
```

```
    det_poni1=0.050,
    det_poni2=0.123,
    det_rotx=np.degrees(-0.023),
    det_roty=np.degrees(-0.5238161921742152),
    det_rotz=np.degrees(0.0),
    energy=energy_eV,
    e_bandwidth=1.0,
    q_hkls=q_values,
    hkls_names=hkls,
)

experiment_3d = polycrystalline.simulate_3d(
    **manual_detector_kwargs,
)

experiment_2d = polycrystalline.simulate_2d(
    **manual_detector_kwargs,
)
```

For direct calls, supply one position list, either `q_hkls` in Å^{-1} or `d_hkls` in Å, and one Miller triplet per position in `hkls_names`. If both position lists are supplied, the current implementation gives `d_hkls` precedence and converts it with $q = 2\pi/d$.

This wavelength corresponds to approximately 8.965 keV. The off-center PONI and nonzero detector rotations intentionally produce an asymmetric detector cut through the diffraction cones.

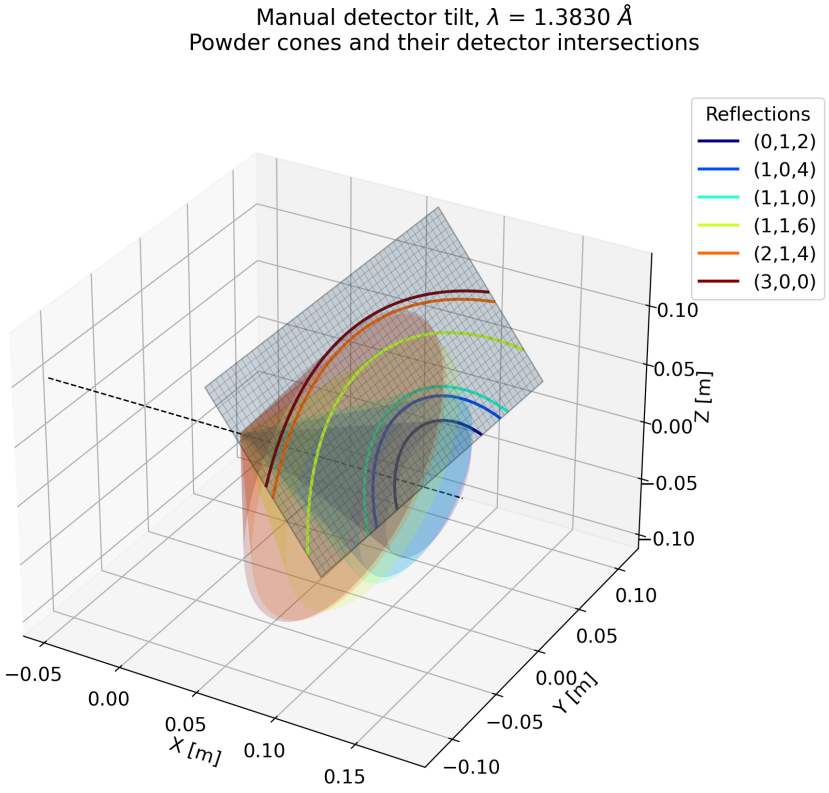

Figure 6.7: Three-dimensional view of the manually defined detector using Rot1 = −0.023, Rot2 = −0.5238161921742152, Rot3 = 0 radians. The curves on the tilted detector plane are the actual cone intersections.

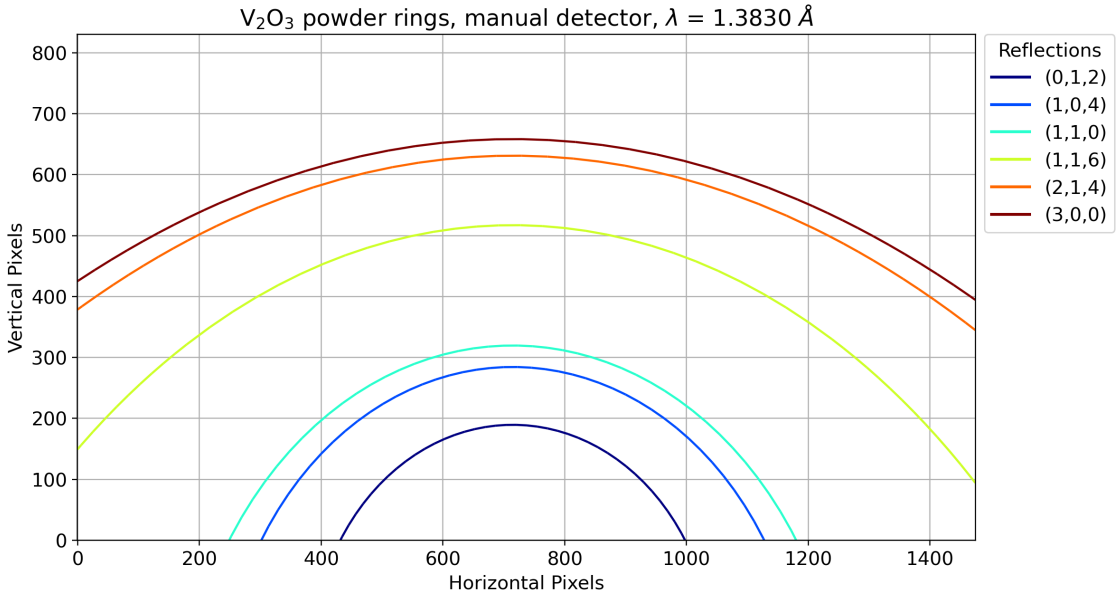

Figure 6.8: Continuous arcs from selected R-3c V_2O_3 powder reflections on the manually defined 831×1475 detector with 172 μm pixels, 0.12 m sample distance, off-center PONI, and wavelength 1.38298 Å.

6.8 Using a PONI detector

Replace the manual geometry arguments with:

```
experiment = polycrystalline.simulate_2d(
    det_type="poni",
    det_poni_file="calibration.poni",
    energy=15000.0,
    d_hkls=d_angstrom,
    hkls_names=hkls,
)
```

The incident energy remains an explicit simulation input. A wavelength stored in the PONI file is parsed as metadata but does not silently replace the high-level `energy` argument.

6.9 Interpreting powder output

A ring outside the detector is not an error: it may follow from energy, detector distance, beam-center position, or the selected q range. Partial rings arise naturally when the detector intercepts only part of a cone or when it is tilted. If all rings are unexpectedly absent, check units first, then detector orientation and reflection values.

The continuous curves show geometric cone–detector intersections; the 2D and 3D routines do not automatically model experimental backgrounds, detector response, texture, finite crystallite size, or all intensity corrections. Their primary purpose is to answer where reflections should intersect the specified detector.

Chapter 7

Diffractometers and motor-chain geometry

7.1 Why use motor chains

Three Euler angles are sufficient for a mathematical orientation but do not necessarily describe a physical instrument. A motor chain names each axis, fixes its origin and reference frame, defines its application order, and separates sample-stage motion from detector-arm motion.

The geometry model contains:

- `Motor`: a named axis, origin, frame, default angle, and metadata;
- `MotorChain`: an ordered list of motors; and
- `DiffractometerGeometry`: independent sample and detector chains.

7.2 Lab-fixed and local axes

A motor with `frame="lab"` keeps its axis fixed in laboratory coordinates. A motor with `frame="local"` inherits the transformations applied by earlier motors in the chain. This distinction is essential for nested cradles such as a kappa stage.

Motor order is list order. Reordering two non-commuting rotations generally changes the result.

7.3 Predefined Euler geometry

```
from trxrdpy.simulation.diffractometers import make_euler_geometry

euler = make_euler_geometry(
    sample_rotation_order="xyz",
    detector_rotation_order="zyx",
    sample_frame="lab",
    detector_frame="lab",
)

sample_angles = {
    "sam_rotx": 2.0,
    "sam_roty": 0.0,
    "sam_rotz": 15.0,
}
detector_angles = {
    "det_rotx": 0.0,
    "det_roty": 3.0,
    "det_rotz": 0.0,
```

```
}
```

With lab-fixed axes, this reproduces the package's Euler-style rotation approach while exposing explicit motor names.

7.4 Predefined kappa geometry

```
from trxrdpy.simulation.diffractometers import make_kappa_geometry

kappa = make_kappa_geometry(
    kappa_tilt_deg=50.0,
    omega_axis="z",
    phi_axis="z",
    two_theta_axis="y",
)

sample_angles = {"omega": 10.0, "kappa": 20.0, "phi": -5.0}
detector_angles = {"tth": 24.0}
```

The default sample chain is omega about a lab-fixed axis, followed by local kappa and phi axes. The detector chain contains one lab-fixed two-theta motor. This is a generic model, not a guarantee that the axes match a particular facility instrument.

7.5 Custom geometry

```
from trxrdpy.simulation.geometry import DiffractometerGeometry

custom = DiffractometerGeometry.from_dict({
    "name": "my_instrument",
    "sample": [
        {
            "name": "omega",
            "axis": "z",
            "origin": [0, 0, 0],
            "frame": "lab",
            "default_angle": 0,
        },
        {
            "name": "chi",
            "axis": [1, 0, 0],
            "origin": [0, 0, 0],
            "frame": "local",
            "default_angle": 0,
        },
    ],
    "detector": [
        {
            "name": "delta",
            "axis": "y",
            "origin": [0, 0, 0],
            "frame": "lab",
            "default_angle": 0,
        },
    ],
```

```
})
```

Axes may use `x`, `-x`, `y`, `-y`, `z`, `-z`, or an explicit three-vector. Origins are three-vectors in meters. Unknown motor names in an angle map raise `KeyError`, which helps catch typographical errors.

7.6 Inspecting and serializing geometry

```
from trxrdpy.simulation.diffractometers import (
    available_diffractometers,
    diffractometer_to_dict,
)

print(available_diffractometers())
print(custom.sample.motor_names)
print(custom.sample.resolved_motors({"omega": 5, "chi": 10}))

geometry_dict = diffractometer_to_dict(custom)
```

The serializer returns JSON-compatible dictionaries. Persist the resulting dictionary with the application's preferred JSON or configuration mechanism. When debugging geometry, `resolved_motors()` exposes each active axis and origin in laboratory coordinates.

Chapter 8

Single-crystal diffraction

8.1 High-level simulation

The main single-crystal entry points create a lattice, generate reflections to `qmax`, apply an orientation, test the Bragg condition, construct the detector, and plot the result. Both 2D and 3D forms are available.

```
from trxrdpy.simulation import single_crystal

simulation_kwargs = dict(
    det_type="manual",
    det_pxsize_h=75e-6,
    det_pxsize_v=75e-6,
    det_ntum_pixels_h=1024,
    det_num_pixels_v=1024,
    det_dist=0.08,  # compact geometry keeps the hit on detector
    det_poni1=0.0384,
    det_poni2=0.0384,
    energy=15000.0,
    e_bandwidth=1.0,
    sam_space_group=227,
    sam_a=5.431,
    sam_rotx=-30.0,
    sam_roty=-20.0,
    sam_rotz=20.0,
    sam_rotation_order="xyz",
    qmax=6.0,
)

experiment_3d = single_crystal.simulate_3d(**simulation_kwargs)
experiment_2d = single_crystal.simulate_2d(**simulation_kwargs)
```

As in the powder interface, the horizontal pixel-count keyword retains the historical spelling `det_ntum_pixels_h`. The sample arguments begin with `sam_`; detector arguments begin with `det_`.

The 3D call visualizes the experiment in laboratory coordinates before the detector projection is inspected. Three-dimensional views are useful for diagnosing orientation and sign conventions before concentrating on detector pixels.

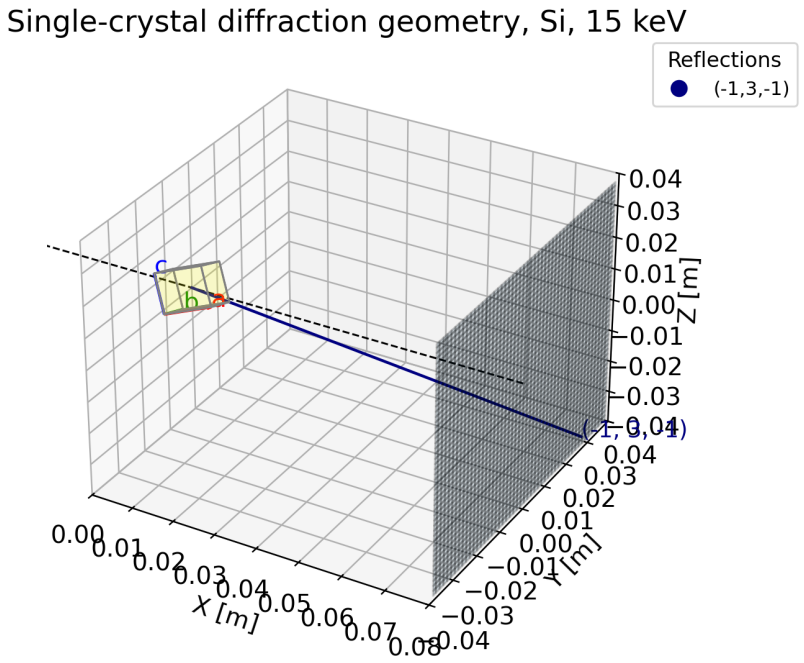

Figure 8.1: Three-dimensional single-crystal silicon experiment showing the incident beam, oriented reciprocal-lattice solution, diffracted ray, and detector plane at 15 keV.

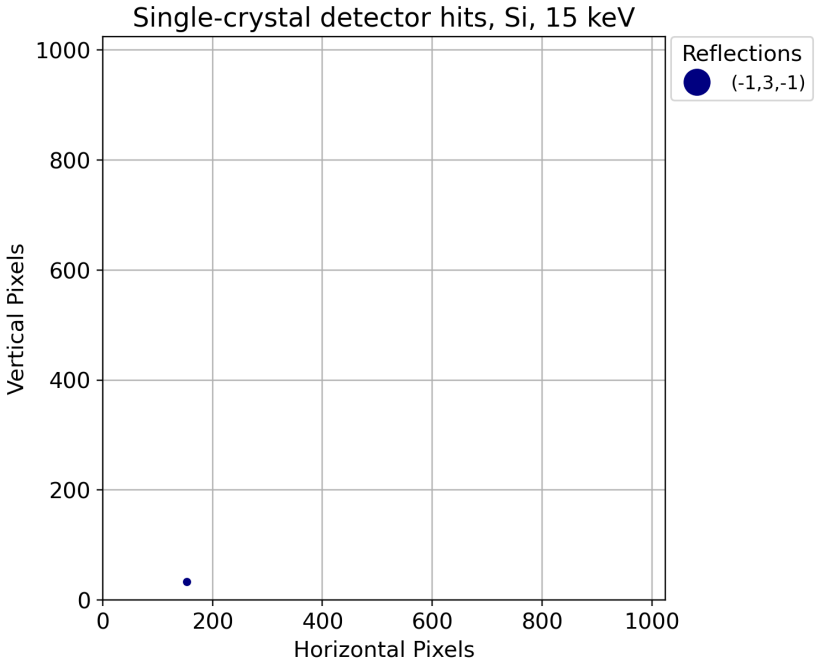

Figure 8.2: Single-crystal silicon reflection projected onto the manual area detector at 15 keV, using the high-level 2D workflow.

8.2 Detector-view scans and intensities

`simulate_2d` and `simulate_3d`, including their geometry-aware variants, accept optional `scan_ranges`. Each dictionary entry maps a parameter to `(start, stop, step magnitude)`. Legacy controls offer beam energy, full relative bandwidth, and sample or detector Euler rotations;

a motor-chain geometry offers the active named motors instead of Euler rotations. The two detector views retain separate GUI scan configurations. Every slider position recomputes the Bragg rays and detector image for that state. Previous and next buttons follow sampled positions, including descending ranges, and stop at the endpoints. A typed value snaps to the nearest sampled position.

```
from trxrdpy.simulation import single_crystal

view = single_crystal.simulate_2d(
    sam_space_group=227, sam_a=5.431, qmax=6.0,
    energy=15000, det_type="manual",
    det_pxsize_h=75e-6, det_pxsize_v=75e-6,
    det_ntum_pixels_h=1024, det_num_pixels_v=1024,
    det_dist=0.08, det_poni1=0.0384, det_poni2=0.0384,
    scan_ranges={"sam_roty": (-5, -25, 5), "energy": (14000, 16000, 500)},
)
```

The *Rotation order* beside the sample Euler fields sets the order for legacy 2D, 3D, reciprocal, and mapping simulations; existing sessions default to `xyz`. Named motor chains use their declared order. Plot titles distinguish entered Euler angles and their order from equivalent fixed-laboratory-axis `xyz` angles inferred for a geometry. Hovering over a detector spot reports HKL, Q components, $|Q|$, laboratory azimuth, and elevation. Reciprocal-space and additional mapping sliders have previous/next buttons as well as numeric boxes; mapping sliders select previously computed slices, while detector-view and compact reciprocal sliders evaluate selected states as needed.

For single-crystal 2D/3D displays, *Consider intensities* requires a CIF with atom sites. Spot colors use relative $|F(hkl)|^2$ with the theoretical allowed-reflection maximum as reference, including allowed reflections outside the current detector view. The same polarization, colormap, limits, and detector noise controls described for powder are available. The 3D legend lists HKLs with relative intensities and can be clicked. The returned experiment exposes `reflection_intensities` and `detector_intensity_image`; the default geometric display remains available when intensity mode is off.

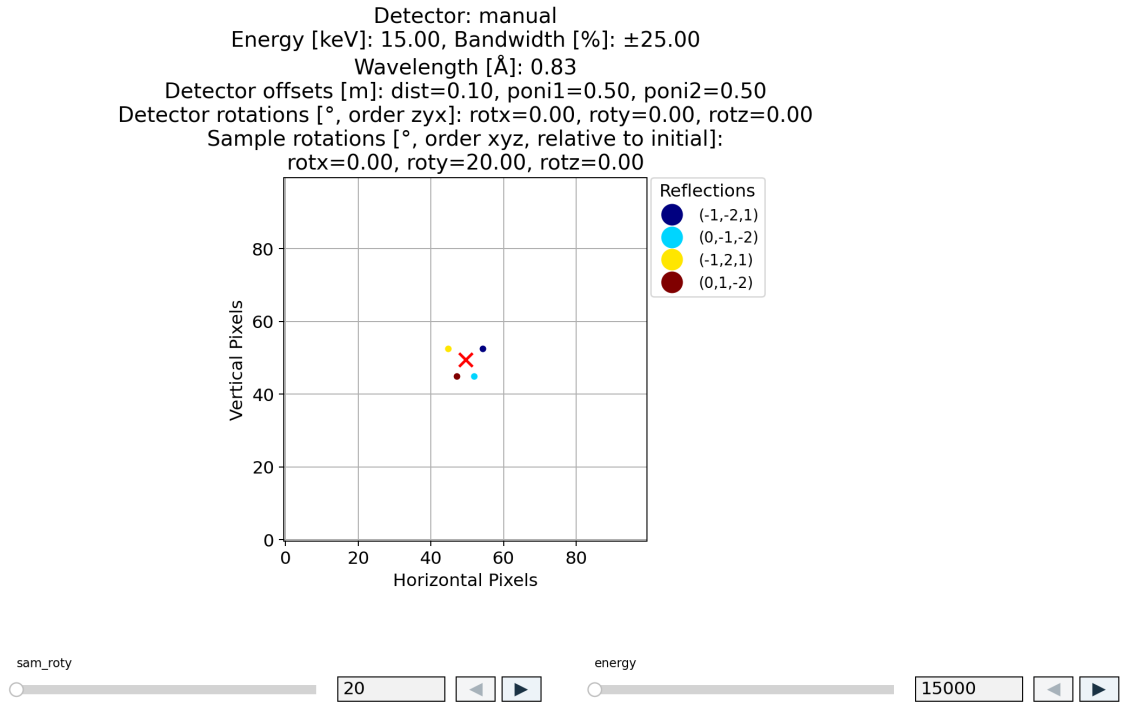

Figure 8.3: Single-crystal 2D detector view with sample-angle and energy scan controls. Previous/next buttons and numeric fields navigate the sampled states.

8.3 Orientation matrices from measured Bragg pixels

Find Orientation Matrix estimates the crystal orientation from measured detector pixels. A project records a lattice, sample goniometer, reusable detector calibrations, beam energy, linked experimental poses, and individual Bragg observations. The GUI procedure is in Section 10.5.

The displayed 3×3 direct-lattice matrix has the real-space basis vectors $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ as its rows, in Å and laboratory axes. The fit also estimates a proper rotation R of the canonical cell basis. At the reference pose, the direct-lattice matrix is $A_{\mathrm{ref}} = A_{\mathrm{cell}} R^{\mathsf{T}}$. At any recorded pose it is $A_{\mathrm{pose}} = A_{\mathrm{ref}} R_{\mathrm{rel}}^{\mathsf{T}}$, where R_{rel} is the sample-motor rotation relative to the reference pose. The mounting matrix at zero sample-motor angles is obtained by undoing the reference pose's motor rotation. The displayed direct-lattice matrices are not reciprocal-lattice UB matrices or pure rotations; identify which form an external program expects before exporting one.

A pose may inherit the energy, detector setup, and motor readings of an earlier parent pose. Sample motor values are either absolute readings or changes from that parent. Every observed peak is associated with one pose and one measured horizontal/vertical pixel. Its index can be fixed, selected from a symmetry family, or inferred from the measured scattering magnitude. Family and unknown assignments can produce several candidate orientations; supplying known indices where possible reduces ambiguity.

Set default horizontal and vertical peak-location uncertainties in pixels; *Apply to all peaks* copies them to existing rows, and a row may then be edited individually. Separate energy (eV), motor (degrees), relative lattice (percent), and shared detector-calibration (pixels) uncertainties contribute to the reciprocal-vector weights. Disabled peak rows remain in the project but do not contribute to the fit.

Fit crystal orientation searches assignments, robustly refines candidate rotations, and ranks solutions by weighted residual. The candidate browser reports RMS pixel error, rotation rank,

approximate local angular uncertainty when estimable, assignment, and per-peak measured-versus-predicted pixels. A rank below three means a rotation remains undetermined; add independent reflections or poses before treating the matrix as unique. Compare symmetry-related candidates and residuals with the diffraction pattern, detector calibration, and expected crystal setting. The reported zero-motor matrix and the direct-lattice matrix at each pose have lattice vectors as rows; they are not themselves pure rotation matrices.

Choose a candidate and the pose to reproduce, then press *Update crystal orientation at selected pose*. The Single Crystal controls receive the fitted orientation and that pose's conditions; run *Detector 2D Simulation* or *Laboratory 3D Simulation* to check the prediction. Save/load the editable project and fitted result as separate JSON files.

For scripts, the orientation fitter is available without Qt. The setup constructors and persistence helpers live in `trxrdpy.simulation.orientation_fit.setup` and `trxrdpy.simulation.orientation_fit.persistence`; the principal fitting call is:

```
from trxrdpy.simulation.orientation_fit import fit_orientation
from trxrdpy.simulation.orientation_fit.persistence import load_experiment

project = load_experiment("orientation_project.json")
result = fit_orientation(project, max_candidates=12)
best = result.candidates[0]
print(best.rank, best.rms_pixel, best.reference_matrix)
for pose_id, matrix in best.pose_matrices.items():
    print(pose_id, matrix)
```

8.4 Geometry-aware simulation

```
from trxrdpy.simulation.diffractometers import make_kappa_geometry

instrument = make_kappa_geometry(kappa_tilt_deg=50.0)

experiment = single_crystal.simulate_2d_with_geometry(
    det_type="manual",
    det_pxsize_h=75e-6,
    det_pxsize_v=75e-6,
    det_ntum_pixels_h=1024,
    det_num_pixels_v=1024,
    det_dist=0.08,
    det_poni1=0.0384,
    det_poni2=0.0384,
    energy=15000.0,
    e_bandwidth=1.0,
    sam_space_group=227,
    sam_a=5.431,
    qmax=6.0,
    geometry=instrument,
    sample_angles={"omega": -30.0, "kappa": 40.0, "phi": 30.0},
    detector_angles={"tth": 0.0},
)
```

Passing `geometry` supplies it to both sample and detector unless `sample_geometry` or `detector_geometry` is set separately. More advanced calls can pass independent motor chains or direct transforms. Avoid combining several geometry routes in one call; the high-level builder applies a defined precedence, but a single explicit route is easier to audit.

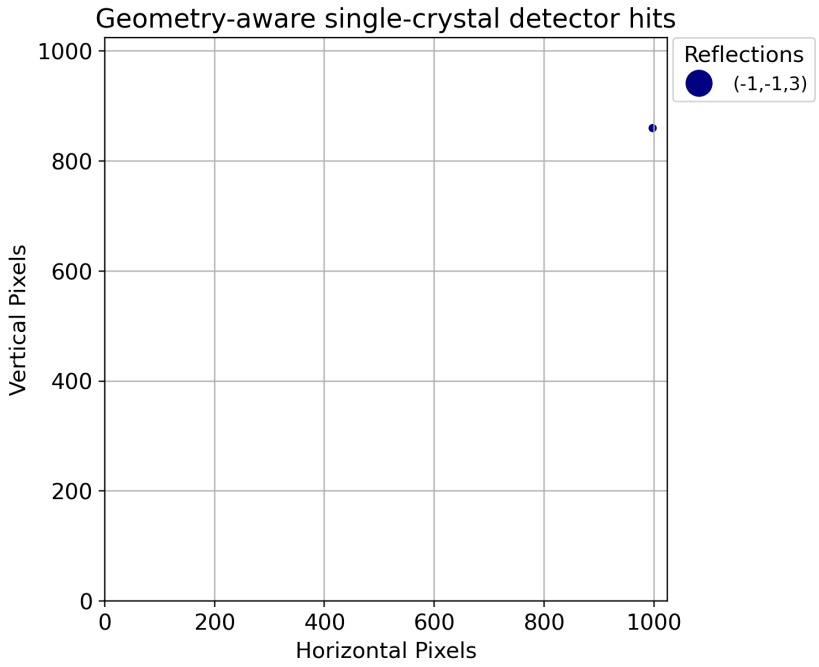

Figure 8.4: Geometry-aware single-crystal detector simulation using named sample and detector motors.

8.5 Explicit additional reflections

The `extra_hkls` argument adds requested Miller indices to the space-group-generated list while preserving first occurrence and removing exact duplicates:

```
experiment = single_crystal.simulate_3d(
    sam_space_group=227,
    sam_a=5.431,
    qmax=6.0,
    energy=15000.0,
    e_bandwidth=1.0,
    sam_rotx=-30.0,
    sam_roty=-20.0,
    sam_rotz=20.0,
    extra_hkls=[[4, 0, 0], [5, 1, 1]],
)
```

Adding an index does not guarantee that it satisfies symmetry, energy, or detector-intersection requirements. Treat this option as an explicit request for evaluation, not as proof of physical observability.

8.6 Searching sample orientations

There are three related routes for sample-orientation searches. The lattice method stores results on an existing object; `sample_rotations_for_Bragg_condition` is a complete legacy convenience workflow; and `scan_two_motors_for_Bragg_condition` scans named motors from a physical chain.

The tracking examples below use the same room-temperature R-3c V_2O_3 reflection set used in the powder chapter:

```
import numpy as np

v2o3_sample = {
    "sam_space_group": 167,
    "sam_a": 4.9537,
    "sam_c": 14.0111,
}

tracked_hkls = np.array([
    [0, 1, 2],  # (012)
    [1, 0, 4],  # (104)
    [1, 1, 0],  # (110)
    [1, 1, 6],  # (116)
    [2, 1, 4],  # (214)
    [3, 0, 0],  # (300)
])
```

8.6.1 Legacy two-angle convenience workflow

The legacy high-level function scans sample `roty` and `rotz` over the same inclusive range, opens a rotation map, and returns a `LatticeStructure` whose `rotations_for_Bragg_condition` attribute contains the accepted orientations:

```
legacy_scan = single_crystal.sample_rotations_for_Bragg_condition(
    **v2o3_sample,
    sam_rotx=-30.0,
    angle_range=(-180, 180, 0.5),
    energy=15000.0,
    e_bandwidth=2.0,
    hkls_names=tracked_hkls,
)
accepted = legacy_scan.rotations_for_Bragg_condition
```

At lattice level, the equivalent operation is `lattice.find_Bragg_orientations(...)`. That method updates the lattice in place rather than returning the accepted mapping directly.

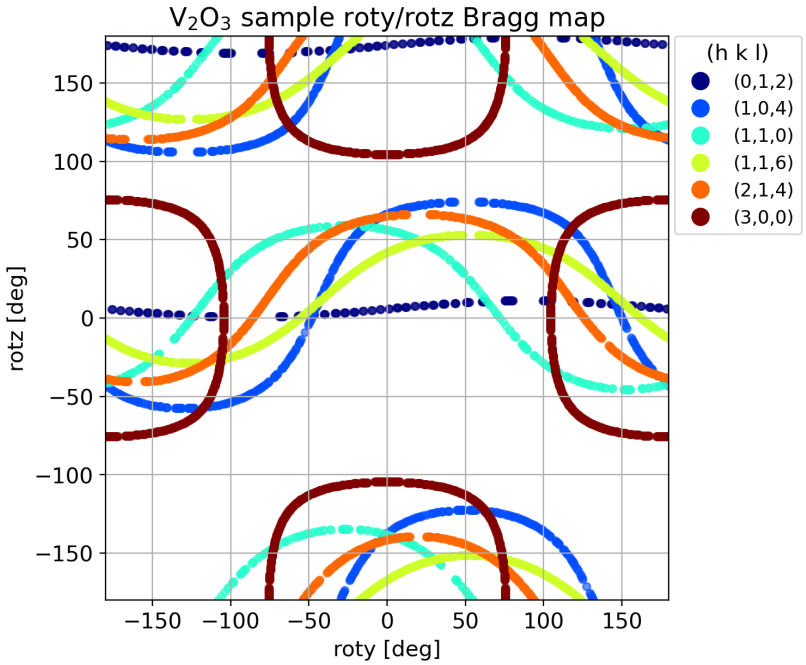

Figure 8.5: Legacy sample `roty`/`rotz` combinations satisfying the Bragg condition for the requested V_2O_3 reflections.

8.6.2 Named-motor two-dimensional scan

Use `scan_two_motors_for_Bragg_condition` when the two variables are real sample motors. The function accepts either a `MotorChain` or a `DiffractometerGeometry`; a supplied geometry takes precedence and its sample chain is scanned.

```
from trxrdpy.simulation.single_crystal import (
    scan_two_motors_for_Bragg_condition,
)

motor_scan = scan_two_motors_for_Bragg_condition(
    motor1_name="omega",
    motor2_name="phi",
    motor1_range=(-180, 180, 0.5),
    motor2_range=(-180, 180, 0.5),
    **v2o3_sample,
    energy=15000.0,
    e_bandwidth=2.0,
    hkls_names=tracked_hkls,
    hkl_equivalent=False,
    geometry=instrument,
    fixed_angles={"kappa": 40.0},
)
```

The returned dictionary maps a stringified Miller index to accepted `(motor1, motor2)` pairs. Set `hkl_equivalent=True` to expand every requested reflection through lattice symmetry before scanning. Search cost grows as the product of both grid sizes, reflection count, and any equivalence expansion.

```
from trxrdpy.simulation.plot import plot_parameter_mapping

plot_parameter_mapping(motor_scan, "omega", "phi")
```

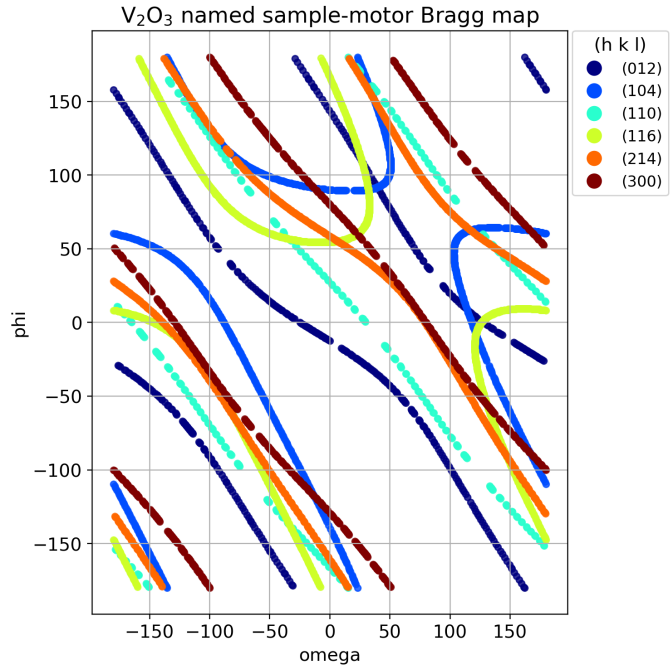

Figure 8.6: Named sample-motor combinations satisfying the Bragg condition for the selected V_2O_3 reflections.

8.7 Scanning two parameters

`scan_two_parameters_for_Bragg_condition` scans any two distinct choices from `rotx`, `roty`, `rotz`, and `energy`. It is therefore useful for both angle–angle maps and energy–angle maps. The sample rotations supplied through `sam_rotx`, `sam_roty`, and `sam_rotz` form the baseline; scanned rotations are added to it.

```
energy_angle_scan = (
    single_crystal.scan_two_parameters_for_Bragg_condition(
        param1_name="roty",
        param2_name="energy",
        param1_range=(-180, 180, 0.5),    # degree increment
        param2_range=(13000, 17000, 100),  # eV
        **v2o3_sample,
        sam_rotx=-30.0,
        sam_roty=-20.0,
        sam_rotz=20.0,
        e_bandwidth=2.0,
        hkls_names=tracked_hkls,
        hkl_equivalent=False,
    )
)

plot_parameter_mapping(energy_angle_scan, "roty", "energy")
```

The output has the same general mapping form as the named-motor scan. Rotation ranges are in degrees; an energy range is in eV. Use physically meaningful bounds and an initial coarse grid, then refine locally.

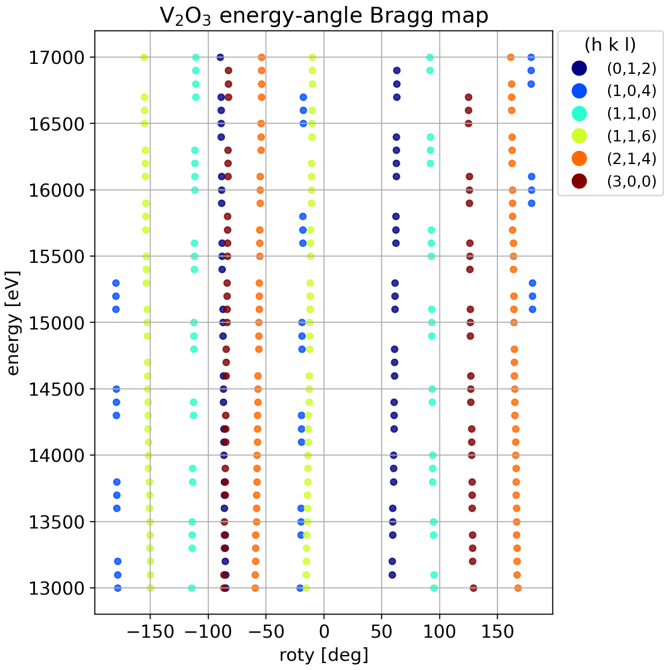

Figure 8.7: Example energy-versus-sample-angle map for the selected V_2O_3 reflections without symmetry-equivalent expansion.

8.8 Mapping display, filtering, and extra slices

The Single Crystal *Mapping display* control renders a two-parameter Bragg scan as Points, Band outlines, or Filled bands. Band modes use occupied cells on the sampled grid, keeping gaps, holes, and disconnected branches. An outline follows the accepted band boundary, not a fitted centre line; its resolution is limited by the scan step. Filled bands merge adjacent occupied cells. The numerical result is not reduced to the displayed shape. Matplotlib places clickable reflection legends beside a square map; Plotly (browser) offers hover values and clickable legends. The selected renderer is saved in the GUI state and can be changed when replotting.

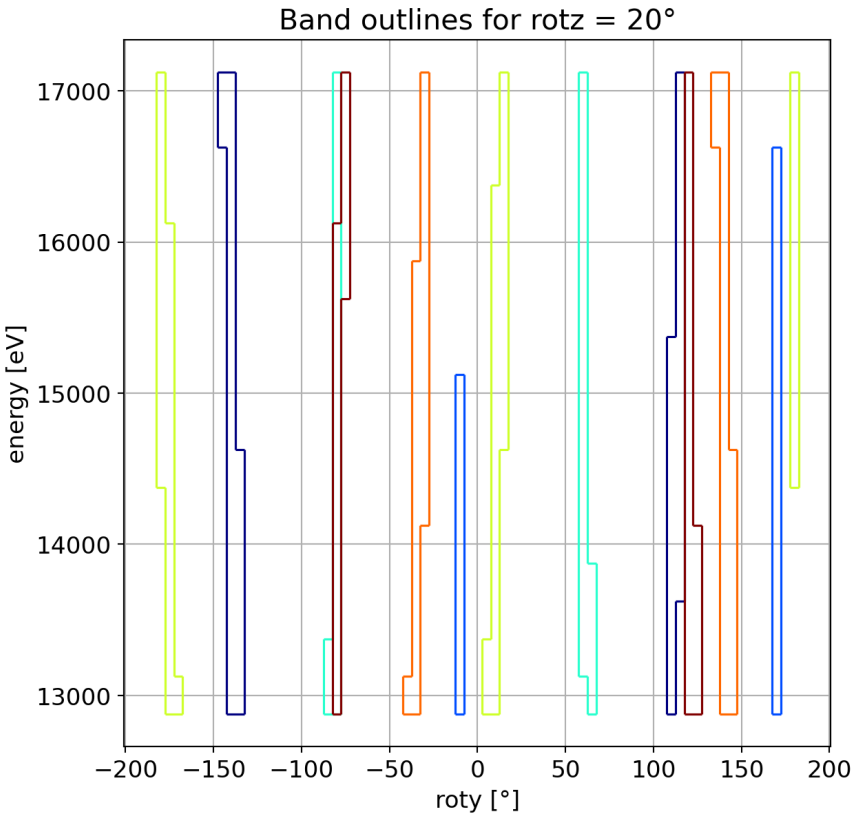

Figure 8.8: Band outlines for six V_2O_3 reflections on a sampled `roty`-versus-energy Bragg map. The contours follow accepted grid cells at 5° and 250 eV steps; empty gaps remain empty.

Require detector hit applies the current detector when drawing a mapping. The GUI saves all Bragg points, then tests central-energy rays against the rectangular detector bounds for the displayed view. Repose the detector and choose *Plot Loaded / Last Results* to see another acceptance without repeating the scan. This test does not model module gaps, dead pixels, or masks. An older result that removed points at calculation time cannot recover them; re-run that scan to obtain a complete map. The low-level scan's `require_detector_hit` argument remains available for compatibility, but complete saved maps are preferable.

For a family of maps, enable *Scan additional parameters* under *Additional Mapping Sliders*. Add start, stop, and step for any unplotted sample rotation or sample-chain motor, energy, or `e_bandwidth`. The two plotted parameters remain fixed; an extra parameter cannot duplicate either axis. Energy is in eV, rotations in degrees, and bandwidth is full $\Delta E/E$ in percent. Values are sampled; the stop is included only if reached by the step. Legacy scans apply the initial sample pose, then combine all scan rotations in *Rotation order*; table-row order does not change that order. Motor-chain scans keep physical chain order and apply unplotted motors as fixed angles for each slice.

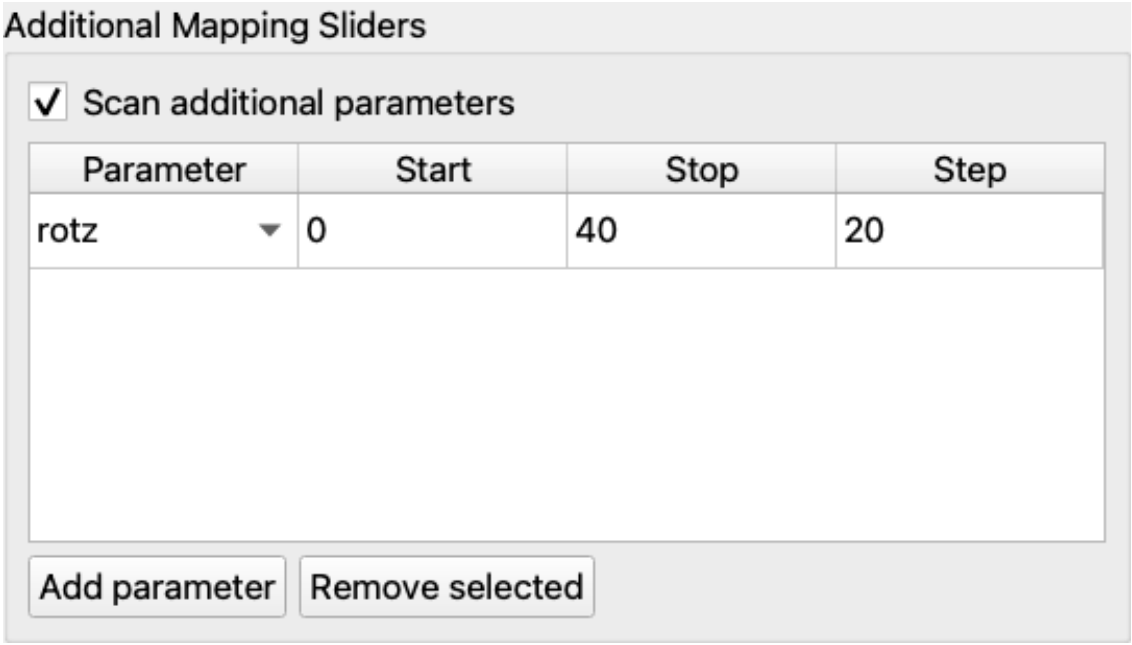

Figure 8.9: Additional Mapping Sliders configured to compute three `rotz` slices at 0, 20, and 40 degrees. The two map axes remain `roty` and energy.

Each slice is computed and retained. Cost therefore multiplies with every extra range; begin with coarse ranges. Sliders, previous/next buttons, and numeric value controls select already computed slices without repeating the Bragg search. Parallel processing distributes mapping rows. *Stop safely* cancels between work units and preserves the previous completed result. Save Results writes every slice to HDF5; Load Results restores slices independently of the current sample inputs. Detector-hit filtering is applied to the displayed slice and leaves the stored Bragg points intact.

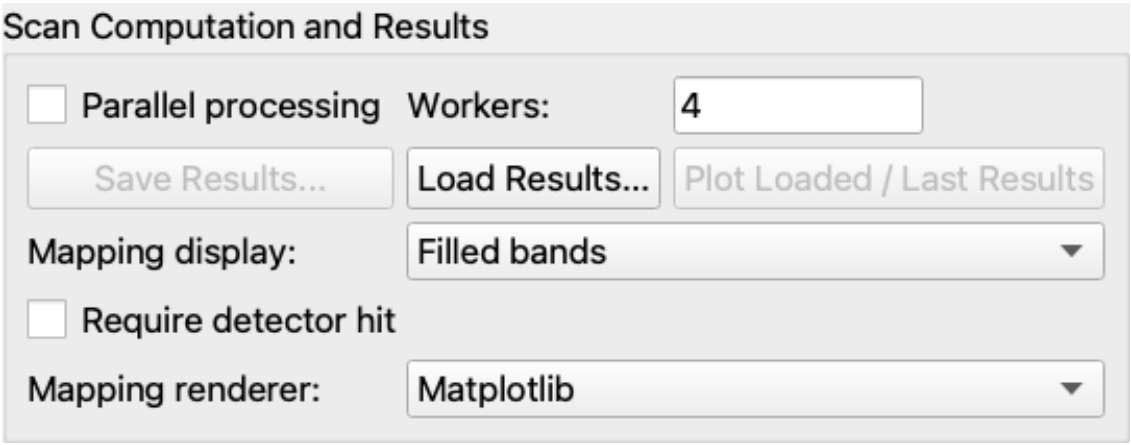

Figure 8.10: Single Crystal result controls with Filled bands selected. Save, Load, replot, detector filtering, and renderer selection operate on the numerical mapping result.

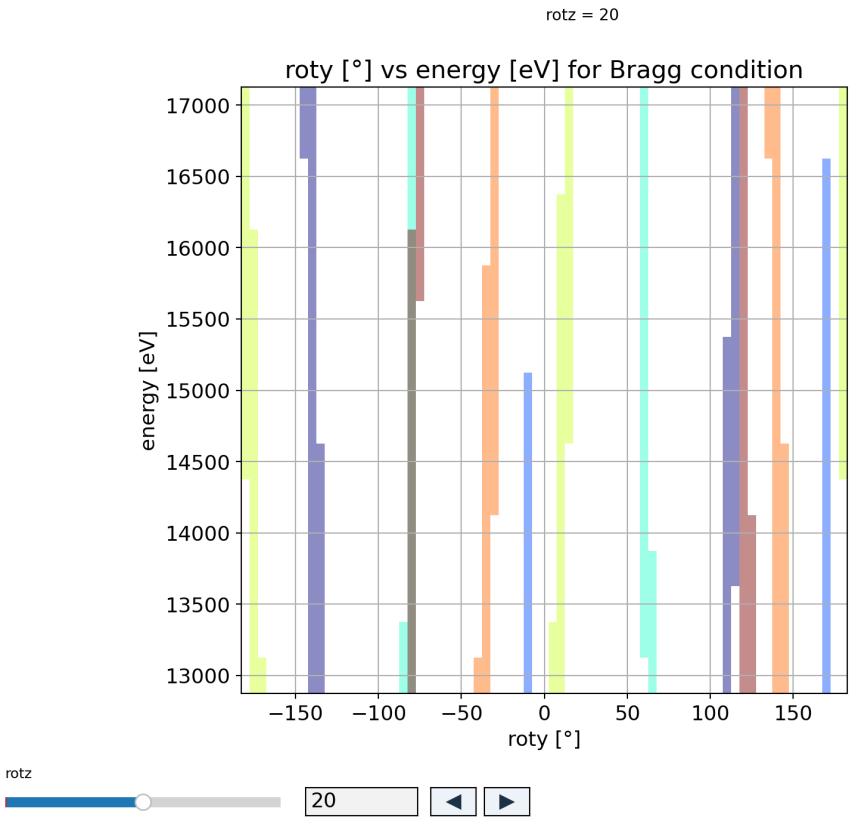

Figure 8.11: The same V_2O_3 Bragg map shown as filled bands at the selected extra `rotz`=20° slice. The slider and numeric box change the displayed computed slice; the full energy bandwidth is 35%.

```
from trxrdpy.simulation import single_crystal
from trxrdpy.simulation.results import (
    SimulationResult, save_result, load_result, plot_result,
)

data = single_crystal.scan_two_parameters_for_Bragg_condition(
    param1_name="roty", param2_name="energy",
    param1_range=(-20, 20, 10),
    param2_range=(10000, 15000, 1000),
    sam_space_group=221, sam_a=4, sam_b=4, sam_c=4,
    sam_alpha=90, sam_beta=90, sam_gamma=90,
    hkls_names=[[-1, 1, 0]],
    extra_scan_ranges={"rotz": (0, 30, 10)},
)
result = SimulationResult("parameter_mapping", data, {})
save_result("mapping_slices.h5", result)
plot_result(load_result("mapping_slices.h5"),
            display_mode="bands", mapping_backend="matplotlib")
```

Without `extra_scan_ranges`, either scan function returns its original HKL-to-points dictionary. With extra ranges, it returns a structured mapping-slice dataset. The same option applies to `scan_two_motors_for_Bragg_condition`, using other named sample motors, energy, or bandwidth. For ordinary maps, `plot_result(result, require_detector_hit=True, detector_obj=det)` filters the view; set `mapping_backend="plotly"` for a browser map. Plotly sliced maps use a local loopback viewer with prepared-frame caching. Keep Python running, replot after changing detector geometry, and save HDF5 for portable numerical results. The browser page for a sliced

map depends on its live Python session.

8.9 Collecting Bragg reflections with detector rotations

Detector-rotation search functions answer a different question from sample-orientation searches: given a crystal state and selected reflections, which detector-arm settings intercept the diffracted rays? The package provides legacy Euler, motor-chain, and geometry-aware variants.

8.9.1 Legacy detector Euler scan

`detector_rotations_collecting_Braggs` scans detector `roty` and `rotz` over one common inclusive range. It returns an `Experiment`, populates successful detector rotations, and opens the legacy rotation map.

```
legacy_detector_scan = (
    single_crystal.detector_rotations_collecting_Braggs(
        det_type="manual",
        det_pxsize_h=75e-6,
        det_pxsize_v=75e-6,
        det_ntum_pixels_h=1024,
        det_num_pixels_v=1024,
        det_dist=0.08,
        det_poni1=0.0384,
        det_poni2=0.0384,
        angle_range=(-45, 45, 5),
        energy=15000.0,
        e_bandwidth=2.0,
        **v2o3_sample,
        sam_rotx=-30.0,
        sam_roty=83.0,
        sam_rotz=50.0,
        hkls=tracked_hkls,
    )
)
```

8.9.2 Detector motor-chain and geometry scans

`detector_rotations_collecting_Braggs_with_chain` accepts arbitrary detector motor names and independent scan ranges. `detector_rotations_collecting_Braggs_with_geometry` is the corresponding convenience wrapper for the detector arm of a `DiffractometerGeometry`.

```
geometry_detector_scan = (
    single_crystal.detector_rotations_collecting_Braggs_with_geometry(
        det_type="manual",
        det_pxsize_h=75e-6,
        det_pxsize_v=75e-6,
        det_ntum_pixels_h=1024,
        det_num_pixels_v=1024,
        det_dist=0.08,
        det_poni1=0.0384,
        det_poni2=0.0384,
        energy=15000.0,
        e_bandwidth=2.0,
        **v2o3_sample,
```

```
        sam_rotx=-30.0,
        sam_roty=83.0,
        sam_rotz=50.0,
        hkls=tracked_hkls,
        geometry=instrument,
        scan_ranges={"tth": (-45, 45, 1)},
    )
)

successful = geometry_detector_scan.success_detector_rotations
```

For the chain form, replace `geometry=instrument` with `detector_motor_chain=...`; use `fixed_detector_angles` for unscanned detector motors. In both modern forms, the returned experiment stores successful configurations by Miller index. Keep the sample orientation fixed and document the detector rotation order or motor chain used.

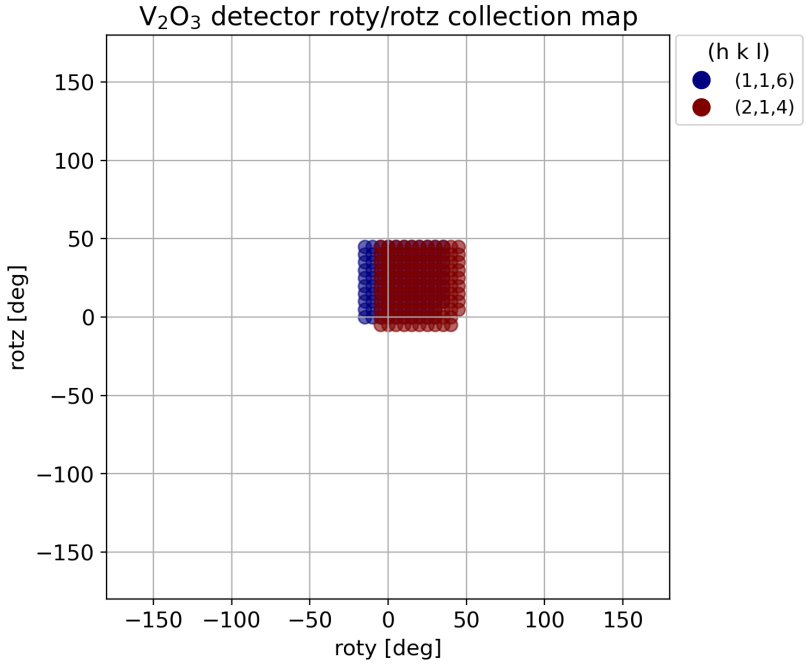

Figure 8.12: Detector-arm settings that intercept the V_2O_3 (116) and (214) Bragg reflections for the fixed sample orientation selected from the requested tracking set.

8.10 Fixed-energy inverse targeting

`target_hkl_near_pixel_fixed_energy` searches for orientations that place one selected reflection near a target detector pixel at fixed energy. It samples the elastic q cone, intersects rays with the detector, retains hits inside a pixel tolerance, and expands the free rotation around each accepted q target.

```
targeting = single_crystal.target_hkl_near_pixel_fixed_energy(
    det_type="manual",
    det_pxsize_h=75e-6,
    det_pxsize_v=75e-6,
    det_ntum_pixels_h=1024,
    det_num_pixels_v=1024,
    det_dist=0.08,
```

```
    det_poni1=0.0384,
    det_poni2=0.0384,
    energy=15000.0,
    **v2o3_sample,
    target_hkl=[1, 0, 4],
    target_pixel=(737, 737),
    pixel_tolerance_px=10.0,
    eta_samples=721,
    phi_samples=181,
    do_detector_plot=True,
    do_2d_plot=True,
    do_3d_plot=True,
)
```

The tested geometry above produces accepted Euler solutions. With an active sample motor chain, the solution object additionally carries ordered `motor_names` and an `(N,M)` array in `motor_angles_deg`.

```
print(targeting.all_pixels[targeting.best_idx])
print(targeting.pixel_error_px[targeting.best_idx])
print(targeting.accepted_mask.sum())

solutions = targeting.solutions
if solutions is not None:
    print(solutions.solution_mode)
    print(solutions.predicted_pixels)
    print(solutions.pixel_error_px)
```

The returned `FixedEnergyTargetingResult` also retains the complete sampled cone, all detector intersections, on-detector and accepted masks, inferred beam center, detector object, and best-hit index. Its `solutions` field is either `None` or a `FixedEnergyAcceptedSolutions` object. Set plotting flags to false when only numerical post-processing is needed.

This is an inverse problem. Multiple orientations can satisfy closely related constraints, and limits or seed choices may affect which families are found. Validate each accepted solution by forward simulation and examine motor feasibility before using it experimentally.

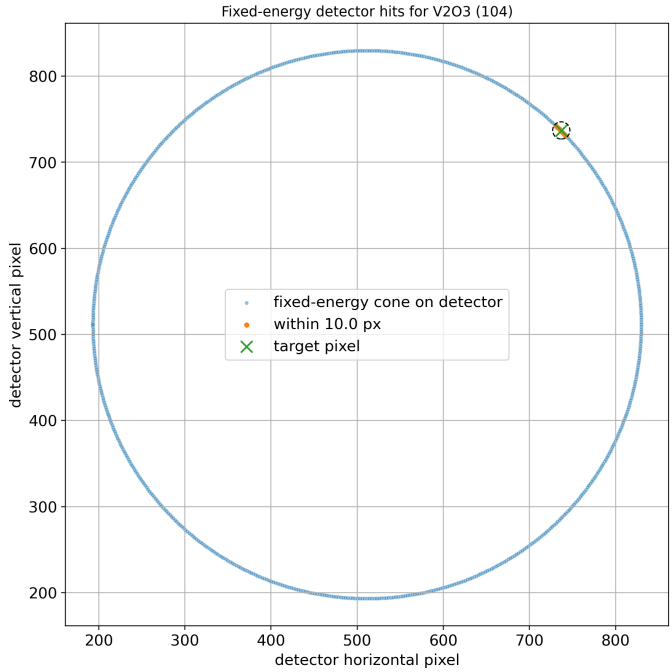

Figure 8.13: Reachable fixed-energy detector hits for V_2O_3 (104), requested target pixel, acceptance radius, and best sampled hit.

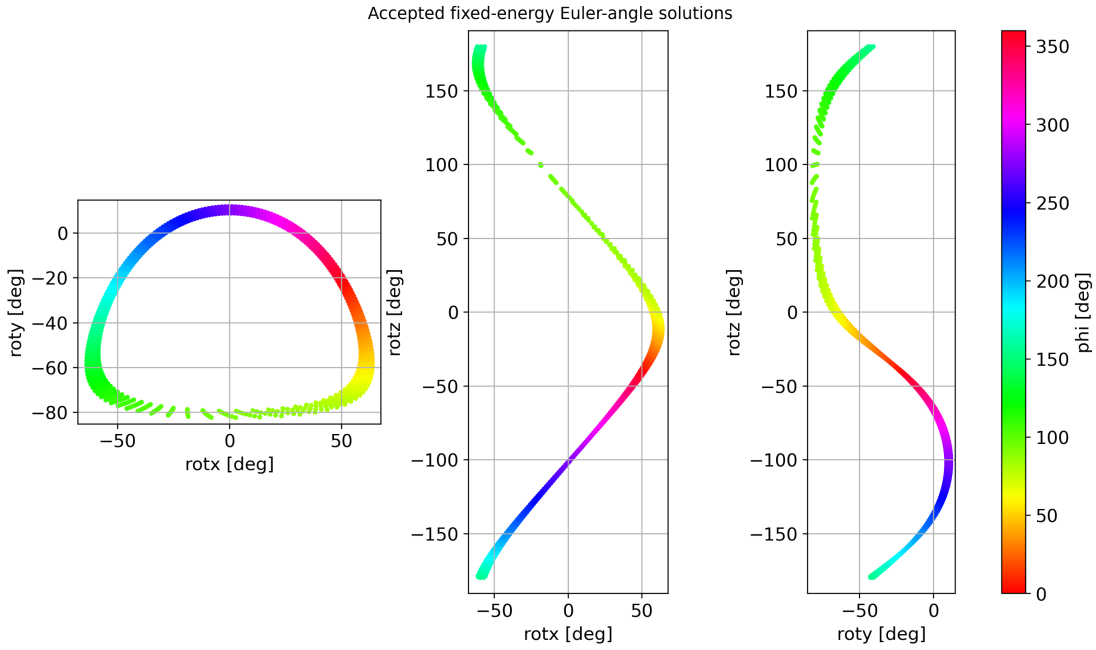

Figure 8.14: Pairwise projections of the accepted Euler-angle or named-motor solution family.

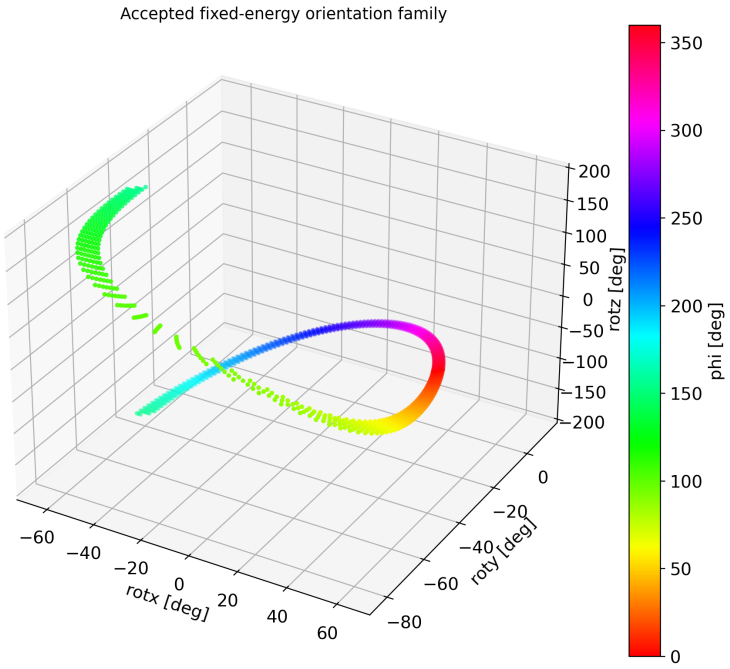

Figure 8.15: Optional three-dimensional view of the accepted orientation family, colored by the free rotation coordinate.

Instrument safety

Geometry solutions are computational results, not collision-checked motion commands. Never transfer angles directly to hardware without instrument limits, collision envelopes, sign conventions, and beamline procedures being independently verified.

8.11 Reciprocal space and Ewald construction

`single_crystal.simulate_reciprocal` builds oriented reflections up to `qmax` and draws the Ewald construction without requiring a detector. The reciprocal origin is excluded. Q is in Å^{-1}, energy in eV, and `e_bandwidth` is the full relative energy width in percent. With the incident beam along $+x$, the central sphere has radius $2\pi/\lambda$ and centre $(-2\pi/\lambda, 0, 0)$ in the same reciprocal-space units. Plotly (browser) is the default renderer; Matplotlib is available with `backend="matplotlib"`. The single-configuration Plotly HTML bundles its JavaScript and works offline.

The plot groups Bragg and non-Bragg reflections, shows HKL and Q in hover information, and provides a Bragg HKL list. Optional bandwidth boundaries and non-Bragg points can be toggled. *Require detector hit* highlights detected Bragg reflections in green while other Bragg reflections remain red; it needs a valid detector and tests central-energy rays against rectangular bounds. Save Results preserves every reflection, including those outside the Bragg condition. Loading and replotting can use a different renderer or current detector without enumerating the lattice again.

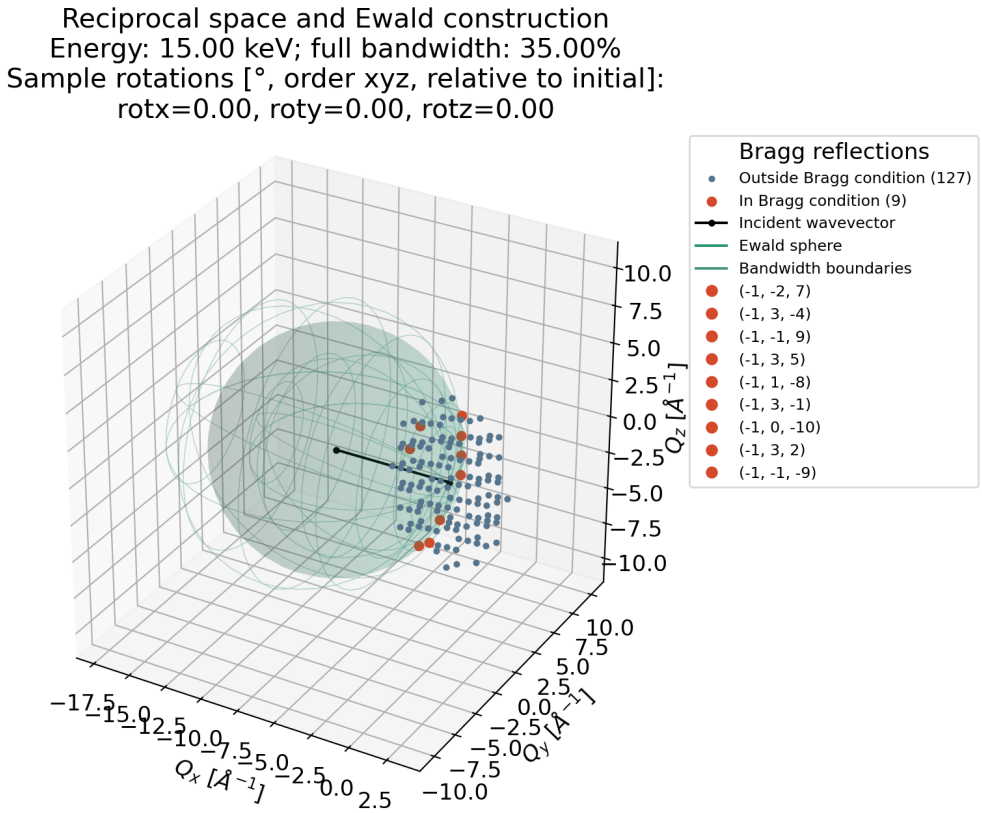

Figure 8.16: Matplotlib Ewald construction for V_2O_3 at 15 keV, $q_{max} = 5$ Å^{-1}, and 35% full bandwidth. Red reflections satisfy the Bragg condition; the central sphere and bandwidth boundaries show the energy tolerance.

```
from trxrdpy.simulation import single_crystal

view = single_crystal.simulate_reciprocal(
    sam_space_group=221, sam_a=4, sam_b=4, sam_c=4,
    sam_alpha=90, sam_beta=90, sam_gamma=90,
    energy=15000, e_bandwidth=2, qmax=5,
    backend="plotly", show=False, html_path="ewald.html",
)
```

In the Single Crystal GUI, enable *Scan configurations* beneath `simulate_reciprocal` to add sampled energy, bandwidth, and pose axes. Legacy geometry accepts `energy`, `e_bandwidth`, `sam_rotx/y/z`, and `det_rotx/y/z`. Geometry-aware mode accepts `sample:<motor>` and `detector:<motor>` instead of Euler axes. Detector scans require a configured detector. Bandwidth must be at least zero and below 200%; for example, 2% means ±1% about the central energy. Unscanned parameters retain their current values. A typed slider value snaps to the nearest sampled point; values outside the saved range are rejected.



Figure 8.17: Single Crystal reciprocal scan configuration with independently sampled energy and sample `roty` ranges. The viewer evaluates the selected configuration on demand.

The compact scan saves one reflection set, axis arrays, and geometry. Selected and neighboring configurations are evaluated as needed, rather than materializing the Cartesian product. Up to eight axes with one million samples each are supported. Parallel processing prepares neighbors in the background; it does not enumerate every combination. Matplotlib and Plotly both provide independent sliders and numeric boxes. Plotly scans run through a loopback-only viewer with a bounded temporary cache. Keep the Python process running while interacting with that browser tab; an exported scan HTML is only a link to the live viewer. Save the HDF5 result and reopen it later for durable access. Close All Plots or closing the GUI shuts down its local viewers, although browser tabs remain open.

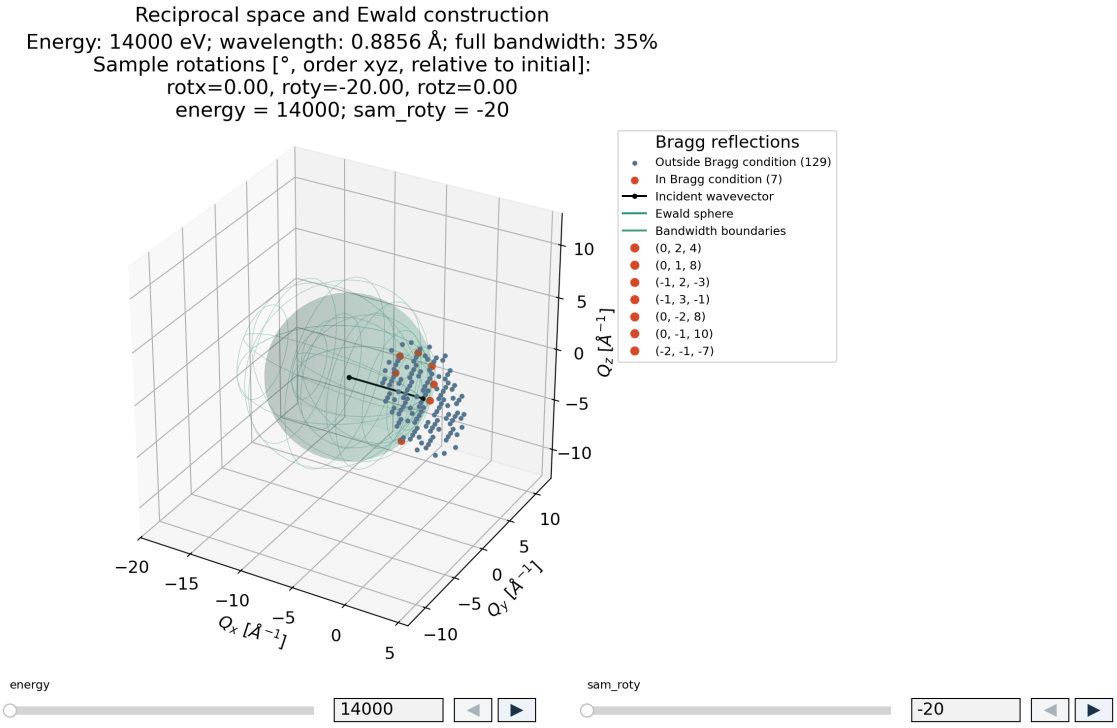

Figure 8.18: Matplotlib view of the compact reciprocal scan at its first sampled point, 14 keV and sample `roty`=-20°. Independent sliders and numeric boxes select other saved-axis values without storing every possible frame.

```
scan = single_crystal.simulate_reciprocal(
    sam_space_group=221, sam_a=4, sam_b=4, sam_c=4,
    sam_alpha=90, sam_beta=90, sam_gamma=90,
    energy=15000, qmax=5, show=False,
    scan_ranges={"energy": (14000, 16000, 500),
                 "sam_roty": (-10, 10, 5)},
)
```

In scripts, `plot.plot_reciprocal(Q_hkls,hkls,wavelength,E_bandwidth,backend="plotly")` accepts matching $N \times 3$ arrays and wavelength in metres. The `simulate_reciprocal` route constructs those arrays from crystallographic input. The GUI's HDF5 Save/Load actions use `results.save_result` and `results.load_result`; they retain the numerical scan, not the viewer cache.

Chapter 9

Plotting and result inspection

9.1 Plot families

The Simulation plotting module provides:

- three-dimensional detector and crystal views;
- two-dimensional powder and single-crystal detector plots;
- diffraction-cone plots;
- one-dimensional powder patterns;
- reciprocal-space views;
- rotation and parameter mappings; and
- fixed-energy detector-hit and motor-family visualizations.

High-level simulation calls normally create the relevant plots automatically. Lower-level functions accept existing Matplotlib axes in several cases, which makes it possible to compose publication or diagnostic figures.

9.2 Separating calculation from presentation

For reusable workflows, retain the returned `Experiment`, lattice, detector, or result object and treat plotting as a separate step. This makes it easier to:

- inspect numerical arrays before display;
- compare several configurations on consistent axes;
- save derived values alongside figures; and
- rerender plots without repeating expensive scans.

9.3 Plot interpretation

Detector plots should be read together with their coordinate labels, image origin, and beam-center convention. Reciprocal-space plots help diagnose whether a missing detector reflection fails the Bragg condition or merely misses the active detector area. Rotation maps reveal families of candidate orientations but do not replace forward validation.

For dense reflection sets, labels and hover annotations can become crowded. Reduce `qmax`, select explicit reflections, or use a coarse view first. The optional `mplcursors` dependency supports interactive hover information in applicable GUI plots.

9.4 Saving figures

Matplotlib figures can be saved using the active figure object:

```
import matplotlib.pyplot as plt

experiment = polycrystalline.simulate_2d(...)
plt.gcf().savefig(
    "figures/powder_2d_rings.png",
    dpi=300,
    bbox_inches="tight",
)
```

The filename matches the generated figure reference in Chapter 6; recompilation inserts it automatically. For workflows that open several figures, inspect `plt.get_fignums()` and save each figure with the filename used by its `\manualfigure` call. For reproducibility, save the input parameters next to the figure. A plot without energy, lattice, detector calibration, orientation, and package version is difficult to reconstruct.

Chapter 10

Simulation graphical interface

10.1 Purpose and architecture

The Simulation GUI exposes the backend workflows without replacing them. Its tabs are Session, Polycrystalline, Single Crystal, and Extra Functions. Session contains state saving/loading, a JSON state-file drop field, notes, and the configuration summary. Extra Functions contains Matrix Rotation, Equivalent Reflections, q / d / Angle Conversion, pyFAI / Fit2D / PONI Geometry, and Photon Attenuation Length. Close All Plots is at the lower right. The computational work remains in the Simulation modules, so a GUI configuration can be translated into a Python workflow when automation is needed.

10.2 Launching the interface

The GUI is launched with the console entry point:

```
trxrdpy-sim-gui
```

The equivalent module invocation is:

```
python -m trxrdpy.simulation.gui.main_window
```

The screenshots in this chapter show the main GUI states and the figures that the same parameter choices produce. The code examples show the corresponding backend calls for the selected tab; use them as the reproducible form of a GUI configuration.

The GUI is most useful when it is treated as a guided parameter editor. A typical session is to select the calculation family, complete only the active controls, run a three-dimensional view to confirm the geometry, and then inspect the detector image or one-dimensional pattern. This order is deliberate: the 3D view shows whether the beam, sample, detector, and reciprocal-space construction are physically reasonable before the detector projection is interpreted as a final result.

10.3 Polycrystalline tab

The powder tab selects `simulate_1d`, `simulate_2d`, or `simulate_3d`. Its controls cover:

- CIF path, space group, cell parameters, and `qmax`;
- beam energy and relative bandwidth;
- manual, PONI, or pyFAI-registered detector input;
- binning, distance, PONI coordinates, Euler angles, and rotation order;

- a 2D/3D reflection source: automatic CIF/lattice families up to `qmax`, or explicit q/d values with Miller-index labels;
- 1D pattern options: horizontal axis, Lorentz-polarization correction, peak FWHM, optional detector coverage, and laboratory azimuth sector;
- 2D/3D relative-intensity display, polarization, colormap, color limits, and optional noise.

For `simulate_1d`, a CIF is required. For 2D and 3D, select *CIF / lattice (auto from qmax)* to generate the reflection families from the CIF; if no CIF is supplied, the entered space group and cell dimensions are used. Set the beam energy, relative bandwidth, and `qmax` before running. Select *Manual q/d + hkls_names* only when you have an explicit reflection list; enter either comma-separated q or d values and one Miller triplet for each position. The GUI hides controls that do not apply to the selected function.

```
from trxrdpy.simulation import polycrystalline
from trxrdpy.simulation.powder_preparation import run_powder

crystal = {"cif_file_path": "cif_files/V2O3_R-3c_room_T.cif"}
settings = dict(
    det_type="rayonixmx170", det_binning=(4, 4),
    det_dist=0.10, det_poni1=0.085, det_poni2=0.085,
    energy=15000.0, e_bandwidth=1.0, qmax=3.5,
)

experiment_3d = run_powder(polycrystalline.simulate_3d, crystal, **settings)
experiment_2d = run_powder(polycrystalline.simulate_2d, crystal, **settings)
```

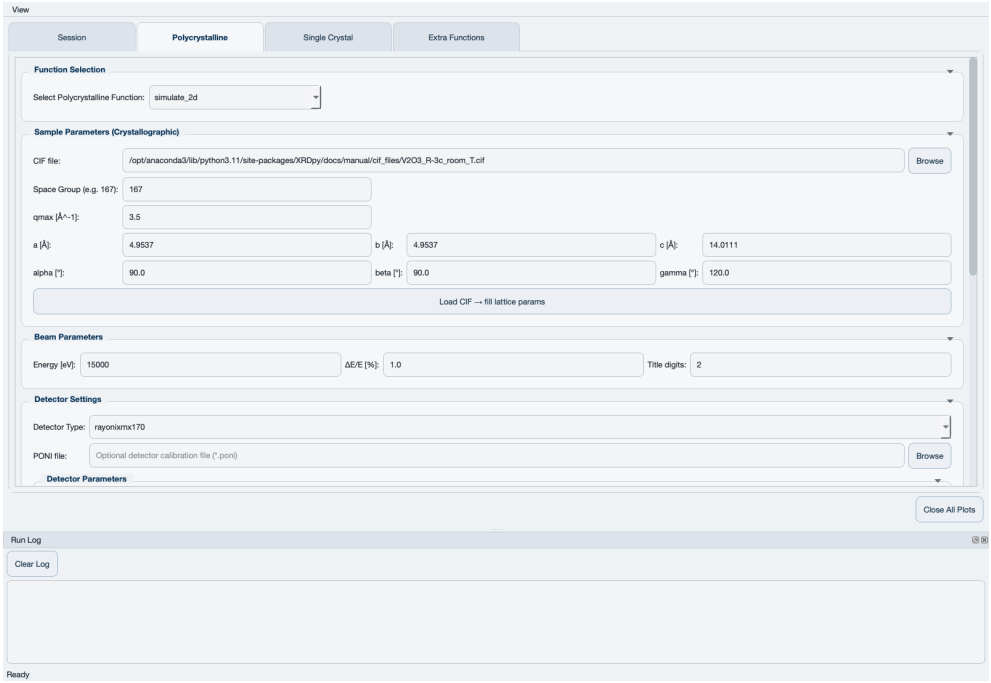

Figure 10.1: Polycrystalline tab set to a 2D simulation from the V_2O_3 CIF, with $q_{max} = 3.5$ Å^{-1}, 15 keV beam energy, and a binned Rayonix MX170 detector.

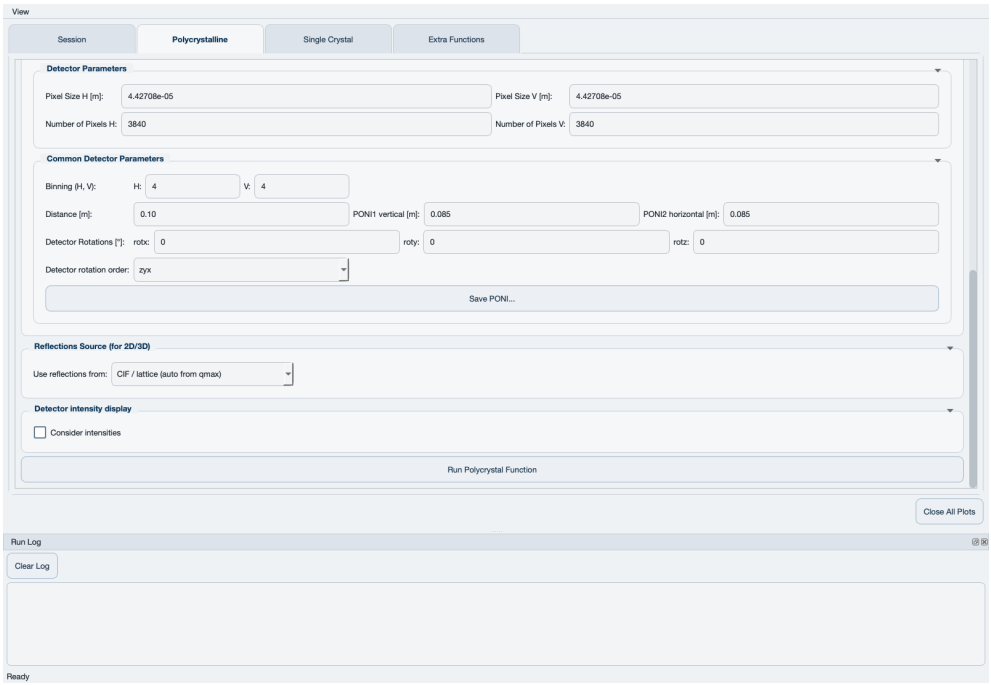

Figure 10.2: Lower part of the same powder tab showing the *CIF / lattice (auto from qmax)* reflection-source selection. The manual q/d list is hidden in this mode.

For a 1D pattern, select `simulate_1d`; 2D/3D reflection controls disappear, and the pattern options offer q, 2θ, or d on the horizontal axis. Set the peak FWHM in the selected axis units or use zero for sticks. Enable *Use detector coverage* to use the current detector geometry and optionally enter an azimuth sector and offset. Detector settings are shared when switching between the powder and single-crystal tabs.

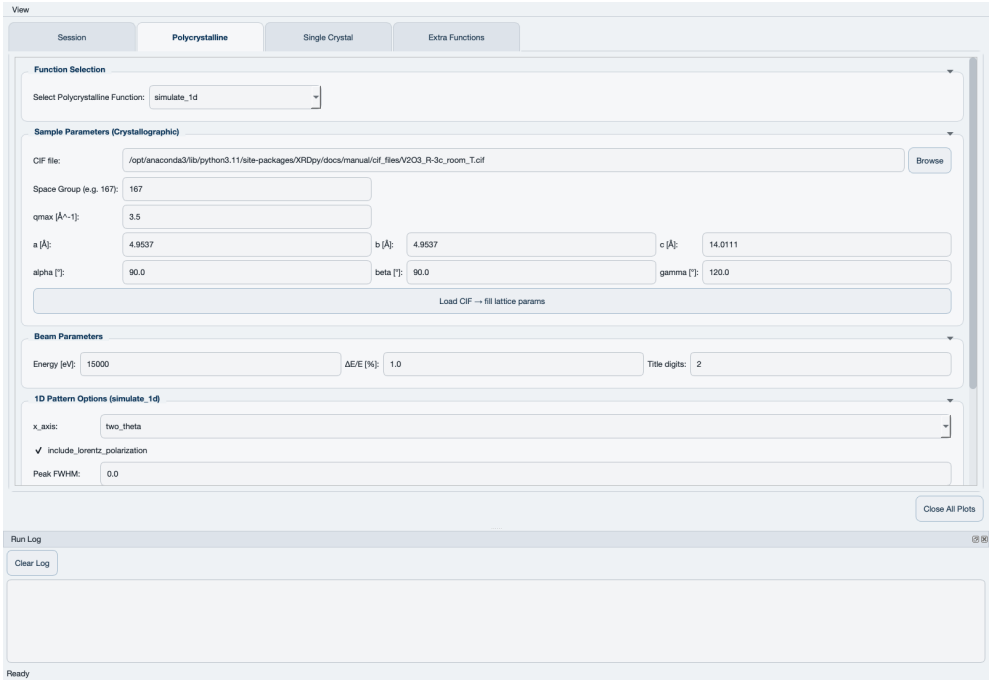

Figure 10.3: The polycrystalline tab in 1D mode, with a CIF input and 2θ selected as the horizontal axis. The axis selector also offers q and d.

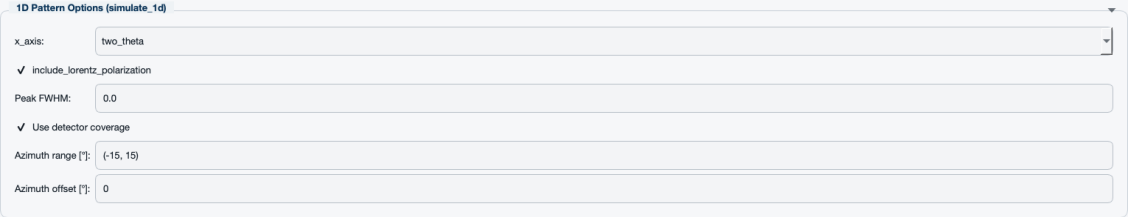

Figure 10.4: One-dimensional pattern controls with detector coverage enabled and a laboratory azimuth sector of $-15°$ to $15°$. The current detector sets the accessible q range.

The corresponding simulation outputs are shown with complete executable examples in Chapter 11. Keeping this chapter focused on GUI state avoids repeating the same detector, 3D, and 1D result figures in two places.

10.4 Single-crystal tab

The single-crystal tab exposes:

- 2D and 3D simulation, each with optional independent scan sliders;
- fitting the crystal orientation matrix from measured Bragg pixels and motor poses;
- fixed-energy reflection targeting near a detector pixel;
- detector-rotation searches for Bragg reflections;
- two-parameter Bragg-condition scans;
- detector, beam, lattice, orientation, and reflection controls;
- legacy Euler, predefined, and custom geometry modes; and
- generated sample and detector motor-angle controls.

The geometry panel distinguishes legacy Euler mode from geometry-aware mode. In geometry-aware mode, motor names, meanings, axes, frames, origins, defaults, and editable angles are presented explicitly.

```
from trxrdpy.simulation import single_crystal
from trxrdpy.simulation.diffractometers import make_kappa_geometry

geometry = make_kappa_geometry(kappa_tilt_deg=50.0)

experiment_3d = single_crystal.simulate_3d_with_geometry(
    det_type="manual",
    det_pxsize_h=75e-6,
    det_pxsize_v=75e-6,
    det_ntum_pixels_h=1024,
    det_num_pixels_v=1024,
    det_dist=0.08,
    det_poni1=0.0384,
    det_poni2=0.0384,
    energy=15000.0,
    e_bandwidth=1.0,
    sam_space_group=227,
    sam_a=5.431,
    qmax=6.0,
    geometry=geometry,
    sample_angles={"omega": -30.0, "kappa": 40.0, "phi": 30.0},
    detector_angles={"tth": 0.0},
)
```

```
experiment_2d = single_crystal.simulate_2d_with_geometry(
    det_type="manual",
    det_pxsize_h=75e-6,
    det_pxsize_v=75e-6,
    det_ntum_pixels_h=1024,
    det_num_pixels_v=1024,
    det_dist=0.08,
    det_poni1=0.0384,
    det_poni2=0.0384,
    energy=15000.0,
    e_bandwidth=1.0,
    sam_space_group=227,
    sam_a=5.431,
    qmax=6.0,
    geometry=geometry,
    sample_angles={"omega": -30.0, "kappa": 40.0, "phi": 30.0},
    detector_angles={"tth": 0.0},
)
```

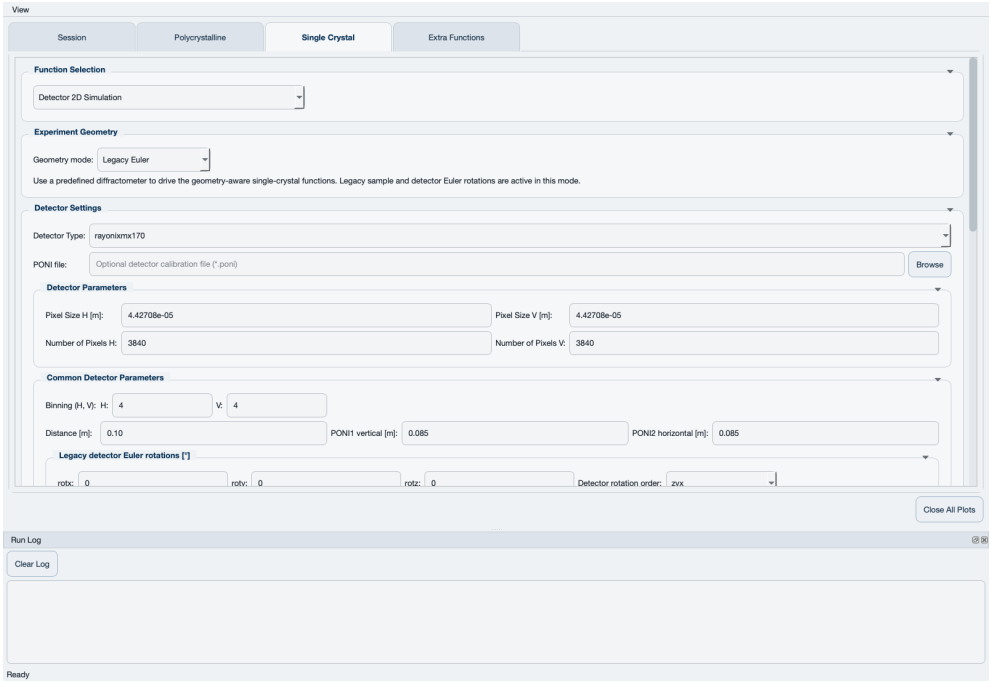

Figure 10.5: Single-crystal Simulation GUI showing geometry selection and generated sample/detector motor controls.

The complete single-crystal examples in Chapter 11 show the generated 3D and detector-projection figures. In GUI use, the same pedagogical order applies: inspect the 3D geometry first, then inspect detector pixels.

10.4.1 Functions and scan controls

The function menu uses descriptive labels: *Laboratory 3D Simulation*, *Detector 2D Simulation*, *Ewald Construction Simulation*, *Find Rotations for Bragg in Detector*, *Detector Rotations Mapping*, *Motors Mapping for Catching Braggs*, and *Find Orientation Matrix*. In the last mode, the orientation editor appears beneath the common lattice, beam, detector, and geometry controls. The full measured-peak workflow and matrix interpretation are in Section 8.3.

Enable *Scan configurations* in *2D Simulation Sliders* or *3D Simulation Sliders* for the corresponding detector view. Add a parameter row and enter start, stop, and a positive step magnitude. The modes keep independent ranges in saved GUI state. Reciprocal-space scans have their own *Scan configurations* group; additional mapping sliders compute and retain all requested map slices. All of these displays offer previous/next buttons beside their sliders and numeric boxes.



Figure 10.6: Independent 2D and 3D detector-simulation range editors in the Single Crystal tab.

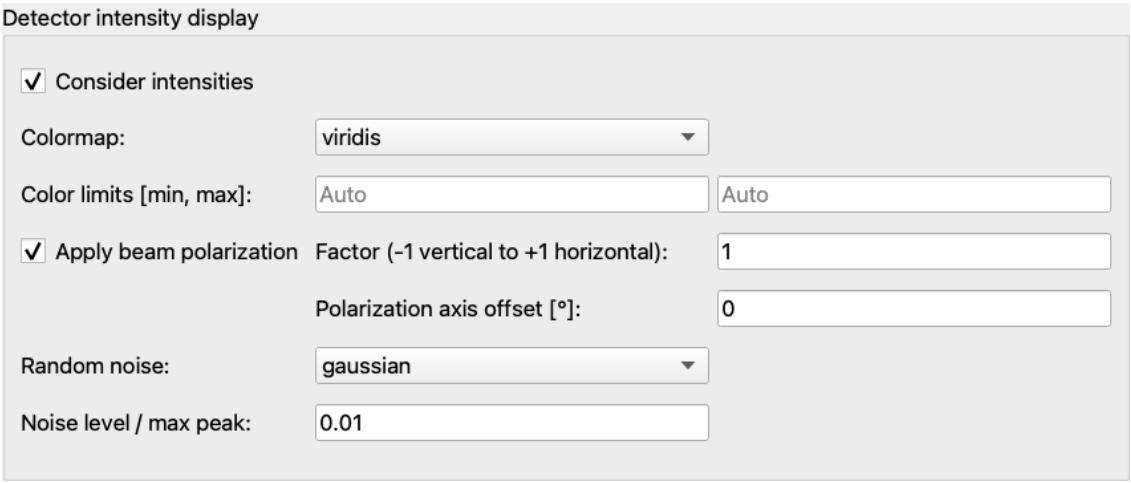

Figure 10.7: Detector intensity controls shared by powder and single-crystal 2D/3D views, including polarization and optional noise.

10.5 Find Orientation Matrix

Select *Find Orientation Matrix* in the Single Crystal function menu when measured Bragg-spot positions are available. The result is a fitted crystal orientation for the lattice, detector calibration,

beam energy, and motor readings recorded in the project. The matrix convention and fitting diagnostics are explained in Section 8.3.

1. Enter the crystal cell or load its CIF. Set the detector calibration, beam energy, and sample goniometer in the common Single Crystal controls. Press *New project from current setup* to capture them as the reference pose.
2. Add a pose for each recorded configuration. *Add pose from selected* links it to a parent. Choose *Absolute readings* for motor positions or *Changes from parent* for increments. Blank cells inherit the parent's conditions. Add another detector setup from the current controls when a pose uses different detector calibration.
3. Add each measured Bragg pixel to its pose. Enter horizontal and vertical pixel coordinates and choose *Exact HKL*, *Any equivalent*, or *Unknown HKL*. *Update q/d from pixels* calculates the observed scattering magnitude and spacing to help assign an index.
4. Enter peak-position uncertainties in pixels. The default values can be copied to all peak rows and then adjusted individually. Energy, motor, lattice, and shared detector-calibration uncertainties have separate fields. Mark an unsuitable peak *No* under *Include?* to leave it in the project without fitting it.
5. Press *Fit crystal orientation*. Inspect candidate rank, RMS pixel difference, assignments, and the measured-versus-predicted residual of each peak. A rank below three means the observations do not determine all rotation directions.
6. Select a candidate and a pose under *Update Single Crystal from fitted candidate*, then press *Update crystal orientation at selected pose*. Run *Detector 2D Simulation* or *Laboratory 3D Simulation* to compare the prediction with the measurements. Save the editable project and fitted result separately if the fit will be revisited.



Figure 10.8: Linked experimental poses and measured Bragg pixels in the Find Orientation Matrix editor. The second pose inherits the detector setup and adds a sample-motor change.

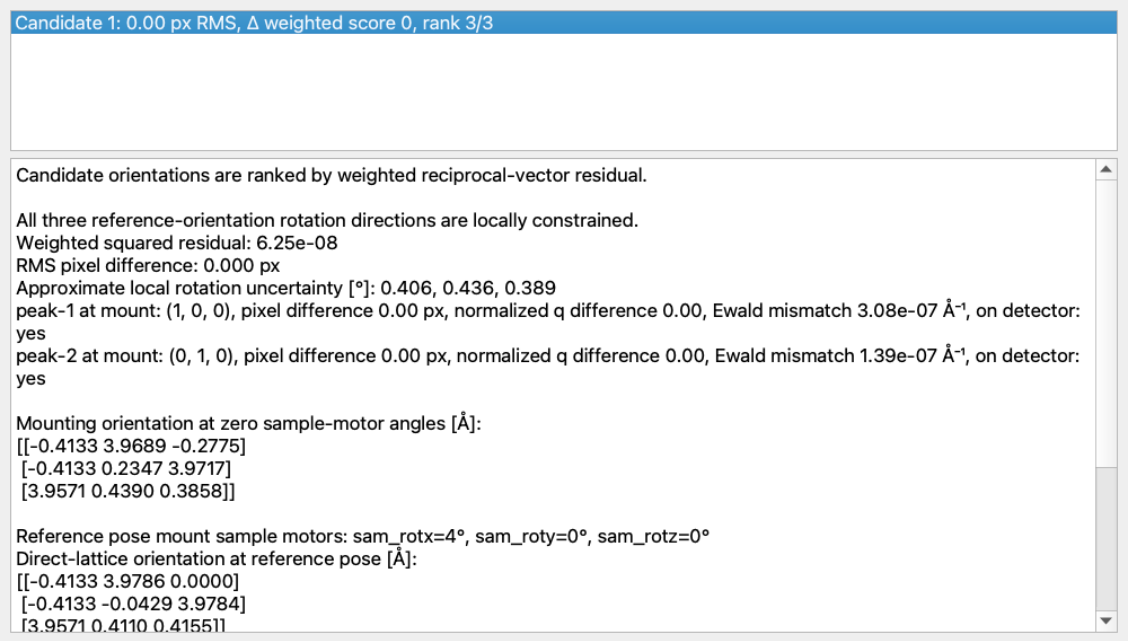

Figure 10.9: A fitted candidate with three constrained rotation directions, the pixel residual for each measured peak, and direct-lattice matrices.

10.6 Extra Functions

The *Extra Functions* tab opens five utilities. They can be used while either simulation tab is selected; each has its own input and result area. The available buttons are *Matrix Rotation*, *Equivalent Reflections*, *q / d / Angle Conversion*, *pyFAI / Fit2D*, and *Photon Attenuation Length*. Their input fields are retained in the saved GUI state.



Figure 10.10: The Extra Functions tab provides five independent utilities. Each button opens the corresponding editor or calculator.

10.6.1 Matrix Rotation

Use *Matrix Rotation* to construct a direct-lattice orientation from unit-cell parameters or a CIF, edit its nine entries, and apply a known sample rotation. *Compute Orientation from Lattice* places the direct-lattice vectors in the editable matrix with rows **a**, **b**, and **c** in Å. Choose *Euler rotations* and set the rotation order and three angles in degrees, or choose *Diffractometer motor chain* for an omega–kappa–phi stage with an explicit kappa tilt. *Apply Rotation* writes a separate result matrix. *Update Orientation Matrix from Result* copies that result back into the editable matrix, allowing another rotation to be applied.

To use the matrix for a single-crystal simulation, press *Import from Rotation Tool* beside the orientation-matrix fields on the Single Crystal tab. The imported entries become the sample's supplied direct-lattice orientation. *Find Orientation Matrix* on that tab is the measured-Bragg

fitting workflow in Section 10.5; it estimates an unknown orientation from observed pixels and recorded poses.

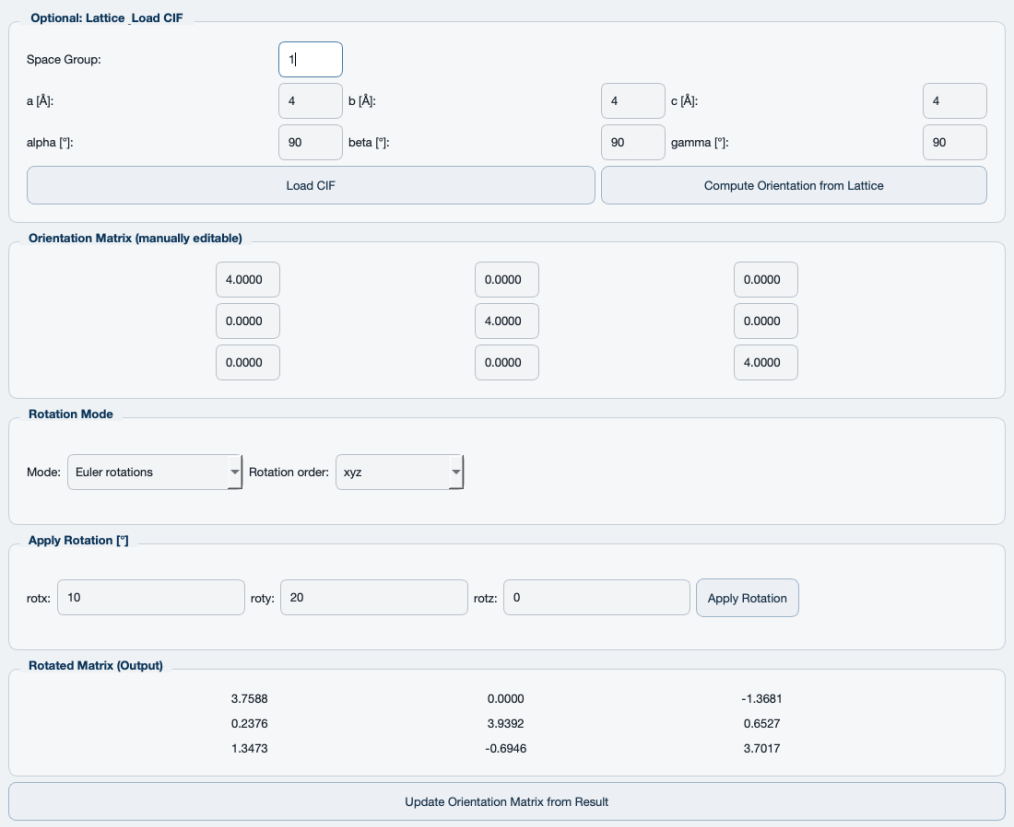

Figure 10.11: The Matrix Rotation window after constructing a cubic direct-lattice matrix and applying a known Euler rotation. The editable input and rotated output are shown separately.

10.6.2 Equivalent Reflections

Enter the space group and unit cell, or press *Use Current Sample* to copy the Single Crystal lattice fields. Enter one nonzero integer HKL triplet, such as `(1, 1, 0)`, or a list such as `[(1, 0, 4), (1, 1, 0)]`. *Find Equivalent Reflections* reports the symmetry-related indices for each input and a count of unique results across the list. Duplicate inputs are ignored. This is useful when a measured spot is identified by a reflection family rather than one indexed member; the orientation fitter also offers an *Any equivalent* identity mode.

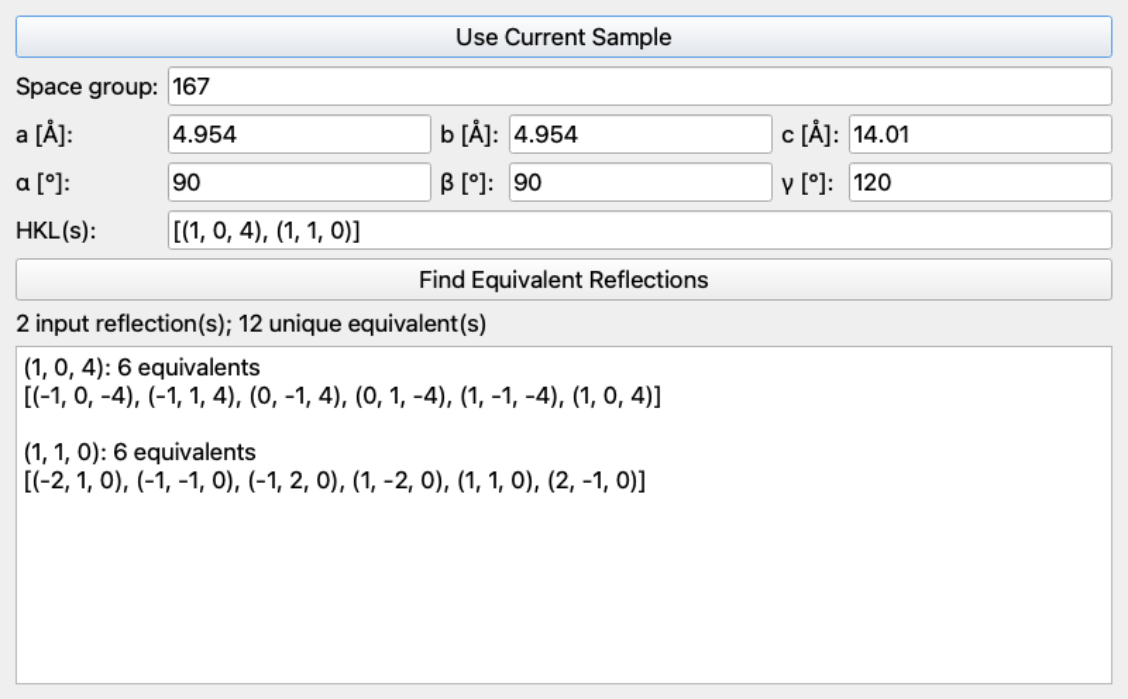

Figure 10.12: Equivalent Reflections for two input HKLs in space group 167, with each family and the unique-reflection count shown in the output panel.

10.6.3 q / d / Angle Conversion

Select an incident energy in keV or wavelength in Å, then choose which of q (Å^{-1}), d (Å), 2θ (degrees), or θ (degrees) is known. Enter its value and press *Convert*; the other three quantities appear together. *Use Current Beam* copies the energy from the active simulation controls. The dialog reports when a scattering vector has no accessible Bragg angle at that wavelength, rather than displaying a misleading angle.

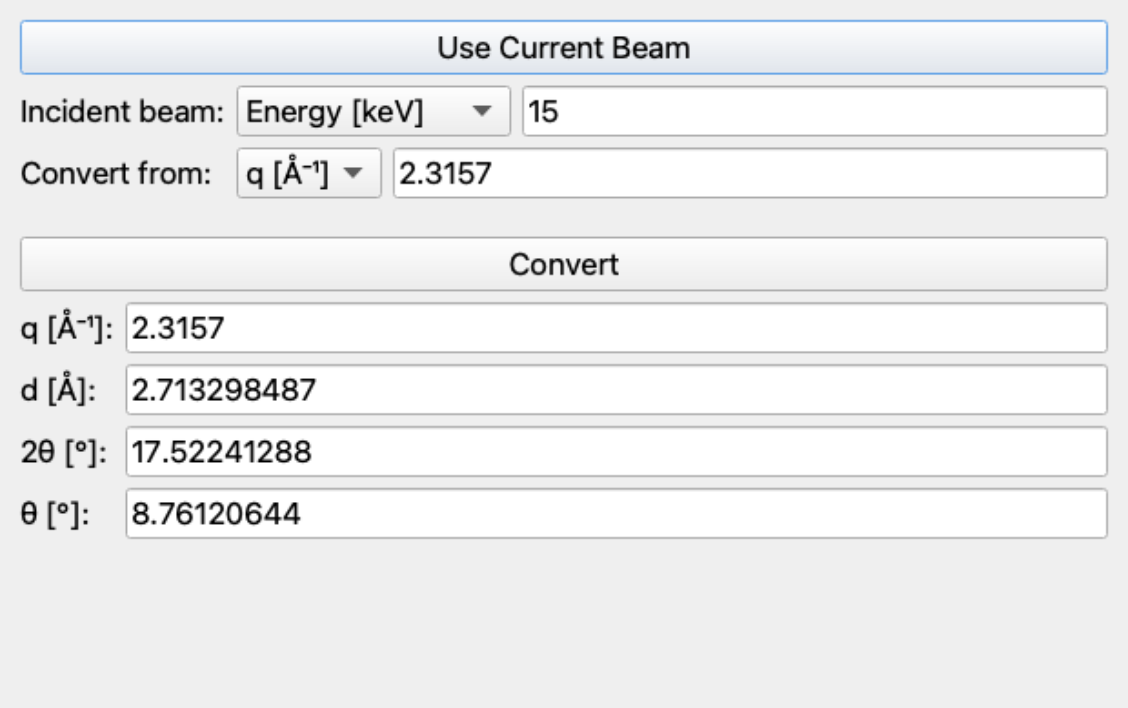

Figure 10.13: q / d / Angle Conversion for $q = 2.3157$ Å^{-1} at 15 keV, reporting d, 2θ, and θ from the same incident beam.

10.6.4 pyFAI / Fit2D geometry

pyFAI / Fit2D loads a PONI calibration or accepts entered geometry and converts in either direction. The pyFAI fields use metres for distance, PONI, and pixel sizes and radians for rotations. Fit2D uses millimetres for direct distance, pixels for beam centre, micrometres for pixel sizes, and degrees for tilt. Read the units beside each field before copying values into another program. Fit2D has no independent pyFAI `rot3`; converting back gives pyFAI's canonical orientation. The converter leaves the active simulation detector as it was. To export the detector currently configured on either simulation tab, use *Save PONI...* under its Common Detector Parameters (Section 5).

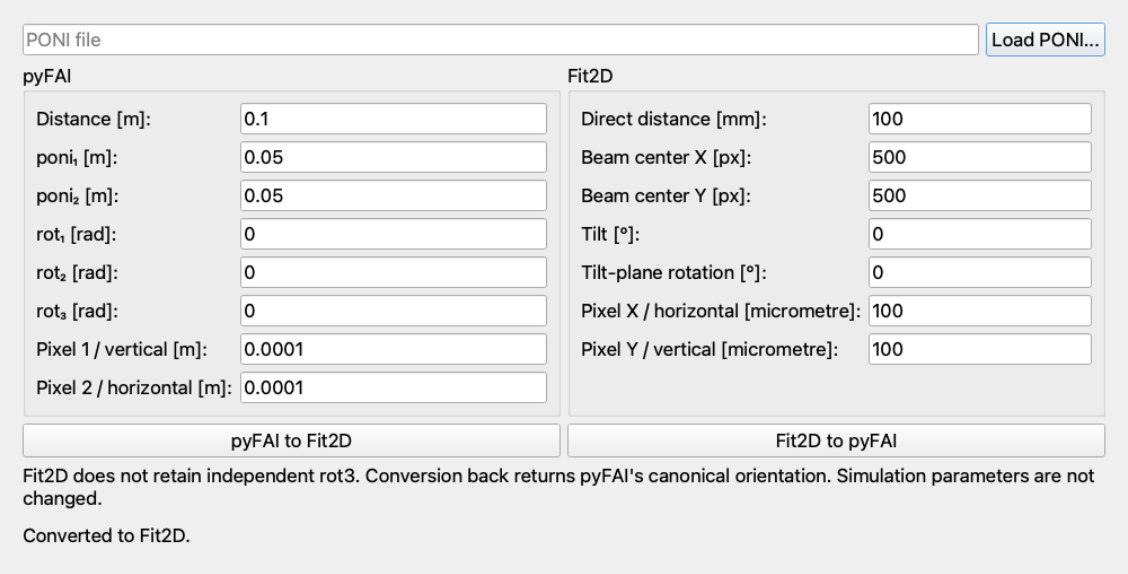

Figure 10.14: The pyFAI / Fit2D converter after converting a 0.10 m, 100 μm-pixel pyFAI geometry to Fit2D distance, centre, tilt, and pixel units.

10.6.5 Photon Attenuation Length

This utility computes offline X-ray optical constants from bundled Henke/CXRO tables. Enter a simple, case-sensitive chemical formula and an explicit density in g/cm^3, or load a supported formula from a CIF and then check its density. Formula parentheses and hydration syntax are not parsed; the Python material class can also accept an element-to-stoichiometry mapping. Energy start, stop, and step are in eV. Choose *Bulk attenuation length* for the $1/e$ intensity path length, or *Normal penetration depth* for the $1/e$ depth normal to a surface at grazing incidence. Incidence angle is measured from the surface in degrees, from 0 to 90. The GUI can scan multiple angles and select whether the plot slider changes angle or photon energy. Output lengths can be shown in metres, nanometres, or micrometres, with an optional logarithmic vertical axis.

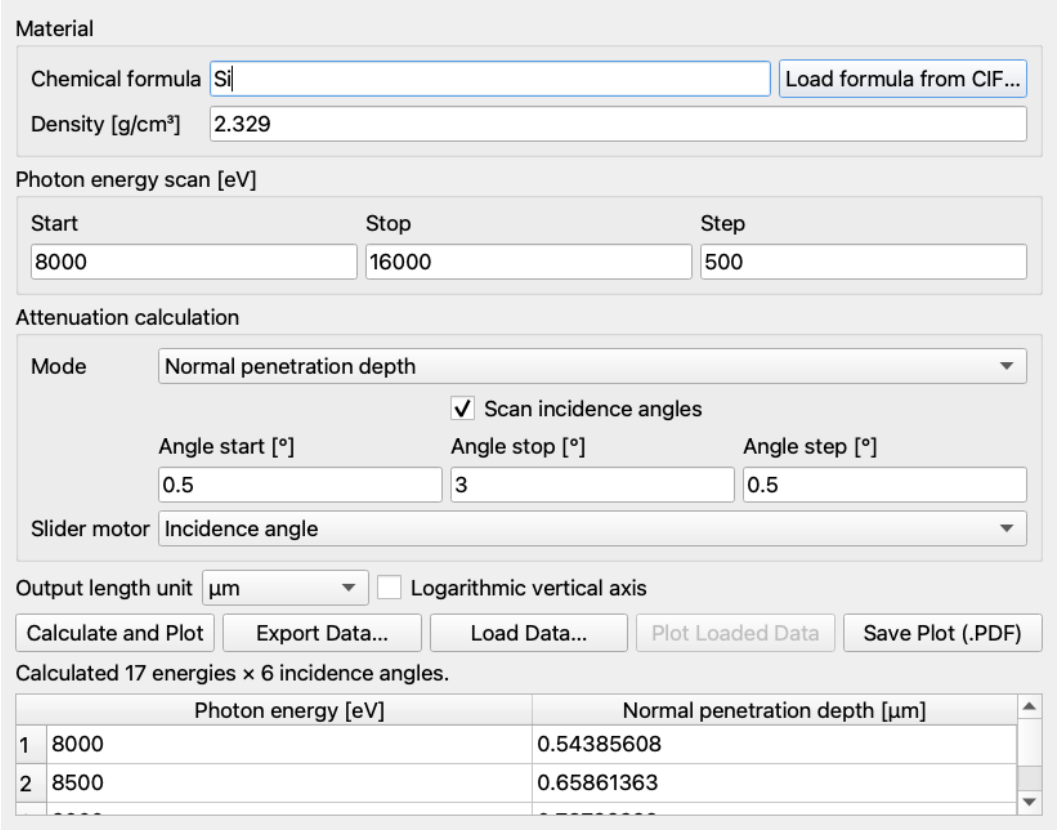

Figure 10.15: Photon Attenuation Length using Si at 2.329 g cm^{-3}, sampled from 8 to 16 keV over six grazing angles. The table follows the selected angle.

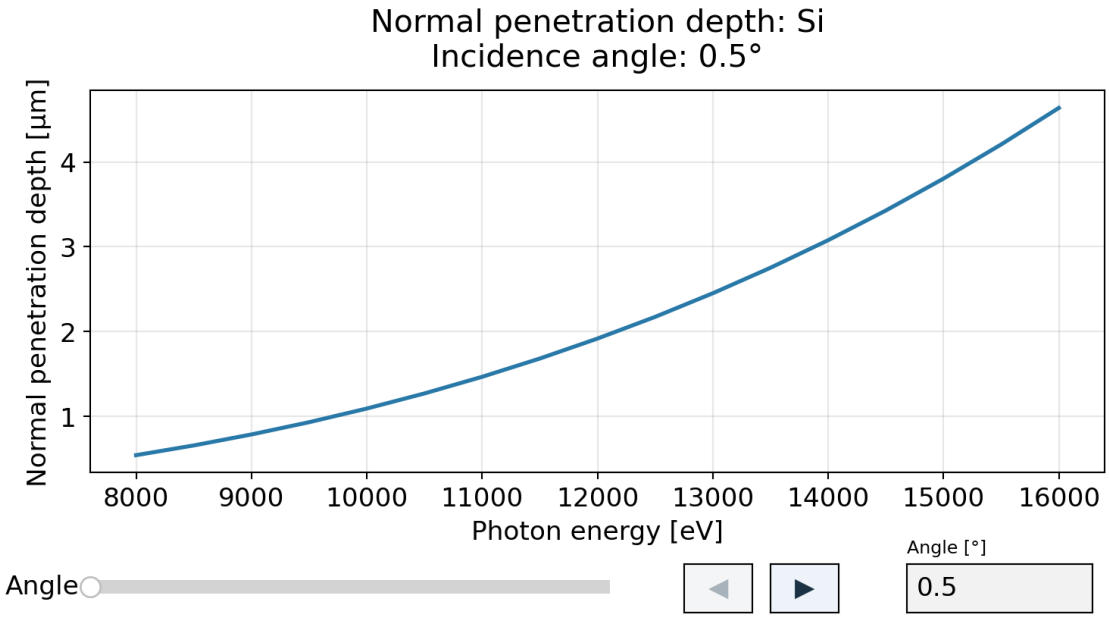

Figure 10.16: Calculated normal $1/e$ penetration depth for Si at a selected 0.5° grazing angle. Previous/next buttons, a slider, and numeric entry select another sampled curve.

The table follows the selected plotted curve. *Export Data...* writes CSV or compressed HDF5; lengths in either file are stored in metres, independent of display units. CSV contains energy, incidence angle, length, and material metadata. HDF5 stores the full angle-by-energy grid and

loads selected curves lazily. *Load Data...* and *Plot Loaded Data* restore saved numerical curves; *Save Plot (.PDF)* saves the currently displayed figure. The utility input fields and plot preferences are included in GUI state, while the calculated grid is kept in its exported data file.

```
from trxrdpy.simulation.attenuation import XRayMaterial

material = XRayMaterial("SrTiO3", density_g_cm3=5.12)
delta, beta = material.optical_constants(15.0)  # energy in keV
bulk_um = material.bulk_attenuation_length(15.0, unit="um")
depth_nm = material.grazing_penetration_depth(
    15.0, grazing_angle_deg=1.0, unit="nm")
```

`optical_constants` returns (δ, β) for $n = 1 - \delta + i\beta$. The default grazing calculation uses the first-order CXRO-style wavevector expression; `exact=True` uses the full complex-index expression. The packaged tables are read locally with interpolation; requests outside their valid energy range, unknown elements, invalid formulae, or nonpositive density are rejected. These are homogeneous-material estimates and do not include surface roughness or multilayer interference.

10.7 Sessions and logs

The GUI maintains session state and supports autosave and restore. Both simulation tabs accept dropped CIF files. Groups can be collapsed without changing their inputs; collapse state, utility inputs, scan settings, renderer selections, and custom orientation matrices survive GUI-state saving. Older saved states remain loadable. Logs and summaries should be retained with significant simulations because they provide a human-readable record of selected functions and parameters. Session recovery is a convenience, not a replacement for a deliberate, version-controlled simulation record.

10.8 Background tasks and reusable simulation results

Both simulation tabs run numerical work in nonmodal background tasks, including powder reflection preparation. A run snapshots its inputs; editing fields or loading a state while it runs does not change that computation. The active Run button is disabled until completion, while other tabs remain usable. Plot creation is returned to the GUI thread. Task dialogs show measured progress when available and a busy indicator when the total is unknown. A multi-slice mapping also shows progress across the full scan with elapsed and approximate remaining time once enough work has finished; terminal-only progress escape sequences are removed from the visible log. Successful tasks close their dialog; errors and cancellations remain visible. *Stop safely* requests cooperative cancellation, waits for active work to finish, and discards an incomplete result while retaining the last completed one. A running numerical solver or native-library call can delay cancellation.

For fixed-energy targeting, detector collection scans, two-parameter Bragg scans, and reciprocal views, *Save Results...* writes numerical HDF5 only when requested. *Load Results...* restores the result without changing current controls or rerunning the simulation; *Plot Loaded / Last Results* uses current plotting options. HDF5 contains numeric data and input metadata rather than Python pickles. In scripts, `results.SimulationResult`, `save_result`, `load_result`, and `plot_result` provide the same route. If `overwrite=False`, saving protects an existing file.

Parallel processing and *Workers* are available for scan workloads. It is off by default; when enabled, four workers are the GUI default. Ordinary two-axis scans distribute independent rows to processes. Legacy Euler targeting can run in parallel, whereas motor-chain inverse targeting

retains serial continuation seeds to preserve solution-branch continuity. Compact reciprocal scans use background preparation for neighboring viewer positions. Small scans may complete faster serially. Use a `if __name__ == "__main__":` guard for scripts that start process workers. Parallel settings persist in GUI state; computed result arrays do not.

Mapping display, detector-hit filtering, and renderer choices are described in the preceding mapping section. For 2D powder and single-crystal detector figures, a red cross marks the direct-beam intersection when the forward beam hits the detector, including tilted or translated geometries. Detector Euler values keep their named axes for every rotation order. 2D/3D titles show entered Euler values and their application order. Geometry views label any inferred equivalent fixed-laboratory-axis xyz rotation explicitly. The Matrix Rotation tool's input mode, rotation order, angles, and result, and custom sample orientation matrices, persist in GUI state.

10.9 GUI operating sequence

1. Select the powder or single-crystal tab and the desired function.
2. Load a CIF or enter the required lattice/reflection values.
3. Enter beam energy and bandwidth.
4. Choose and validate detector input.
5. Choose legacy or geometry-aware rotations.
6. Enter scan or targeting parameters when applicable.
7. For 2D/3D families, run or inspect the 3D view first so the beam, sample, reciprocal-space object, and detector plane can be checked together.
8. Inspect the detector projection or one-dimensional pattern.
9. Check the summary and log area for the exact function family and parameter values.
10. Save the result figures and the parameter record before changing the configuration.

If a GUI result appears inconsistent, reproduce a minimal version through the Python API. Explicit keyword arguments make unit and convention errors easier to identify.

Chapter 11

Complete simulation examples

11.1 Example data files

Files needed to run the examples are kept with the manual rather than referred to by generic local paths. The current data set is:

`cif_files/V2O3_R-3c_room_T.cif` Corundum-type V_2O_3 at 301 K, space group R-3c (No. 167), with lattice parameters $a = b = 4.9537$ Å, $c = 14.0111$ Å, and $\alpha = \beta = 90°$, $\gamma = 120°$.

The package selects the first CIF data block containing a complete non-zero unit cell. Single-block example files are nevertheless preferable because the intended phase remains explicit to both readers and software.

11.2 Example A: lattice and detector inspection

This example constructs the two central objects without running a high-level simulation:

```
from trxrdpy.simulation.sample import LatticeStructure
from trxrdpy.simulation.detector import Detector
from trxrdpy.simulation.utils import energy_to_wavelength

lattice = LatticeStructure(space_group=227, a=5.431)
lattice.create_possible_reflections(qmax=5.0)
lattice.calculate_q_hkls()
lattice.calculate_d_hkls()
lattice.apply_rotation(rotx=-30, roty=-20, rotz=20)
lattice.check_Bragg_condition(
    wavelength=energy_to_wavelength(15000.0),
    e_bandwidth=1.0,
)

det = Detector(
    detector_type="manual",
    pxsize_h=75e-6,
    pxsize_v=75e-6,
    num_pixels_h=512,
    num_pixels_v=512,
    dist=0.30,
    poni1=0.0192,
    poni2=0.0192,
)
det.calculate_lab_grid()
```

```
print("Allowed reflections:", len(lattice.allowed_hkls))
print("Bragg reflections:", lattice.hkls_in_Bragg_condition)
print("Detector grid:", det.lab_grid.shape)
```

This is a useful first diagnostic because it separates crystallographic reflection generation from detector intersection.

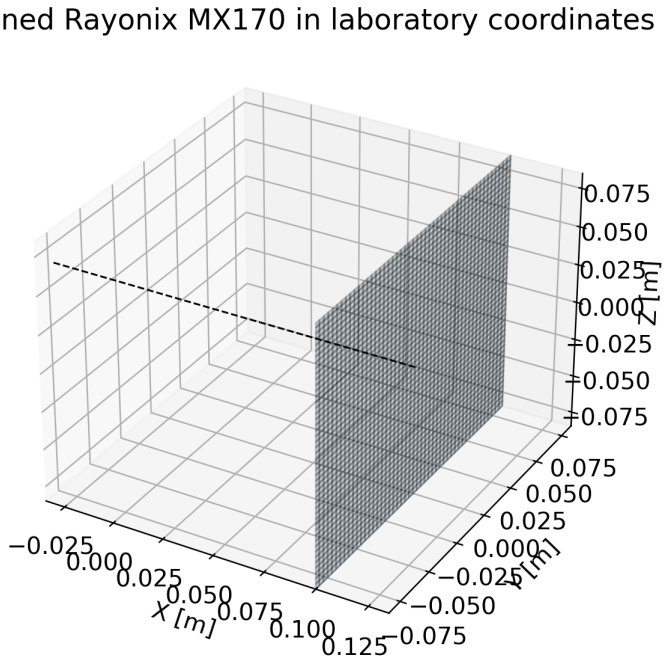

Figure 11.1: Detector laboratory-coordinate grid used as a first geometry diagnostic before running full diffraction simulations.

11.3 Example B: powder detector prediction

```
from trxrdpy.simulation import polycrystalline
from trxrdpy.simulation.powder_preparation import run_powder

crystal = {"cif_file_path": "cif_files/V2O3_R-3c_room_T.cif"}
settings = dict(
    det_type="rayonixmx170",
    det_binning=(4, 4),
    det_dist=0.10,
    det_poni1=0.085,
    det_poni2=0.085,
    energy=15000.0,
    e_bandwidth=1.0,
    qmax=3.5,
)

exp_3d = run_powder(polycrystalline.simulate_3d, crystal, **settings)
exp_2d = run_powder(polycrystalline.simulate_2d, crystal, **settings)

print(exp_2d.detector.num_pixels_h, exp_2d.detector.num_pixels_v)
```

The pyFAI registry supplies the Rayonix MX170 pixel size and native shape. The binning preserves the physical detector extent while reducing the calculation to 960×960 effective pixels.

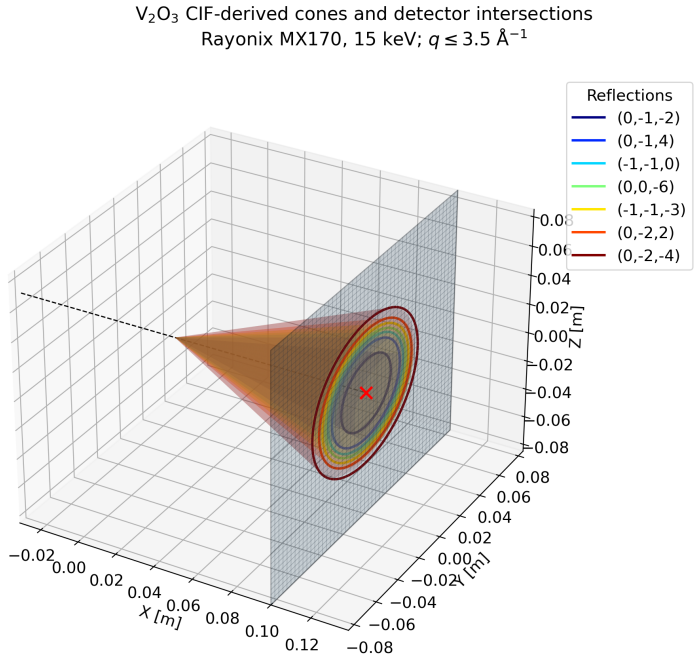

Figure 11.2: Complete simulation example B: CIF-derived R-3c V_2O_3 cone surfaces and their detector-intersection curves through $q = 3.5$ Å^{-1}.

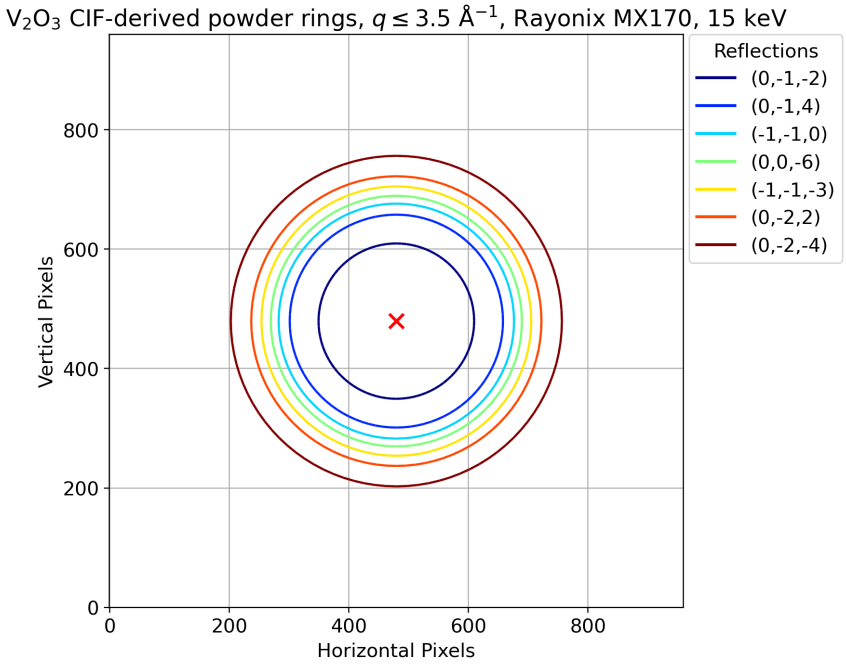

Figure 11.3: Complete simulation example B: the same cone intersections projected as continuous detector-clipped rings.

11.4 Example C: manual detector from calibration values

```
import numpy as np
from trxrdpy.simulation.polycrystalline import simulate_2d, simulate_3d
```

```
hkls = np.array([
    [0, 1, 2],
    [1, 0, 4],
    [1, 1, 0],
    [1, 1, 6],
    [2, 1, 4],
    [3, 0, 0],
])
q = np.array([1.7174, 2.3157, 2.5368,
              3.6979, 4.2700, 4.3938])

wavelength_m = 1.3829804621662048e-10
energy_eV = 12398.419843320026 / (wavelength_m * 1e10)

exp_3d = simulate_3d(
    det_type="manual",
    det_pxsize_h=0.000172,
    det_pxsize_v=0.000172,
    det_ntum_pixels_h=1475,
    det_num_pixels_v=831,
    det_dist=0.12,
    det_poni1=0.050,
    det_poni2=0.123,
    det_rotx=np.degrees(-0.023),
    det_roty=np.degrees(-0.5238161921742152),
    det_rotz=np.degrees(0.0),
    energy=energy_eV,
    q_hkls=q,
    hkls_names=hkls,
)

exp_2d = simulate_2d(
    det_type="manual",
    det_pxsize_h=0.000172,
    det_pxsize_v=0.000172,
    det_ntum_pixels_h=1475,
    det_num_pixels_v=831,
    det_dist=0.12,
    det_poni1=0.050,
    det_poni2=0.123,
    det_rotx=np.degrees(-0.023),
    det_roty=np.degrees(-0.5238161921742152),
    det_rotz=np.degrees(0.0),
    energy=energy_eV,
    q_hkls=q,
    hkls_names=hkls,
)

print(f"Energy: {energy_eV:.3f} eV")
print(exp_2d.detector.num_pixels_h, exp_2d.detector.num_pixels_v)
```

This example keeps the detector definition close to the calibration fields: distance, PONI coordinates, rotations, wavelength, pixel size, and maximum shape. Convert PONI-file rotations from radians before passing them to the current high-level simulation API.

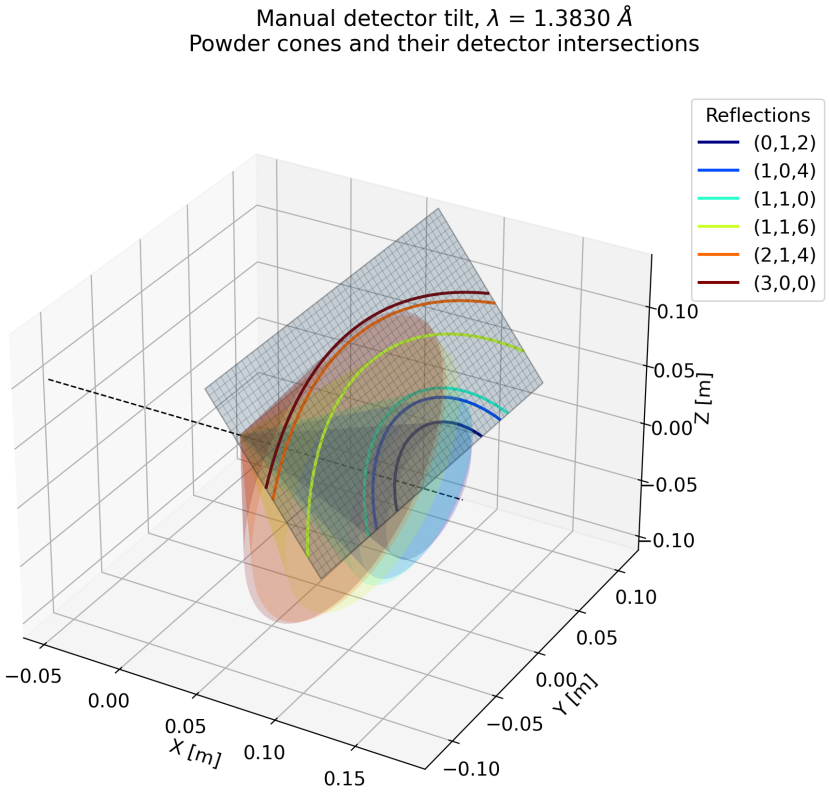

Figure 11.4: Complete simulation example C: three-dimensional powder-cone geometry with the manually defined tilted detector.

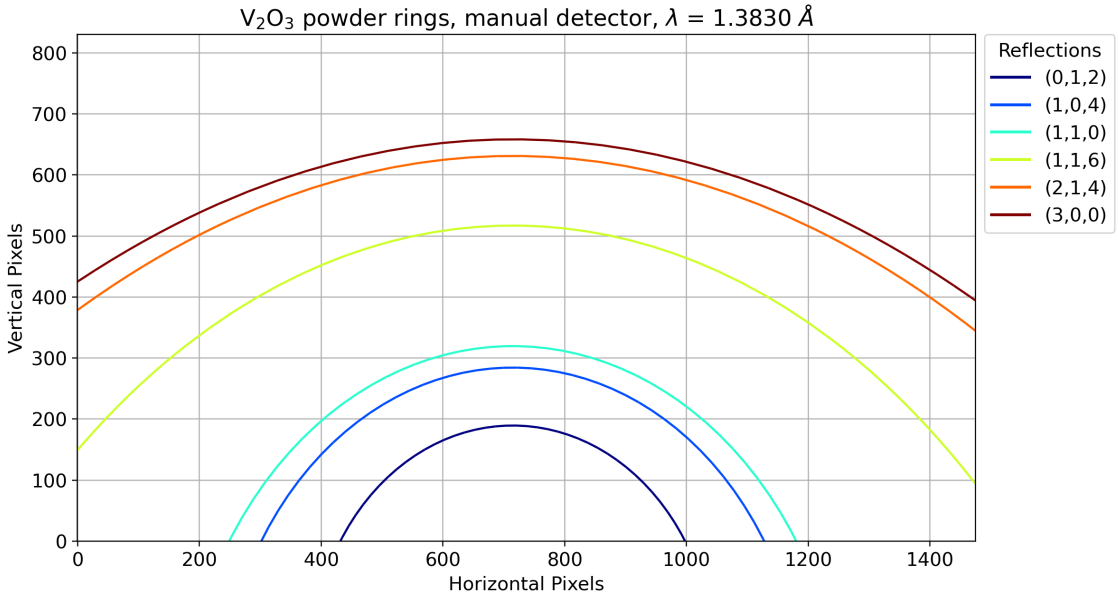

Figure 11.5: Complete simulation example C: detector projection from the same manually defined geometry.

11.5 Example D: geometry-aware single crystal

```
from trxrdpy.simulation.diffractometers import make_kappa_geometry
from trxrdpy.simulation.single_crystal import (
    simulate_2d_with_geometry,
    simulate_3d_with_geometry,
)

geom = make_kappa_geometry(
    kappa_tilt_deg=50.0,
    sample_defaults={"omega": 0, "kappa": 0, "phi": 0},
    detector_defaults={"tth": 0},
)

simulation_kwargs = dict(
    det_type="manual",
    det_pxsize_h=75e-6,
    det_pxsize_v=75e-6,
    det_ntum_pixels_h=1024,
    det_num_pixels_v=1024,
    det_dist=0.08,
    det_poni1=0.0384,
    det_poni2=0.0039,
    energy=15000.0,
    e_bandwidth=1.0,
    sam_space_group=227,
    sam_a=5.431,
    qmax=5.0,
    geometry=geom,
    sample_angles={"omega": -30, "kappa": 40, "phi": 30},
    detector_angles={"tth": -18},
)

experiment_3d = simulate_3d_with_geometry(**simulation_kwargs)
experiment_2d = simulate_2d_with_geometry(**simulation_kwargs)
```

The example encodes the instrument motions by name. Both calls consume the same parameter dictionary, so every reflection displayed on the active area in the detector projection belongs to the three-dimensional geometry shown immediately before it. Before applying the example to a real diffractometer, replace the generic axes and origins with the instrument definition.

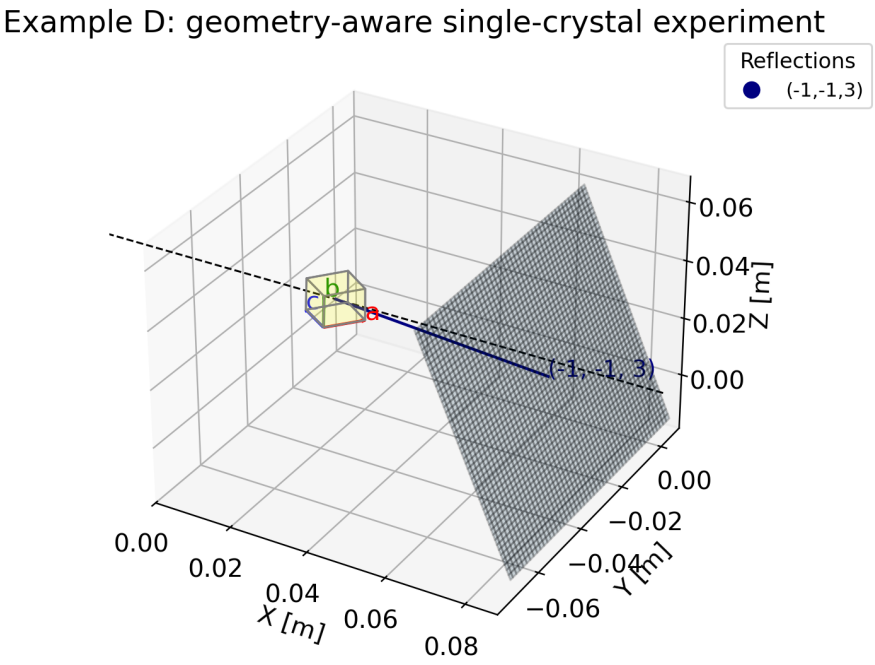

Figure 11.6: Complete simulation example D: three-dimensional single-crystal geometry for the named kappa sample motions and the detector arm at `tth=-18` degrees.

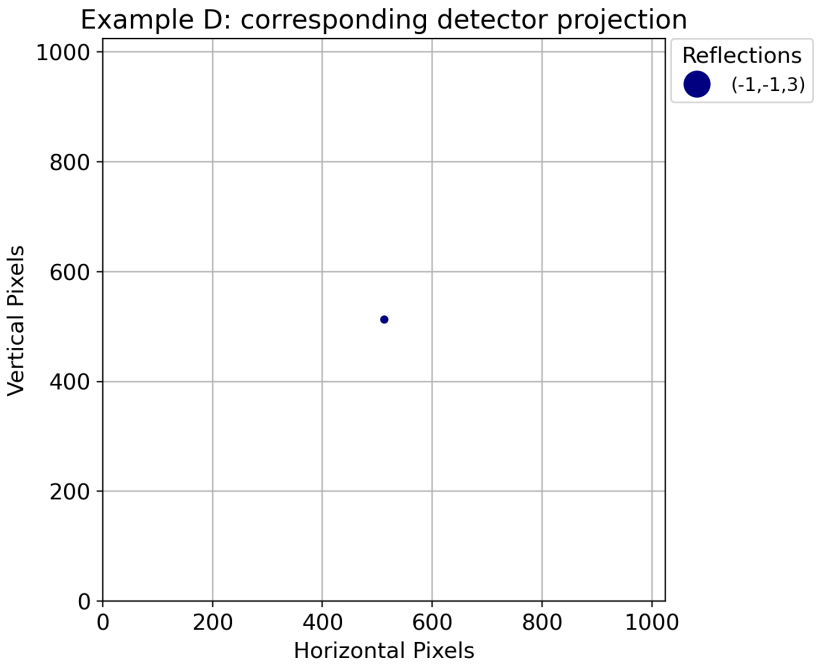

Figure 11.7: Complete simulation example D: detector projection generated from exactly the same geometry and motor angles as Figure 11.6.

11.6 Example E: reproducible parameter record

Save a plain dictionary beside numerical or graphical results:

```
import json
```

```
import trxrdpy

record = {
    "package": "trxrdpy",
    "model": "polycrystalline.simulate_2d",
    "energy_eV": 15000.0,
    "bandwidth_percent": 1.0,
    "detector": {
        "type": "rayonixmx170",
        "distance_m": 0.10,
        "poni1_m": 0.085,
        "poni2_m": 0.085,
        "binning_hv": [4, 4],
    },
    "reflection_units": "q in inverse angstrom",
    "q_hkls": q.tolist(),
    "hkls": hkls.tolist(),
}

with open("simulation_parameters.json", "w", encoding="utf-8") as handle:
    json.dump(record, handle, indent=2)
```

If an installed version attribute is unavailable, record the distribution version using `importlib.metadata.version("trxrdpy")`. Include the CIF or its persistent identifier, PONI file or checksum, geometry definition, rotation conventions, and script revision for serious work.

Chapter 12

Simulation API reference

12.1 High-level modules

Callable	Purpose
`polycrystalline.simulate_1d`	Powder pattern from CIF; optional detector-limited coverage and azimuth sectors.
`polycrystalline.simulate_2d`	Draw continuous detector-clipped rings from explicit q/d reflections.
`polycrystalline.simulate_3d`	Display cone surfaces and their detector-intersection curves in 3D.
`powder_preparation.run_powder`	Derive CIF/lattice reflection families through `qmax`, then run the selected 2D/3D powder function.
`single_crystal.simulate_2d`	Single-crystal detector simulation with optional intensity and configuration sliders.
`single_crystal.simulate_3d`	Single-crystal 3D simulation with optional intensity and configuration sliders.
`single_crystal.simulate_2d_with_geometry`	Single-crystal detector simulation with motor chains or transforms.
`single_crystal.simulate_3d_with_geometry`	Single-crystal 3D simulation with motor chains or transforms.
`single_crystal.simulate_reciprocal`	Reciprocal-lattice and Ewald view, with optional compact parameter scans.
`single_crystal.sample_rotations_for_Bragg_condition`	Legacy sample `roty`/`rotz` orientation scan and rotation map.
`single_crystal.scan_two_motors_for_Bragg_condition`	Geometry-aware two-motor scan.
`single_crystal.scan_two_parameters_for_Bragg_condition`	Legacy/general two-parameter Bragg map.
`single_crystal.detector_rotations_collecting_Braggs`	Legacy detector `roty`/`rotz` collection scan.
`single_crystal.detector_rotations_collecting_Braggs_with_chain`	Arbitrary detector motor-chain collection scan.
`single_crystal.detector_rotations_collecting_Braggs_with_geometry`	Diffractometer detector-arm collection scan.
`single_crystal.target_hkl_near_pixel_fixed_energy`	Inverse orientation targeting for a reflection and detector pixel.
`orientation_fit.fit_orientation`	Refine ranked mounting orientations from measured Bragg pixels at linked experimental poses.

12.2 Core classes

Class	Role
`cif.Cif`	Validated extraction of cell, space group, and fractional coordinates.
`sample.LatticeStructure`	Direct/reciprocal lattice, reflections, orientation, Bragg tests, and powder data.
`detector.Detector`	Detector pixels, calibration, rotations, transforms, and lab grid.
`experiment.Experiment`	Combined beam, lattice, detector, diffraction directions, pixel positions, and plots.
`geometry.Motor`	One named axis rotation with origin and frame.
`geometry.MotorChain`	Ordered instrument rotations evaluated by motor-name angle maps.
`geometry.DiffractometerGeometry`	Paired sample-stage and detector-arm chains.
`poni.PoniGeometry`	Normalized immutable values parsed from a PONI file.
`utils.AxisRotation`	General axis-angle rotation object.
`utils.RotationChain`	Ordered general rotation composition.
`single_crystal.` `FixedEnergyTargetingResult`	Complete fixed-energy cone, detector-intersection, mask, best-hit, and solution result.
`single_crystal.` `FixedEnergyAcceptedSolutions`	Accepted Euler or named-motor orientation family and predicted detector pixels.
`results.SimulationResult`	Portable numeric targeting, mapping, detector-scan, or reciprocal result.
`orientation_fit.` `OrientationExperiment`	Editable lattice, detector, pose, uncertainty, and measured-peak project.
`orientation_fit.` `OrientationFitResult`	Ranked fitted candidates and exact source-project snapshot.
`attenuation.XRayMaterial`	Offline optical constants and bulk/grazing attenuation lengths from material composition and density.

12.3 Geometry factories

`make_euler_geometry` Independent three-axis sample and detector chains using selectable Cartesian order and frame.
`make_legacy_euler_geometry` Alias of `make_euler_geometry`.
`make_kappa_geometry` Generic omega–kappa–phi sample stage and single-circle detector arm.
`make_diffractometer` Registry factory for predefined geometries.

12.4 Common utility functions

Function family	Purpose
`energy_to_wavelength`, `wavelength_to_energy`	Beam conversion between eV and meters.
`q_to_two_theta`, `d_to_two_theta`	Diffraction-coordinate conversion.

`axis_angle_to_matrix`, `euler_to_matrix`, `matrix_to_euler`	Rotation representations.
`make_transform`, `compose_transforms`, `invert_transform`	Homogeneous transformations.
`apply_rotation_matrix`, `apply_transform`	Apply orientations or transforms to arrays.
`diffractometer_to_dict` and related serializers	Convert geometry objects to JSON-compatible dictionaries.
`poni.write_poni_file`	Export flat pyFAI geometry as a PONI 2.1 calibration file.
`results.save_result`, `results.load_result`, `results.plot_result`	Save numeric scan results in HDF5 and replot without recomputation.
`orientation_fit.persistence.save_experiment`, `load_experiment`	Save and restore measured-peak orientation projects as JSON.
`orientation_fit.persistence.save_fit_result`, `load_fit_result`	Save and restore ranked orientation candidates as JSON.

12.5 Return objects and cached state

Many methods update object attributes instead of returning a new array. Examples include `Detector.calculate_lab_grid()`, `LatticeStructure.calculate_q_hkls()`, and `LatticeStructure.check_Bragg_condition()`. Read the documented attribute after the method call.

High-level simulations generally return an `Experiment`; powder 1D and search workflows instead return documented dictionaries or dataclasses whose named fields should be inspected directly.

Chapter 13

Validation, reproducibility, and troubleshooting

13.1 Validation hierarchy

Validate a simulation from simple quantities to complex output:

1. Confirm energy–wavelength conversion.
2. Confirm cell parameters, symmetry, and several known d spacings.
3. Confirm allowed reflections and equivalent-reflection behavior.
4. Confirm detector size, physical extent, distance, and beam center.
5. Confirm zero-angle geometry in 3D.
6. Apply one motor at a time and check its axis and sign.
7. Confirm a known reflection or calibrant pattern.
8. Only then run multidimensional scans or inverse targeting.

13.2 Common problems

13.2.1 Import fails

Confirm that installation and execution use the same Python interpreter. Use `python -m pip show trxrdpy` and print `sys.executable`. GUI import failures often indicate that the `gui` extra was not installed.

13.2.2 CIF cannot be read

Check the path, required cell fields, `_space_group_IT_number`, and atom-site fractional columns. If the file contains several blocks, remember that the first complete non-zero cell is selected.

13.2.3 No reflections satisfy Bragg condition

Check energy in eV, wavelength in meters, q in Å^{-1}, lattice orientation, `qmax`, and bandwidth in percent. Visualize reciprocal space before changing tolerances.

13.2.4 No reflections appear on the detector

A reflection may satisfy Bragg but miss the active detector. Check detector distance, dimensions, PONI coordinates, orientation, and image conventions. Use the 3D plot to distinguish a Bragg failure from an interception failure.

13.2.5 Powder rings are displaced or mirrored

Check PONI axis mapping, pixel order, image origin, horizontal sign, and detector rotations. Do not correct a convention mismatch by arbitrarily changing the beam center.

13.2.6 Geometry scan is unexpectedly slow

The number of evaluations grows multiplicatively with scan dimensions. Reduce reflection count, use coarser steps, narrow the range, and refine only around candidates. Avoid creating a full-resolution detector grid inside an unnecessary inner loop.

13.2.7 Changing angles has no effect

For a detector, call `calculate_lab_grid()` after changing angles. Also check whether a custom transform is active; it takes precedence over legacy Euler angles. Call `clear_transform()` to restore the Euler path.

13.2.8 Unexpected lattice state after repeated rotations

Check `mode`. Absolute rotations start from the initial orientation; relative rotations accumulate from the current one. Record the initial orientation and avoid mixing the two modes unintentionally.

13.3 Reproducibility record

For each published or operational simulation, retain:

- XRDpy version and Python environment;
- source script or GUI session;
- CIF and its source or checksum;
- detector type, PONI file, and binning;
- energy and bandwidth;
- coordinate definitions and rotation orders;
- diffractometer geometry and motor-angle maps;
- reflection selection and `qmax`;
- scan bounds, steps, seeds, and acceptance settings; and
- numerical results before graphical post-processing.

13.4 Known interface cautions

- The PyPI and import name is `trxrdpy`, not `xrdpy`.
- The high-level horizontal pixel-count keyword is currently spelled `det_ntum_pixels_h`.
- Several calculation methods store their result on the object and return `None`.
- A PONI file's wavelength metadata does not replace every explicit beam-energy argument.
- Generic predefined geometries must be validated before representing a real instrument.
- Analysis modules are independent of the Simulation workflow described here.

Part II

Analysis

Chapter 14

Analysis branch overview

14.1 Scope of the Analysis branch

The Analysis branch is the experimental-data half of XRDpy. It does not require the Simulation branch and it does not assume that a simulated pattern is available. Its job is to take beamline data and reduce it to reproducible scientific summaries: corrected detector images, azimuthally integrated one-dimensional patterns, fitted peak parameters, differential intensity traces, and publication-ready figures or tables.

The package is organized around the fact that pump-probe diffraction experiments have two kinds of complexity. The first is facility-specific: every beamline stores raw detector frames, timing information, metadata, and dark/reference conditions differently. The second is facility-independent: once detector geometry has been validated with a representative image and the selected source has been reduced to standardized `xy` patterns, plotting, differential analysis, and peak fitting are mostly the same. The manual therefore treats facility data reduction, final-pattern production, and shared analysis as separate layers.

Facility preparation
: The facility modules know how to read the raw beamline products. They resolve scan or run identifiers, apply timing-reference information, reject invalid shots, and create dark or reference images. The default route also averages detector frames into standardized two-dimensional arrays. FemtoMAX and SACLA can instead preserve metadata-selected frame identity for single-shot one-dimensional integration, but both still require a representative two-dimensional image for calibration.

Shared reduction and analysis
: The shared modules know how to work with calibrated images and `xy` patterns. This layer contains detector/cake diagnostics, pyFAI-based azimuthal integration, one-dimensional pattern visualization, differential analysis, and peak fitting. Final FemtoMAX and SACLA patterns may be integrated from representative two-dimensional images or aggregated from a compatible single-shot one-dimensional cache; both routes produce the same standardized `xy_files` products.

GUI orchestration
: The Analysis GUI is not a separate scientific method. It is an interface that collects parameters and calls the same backend routines. Its value is session management, path consistency, form validation, and a single workflow for users who prefer interactive execution.

14.2 Supported facilities

The Analysis branch contains dedicated namespaces for ESRF ID09, Max IV FemtoMAX, and SPring-8 / SACLA. These names are not simple labels; each namespace reflects a different raw-data

model.

FemtoMAX is handled through a wrapper layer that accepts modern explicit path objects while remaining compatible with local configuration-driven workflows. The beamline and MAX IV context are described in Refs. [4, 5]. In practice, users may still keep experiment-specific defaults in a local `config.py` or equivalent setup file, but the reduction functions should receive resolved paths explicitly when a workflow is documented. The module resolves timing-reference pings and builds standardized metadata HDF5 files. It can then export averaged two-dimensional images for dark, delay, and fluence workflows or integrate metadata-selected detector frames into the FemtoMAX single-shot one-dimensional cache. A representative dark or calibration image remains necessary for detector calibration in either case.

ESRF ID09 uses BLISS/txs raw data. Time-resolved ID09 pump-probe operation and chopper-based timing infrastructure are described in Refs. [1, 2, 3]. The ID09 routines open the BLISS dataset, select frames by delay token, average selected frames, and write standardized dark or delay-resolved images. ID09 also has an integration layer that understands ID09 delay-token conventions and cached delay points.

SACLA support is more facility-legacy and infrastructure-dependent. The facility context and hard-X-ray XFEL timing diagnostics are described in Refs. [6, 7, 8]. The code relies on SACLA database and timing utilities, reads tag-level metadata, applies shutter and beam-status filters, constructs delay lists, creates background or dark images, and can process large runs in chunks suitable for HPC execution. The SACLA integration namespace exposes both the shared representative-image workflow and single-shot integration of metadata-selected run/tag pairs. Raw frame and legacy pulse-metadata access use direct `stpy` and `dbpy` API calls; aggregation of an existing cache does not require those facility modules.

Because these facilities differ substantially, raw-data preparation is selected by facility. Identify the facility first, create the correct intermediate products, and only then move into the shared calibration, integration, differential-analysis, and fitting chapters.

14.3 Analysis data flow

The full analysis path is a staged pipeline. A user normally starts by defining where the experiment lives and which facility produced the data. Every facility route must produce or locate a representative two-dimensional detector image for calibration. Final pattern production then follows either the default representative-image route or, for FemtoMAX and SACLA, the single-shot one-dimensional route. The downstream `xy_files` interface is deliberately identical.

1. define the experiment paths and facility;
2. create or locate metadata, dark frames, and a representative two-dimensional calibration image;
3. validate detector calibration, PONI files, masks, cakes, and azimuthal conventions using that image;
4. select representative two-dimensional integration or, where supported, single-shot one-dimensional production and aggregation;
5. write or refresh the standardized final `xy` patterns;
6. inspect absolute and differential patterns;
7. calculate differential integrals or fit selected peaks;
8. summarize delay, fluence, or multi-experiment trends; and
9. export figures, tables, and reproducibility records.

The important practical point is that calibration and final-pattern production are related but distinct. Calibration always uses a representative two-dimensional detector image. After the

PONI file, mask, cake, and azimuthal convention have been validated, the optional single-shot route integrates metadata-selected raw frames separately and aggregates the available single-shot patterns. If either route fails before the final `xy_files` handoff, the likely problem is raw data, metadata, timing, path layout, detector geometry, or integration settings. Viewer, differential, and fitting failures occur after that common handoff.

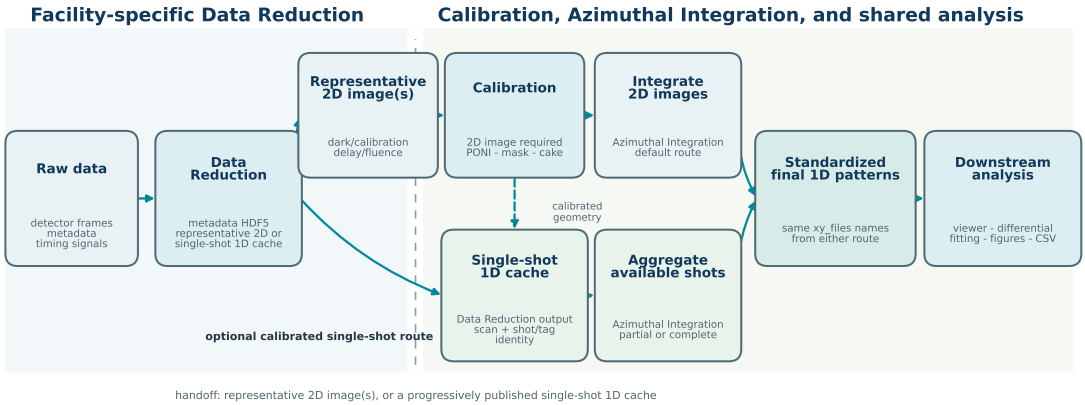

Figure 14.1: Analysis data flow with the two final-pattern production routes. Calibration always uses a representative two-dimensional detector image. The default route integrates representative dark, delay, or fluence images; the optional single-shot route integrates metadata-selected detector frames into a separate cache and aggregates the shots currently available. Both routes write the same final `xy_files` products for viewing, differential analysis, fitting, and export.

14.4 Programmatic and GUI routes

Programmatic workflows are the reference implementation for reproducible analysis. They expose explicit paths, scan identifiers, q ranges, azimuthal windows, normalization settings, and output names. They are best for scripts, publications, and batch processing.

The GUI is useful when parameter choices are still being explored. It keeps the same state across tabs, logs backend calls, and helps users avoid inconsistent path and facility settings. A good practical workflow is to use the GUI to inspect detector images, cakes, and initial fits, then transfer the final parameter values into a scripted workflow for reproducibility.

When documenting or publishing an analysis, report the backend function and the parameter values. A GUI screenshot is useful for communication, but it is not a reproducibility record by itself.

Chapter 15

Data organization and file conventions

15.1 Experiment root and analysis root

Analysis functions distinguish raw inputs from generated products. The central object is `trxrdpy.analysis.common.paths.AnalysisPaths`. It stores one experiment root, a raw-data subdirectory, and an analysis-output subdirectory. The resulting `raw_root` is where facility readers look for beamline files; the resulting `analysis_root` is where XRDpy writes processed images, cached `xy` files, fit tables, and figures.

The preferred style is to pass `paths=AnalysisPaths(...)` explicitly. Many functions also support legacy arguments such as `path_root`, `raw_subdir`, and `analysis_subdir`. These routes are equivalent only if they resolve to the same filesystem locations. For reproducibility, avoid relying on the current working directory; make the raw and analysis roots visible in the script.

The `AnalysisPaths` class does not create directories by itself. It only resolves locations. Directory creation occurs in the facility or analysis routines when outputs are written.

`experiment_root/`	Experiment-level root folder.
`RAW_DATA/`	Beamline raw files, scans, runs, or BLISS/SACLA/FemtoMAX inputs.
`calibration/`	Shared calibration files.
`detector.poni`	pyFAI detector geometry.
`mask.edf`	Detector mask.
`analysis/`	Generated and reusable analysis products.
`<sample>/temperature_<T>K/`	Sample and temperature branch.
`dark/<scan_tag>/`	Dark or calibration branch.
`2D_images/`	Averaged dark or calibration images.
`single_shot_1D_patterns/<azimuth>/`	Optional FemtoMAX or SACLA per-shot dark patterns.
`xy_files/`	Dark/calibration one-dimensional patterns.
`metadata/`	Facility metadata and provenance.
`figures/`	Detector, cake, fit, and diagnostic figures.
`excitation_wl_<wl>nm/delay/`	Delay-scan branch.
`fluence_<F>mJ/time_window_<tw>fs/`	One fluence and integration-time-window branch.
`2D_images/`	Delay-resolved averaged images.
`single_shot_1D_patterns/`	Optional per-shot delay patterns, organized by azimuth and then delay. Each filename retains scan and shot identifiers (FemtoMAX) or run and tag identifiers (SACLA).
`xy_files/`	Cached `q, intensity` patterns.
`fitting/`	Peak-fit CSV tables.
`figures/`	Viewer, differential, and fit plots.
`excitation_wl_<wl>nm/fluence/`	Fluence-scan branch.
`delay_<d>fs/time_window_<tw>fs/`	One delay and integration-time-window branch with the same standard outputs. Its optional cache uses the same azimuth-first layout with one fluence subdirectory per condition.

Figure 15.1: Typical Analysis directory tree. Facility-specific raw data are kept below the raw root, while the analysis root stores representative images, optional single-shot one-dimensional caches, final `xy` files, metadata, fit tables, and figures using sample, temperature, excitation, fluence, delay, and time-window tags.

15.2 Scan specifications and tags

Scan identity appears throughout the Analysis branch. For simple workflows a scan may be a single integer. For combined dark scans or averaged references it may be a list of integers. For cached outputs it may be a string such as `scan_167246` or a combined scan tag. Facility modules may also require a dataset, run number, BLISS scan number, or SACLA tag list.

The package uses stable scan tags to make filenames predictable. A single scan can be represented as a scan tag; a group of scans can be represented as a combined scan tag. These tags matter because later steps may reuse cached `xy` files or fit CSV files rather than recomputing them. If a user changes from scan `7` to scans `[7, 8]` but reuses an old output path, the analysis can silently compare the wrong products. Good examples show both the human scan selection and the tag or output folder it creates.

15.3 Standardized intermediate products

The shared pipeline is built around a small number of intermediate products. Keeping these products standardized is what allows different beamline preparations to use common integration, plotting, differential-analysis, and fitting code.

Metadata files
: Facility data reduction may write HDF5 or CSV metadata describing scan or run identity, frame validity, shot/tag identity, delay bins, fluence values, temperature, excitation wavelength, and timing windows. These files are part of the scientific record, not temporary implementation details. For the single-shot route, the metadata HDF5 is the authority for condition membership.

Representative two-dimensional image arrays
: Facility routines write averaged images, typically as NumPy arrays, for calibration and, in the default route, for dark conditions, delay points, or fluence points. A representative image is always required to validate the PONI file, mask, detector/cake display, and azimuthal convention. Producing every final-condition image is optional when the supported single-shot route is selected.

Single-shot one-dimensional cache
: FemtoMAX and SACLA can integrate each metadata-selected frame independently into a separate, resumable cache. Files retain scan/run and shot/tag identity, are published atomically, and carry an integration-settings fingerprint. This cache is an intermediate source for aggregation; it is not a second family of final patterns.

Final one-dimensional `xy` patterns
: Azimuthal Integration writes two-column text files. The first column is the radial coordinate, normally q in $Å^{-1}$, and the second column is intensity. Representative-image integration and single-shot aggregation write the same final paths and filenames, so plotting and fitting are independent of the selected source.

Result tables
: Differential analysis and peak fitting write CSV tables. These tables are the numerical outputs used for downstream plotting, error checking, and publication figures.

15.4 Reproducibility records

Every complete analysis records the raw-data selection, facility, sample name, temperature, excitation wavelength, fluence, time window, dark or reference selection, PONI file, mask file,

azimuthal offset, polarization factor, q normalization range, azimuthal windows, fitting windows, final-pattern source, output directory, and package version. A single-shot analysis additionally records the metadata HDF5 file, cache location, settings fingerprint inputs, production chunking or worker settings, and whether the reported final patterns were refreshed from a partial or complete cache.

This information is not optional bookkeeping. Time-resolved diffraction results are sensitive to reference choice, azimuthal sector, mask, q range, and normalization. Two analyses can use the same raw scan and produce different conclusions if these values differ. Manual examples must therefore let the user reconstruct the path from raw data to final plot.

Chapter 16

Facility-specific data reduction

Facility boundary

Facility modules are responsible for reaching a shared representation. The shared routines do not need to know the full raw-data layout of each beamline.

The examples in this chapter are launch examples. They show where each facility-specific backend is called and which products are expected before the workflow moves to shared calibration, integration, differential analysis, or fitting.

16.1 Max IV FemtoMAX

FemtoMAX is a time-resolved hard X-ray beamline at MAX IV Laboratory in Lund, Sweden [4, 5]. In the context of this manual, it represents synchrotron pump-probe experiments where detector images must be associated with timing-reference information before they can be averaged into delay or fluence conditions. The relevant facility-specific issues are therefore path layout, scan numbering, ping references, delay-bin definitions, and the distinction between dark, delay, and fluence scans.

FemtoMAX is the most modern facility wrapper in the Analysis branch. The user-facing modules construct an experiment object, resolve paths, load timing-reference information, create metadata HDF5 files, and expose both supported products: averaged two-dimensional detector images and a metadata-selected single-shot one-dimensional cache. The wrapper accepts either an `AnalysisPaths` object or explicit path arguments. If a local `config.py` is used to collect site- or proposal-specific defaults, treat it as a convenience layer that prepares those values, not as the scientific record. The script or notebook should still expose the resolved raw path, analysis path, scan numbers, ping-reference table, selected conditions, and final-pattern source.

The FemtoMAX workflow begins with a scan or scan collection and, for scans using ping timing, a timing-reference table. The packaged reference table can be used by default, or a custom CSV can be supplied. The reference table is validated before use; overlapping scan ranges, missing columns, and malformed ping values are rejected. The `ping2_ref_s` and `ping4_ref_s` columns are values in seconds and should retain every meaningful measured digit; do not round them before saving the CSV. XRDpy reads these references and promotes the raw ping arrays to 64-bit precision before subtraction, then converts the corrected delays to femtoseconds for bin assignment. Metadata created by an older release without this precision marker must be recreated with `overwrite=True` before image or single-shot production. The timing reference is used to center corrected delay distributions and to define which frames belong to each delay bin. Optional per-scan delay assignments bypass this timing step only for the explicitly listed scans, as described below.

FemtoMAX distinguishes three scan types. A `dark` scan creates a selection without pump metadata. A `delay` scan uses excitation wavelength, fluence, and a time window to group frames by corrected delay. A `fluence` scan is organized at one or more explicit selected delays, with fluence values aligned to scans. Each selection can feed averaged-image export or single-shot integration after calibration. The code intentionally rejects `selected_delays="auto"` for fluence exports, because a fluence series must be associated with a known delay.

The normal sequence is to inspect timing quality with `plot_pings_distribution` and create metadata with `create_h5_files`. From that metadata, two one-dimensional production routes are available. The default route exports averaged images with `generate_2D_imgs` and then integrates those representative images. The optional FemtoMAX single-shot route integrates every metadata-selected detector frame separately and can refresh the final one-dimensional patterns from whichever completed shots are already available. Both routes write the same final filenames below `xy_files`, so the viewer, differential-analysis, and fitting stages are unchanged.

16.1.1 Optional scan-delay assignments

When the timing tool is unreliable for particular scans, use `scan_delay_overrides_fs` to assign their delays explicitly. The default is `None`; there is no automatic long-delay threshold. This option is accepted by `plot_pings_distribution`, `create_h5_files`, `generate_2D_imgs`, and the underlying `Experiment` constructor. Python values are integer femtoseconds; 200 ns is 200 000 000 fs. Every assigned scan must also appear in `scans`. Repeated scan numbers are processed once, and conflicting assignments supplied as scan-delay pairs are rejected.

```
from pathlib import Path
from trxrdpy.analysis.common.paths import AnalysisPaths
from trxrdpy.analysis.MaxIV_FemtoMAX import datared

paths = AnalysisPaths(
    path_root=Path("/path/to/FemtoMAX2026"),
    raw_subdir="raw", analysis_subdir="analysis",
)
scans = [167298, 167299, 167300, 167301, 167302]
overrides_fs = {
    167300: 200_000_000,  # 200 ns
    167301: 200_000_000,  # another scan at 200 ns
    167302: 500_000_000,  # 500 ns
}
datared.create_h5_files(
    scans=scans, sample_name="sample", temperature_K=300,
    excitation_wl_nm=1500, fluence_mJ_cm2=15,
    time_window_fs=750, scan_type="delay",
    selected_delays="auto", delay_source="avg",
    scan_delay_overrides_fs=overrides_fs,
    ping_reference_path="/path/to/ping_references.csv",
    paths=paths, overwrite=True,
)
```

Here scans 167298 and 167299 retain normal ping correction and time-window sorting. All detector shot indices from each assigned scan are placed at its declared delay without ping-based rejection; missing or invalid pings do not discard those shots. The detector dataset shape supplies the shot count without reading image pixels at this stage. Existing detector-frame validity checks still apply during image or single-shot production.

For delay scans, the assigned delays are added to the regular auto-discovered or explicitly selected delay points. They are not shifted by automatic clustering, and assigned shots are not copied

into neighboring time windows. Scans at the same declared delay share a delay group. The usual `nb_shot_threshold`, when supplied, applies to the resulting total counts. For fluence scans, assigned delays must equal the explicit fixed delay of that metadata file; prepare distinct fixed delays separately and retain the scan-to-fluence mapping. Dark reduction ignores delay assignments.

Only unassigned scans require ping-reference coverage. An entirely assigned selection needs neither a ping-reference CSV nor raw ping datasets. Timing diagnostics label assigned traces as *assigned delay*: their constant values are not measured timing distributions or estimates of timing jitter.

Both timing paths produce the same `/delays/<delay>fs/scans/<scan>/indices` structure. Per-scan `timing_source` provenance records `ping` or `manual`; assigned scans also record `assigned_delay_fs`. The `/meta` group retains the complete override mapping. Ping diagnostic arrays contain only ping-timed shots, never fabricated manual measurements. Representative-image export, single-shot integration, final-pattern aggregation, visualization, differential analysis, and fitting use the standard metadata selection without another timing-mode option.

Regenerate products after changing timing assignments

Reusing metadata with a different override mapping is rejected. Recreate the metadata with `overwrite=True` and regenerate the dependent products. Changing a scan's delay can leave old image, shot-cache, or `xy` files under its previous delay name: overwrite replaces matching filenames, not obsolete delay folders. Use a fresh analysis subdirectory for a revised assignment, or deliberately remove the superseded derived products before rebuilding. Do not replace metadata while a production job is using it. Existing metadata without override fields continues to represent the ordinary ping-timing workflow, subject to the existing ping-reference precision checks.

16.1.2 FemtoMAX delay-scan 2D image production

The example below shows the FemtoMAX reduction call used for a DET58 delay scan at 300 K, 1500 nm, and 52 mJ cm^{-2}. The first call plots the corrected ping distribution for the selected scans. The second call creates or validates the metadata HDF5 file and exports averaged two-dimensional images into the standardized analysis tree.

The delay source is `p2`. The selected delays are explicit because these values define the image folders that the later shared azimuthal-integration functions read. The same call can be run on a workstation or cluster node that has access to the raw FemtoMAX files.

```
from pathlib import Path

import numpy as np

from trxrdpy.analysis.common.paths import AnalysisPaths
from trxrdpy.analysis.MaxIV_FemtoMAX import datared as femtomax_datared

paths = AnalysisPaths(
    path_root=Path("/path/to/FemtoMAX2026"),
    raw_subdir="raw",
    analysis_subdir="analysis",
)

sample_name = "DET58"
temperature_K = 300
excitation_wl_nm = 1500
```

```
fluence_mJ_cm2 = 52
time_window_fs = 1000
scan_type = "delay"
delay_source = "p2"
nb_shot_threshold = None
overwrite = True

scans = np.arange(181060, 181092 + 1)
selected_delays = [
    -98972, -49132, -32079, -23519, -15817, -12481,
    -11000, -9448, -8190, -6684, -5268, -2871,
    -1536, 1253, 2622, 4090, 6000, 8732, 10792,
    12662, 15292, 17528, 19314, 21927, 26283,
    30691, 40272, 57032, 84809, 200391,
]

femtomax_datared.plot_pings_distribution(
    scans=scans,
    mode="overlay",
    delay_source=delay_source,
    unit="fs",
    view="scatter",
    require_both=True,
    paths=paths,
)

experiment, exported = femtomax_datared.generate_2D_imgs(
    scans=scans,
    sample_name=sample_name,
    temperature_K=temperature_K,
    excitation_wl_nm=excitation_wl_nm,
    fluence_mJ_cm2=fluence_mJ_cm2,
    time_window_fs=time_window_fs,
    scan_type=scan_type,
    selected_delays=selected_delays,
    delay_source=delay_source,
    require_both=True,
    nb_shot_threshold=nb_shot_threshold,
    overwrite=overwrite,
    batch_size=500,
    use_parallel=True,
    max_workers=5,
    chunk_size=1,
    start_method="spawn",
    paths=paths,
)
```

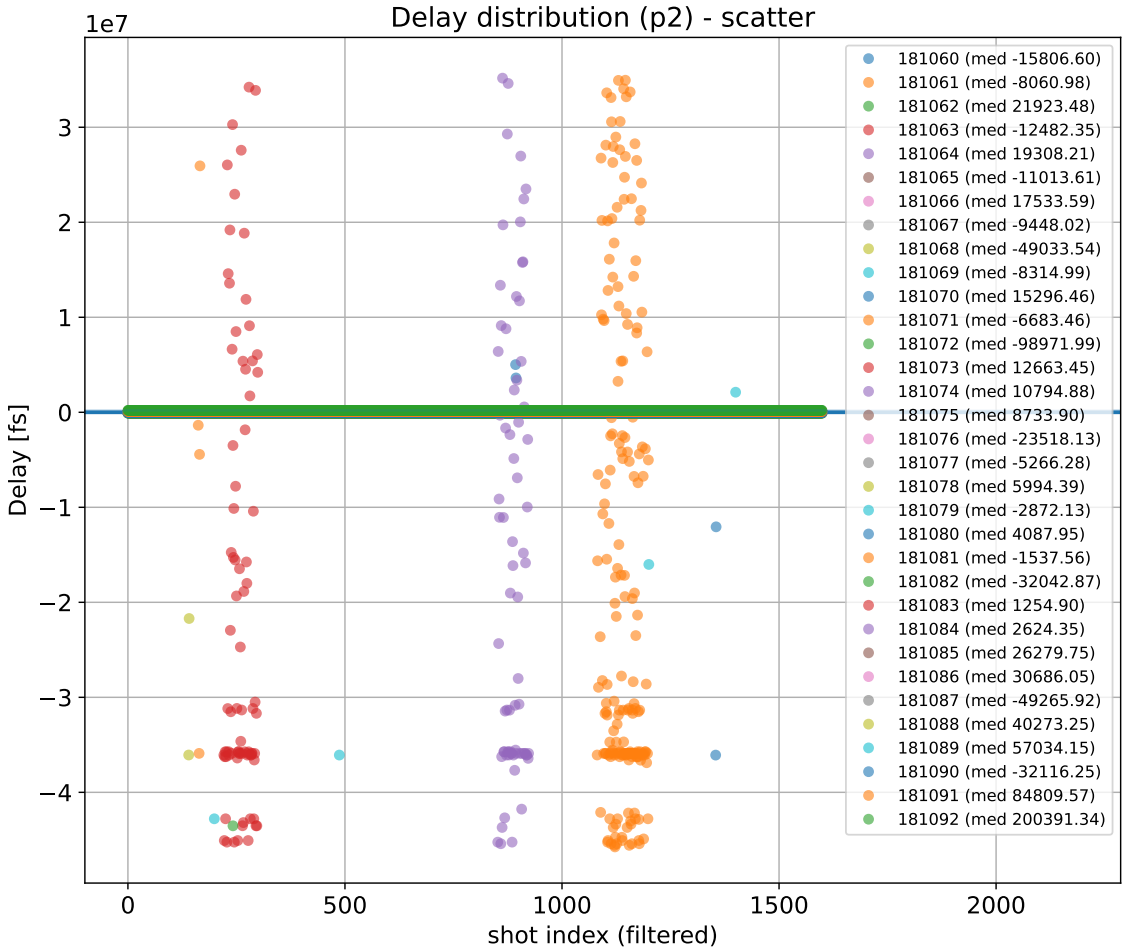

Figure 16.1: FemtoMAX DET58 `p2` timing distribution for scans 181060–181092, shown over the full delay range.

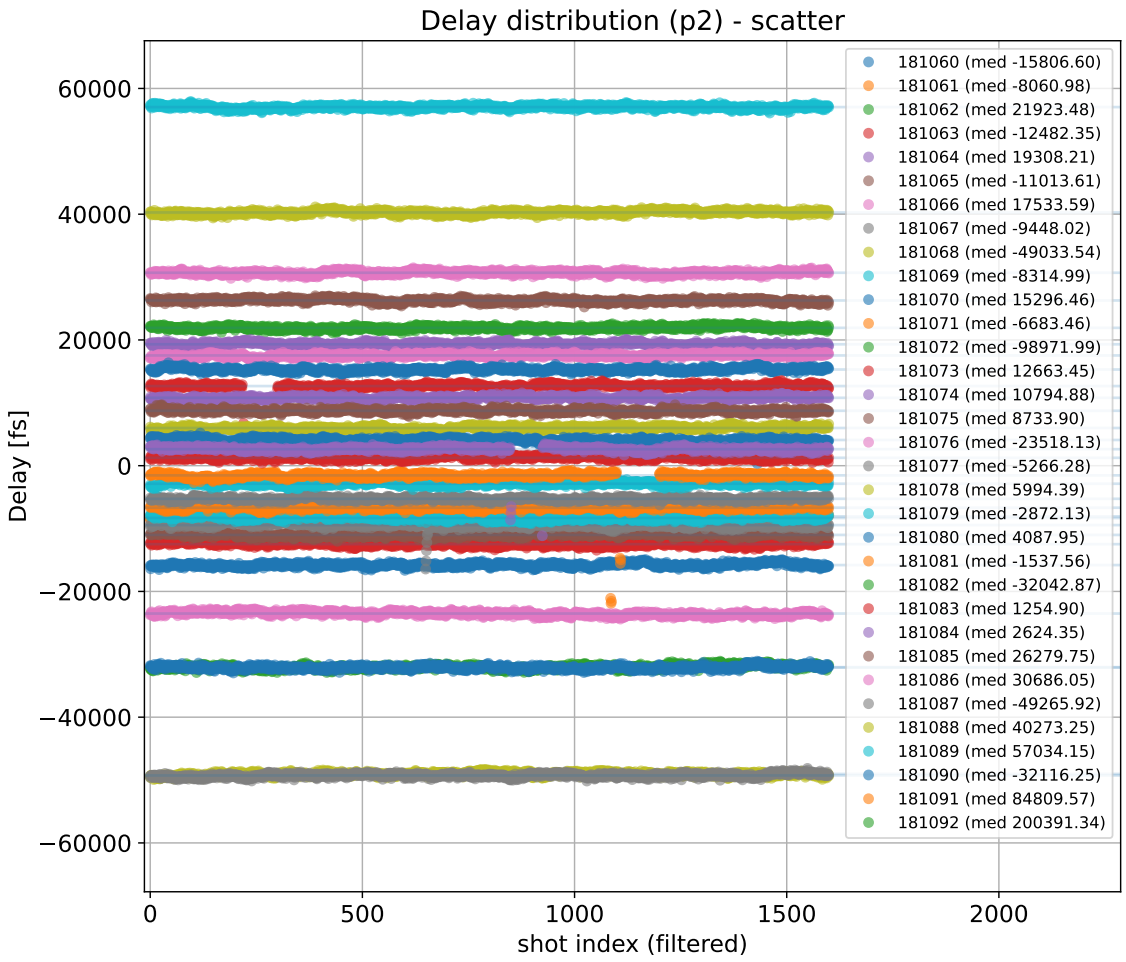

Figure 16.2: FemtoMAX DET58 `p2` timing distribution with the vertical axis restricted to the central delay region, making the main scan-to-scan timing structure visible.

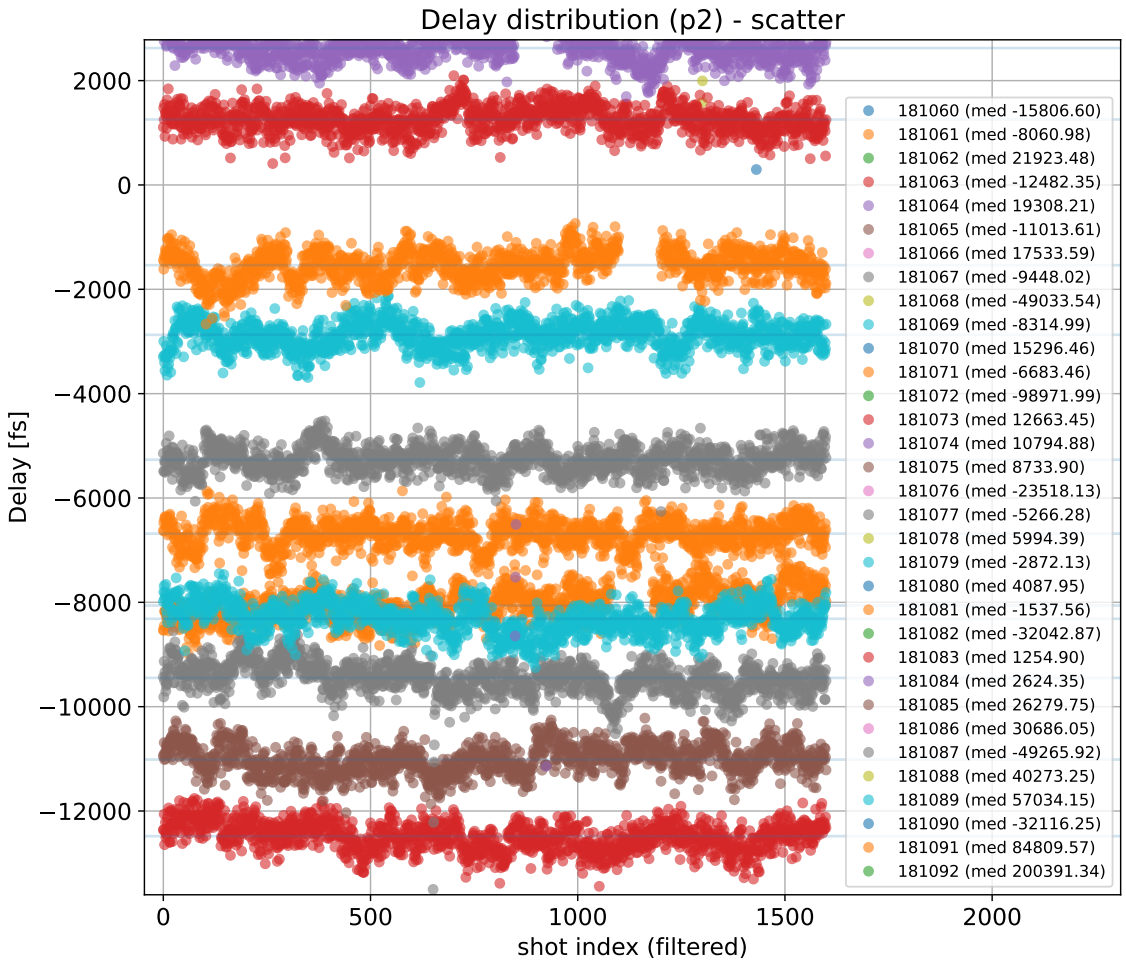

Figure 16.3: FemtoMAX DET58 `p2` timing distribution zoomed around the near-time-zero region, where the shot-to-shot timing jitter is visible on the femtosecond scale.

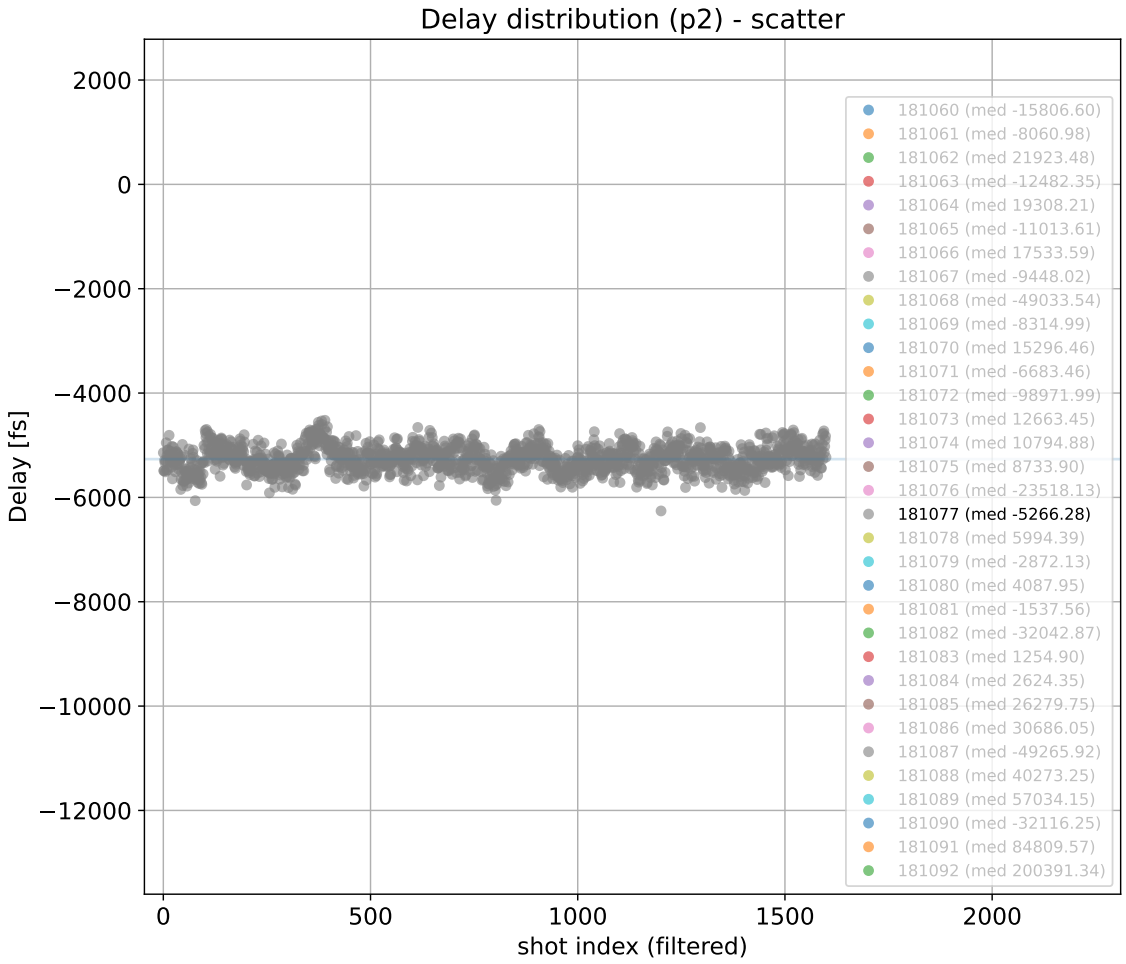

Figure 16.4: FemtoMAX DET58 `p2` timing distribution for the isolated scan 181077, used to inspect the local timing spread around the −5266.28 fs median delay.

16.2 ESRF ID09

ID09 is an ESRF beamline context associated here with time-resolved diffraction and scattering experiments at the European Synchrotron Radiation Facility in Grenoble, France [1, 2, 3]. The practical consequence for XRDpy users is that the raw data arrive through the ESRF data stack rather than through the FemtoMAX or SACLA file models. The module therefore focuses on BLISS datasets, txs delay metadata, scan keys, raw sample naming, and delay-token normalization.

The ESRF ID09 analysis namespace is built around BLISS/txs data access. The optional `pytxs` dependency is the ID09 local analysis tool used by XRDpy for parts of the raw-data handling layer; it is distributed separately as `pytxs` on PyPI [17]. The reduction functions open a BLISS dataset file located in the ID09 raw-data tree, select a scan key such as `<scan>.1`, read delay metadata, and average detector frames matching selected delay tokens. The raw sample name can be different from the analysis-facing sample name, so the functions support a `raw_sample_name` override.

ID09 delay handling is token-based. The raw metadata delays are formatted through txs utilities into canonical strings, and user selections are normalized to the same representation. This matters because the same physical delay may appear as a string token, a byte string, or a numeric value depending on where it enters the workflow. The reduction code standardizes these representations

before selecting frames.

The function `get_2D_img` averages frames for one delay and returns the image without writing it. `create_dark_from_ref_delay` averages a reference-delay selection and writes it into the standardized dark-image structure. `create_final_2D_images` exports averaged detector images for all or selected delay points, converts delay tokens to femtoseconds, and writes the output using the shared delay-series naming convention.

The ID09 azimuthal-integration module adds ID09-specific logic on top of this prepared-image layer. It resolves calibration paths, lists available cached delay points, integrates selected delays, plots absolute and differential one-dimensional patterns, and can create a fluence scan from a set of delay scans. This makes ID09 slightly different from FemtoMAX and SACLA: it has both facility-specific image preparation and facility-specific integration conveniences.

16.2.1 ID09 2D image production example

The ID09 preparation example starts from a BLISS dataset and scan number. The reference-delay image is written as a standardized dark image, and selected laser-on delays are written as standardized delay images. Downstream chapters can then use the cached `xy` files if they already exist, or integrate from these two-dimensional images if the cache is missing.

```
from pathlib import Path

from trxrdpy.analysis.common.paths import AnalysisPaths
from trxrdpy.analysis.ESRF_ID09 import datared as id09_datared

paths = AnalysisPaths(
    path_root=Path("/path/to/ESRF/ID09/proposal"),
    raw_subdir="RAW_DATA",
    analysis_subdir="analysis",
)

dark_path = id09_datared.create_dark_from_ref_delay(
    sample_name="NiS2",
    raw_sample_name="NiS2",
    dataset=1,
    scan_nb=7,
    delay_ref="-5ns",
    temperature_K=300,
    paths=paths,
    overwrite=True,
)

delay_image_paths = id09_datared.create_final_2D_images(
    sample_name="NiS2",
    raw_sample_name="NiS2",
    dataset=1,
    scan_nb=7,
    temperature_K=300,
    excitation_wl_nm=1400.0,
    fluence_mJ_cm2=10.7,
    time_window_fs=100000,
    delays=["100ps", "500ps", "1ns"],
    paths=paths,
    overwrite=True,
)
```

16.3 SPring-8 / SACLA

SACLA is the X-ray free-electron laser facility operated at the RIKEN SPring-8 Center in Harima, Japan, next to the SPring-8 synchrotron [6, 7]. The experiments represented by this namespace are closer to XFEL-style shot or tag processing than to a simple synchrotron image stack: each detector frame must be interpreted together with facility tags, timing metadata, shutter state, beam status, and background or laser-off information.

The SACLA reduction code reflects a more legacy and facility-dependent environment. It uses SACLA-specific packages such as `stpy` and `dbpy`, and it bootstraps paths from environment variables: `XRDPY_PATH_ROOT`, `XRDPY_ANALYSIS_SUBDIR`, and `XRDPY_TIME_METADATA_SUBDIR`. This is different from the more self-contained FemtoMAX wrapper, so SACLA preparation is best treated as a beamline-environment workflow.

SACLA metadata are tag-based. The reduction reads tag lists and synchronized facility parameters, then merges them with timing-tool CSV metadata. For delay and fluence scans it filters invalid shots using X-ray shutter status, laser shutter status, and beam-status flags. The delay calculation combines timing-edge information and programmed motor position, with timing diagnostics related to the branching method described in Ref. [8]. In the current implementation the timing-edge contribution is scaled by -2.7 and the programmed delay motor by 6.67, producing a delay column in femtoseconds.

The SACLA preparation layer supports creating delay lists, processing background runs, creating dark images from laser-off frames, creating final two-dimensional images, and producing a single-shot one-dimensional cache from metadata-selected run/tag pairs. Because SACLA datasets can be large, representative-image production remains chunked and single-shot production uses a dedicated PBS array sender. Both routes preserve the facility access model: direct `stpy` frame reads and batched `dbpy` metadata access where legacy metadata requires it. After calibration, users may integrate corrected representative images or aggregate the compatible completed shot files into the same final `xy_files` products.

For SACLA, document the reduction environment carefully. The database access layer, timing metadata folder, run number, beamline identifier, delay-bin definition, and background/dark strategy are all part of the analysis provenance.

16.3.1 SACLA 2D image production example

SACLA preparation depends on the local SACLA environment. Set the required path environment before importing the SACLA reduction module, create metadata for the selected run or run group, process the no-X-ray background run when one is used, and then create the final delay, fluence, laser-off, or differential image product.

```
import os

os.environ["XRDPY_PATH_ROOT"] = "/path/to/SACLA/proposal"
os.environ["XRDPY_ANALYSIS_SUBDIR"] = "analysis"
os.environ["XRDPY_TIME_METADATA_SUBDIR"] = "TM_data"

from trxrdpy.analysis.Spring8_SACLA import datared as sacla_datared

metadata_h5 = sacla_datared.create_metadata(
    bl=3,
    run=[1466583, 1466578],
    sample_name="sample",
    temperature_K=300,
```

```
    scan_type="delay",
    time_window_fs=250,
    excitation_wl_nm=800,
    fluence_mJ_cm2=1.0,
    time_step=250,
    overwrite=True,
)

sacla_datared.process_background_run(
    bl=3,
    run=1466500,
    overwrite=True,
)

delay_image = sacla_datared.create_final_2D_images(
    bl=3,
    scan_type="delay",
    metadata_h5_path=metadata_h5,
    delay=1000,
    background=1466500,
    detector_id="MPCCD-8N0-3-002",
    threshold_counts=40,
    save_laser_off=True,
    overwrite=True,
)
```

The SACLA single-shot production and aggregation interface is documented in Section 18.2. The one-dimensional viewer, differential, fitting, and multi-experiment analysis examples are presented later in Chapter 21, after the shared analysis pipeline chapters.

16.4 Facility comparison

The table below summarizes the practical differences between the three facility layers. It is not meant to hide the details; it is meant to show where each facility enters the shared workflow.

Facility	Raw input concept	Main preparation output	Shared handoff
FemtoMAX	scans plus ping references	metadata HDF5; averaged 2D arrays or single-shot 1D cache	identical final `xy_files` from either route
ESRF ID09	delay-resolved scan source	dark/final images and cached delay patterns	ID09 integration; no single-shot 1D mode
SACLA	beamline run/tag data	metadata HDF5; corrected 2D arrays or single-shot 1D cache	identical final `xy_files` from either route

Chapter 17

Calibration, masks, and detector diagnostics

17.1 Calibration inputs

Calibration and integration require a consistent detector geometry. In practice this means more than having a PONI file. The user must know which detector image is being integrated, which mask is being applied, how detector pixels are displayed, and how the package's azimuthal convention maps onto pyFAI's convention.

- a PONI file;
- an optional detector mask;
- a calibration or dark image;
- a radial coordinate convention; and
- an azimuthal coordinate convention.

The calibration module can discover or accept explicit PONI and mask paths. EDF masks and related detector-image files are read through fabio where appropriate [11, 12]. The compatibility loader can patch narrowly scoped legacy PONI issues, such as unsupported PONI-version syntax or detector `orientation` metadata. A load is accepted only when pyFAI has populated both detector pixel sizes; this catches older pyFAI releases that return an integrator but defer failure until the first image is integrated. Compatibility copies are published atomically and an identical existing copy is reused, so concurrent processes cannot observe a partly written PONI file. This patching is intentionally conservative and records the changes applied. A patched PONI file makes pyFAI loading possible; it does not prove that the experiment geometry is scientifically correct.

The single-shot one-dimensional mode does not replace this calibration stage. Before integrating raw frames shot by shot at FemtoMAX or SACLA, create or locate the representative dark or calibration two-dimensional image and complete the same detector/cake, PONI, mask, and azimuthal-convention checks used by the representative-image workflow. The resulting calibrated geometry is then reused for every single-shot integration.

The parameter `azim_offset_deg` is central. It maps the package display-coordinate azimuth convention to the pyFAI coordinate convention. The default value in many workflows is $-90°$, but verify this against a calibration image or a known anisotropic feature. The optional `polarization_factor` follows pyFAI's convention and must be either `None` or a finite number between -1 and 1.

17.2 Detector and cake diagnostics

Detector and cake plots are the first quality-control step after path and calibration setup. The detector panel shows the image in pixel coordinates. The cake panel shows the same image after pyFAI remapping into radial coordinate and azimuth. If the PONI file, mask, axis convention,

or azimuthal offset is wrong, the cake plot usually exposes the problem before it contaminates one-dimensional integrations.

The function `calibration.plot_detector_and_cake` computes this diagnostic. It supports independent detector and cake color limits, logarithmic display, optional detector-axis flips, row-wise normalization over a q interval, explicit radial and azimuthal ranges, and saving. Axis flips affect only the displayed detector panel; they do not change the integration arrays. This distinction is important because display correction is not the same as changing the scientific geometry.

The example in Figure 17.1 uses the ESRF ID09 NiS2 dark scan at 300 K with the corresponding room-temperature PONI file and EDF mask. The plotted settings follow the saved GUI state for this dataset: the EDF mask is applied, the detector display uses the saved y-axis flip, the detector color limits are $(0, 100)$, and the cake color limits are $(0, 2)$. These are display choices for inspection; they do not modify the calibrated geometry used later for integration.

```
from pathlib import Path

from trxrdpy.analysis import calibration

fig, axes, data = calibration.plot_detector_and_cake(
    sample_name="NiS2",
    scan=7,
    temperature_K=300,
    npt_rad=1000,
    npt_azim=360,
    azimuthal_range=(-90.0, 90.0),
    normalize=True,
    q_norm_range=(2.9308, 3.2827),
    use_mask=True,
    poni_path=Path("/path/to/NiS2_Room_T.poni"),
    mask_edf_path=Path("/path/to/Mask_NiS2_Room_T.edf"),
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    detector_clim=(0, 100),
    cake_clim=(0, 2),
    invert_detector_y=True,
    save=True,
    path_root=Path("/path/to/ESRF2023"),
    analysis_subdir="analysis",
)
```

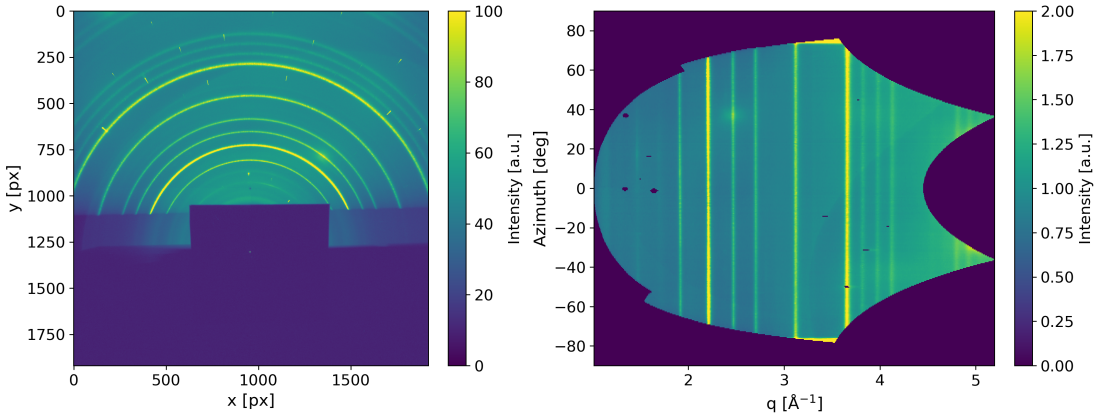

Figure 17.1: ID09 NiS2 detector image and two-dimensional cake for the 300 K dark scan, using the saved GUI display settings: detector y-axis flip, EDF mask, detector color limits $(0, 100)$, and cake color limits $(0, 2)$.

17.3 Azimuthal windows

Many workflows operate over azimuthal windows rather than over the full detector. Windows are used to separate anisotropic scattering, avoid detector artifacts, or compare symmetry-related sectors. The package supports two common representations. Edge-based windows use an ordered list of azimuthal edges and create adjacent sectors. Explicit window lists use individual (ϕ_0, ϕ_1) pairs.

Calibration and integration routines can also include a full-range pattern in addition to segmented sectors. The full-range pattern is convenient for quick inspection, but sector-resolved patterns are often more diagnostic. If a sector is used for differential analysis or fitting, the sector definition must be reported with the result. A peak amplitude integrated over $-90°$ to $90°$ is not directly comparable to one integrated over a narrower sector unless the normalization and interpretation are explicit.

Figure 17.2 uses the same NiS2 calibration context as the detector/cake diagnostic. The full range is $(-90°, 90°)$, and the segmented windows follow the saved GUI edge list $[-90, -70, -50, -30, -10, 10, 30, 50, 70, 90]$. The function `calibration.plot_cake_azimuthal_windows` computes the cake with the same pyFAI path as `calibration.plot_detector_and_cake`, overlays adjacent azimuthal sectors, and optionally adds the sector side bar used in the figure.

```
from trxrdpy.analysis import calibration

fig, axes, data = calibration.plot_cake_azimuthal_windows(
    sample_name="NiS2",
    scan=7,
    temperature_K=300,
    npt_rad=1000,
    npt_azim=360,
    azimuthal_range=(-90.0, 90.0),
    normalize=True,
    q_norm_range=(2.9308, 3.2827),
    use_mask=True,
    poni_path="/path/to/NiS2_Room_T.poni",
    mask_edf_path="/path/to/Mask_NiS2_Room_T.edf",
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    azimuthal_edges=[-90, -70, -50, -30, -10, 10, 30, 50, 70, 90],
```

```
    full_range=(-90, 90),
    cake_clim=(0, 2),
    show_side_bar=True,
    save=True,
    path_root="/path/to/ESRF2023",
    analysis_subdir="analysis",
)
```

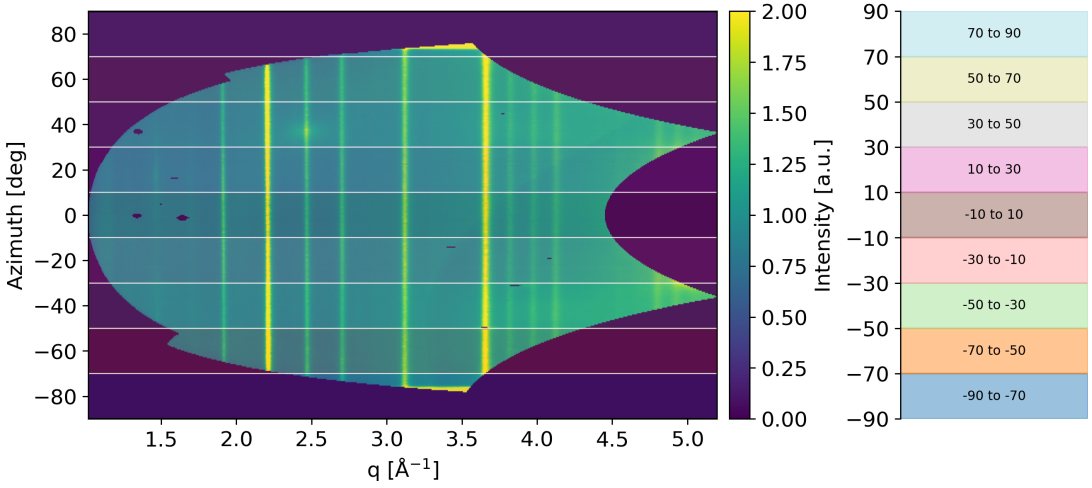

Figure 17.2: ID09 NiS2 cake with the saved segmented azimuthal windows overlaid. The side bar lists each sector from the GUI edge definition, while the full $(-90°, 90°)$ range is retained as the reference full-range integration window.

17.4 Calibration peak fitting

Calibration peak fitting quantifies whether a calibration or dark image behaves consistently across azimuth. The function `calibration.do_peak_fitting` integrates the calibration image into one-dimensional patterns, fits a linear background plus pseudo-Voigt peak in each azimuthal window, and writes a CSV table of fit parameters and quality metrics. Choose and record the fitting range, pseudo-Voigt fraction, normalization range, and fit method.

The most useful diagnostic is often not the individual fit overlay, but the trend of fitted peak position, FWHM, amplitude, or area versus azimuth. Smooth trends can indicate geometry or sample anisotropy; abrupt jumps usually indicate bad sectors, masking problems, or a fitting range that is too narrow. The functions `plot_property_vs_azimuth`, `plot_1D_plus_fit`, and `compare_1D_patterns` support this review.

```
from trxrdpy.analysis import calibration

fit_table = calibration.do_peak_fitting(
    sample_name="NiS2",
    scan=7,
    temperature_K=300,
    q_fit_range=(3.11, 3.135),
    azimuthal_ranges=[-90, -70, -50, -30, -10, 10, 30, 50, 70, 90],
    include_full=True,
    full_range=(-90, 90),
    npt=1000,
    normalize=True,
```

```
    q_norm_range=(2.9308, 3.2827),
    poni_path="/path/to/NiS2_Room_T.poni",
    mask_edf_path="/path/to/Mask_NiS2_Room_T.edf",
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    out_csv_name="peak_fits.csv",
    path_root="/path/to/ESRF2023",
    analysis_subdir="analysis",
)

fig_pos, ax_pos = calibration.plot_property_vs_azimuth(
    "NiS2", 7, 300,
    _property="pv_center",
    out_csv_name="peak_fits.csv",
    ylim=(3.11, 3.135),
    path_root="/path/to/ESRF2023",
    analysis_subdir="analysis",
)

fig_fwhm, ax_fwhm = calibration.plot_property_vs_azimuth(
    "NiS2", 7, 300,
    _property="pv_fwhm",
    out_csv_name="peak_fits.csv",
    ylim=(0.01, 0.06),
    path_root="/path/to/ESRF2023",
    analysis_subdir="analysis",
)
```

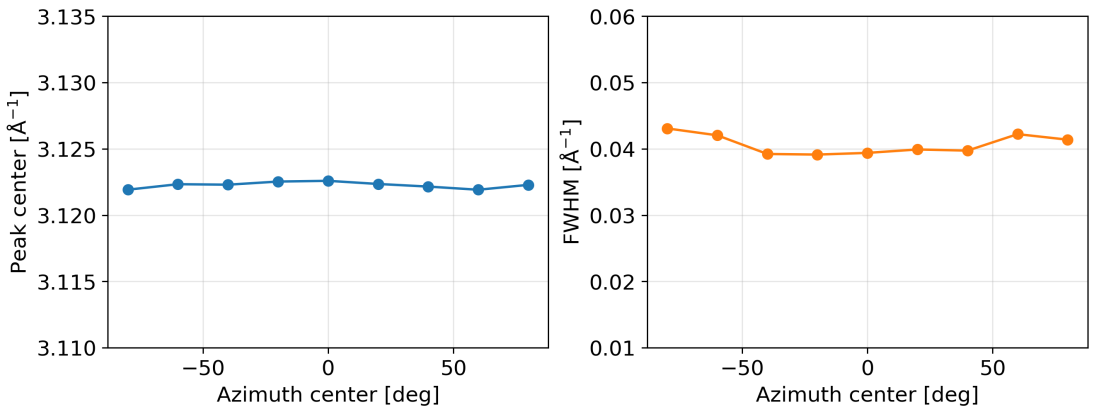

Figure 17.3: ID09 NiS2 calibration peak properties versus azimuthal sector for the 300 K dark scan. The full-range sector is excluded from the trend so the segmented azimuth windows can be compared directly.

17.5 Cake azimuthal-distribution analysis

The calibration image can also be used to quantify how intensity in a selected q band is distributed over azimuth. This is different from fitting a peak independently in each azimuthal sector. Instead, the workflow starts from a two-dimensional cake, integrates a narrow q band for every azimuthal bin, subtracts a scaled background band, and normalizes the remaining signal into an azimuthal fraction or percentage.

The user-facing function is `calibration.analyze_cake_azimuthal_distribution`. It uses the same

calibration context as the detector/cake diagnostic: sample name, scan, temperature, PONI path, mask path, radial binning, azimuthal range, normalization range, azimuthal offset, and optional polarization correction. The scientific selectors are:

- `q_value`: center of the signal q band in Å^{-1};
- `q_width`: full width of the signal q band;
- `bg_mode`: background placement, one of `left`, `right`, `average`, or `manual`;
- `bg_q_range`: explicit background interval used when `bg_mode="manual"`;
- `phi_windows`: optional $(\phi_{\text{center}}, \phi_{\text{halfwidth}})$ selectors used to summarize selected angular sectors; and
- `mirror_mode`: `none`, `separate`, or `together`, controlling whether positive and negative angular sectors are treated independently or combined.

The signal band is interpreted as $q_{\text{value}} \pm q_{\text{width}}/2$. For automatic background modes, `left` uses the adjacent lower-q band, `right` uses the adjacent higher-q band, and `average` averages the scaled lower- and higher-q backgrounds. Manual background mode is useful when nearby peaks, fluorescence structure, or detector artifacts make the adjacent bands unsuitable. The selected background is scaled to the signal-band width before subtraction.

```
from trxrdpy.analysis import calibration

result = calibration.analyze_cake_azimuthal_distribution(
    sample_name="sample",
    scan=167246,
    temperature_K=300,
    q_value=2.2038,
    q_width=0.0757,
    bg_mode="right",
    phi_windows=[(0, 10)],
    mirror_mode="none",
    npt_rad=1000,
    npt_azim=360,
    azimuthal_range=(-90, 90),
    normalize=True,
    q_norm_range=(2.9308, 3.2827),
    use_mask=True,
    save=True,
)

profile = result["profile_df"]
summary = result["summary_df"]
```

The returned `profile_df` contains one row per azimuthal bin. The main columns are `azimuth_deg`, `full_intensity`, `background_raw`, `background_scaled`, `sample_intensity`, `fraction`, and `percent`. Metadata columns record the signal q limits, background mode, background range, scale factor, and number of q bins used. The returned `summary_df` contains one row per requested phi selector and reports the corrected intensity sum, fraction, and percent in that angular window.

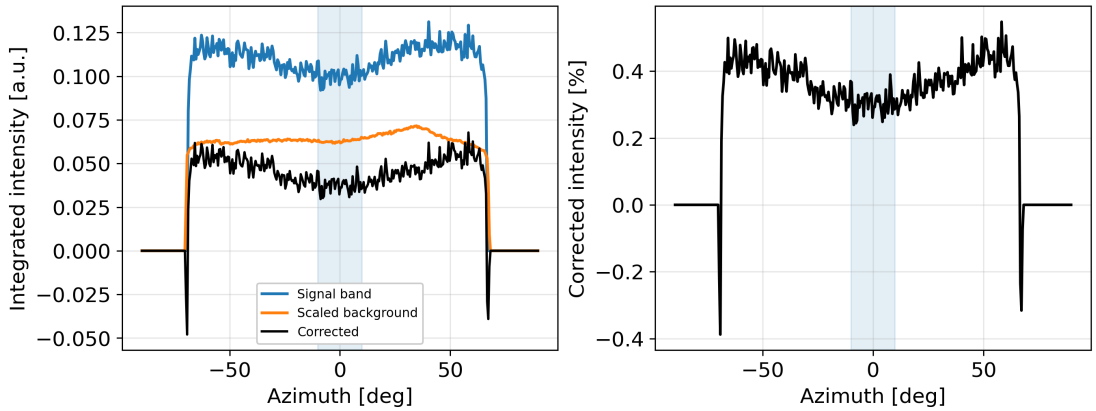

Figure 17.4: ID09 NiS2 cake azimuthal-distribution diagnostic for $q = 2.2038$ Å^{-1} with a 0.0757 Å^{-1} band and the background band placed on the high-q side. The left panel compares the signal-band integral, scaled background, and corrected response; the right panel shows the normalized corrected distribution with the selected phi window highlighted.

When called from scripts, the function can create Matplotlib figures directly. When called from the Analysis GUI, the expensive cake calculation is run with `make_plots=False`; the GUI then calls `calibration.plot_cake_azimuthal_distribution_profiles` on the main Qt thread. This split is intentional because pyFAI computation is safe to run in a worker, while Matplotlib window creation belongs on the GUI thread.

If `save=True`, the workflow writes the profile and summary tables as CSV files in the selected figures directory, together with the profile and normalized-distribution figures. Treat those CSV files as numerical outputs, not only as plotting byproducts. They define the q band, background treatment, selected phi sectors, and integrated fractions used in later interpretation.

Chapter 18

Azimuthal integration and standardized 1D patterns

18.1 Shared 2D integration workflow

The shared azimuthal-integration API is implemented in `trxrdpy.analysis._shared_2d.azimint` and reusable classes in `trxrdpy.analysis.common.azimint_utils`. It is the common route for beamlines whose preparation stage produces standardized two-dimensional images. FemtoMAX and SACLA expose this layer through their facility namespaces, and ID09 has additional facility-specific integration utilities.

The integration functions create `AzimIntegrator` objects configured with a PONI file, EDF mask, radial bin count, normalization setting, q normalization range, azimuthal offset, and optional polarization correction. Dataset classes such as `DarkDataset`, `DelayDataset`, and `FluenceDataset` describe where the input two-dimensional image is located and where `xy` cache files are written.

The shared workflow uses the same conceptual parameters for dark, delay, and fluence datasets:

- image source;
- reference or dark selection;
- azimuthal window;
- q or two-theta limits;
- normalization range;
- polarization correction; and
- cache overwrite behavior.

Existing `xy` files are reused unless overwrite is requested. This is a major performance advantage, but it also means that changes to PONI files, masks, azimuthal windows, radial bin counts, or normalization settings require attention. If the integration settings change, regenerate the corresponding `xy` cache.

```
from pathlib import Path
import numpy as np

from trxrdpy.analysis.common.paths import AnalysisPaths
from trxrdpy.analysis.MaxIV_FemtoMAX import azimint as femtomax_azimint

paths = AnalysisPaths(
    path_root=Path("/path/to/FemtoMAX/proposal"),
    analysis_subdir="analysis",
)

integrator, datasets = femtomax_azimint.integrate_delay_1d(
```

```
    sample_name="sample",
    temperature_K=300,
    excitation_wl_nm=800.0,
    fluence_mJ_cm2=1.5,
    time_window_fs=250,
    delays_fs=[-1000, 0, 1000, 5000],
    poni_path="/path/to/detector.poni",
    mask_edf_path="/path/to/mask.edf",
    azimuthal_edges=np.array([-90, -45, 0, 45, 90]),
    include_full=True,
    full_range=(-90, 90),
    npt=1000,
    normalize=True,
    q_norm_range=(2.65, 2.75),
    overwrite_xy=False,
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    paths=paths,
)
```

18.2 Single-shot 1D integration

FemtoMAX and SACLA can bypass representative delay, fluence, and dark two-dimensional image production after the metadata HDF5 has been created and calibration has been completed with a representative two-dimensional image. The function `integrate_single_shot_1d` reads the detector-frame identities already selected in the metadata file and integrates those frames separately. It does not repeat timing correction or delay/fluence-bin selection. The metadata HDF5 remains the authority for which frame belongs to each dark, delay, or fluence condition. FemtoMAX identities are scan numbers plus zero-based detector-frame indices; SACLA identities are run numbers plus event tags.

The single-shot cache is separate from the final cache. Within the experiment analysis directory, files are organized first by azimuthal window and then by delay or fluence. Scan/run identity remains in every filename, so no redundant scan subdirectory is added. Dark data do not have a delay or fluence layer:

```
single_shot_1D_patterns/
  -90_90/
    delay_100fs/
      <final_stem>_scan181060_shot42.xy
      <final_stem>_scan1466583_tag275628805.xy

single_shot_1D_patterns/
  -90_90/
    fluence_5p0mJ/
      <final_stem>_scan181060_shot42.xy
      <final_stem>_scan1466583_tag275628805.xy

single_shot_1D_patterns/
  -90_90/
    <final_dark_stem>_scan181060_shot42.xy
    <final_dark_stem>_scan1466583_tag275628805.xy
```

For FemtoMAX, the `shot` value is the zero-based detector-frame index stored in the metadata HDF5 `indices` dataset. For SACLA, the `tag` value is the event tag stored in the per-run `tags`

dataset. The filename begins with the exact final-pattern stem, including the azimuthal tag, and appends the scan/run and shot/tag identifiers at the end. This keeps every file independently identifiable while the directory hierarchy supports efficient discovery and aggregation. FemtoMAX aggregation and resume also recognize caches made by the earlier layout that placed the same filenames below `scan_*` subdirectories.

Each single-shot file is published with an atomic rename only after both columns have been written. It also contains a settings fingerprint derived from the PONI file, detector mask, radial binning, polarization factor, azimuthal offset, and azimuthal window. New FemtoMAX files include the corresponding settings as a second provenance header, allowing an incompatibility report to name each differing field rather than showing only two hashes. The SACLA fingerprint additionally records the background image, detector identifier, beamline, low-count threshold, pulse-intensity column, and whether pulse normalization applies. Aggregation validates representative fingerprints before announcing selected delay or fluence groups as available, then rejects any incompatible file encountered during reduction. Overwrite-disabled FemtoMAX production also refuses to resume into a directory whose existing representative file has another fingerprint. Existing compatible single-shot files are skipped unless `overwrite=True` is requested.

Production remains incremental even when I/O is optimized. FemtoMAX reads sorted selected frames in small HDF5 batches controlled by `read_batch_size` (default 16), but publishes each integrated shot separately as soon as it has been processed. Worker chunks are assembled separately for each delay or fluence and ordered round-robin, so every condition receives an early statistical subset before later chunks improve the statistics. When the run contains at least as many raw scans as workers, scan-affine lanes assign each raw file to one worker while preserving this round-robin order within each lane. The worker retains both the read-only HDF5 handle and detector dataset, preventing the same scan from being reopened for every chunk. `work_chunk_size` controls the coarser chunk size without changing batch-level progress reporting. If every requested output already exists and overwrite is disabled, the raw scan file is not reopened. A safe stop finishes the active HDF5 batch and atomic file publication; relaunching with overwrite disabled skips completed files and resumes missing shots. Hidden temporary names left by an interrupted atomic write are ignored by cache discovery; production does not recursively scan a potentially million-file tree merely to remove them. Fresh or only partly populated caches also skip per-file existence probes for delay/window directories that do not exist. SACLA keeps detector access serial because each run uses a stateful `stpy.StorageReader/StorageBuffer` pair; the pair is reused for the full run, pulse intensities are requested once per run when needed, and a complete cache does not initialize `stpy` at all. In both facilities the radial-to-two-theta coordinate is reused for subsequent shots with the same integration fingerprint.

Single-shot production performs substantially more work than representative-image integration. Each selected frame is integrated once for every requested azimuthal window and produces one independent XY file per window. For example, six segmented windows plus the full window produce seven integrations and seven files per shot; 142,754 selected shots therefore produce 999,278 patterns. The terminal start message reports both pending shots and pending patterns so this expansion is explicit. The package retains one pyFAI sparse integration engine per azimuthal window, avoiding lookup-table reconstruction when windows alternate, and writes compact twelve-significant-digit text while preserving the standard two-column XY format. On a parallel filesystem, creating and atomically publishing this number of small text files can itself be a major cost. Even with these optimizations, this route cannot approach the runtime of integrating a few representative averaged images because it intentionally preserves every selected shot. Request only the azimuthal windows needed for the on-the-fly analysis; runtime and file count scale approximately with their number.

Single-shot intensities are intentionally stored without q-range normalization. The available shots are averaged first, and the requested normalization is then applied once to the final pattern. This

preserves the order used by the representative-image route: average the selected detector response, integrate linearly, and normalize the resulting aggregate.

```
from pathlib import Path
import numpy as np

from trxrdpy.analysis.common.paths import AnalysisPaths
from trxrdpy.analysis.MaxIV_FemtoMAX import azimint as femtomax_azimint

paths = AnalysisPaths(
    path_root=Path("/path/to/FemtoMAX/proposal"),
    raw_subdir="raw",
    analysis_subdir="analysis",
)
metadata_h5 = Path(
    "/path/to/the/metadata_file_created_by_create_h5_files.h5"
)

# Long-running production step. Completed files become available atomically.
report = femtomax_azimint.integrate_single_shot_1d(
    metadata_h5_path=metadata_h5,
    poni_path="/path/to/detector.poni",
    mask_edf_path="/path/to/mask.edf",
    azimuthal_edges=np.array([-90, -45, 0, 45, 90]),
    include_full=True,
    full_range=(-90, 90),
    npt=1000,
    overwrite=False,
    read_batch_size=16,
    work_chunk_size=64,
    use_parallel=True,
    max_workers=4,
    start_method="spawn",
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    paths=paths,
)

# Fast refresh step. It uses all compatible files currently available.
integrator, datasets = femtomax_azimint.integrate_delay_1d(
    source="single_shot_1d",
    metadata_h5_path=metadata_h5,
    sample_name="sample",
    temperature_K=300,
    excitation_wl_nm=800.0,
    fluence_mJ_cm2=1.5,
    time_window_fs=250,
    delays_fs="all",
    poni_path="/path/to/detector.poni",
    mask_edf_path="/path/to/mask.edf",
    azimuthal_edges=np.array([-90, -45, 0, 45, 90]),
    include_full=True,
    full_range=(-90, 90),
    npt=1000,
    normalize=True,
    q_norm_range=(2.65, 2.75),
    overwrite_xy=True,
    use_parallel=True,
    max_workers=4,
```

```
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    paths=paths,
)
```

FemtoMAX single-shot production uses process parallelism when `use_parallel=True`. Each process constructs its own pyFAI integrator once, keeps one sparse engine for every requested azimuthal window, and retains its assigned read-only HDF5 detector datasets. This avoids shared HDF5 state while also avoiding repeated geometry, sparse-lookup, file-open, and dataset-discovery work. `read_batch_size` controls the number of selected frames read per HDF5 operation, `work_chunk_size` controls round-robin scheduling granularity, and `max_workers` controls concurrent integration processes. The Analysis GUI exposes dedicated *parallel processing*, *Parallel workers*, *Shots per worker task*, and *Start method* controls in Single-Shot 1D Production. The `spawn` method remains the default. Progress is reported after each HDF5 batch to both the nonmodal task dialog and the launching terminal.

Final-pattern refresh discovers a snapshot of completed files rather than assuming that every metadata-selected delay or fluence has already been produced. With an `"all"` selector, only groups having completed files for every requested azimuthal window are aggregated; incomplete groups are left for a later refresh. A hidden incremental accumulator records the compatible files already reduced for each group and window. Subsequent refreshes validate the file snapshot and parse only newly completed `xy` files before atomically replacing the standard final pattern. Final integration accepts `use_parallel` and `max_workers` for both input routes. Representative-image integration schedules the missing image/azimuthal-window patterns on worker threads, with a separate pyFAI integrator in each worker. Worker geometries are initialized serially before threaded calculation to remain compatible with older pyFAI geometry caches. Each representative two-dimensional image is loaded only once and shared read-only among its window tasks; image batches remain bounded so several large detector arrays are not loaded unnecessarily. This also uses the requested workers for a dark image, one selected delay, or one fluence whenever several azimuthal windows must be produced. Single-shot refresh assigns independent completed delay or fluence groups to workers; when only one group is selected, the worker budget is instead used for bounded concurrent shot-file reads. These levels are not nested, so the requested worker limit remains the total concurrency budget.

The same `source="single_shot_1d"` dispatch is accepted by the FemtoMAX and SACLA dark and fluence `integrate_*_1d` functions. Repeating the refresh with `overwrite_xy=True` replaces the same quasi-final or final `xy_files` as statistics improve; no second family of downstream filenames is created. The default `source="representative_2d"` retains the established representative-image workflow.

For SACLA, the production step uses the same frame-level corrections as representative-image creation. A processed no-X-ray background is subtracted first when requested, pixels below `threshold_counts` are then set to zero, and delay/fluence shots are divided by their pulse intensity before integration. Dark shots are not pulse-normalized. New metadata HDF5 files store `pulse_intensity` arrays aligned with their selected `tags`; older metadata remains usable through one direct batched `dbpy` lookup per run. Detector images are read with direct `stpy.StorageReader` and `stpy.StorageBuffer` calls.

```
from trxrdpy.analysis.Spring8_SACLA import azimint as sacla_azimint

report = sacla_azimint.integrate_single_shot_1d(
    metadata_h5_path="/path/to/analysis/.../metadata/selection.h5",
    poni_path="/path/to/detector.poni",
    mask_edf_path="/path/to/mask.edf",
    azimuthal_edges=np.array([-90, -45, 0, 45, 90]),
```

```
    include_full=True,
    npt=1000,
    beamline=3,
    detector_id="MPCCD-8N0-3-002",
    background=1466500,
    threshold_counts=40,
    overwrite=False,
    chunk_id=1,
    n_chunks=1,
    paths=paths,
)

integrator, datasets = sacla_azimint.integrate_delay_1d(
    source="single_shot_1d",
    metadata_h5_path="/path/to/analysis/.../metadata/selection.h5",
    sample_name="sample",
    temperature_K=300,
    excitation_wl_nm=1500,
    fluence_mJ_cm2=20,
    time_window_fs=250,
    delays_fs="all",
    poni_path="/path/to/detector.poni",
    mask_edf_path="/path/to/mask.edf",
    azimuthal_edges=np.array([-90, -45, 0, 45, 90]),
    npt=1000,
    normalize=True,
    q_norm_range=(2.65, 2.75),
    overwrite_xy=True,
    beamline=3,
    detector_id="MPCCD-8N0-3-002",
    background=1466500,
    threshold_counts=40,
    paths=paths,
)
```

The SACLA production step must run in an environment where the facility `stpy` package is available; legacy metadata without stored pulse intensities also requires `dbpy`. Large productions retain the facility scheduler model instead of starting local Python worker processes. In the Analysis GUI, the Data Reduction action submits the packaged `pbs/single_shot_1d_job_sender.sh` as a PBS array using the requested number of chunks and returns immediately with the scheduler job identifier. Each task passes its one-based `chunk_id` and common `n_chunks` to the integration backend. Metadata-selected `(run, tag)` identities are partitioned deterministically, array tasks own disjoint output files, and every file is published atomically.

```
export XRDPY_ENV_SETUP=/home/user/main.bashrc
export XRDPY_PATH_ROOT=/UserData/user/experiment
export XRDPY_METADATA_H5=/UserData/user/experiment/analysis/.../selection.h5
export XRDPY_PONI_PATH=/UserData/user/experiment/calibration/detector.poni
export XRDPY_MASK_PATH=/UserData/user/experiment/calibration/mask.edf
export XRDPY_N_CHUNKS=20
export XRDPY_AZIMUTHAL_EDGES="-90 -45 0 45 90"

qsub /path/to/trxrdpy/analysis/Spring8_SACLA/pbs/single_shot_1d_job_sender.sh
```

For manual submission, the PBS array range and `XRDPY_N_CHUNKS` must agree; the GUI sets both values from its *PBS array chunks* field. Once compatible shot patterns exist, aggregation reads only the HDF5 selection and completed cached `xy` files and can therefore run in the normal

analysis environment while array tasks continue producing additional shots.

Facility availability

The single-shot 1D integration and aggregation mode described in this section is implemented for the FemtoMAX and SACLA pipelines. It is not available for the ESRF ID09 pipeline, which continues to use its facility-specific prepared-image and cached-pattern workflow.

18.3 Delay-scan patterns

Delay-scan integration creates a time series of final one-dimensional patterns from either delay-resolved representative images or, for FemtoMAX and SACLA, the compatible completed files in a single-shot cache. The function `integrate_delay_1d` accepts one delay, a list of delays, or `"all"`. Representative-image selection discovers available images from the standardized analysis tree. Single-shot selection discovers only condition groups that currently contain compatible completed patterns for every requested azimuthal window; it does not assume that all metadata-selected groups have already been produced. Both routes normalize delay selection to integer femtoseconds and write the same final filenames.

Plotting functions can show absolute patterns, difference patterns relative to a reference, or both. A reference may be a selected delay, a dark pattern, or another supported reference specification depending on the facility wrapper. The reference choice is part of the scientific result. For example, subtracting a negative-delay reference and subtracting a dark pattern answer different questions.

When interpreting delay patterns, inspect the absolute patterns before the differences. A difference pattern can look clean even when the absolute pattern contains a masked-detector artifact, a normalization problem, or an unexpected baseline. The robust sequence is detector/cake diagnostic, absolute pattern inspection, reference selection, then differential plotting.

Figure 18.1 uses the ESRF ID09 NiS2 viewer dataset and is generated through the ID09 one-dimensional viewer backend. The cached `xy` files are loaded with the saved PONI geometry so the horizontal axis is displayed as q. The -5 ns reference is displayed at 0 ns after applying the saved $+5$ ns delay offset, matching the GUI convention.

```
from trxrdpy.analysis.ESRF_ID09 import azimint as id09_azimint

fig, axes = id09_azimint.plot_1D_abs_and_diffs_delay(
    sample_name="NiS2",
    raw_sample_name="NiS2",
    dataset=1,
    scan_nb=7,
    temperature_K=300,
    excitation_wl_nm=1400.0,
    fluence_mJ_cm2=10.7,
    time_window_fs=100000,
    delays_fs="all",
    ref_type="delay",
    ref_value=-5000000,
    ref_delay="-5ns",
    path_root="/path/to/ESRF2023",
    raw_subdir="RAW_DATA",
    analysis_subdir="analysis",
    poni_path="/path/to/NiS2_Room_T.poni",
    mask_edf_path="/path/to/Mask_NiS2_Room_T.edf",
```

```
    azim_window=(-90.0, 90.0),
    npt=1000,
    q_norm_range=(2.9308, 3.2827),
    normalize=True,
    compute_if_missing=False,
    xlim=(1.5, 4.5),
    fs_or_ps="ns",
    delay_offset_fs=5000000,
    polarization_factor=0.99,
    save_plots=True,
)
```

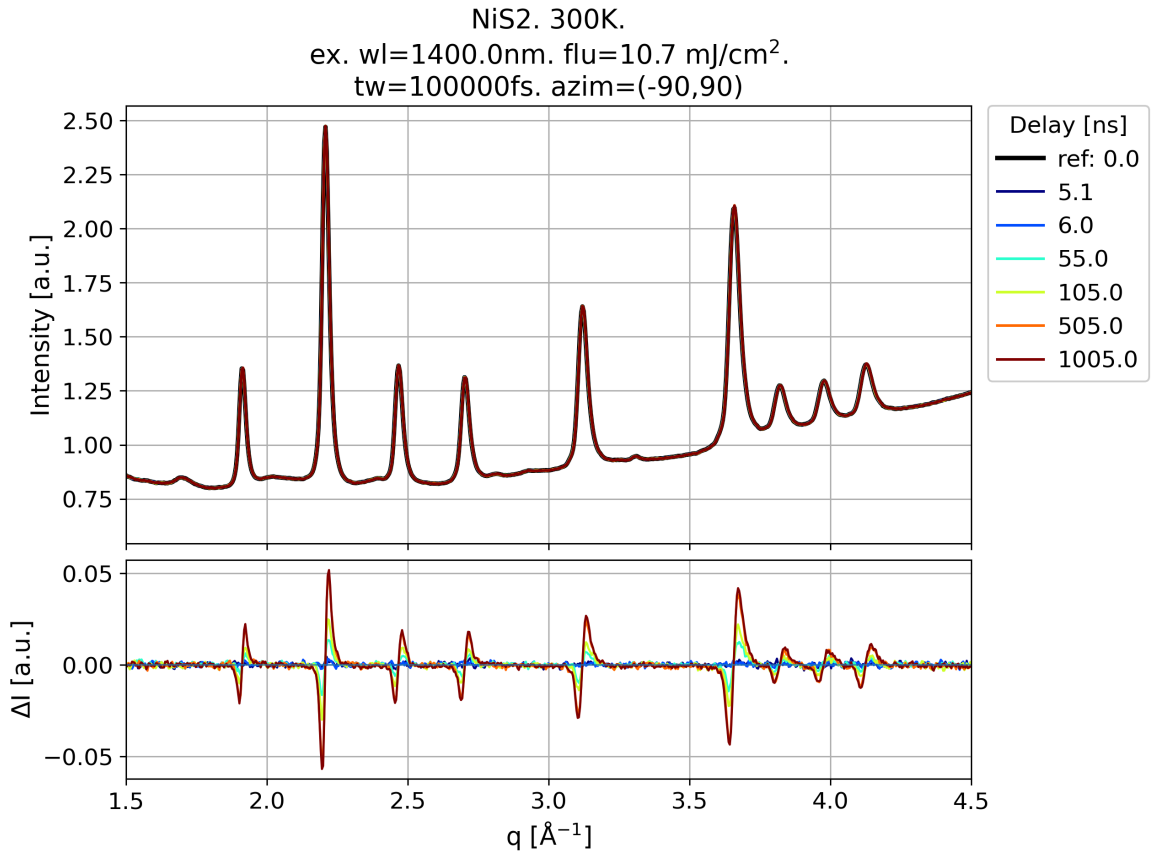

Figure 18.1: ID09 one-dimensional viewer example for NiS2 at 300 K. The top panel compares absolute full-azimuth patterns at the negative-delay reference and selected laser-on delays; the bottom panel shows differences relative to the −5 ns pattern after the saved +5 ns display offset.

18.4 Fluence-scan patterns

Fluence-scan integration compares one-dimensional patterns at different pump fluences, usually at a fixed delay. The dataset identity therefore includes sample name, temperature, excitation wavelength, fluence, time window, and delay. The package normalizes fluence labels and constructs conventional output paths so that fluence series can be reloaded for plotting, differential analysis, or fitting.

A fluence series is not just another delay series. In a delay scan the independent variable is time at fixed excitation condition. In a fluence scan the independent variable is excitation density, and

the selected delay defines the time slice being compared. Captions and filenames must make that fixed-delay condition explicit.

```
from trxrdpy.analysis.MaxIV_FemtoMAX import azimint as femtomax_azimint

fig, axes = femtomax_azimint.plot_1D_abs_and_diffs_fluence(
    sample_name="sample",
    temperature_K=300,
    excitation_wl_nm=800.0,
    delay_fs=1000,
    time_window_fs=250,
    fluences_mJ_cm2=[0.5, 1.0, 2.0, 4.0],
    ref_type="dark",
    ref_value="scan_12344",
    poni_path="/path/to/detector.poni",
    mask_edf_path="/path/to/mask.edf",
    azim_window=(-90.0, 90.0),
    npt=1000,
    normalize=True,
    q_norm_range=(2.65, 2.75),
    compute_if_missing=True,
    overwrite_xy=False,
    xlim=(1.5, 4.5),
    fluence_digits=3,
    save_plots=True,
    path_root="/path/to/FemtoMAX/proposal",
    analysis_subdir="analysis",
)
```

18.5 Quality checks before fitting

Before differential analysis or fitting, verify:

- stable q grids or correctly resampled patterns;
- acceptable signal-to-background ratio;
- consistent normalization;
- absence of masked-detector artifacts in the integrated windows; and
- correct reference selection.

These checks are faster than debugging failed fits later. A good rule is that a peak must be visually identifiable in the integrated patterns before fitting is attempted. If a peak is only visible after aggressive subtraction or normalization, the fitting model and uncertainty estimate need extra scrutiny.

Chapter 19

Differential analysis

19.1 Peak and background specifications

Differential analysis summarizes changes in selected q regions without necessarily fitting a full peak model. A peak specification defines the q interval of interest and how the background region is selected. The background can be placed before or after the peak window, or otherwise specified by the analysis utilities. This makes the result easier to interpret than a black-box integral: the user can state exactly which q interval contributed to the signal and which interval estimated the background.

The differential routines operate on differences relative to a reference. As in the integration chapter, reference choice matters. A dark reference, a negative-delay reference, and an average of multiple reference delays can produce different physical interpretations.

19.2 Delay differential traces

The main delay differential entry point, `differential_analysis.plot_differential_integrals`, computes signed ΔI and absolute $|\Delta I|$ integrals for a selected peak region and matched background. Error bars, when requested, are derived from the background response at the same delay. This gives a direct visual check of whether the peak-region response is larger than the local background variation.

Delay traces can be plotted in femtoseconds or converted to other time units. A display offset can be applied when the experimental time zero is refined after reduction. The output is both a table and a figure, so the numerical trace can be reused for further analysis.

Figure 19.1 uses the ID09 NiS2 delay dataset shown in the one-dimensional viewer example. The selected peak is the (202) region, integrated over $q = (3.0182, 3.2232)$ Å^{-1}, with the matched background placed after the peak window. The reference is the -5 ns pattern, and the displayed delay axis includes the saved $+5$ ns offset.

```
from trxrdpy.analysis import differential_analysis

peak_specs = {
    "202": {
        "q_range": (3.0182, 3.2232),
        "bg_mode": "after",
    }
}

df, fig = differential_analysis.plot_differential_integrals(
    sample_name="NiS2",
```

```
    temperature_K=300,
    excitation_wl_nm=1400.0,
    fluence_mJ_cm2=10.7,
    time_window_fs=100000,
    delays_fs="all",
    ref_type="delay",
    ref_value=-5000000,
    poni_path="/path/to/NiS2_Room_T.poni",
    mask_edf_path="/path/to/Mask_NiS2_Room_T.edf",
    azim_window=(-90.0, 90.0),
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    peak="202",
    peak_specs=peak_specs,
    npt=1000,
    normalize_xy=True,
    q_norm_range=(2.9308, 3.2827),
    compute_if_missing=False,
    unit="ns",
    delay_offset_fs=5000000,
    show_errorbars=True,
    save=True,
    path_root="/path/to/ESRF2023",
    analysis_subdir="analysis",
)
```

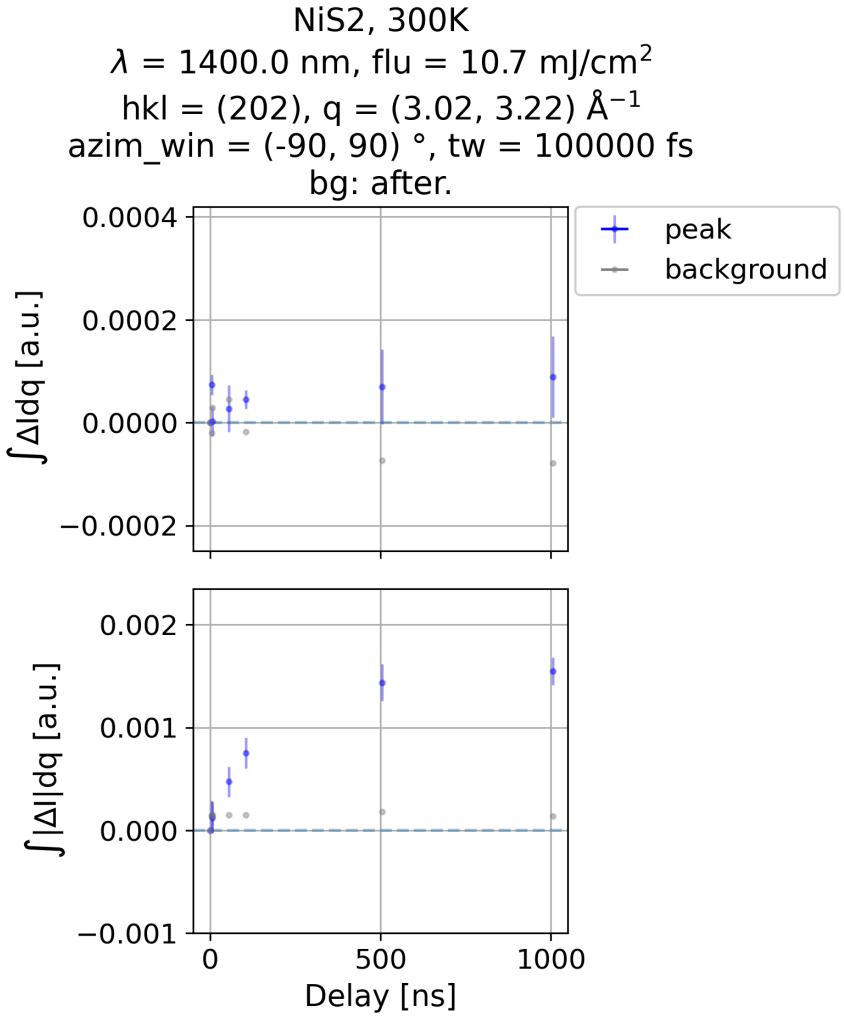

Figure 19.1: ID09 NiS2 differential-integral example for the (202) peak region. The upper panel shows signed $\int \Delta I dq$, and the lower panel shows $\int |\Delta I| dq$; the gray background trace provides the error-bar estimate for the blue peak-region response.

The same delay-domain differential trace can be transformed with `differential_analysis.plot_differential_fft`.

```
df, (fft_peak, fft_background), fig = differential_analysis.plot_differential_fft(
    sample_name="NiS2",
    temperature_K=300,
    excitation_wl_nm=1400.0,
    fluence_mJ_cm2=10.7,
    time_window_fs=100000,
    delays_fs="all",
    ref_type="delay",
    ref_value=-5000000,
    poni_path="/path/to/NiS2_Room_T.poni",
    mask_edf_path="/path/to/Mask_NiS2_Room_T.edf",
    azim_window=(-90.0, 90.0),
    peak="202",
    peak_specs=peak_specs,
    region="peak",
    kind="diff",
    time_window_select_ps=(0, 1000),
    poly_order=1,
    freq_unit="cm^-1",
    compute_if_missing=False,
    save=True,
    path_root="/path/to/ESRF2023",
    analysis_subdir="analysis",
)
```

19.3 Fluence differential traces

Fluence differential traces summarize the same kind of integrated intensity change, but as a function of pump fluence. They are useful for identifying thresholds, saturation, or non-linear response. As with fluence fitting, the fixed delay must be stated. If the fixed delay changes, the fluence trace is a different experiment.

```
peak_specs = {"116": {"q_range": (3.55, 3.75), "bg_mode": "after"}}

df, fig = differential_analysis.plot_differential_integrals_fluence(
    sample_name="DET58_2",
    temperature_K=80,
    excitation_wl_nm=1400.0,
    delay_fs=500000,
    time_window_fs=100000,
    fluences_mJ_cm2=[1.3, 2.29, 5.49, 13.9],
    ref_type="dark",
    ref_value="scan_7",
    poni_path="/path/to/DET58_80K_2_0001_0035.poni",
    mask_edf_path="/path/to/DET58_80K_mask.edf",
    azim_window=(-90.0, 90.0),
    azim_offset_deg=90.0,
    polarization_factor=0.99,
    peak="116",
    peak_specs=peak_specs,
    npt=1000,
    normalize_xy=True,
    q_norm_range=(2.65, 2.75),
    compute_if_missing=True,
```

```
    show_errorbars=True,
    save=True,
    path_root="/path/to/ESRF2026/March",
    analysis_subdir="analysis",
)
```

19.4 Multi-experiment comparison

Multi-experiment differential analysis compares traces from several experiments or conditions. Each experiment can carry its own path configuration, or the function can receive a shared path configuration. The key requirement is explicit labeling: sample name, temperature, excitation wavelength, fluence, time window, reference choice, and azimuthal window must be visible either in the plot legend or in the saved metadata.

Comparisons can be made on an absolute scale or after normalization. Absolute-scale comparisons preserve amplitude information but require consistent integration and normalization. Shape-normalized comparisons are useful for timing or frequency comparisons, but they do not support claims about absolute intensity differences.

```
base_experiment = {
    "sample_name": "DET58_2",
    "temperature_K": 80,
    "excitation_wl_nm": 1400.0,
    "time_window_fs": 100000,
    "ref_type": "dark",
    "ref_value": "scan_7",
}

experiments = [
    {**base_experiment, "label": "1.3 mJ/cm^2", "fluence_mJ_cm2": 1.3},
    {**base_experiment, "label": "13.9 mJ/cm^2", "fluence_mJ_cm2": 13.9},
]

result = differential_analysis.plot_differential_integrals_multi(
    experiments=experiments,
    delays_fs="all",
    poni_path="/path/to/DET58_80K_2_0001_0035.poni",
    mask_edf_path="/path/to/DET58_80K_mask.edf",
    azim_window=(-90.0, 90.0),
    azim_offset_deg=90.0,
    polarization_factor=0.99,
    peak="116",
    peak_specs=peak_specs,
    npt=1000,
    normalize_xy=True,
    q_norm_range=(2.65, 2.75),
    compute_if_missing=True,
    unit="ps",
    show_errorbars=True,
    save=True,
    path_root="/path/to/ESRF2026/March",
    analysis_subdir="analysis",
)
```

Chapter 20

Peak fitting

20.1 Fitting philosophy

Peak fitting is a model-based compression of the one-dimensional pattern. It is never the first diagnostic. First verify the detector/cake geometry, then inspect absolute and differential patterns, and only then fit peaks. The fit is useful when a peak can be described by a stable model over a defined q interval and when the fitted parameters have a physical interpretation.

The fitting utilities use peak specifications: each named peak defines a q range and optional model settings. Delay and fluence fitting routines then apply those specifications to every selected delay or fluence point and every selected azimuthal group. The default model is based on a pseudo-Voigt peak plus background handling implemented through lmfit models [16]. The user controls the q window, pseudo-Voigt fraction, fitting method, azimuthal treatment, reference behavior, and whether missing `xy` files may be computed on demand.

20.2 Delay peak fitting

The main delay fitting entry point is `fitting.run_delay_peak_fitting`. It locates the selected delay patterns, optionally integrates missing `xy` files from two-dimensional images, fits each requested peak, and writes a CSV table. The output can include reference rows, and reference values can be combined or kept separate depending on the analysis question.

Azimuthal handling is explicit. With `phi_mode="separate_phi"`, sectors are fit independently. With `phi_mode="phi_avg"`, symmetry-related or selected sectors can be reduced before fitting, using `phi_reduce="sum"` or `"mean"`. These choices affect amplitudes and areas, so they must be included in filenames and captions. The code tags output CSV names with the azimuthal mode to reduce accidental reuse of incompatible results.

Diagnostic fit figures are optional because a full delay series can produce many plots. During method development, saving or showing fit overlays is useful. Once the model is validated, the CSV table and evolution plots are usually the main outputs.

The ID09 fitting examples in this section use the 2026 DET58_2 dataset at 80 K and 1400 nm excitation with a 100 ps time window. The delay comparison follows the saved multi-delay fitting state and uses the available local fluence folders from 0.9 to 13.9 mJ cm^{-2}. The position and FWHM evolutions are plotted separately using `fitting.plot_time_evolution_multi`; the display then uses a logarithmic delay axis to match the GUI view.

```
from trxrdpy.analysis import fitting

overlay = fitting.plot_fit_overlay_from_csv(
    sample_name="DET58_2",
```

```
    temperature_K=80,
    excitation_wl_nm=1400.0,
    fluence_mJ_cm2=13.9,
    time_window_fs=100000,
    peak="110",
    delay_fs=500000,
    group="Full",
    phi_mode="phi_avg",
    phi_reduce="sum",
    csv_path="/path/to/peak_fits_delay_phiavg_sum.csv",
    ensure_csv=False,
    show=False,
    poni_path="/path/to/DET58_80K_2_0001_0035.poni",
    mask_edf_path="/path/to/DET58_80K_mask.edf",
    azim_offset_deg=90.0,
    compute_if_missing=False,
    path_root="/path/to/ESRF2026/March",
    analysis_subdir="analysis",
)
```

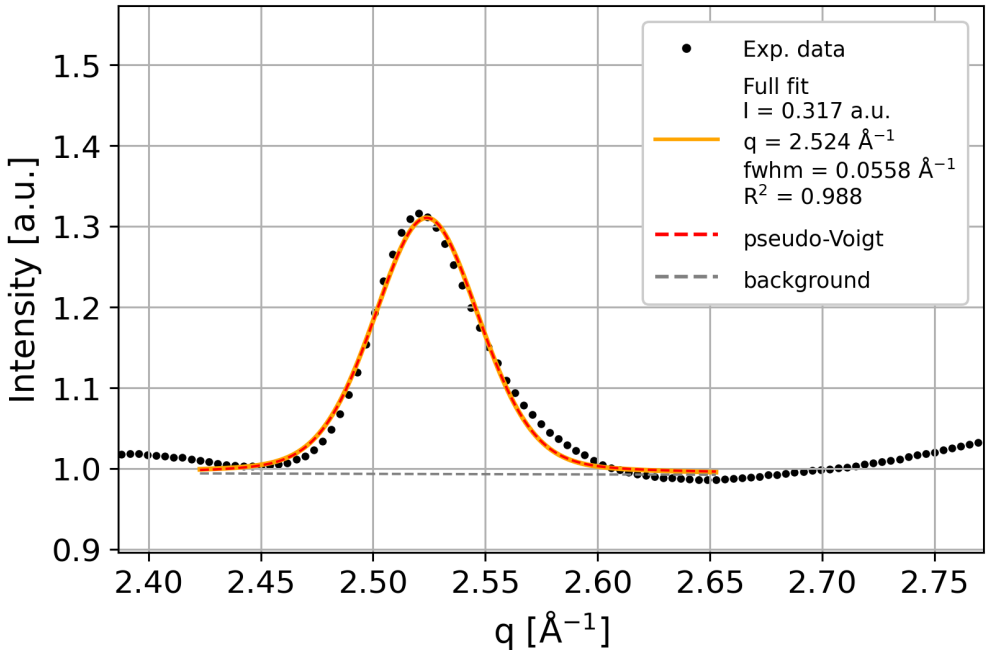

Figure 20.1: ID09 DET58_2 delay-fit overlay reconstructed from the saved fit CSV for the (110) peak at 500 ps and 13.9 mJ cm^{-2}. The plot shows the experimental points, pseudo-Voigt component, background, and total fit for the full azimuthal group after `phi_avg` summation.

```
experiments = [
    {
        "label": "V2O3, 80, 1400, 1.3, 100000",
        "sample_name": "DET58_2",
        "temperature_K": 80,
        "excitation_wl_nm": 1400.0,
        "fluence_mJ_cm2": 1.3,
        "time_window_fs": 100000,
        "phi_mode": "phi_avg",
        "phi_reduce": "sum",
        "ref_type": "dark",
        "csv_path": "/path/to/fluence_1p3mJ/peak_fits_delay_phiavg_sum.csv",
```

```
    },
    {
        "label": "V2O3, 80, 1400, 13.9, 100000",
        "sample_name": "DET58_2",
        "temperature_K": 80,
        "excitation_wl_nm": 1400.0,
        "fluence_mJ_cm2": 13.9,
        "time_window_fs": 100000,
        "phi_mode": "phi_avg",
        "phi_reduce": "sum",
        "ref_type": "dark",
        "csv_path": "/path/to/fluence_13p9mJ/peak_fits_delay_phiavg_sum.csv",
    },
]

position_result = fitting.plot_time_evolution_multi(
    experiments=experiments,
    peak="116",
    _property="hkl_pos",
    unit="ps",
    phi_mode="phi_avg",
    phi_reduce="sum",
    phi_window="Full",
    as_lines=True,
    show_baseline_sigma=True,
    baseline_mode="errorbar",
    cmap="jet",
    show=False,
)
position_result["ax"].set_xscale("log")

fwhm_result = fitting.plot_time_evolution_multi(
    experiments=experiments,
    peak="116",
    _property="hkl_fwhm",
    unit="ps",
    phi_mode="phi_avg",
    phi_reduce="sum",
    phi_window="Full",
    as_lines=True,
    show_baseline_sigma=True,
    baseline_mode="errorbar",
    cmap="jet",
    show=False,
)
fwhm_result["ax"].set_xscale("log")
```

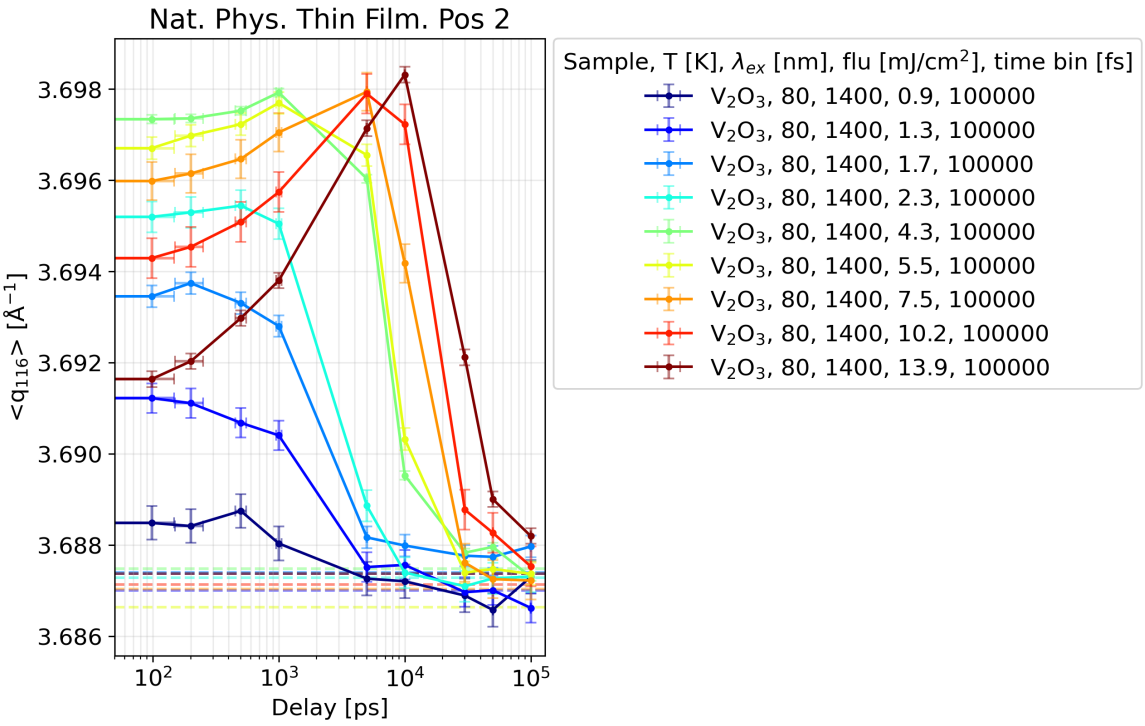

Figure 20.2: ID09 DET58_2 fitted (116) position versus delay for the local delay-scan fluence series, generated with the existing multi-experiment fitting plotting facility. The delay axis is displayed logarithmically, matching the GUI view.

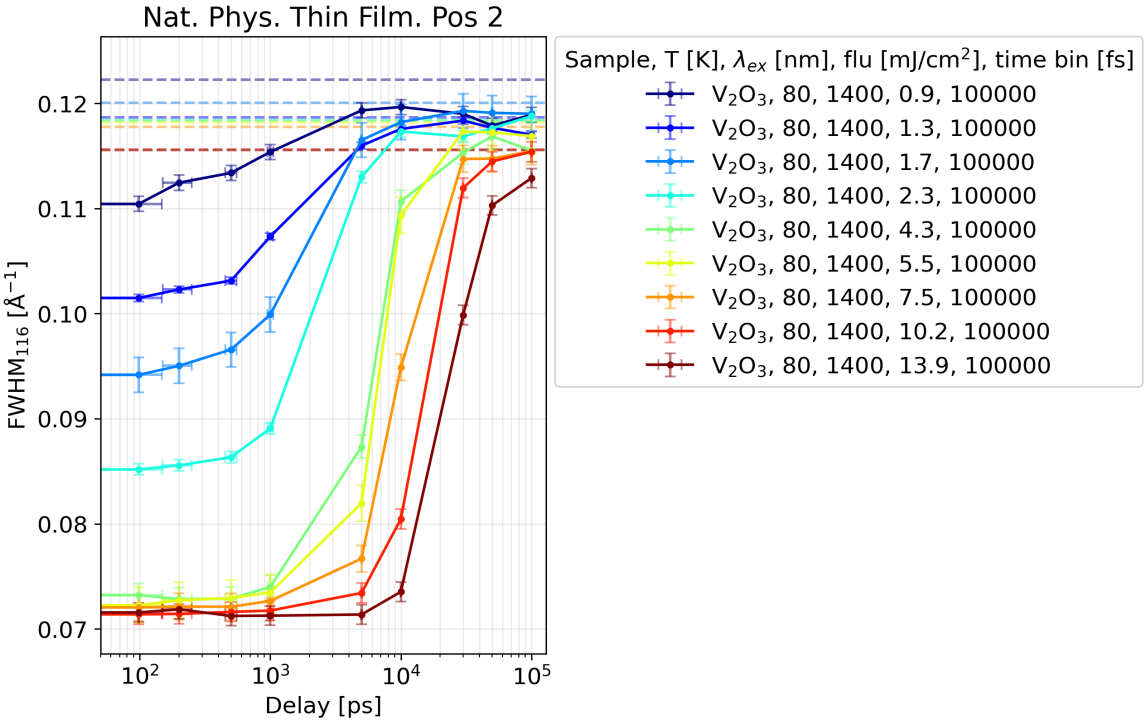

Figure 20.3: ID09 DET58_2 fitted (116) FWHM versus delay for the local delay-scan fluence series, generated with the existing multi-experiment fitting plotting facility. The delay axis is displayed logarithmically, matching the GUI view.

20.3 Fluence peak fitting

Fluence peak fitting follows the same model logic as delay fitting, but the independent variable is fluence rather than time. The fluence fitter resolves fluence-specific `xy` files, writes fluence-specific CSV tables, and provides evolution plots as a function of excitation fluence.

The main interpretive risk is confusing fluence dependence with time dependence. Captions and filenames must always state the fixed delay used for the fluence series. If multiple delays are analyzed as separate fluence series, give each delay its own output path or clearly tagged CSV file.

The fluence example uses the shared 2026 DET58_2 fixed-delay folders at 500 ps, 5 ns, and 10 ns. Each curve is loaded from its corresponding `peak_fits_fluence_phiavg_sum.csv` file, and the plotted quantity follows the GUI setting for the shared state: (116) FWHM in the full `phi_avg` group.

```
from trxrdpy.analysis import fitting

experiments = [
    {
        "label": "500 ps",
        "sample_name": "DET58_2",
        "temperature_K": 80,
        "excitation_wl_nm": 1400.0,
        "delay_fs": 500000,
        "time_window_fs": 100000,
        "phi_mode": "phi_avg",
        "ref_type": "dark",
        "csv_path": "/path/to/delay_500000fs/peak_fits_fluence_phiavg_sum.csv",
    },
    {
        "label": "10 ns",
        "sample_name": "DET58_2",
        "temperature_K": 80,
        "excitation_wl_nm": 1400.0,
        "delay_fs": 10000000,
        "time_window_fs": 100000,
        "phi_mode": "phi_avg",
        "ref_type": "dark",
        "csv_path": "/path/to/delay_10000000fs/peak_fits_fluence_phiavg_sum.csv",
    },
]

fig, ax, saved_path = fitting.plot_fluence_evolution_multi(
    experiments=experiments,
    peak="116",
    prop="hkl_fwhm",
    group_by="phi_label",
    group="Full",
    fluence_unit="mJ/cm$^2$",
    only_success=True,
    include_reference=False,
    legend_title="Delay",
    as_lines=True,
    show=False,
    save=True,
)
```

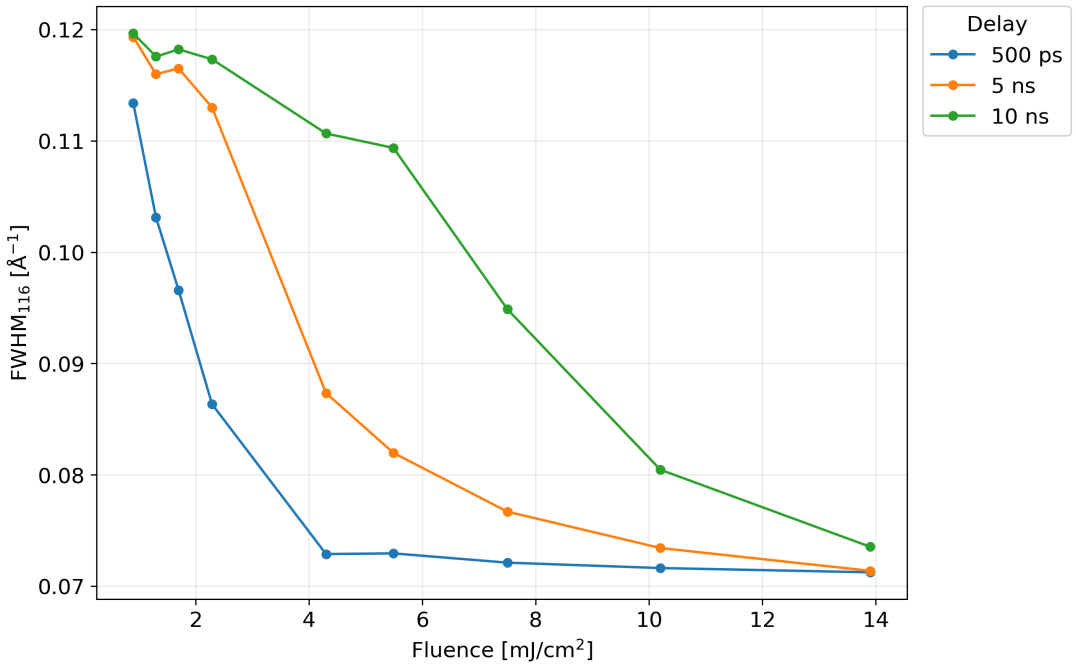

Figure 20.4: ID09 DET58_2 fitted (116) FWHM versus fluence for three fixed-delay fluence scans. The fixed delay is encoded by the curve label, so the figure should not be interpreted as a time trace.

20.4 Fit outputs and diagnostics

Fit CSV files are the numerical record of the fitting step. They normally include experiment identity, independent-variable value, peak name, azimuthal group, best-fit parameters, derived width or area values, and quality metrics such as R^2 where available. Failed fits remain visible in the table rather than being silently dropped, because missing points can bias time or fluence trends.

The overlay functions can reconstruct diagnostic plots from saved CSV files. This is useful when a user wants to inspect one suspicious point without rerunning the entire fit series. The correct workflow is to keep the CSV, the peak specification, and the integration settings together.

20.5 Displaying fitted-property changes

Fitting Analysis evolution plots have three display choices. Leave both display-mode boxes unchecked for absolute fitted properties with physical units. *Normalize (0–1)* displays $(P - P_{\mathrm{ref}})/(P_{\max} - P_{\mathrm{ref}})$. *Relative variation (%)* displays $100(P - P_{\mathrm{ref}})/P_{\mathrm{ref}}$. These modes are mutually exclusive. The selected reference is mapped to zero; axes for transformed values omit the original physical unit. A missing reference, zero reference for relative variation, or zero normalization span raises an error instead of producing a misleading curve.

Reference lines and existing baseline error bars use the same transformation. The reference estimate is treated as fixed while scaling the baseline spread; this does not create fit-parameter confidence intervals. For a single experiment, the reference comes from its series controls. Each entry in a multi-experiment plot uses its own reference, and merged delay entries retain their pooled negative-delay baseline. The reference must exist in the fitting CSV. Changing the display reference does not refit the peaks or rewrite that CSV.

In a multi-experiment evolution plot, each entry may set an *Azimuthal selection* independently. *Full* selects the full group, a number such as `30` selects a centre for phi-averaged fitting, and an interval such as `(-15, 15)` selects a sector for separate-phi fitting. Leaving an entry blank uses the shared selection. The API descriptor key is `phi_window`. Multiple-fluence evolution also accepts an optional *Colormap*; blank retains the previous categorical colors, while a Matplotlib name such as `viridis` selects that map. These display controls and per-entry selections are saved in GUI states, including when reopening older states.

```
from trxrdpy.analysis import fitting

# Each entry identifies its fitting CSV and may select its own sector.
experiments = [
    {"label": "sample A", "csv_path": "/path/to/a.csv",
     "phi_window": "Full", "ref_type": "dark"},
    {"label": "sample B", "csv_path": "/path/to/b.csv",
     "phi_window": (-15, 15), "ref_type": "dark"},
]
# Pass the experiment identifiers and other required fitting options for
# your dataset, as in the complete examples above.
```

The delay and fluence evolution functions expose `norm_min_max` and `relative_variation`; multi-experiment functions accept per-entry `phi_window`. The multi-fluence function additionally accepts `cmap`. Keep the fitting CSV and selected display settings with any exported figure so that a transformed trend can be reconstructed.

Chapter 21

Facility-specific worked analysis examples

The shared chapters above define the common analysis pipeline: detector diagnostics, azimuthal integration, differential analysis, and peak fitting. The examples in this chapter apply those shared tools to facility-specific datasets after the facility preparation step has already produced corrected two-dimensional images or cached one-dimensional `xy` files.

21.1 Max IV FemtoMAX

21.1.1 FemtoMAX single-delay-scan example

This example follows a FemtoMAX DET58 delay scan at 300 K, 1500 nm, and 52 mJ cm^{-2}. The reduction step has already produced averaged two-dimensional images and cached one-dimensional `xy` files for a 1000 fs time window. The reference used for the delay scan is not a dark scan; it is the −98972 fs delay point. For display, a +4000 fs offset is applied, so the reference appears at −94.97 ps.

21.1.1.1 Detector and 2D cake diagnostic from the FemtoMAX dark scan

The calibration diagnostic starts from dark scan 180951. The detector image is plotted with the detector y axis inverted, the detector color scale limited to $(0, 0.05)$, and the cake color scale limited to $(0, 2)$. The cake is normalized over $q = (1.9, 2.0)$ $\mathrm{Å}^{-1}$.

```
from pathlib import Path

from trxrdpy.analysis import calibration

root = Path("/path/to/FemtoMAX2026")
poni_path = root / "calibration/DET58_180951.poni"
mask_path = root / "calibration/DET58_180951_mask.edf"

fig, axes, data = calibration.plot_detector_and_cake(
    sample_name="DET58",
    scan=180951,
    temperature_K=300,
    npt_rad=1000,
    npt_azim=360,
    azimuthal_range=(-90.0, 90.0),
    normalize=True,
    q_norm_range=(1.9, 2.0),
    use_mask=True,
    poni_path=str(poni_path),
```

```
    mask_edf_path=str(mask_path),
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    detector_clim=(0.0, 0.05),
    cake_clim=(0.0, 2.0),
    invert_detector_y=True,
    save=True,
    path_root=root,
    analysis_subdir="analysis",
)
```

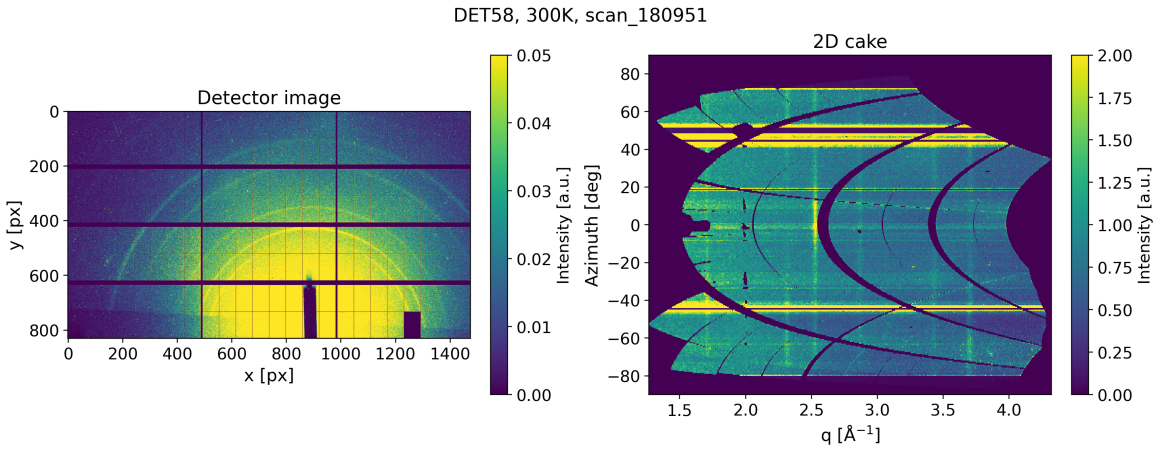

Figure 21.1: FemtoMAX DET58 dark-scan detector image and 2D cake diagnostic for scan 180951. The detector panel uses the inverted y-axis convention used in the GUI state, and the cake panel uses the normalized q-azimuth representation used for later integration checks.

21.1.1.2 One-dimensional viewer for the FemtoMAX delay scan

The one-dimensional viewer compares all cached delay patterns against the selected delay reference. The absolute-pattern and differential-pattern y limits are passed directly to the plotting function, so the figure can be reproduced from the GUI without manual Matplotlib edits after plotting.

```
from pathlib import Path

from trxrdpy.analysis.MaxIV_FemtoMAX import azimint as femtomax_azimint

root = Path("/path/to/FemtoMAX2026")
poni_path = root / "calibration/DET58_180951.poni"
mask_path = root / "calibration/DET58_180951_mask.edf"

q_ref, I_ref, fig, axes = femtomax_azimint.plot_1D_abs_and_diffs_delay(
    sample_name="DET58",
    temperature_K=300,
    excitation_wl_nm=1500.0,
    fluence_mJ_cm2=52.0,
    time_window_fs=1000,
    delays_fs="all",
    ref_type="delay",
    ref_value=-98972,
    poni_path=str(poni_path),
    mask_edf_path=str(mask_path),
    azim_window=(-90.0, 90.0),
```

```
    npt=1000,
    normalize=True,
    q_norm_range=(1.9, 2.0),
    compute_if_missing=False,
    overwrite_xy=False,
    xlim=(1.5, 4.0),
    ylim_top=(0.3285, 1.5136),
    ylim_diff=(-0.55, 0.55),
    fs_or_ps="ps",
    digits=2,
    delay_offset_fs=4000.0,
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    save_plots=True,
    from_2D_imgs=False,
    path_root=root,
    analysis_subdir="analysis",
)
```

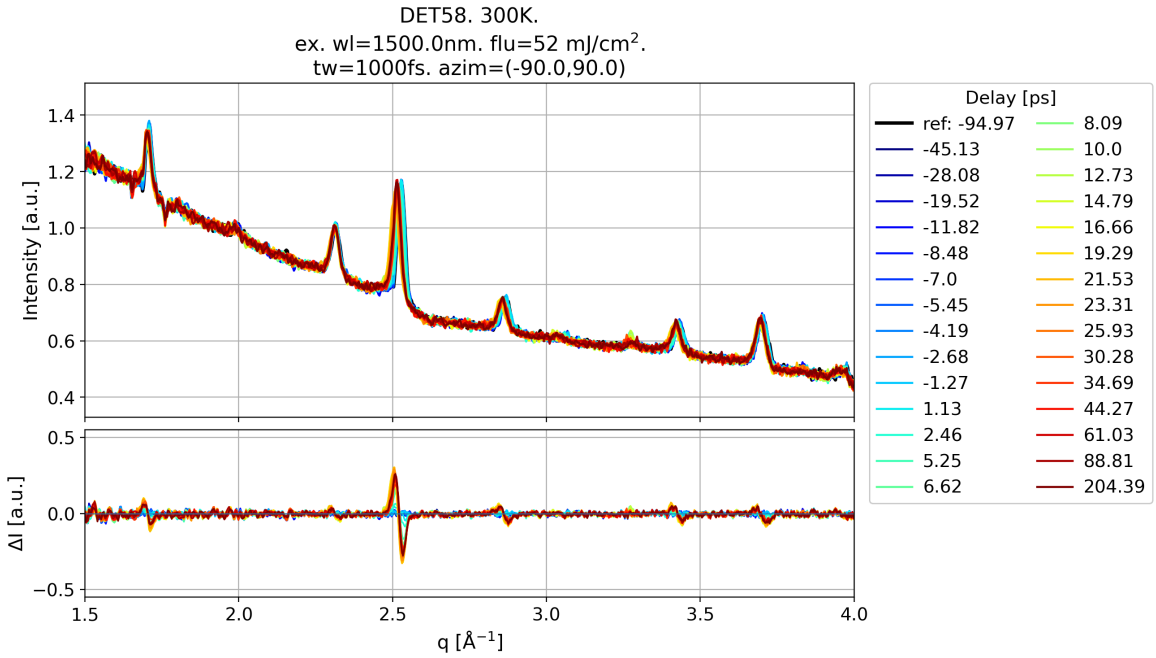

Figure 21.2: FemtoMAX DET58 one-dimensional viewer example for the 300 K, 1500 nm delay scan. The reference is the −98972 fs delay pattern, displayed as −94.97 ps after the +4000 fs offset.

21.1.1.3 Differential-integral analysis for the FemtoMAX (110) peak

The differential-integral plot uses the (110) peak over $q = (2.4584, 2.5733)$ Å^{-1}, with the matched background window placed after the peak. The displayed delay axis and both y limits are provided as plotting arguments.

```
from pathlib import Path

from trxrdpy.analysis import differential_analysis

root = Path("/path/to/FemtoMAX2026")
```

```
poni_path = root / "calibration/DET58_180951.poni"
mask_path = root / "calibration/DET58_180951_mask.edf"

peak_specs = {
    "110": {"q_range": (2.4584, 2.5733), "bg_side": "right"},
}

df, fig = differential_analysis.plot_differential_integrals(
    sample_name="DET58",
    temperature_K=300,
    excitation_wl_nm=1500.0,
    fluence_mJ_cm2=52.0,
    time_window_fs=1000,
    delays_fs="all",
    ref_type="delay",
    ref_value=-98972,
    poni_path=str(poni_path),
    mask_edf_path=str(mask_path),
    azim_window=(-90.0, 90.0),
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    peak="110",
    peak_specs=peak_specs,
    npt=1000,
    normalize_xy=True,
    q_norm_range=(1.9, 2.0),
    compute_if_missing=False,
    overwrite_xy=False,
    unit="ps",
    delay_offset_fs=4000.0,
    show_errorbars=True,
    errorbar_scale=1.0,
    xlim=(-15.0, 65.0),
    ylim_signed=(-0.008, 0.008),
    ylim_abs=(-0.0027, 0.018),
    save=True,
    path_root=root,
    analysis_subdir="analysis",
)
```

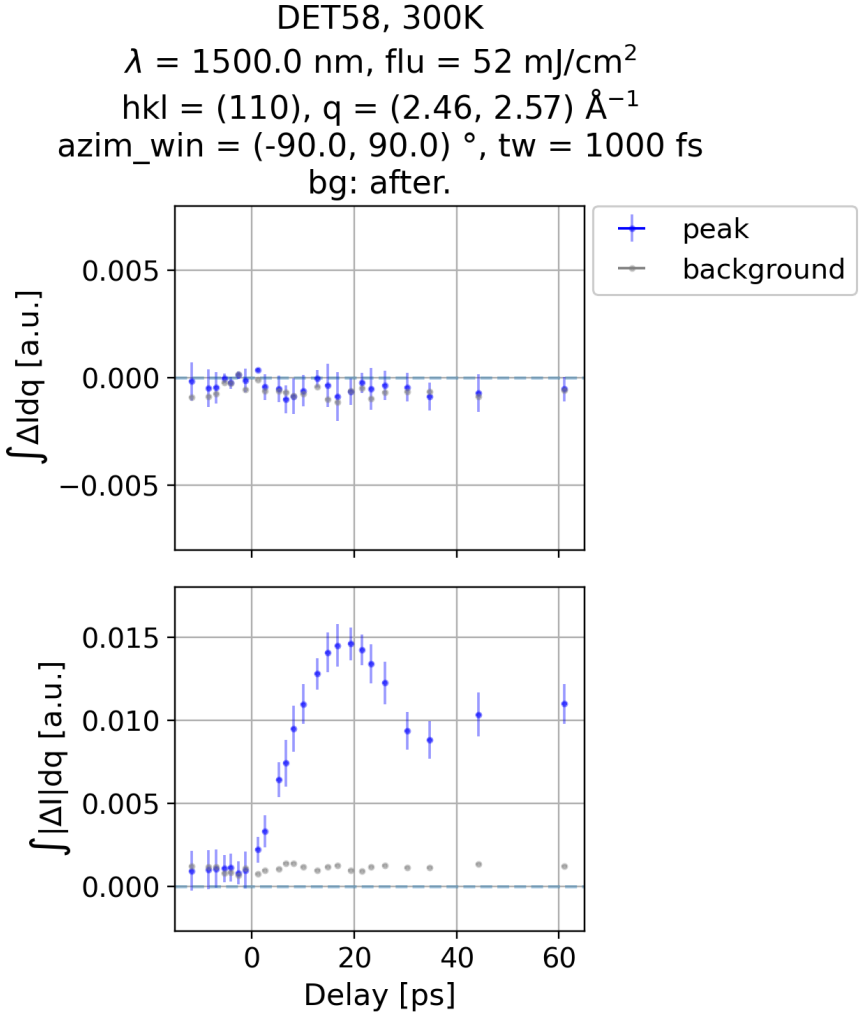

Figure 21.3: FemtoMAX DET58 differential-integral example for the (110) peak region. The upper panel shows signed $\int \Delta I dq$, and the lower panel shows $\int |\Delta I| dq$ over the displayed -15 to 65 ps window.

21.1.1.4 Fitting analysis for different FemtoMAX azimuthal sectors

The fitting example reads the existing `peak_fits_delay_phiavg_sum.csv` table and plots the fitted (110) peak position for the full azimuthal range and the $|\Phi| = 60°, 30°, 0°$ sector groups. The dashed horizontal lines are the reference values from the selected delay reference.

```
from pathlib import Path

from trxrdpy.analysis import fitting

root = Path("/path/to/FemtoMAX2026")
csv_path = (
    root / "analysis/DET58/temperature_300K/excitation_wl_1500nm"
    / "delay/fluence_52p0mJ/time_window_1000fs"
    / "fitting/peak_fits_delay_phiavg_sum.csv"
)

out = fitting.plot_time_evolution(
    sample_name="DET58",
    temperature_K=300,
    excitation_wl_nm=1500.0,
    fluence_mJ_cm2=52.0,
    time_window_fs=1000,
    peak="110",
    _property="hkl_pos",
    unit="ps",
    group_by="azim_range_str",
    groups=["Full", 60, 30, 0],
    only_success=True,
    include_reference=True,
    as_lines=True,
    delay_offset_fs=4000.0,
    show_baseline_sigma=True,
    baseline_sigma=1.0,
    baseline_alpha=1.0,
    baseline_mode="errorbar",
    xlim=(-15.0, 65.0),
    ylim=(2.50, 2.535),
    csv_path=str(csv_path),
    phi_mode="phi_avg",
    phi_reduce="sum",
    save=True,
    path_root=root,
    analysis_subdir="analysis",
)
```

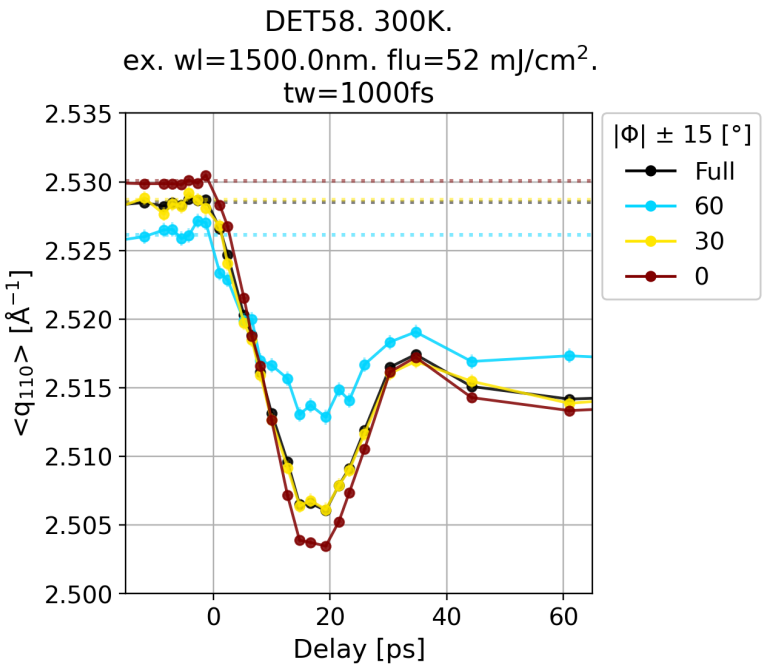

Figure 21.4: FemtoMAX DET58 fitted (110) peak position versus delay for different symmetric azimuthal sectors, generated from the existing `peak_fits_delay_phiavg_sum.csv` file.

21.2 SPring-8 / SACLA

21.2.1 SACLA delay-scan examples from cached one-dimensional data

Once the SACLA preparation step has produced corrected two-dimensional images or cached one-dimensional `xy` files, the downstream analysis uses the shared two-dimensional integration backend exposed through `trxrdpy.analysis.Spring8_SACLA.azimint`. The examples below use a DET70 delay scan at 300 K and 1500 nm. The local folders are stored as 25 and 10 mJ cm^{-2}, while the GUI display applies a fluence scale of 0.4. Therefore the plotted labels appear as 10 and 4 mJ cm^{-2}. This scale is a display convention only; the data lookup still uses the folder fluence.

21.2.1.1 One-dimensional viewer for a SACLA delay scan

The one-dimensional viewer compares cached delay patterns against a dark reference and plots both the absolute patterns and their differences. In this example the reference is dark scan 1466609, the integration uses the full $(-90°, 90°)$ azimuthal range, and the displayed delay axis includes a $+9.6$ ps offset.

```
from pathlib import Path

from trxrdpy.analysis.Spring8_SACLA import azimint as sacla_azimint

root = Path("/path/to/SACLA2024")
poni_path = root / "calibration/DET70_1466610.poni"
mask_path = root / "calibration/DET70_300K_mask.edf"

q_ref, I_ref, fig, axes = sacla_azimint.plot_1D_abs_and_diffs_delay(
    sample_name="DET70",
    temperature_K=300,
    excitation_wl_nm=1500.0,
```

```
    fluence_mJ_cm2=25.0,
    time_window_fs=250,
    delays_fs="all",
    ref_type="dark",
    ref_value=1466609,
    poni_path=str(poni_path),
    mask_edf_path=str(mask_path),
    azim_window=(-90.0, 90.0),
    npt=1000,
    normalize=True,
    q_norm_range=(2.65, 2.75),
    compute_if_missing=True,
    overwrite_xy=False,
    xlim=(1.5, 4.0),
    fs_or_ps="ps",
    digits=2,
    delay_offset_fs=9600.0,
    fluence_scale=0.4,
    max_curves=30,
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    save_plots=True,
    from_2D_imgs=False,
    path_root=root,
    analysis_subdir="analysis",
)
```

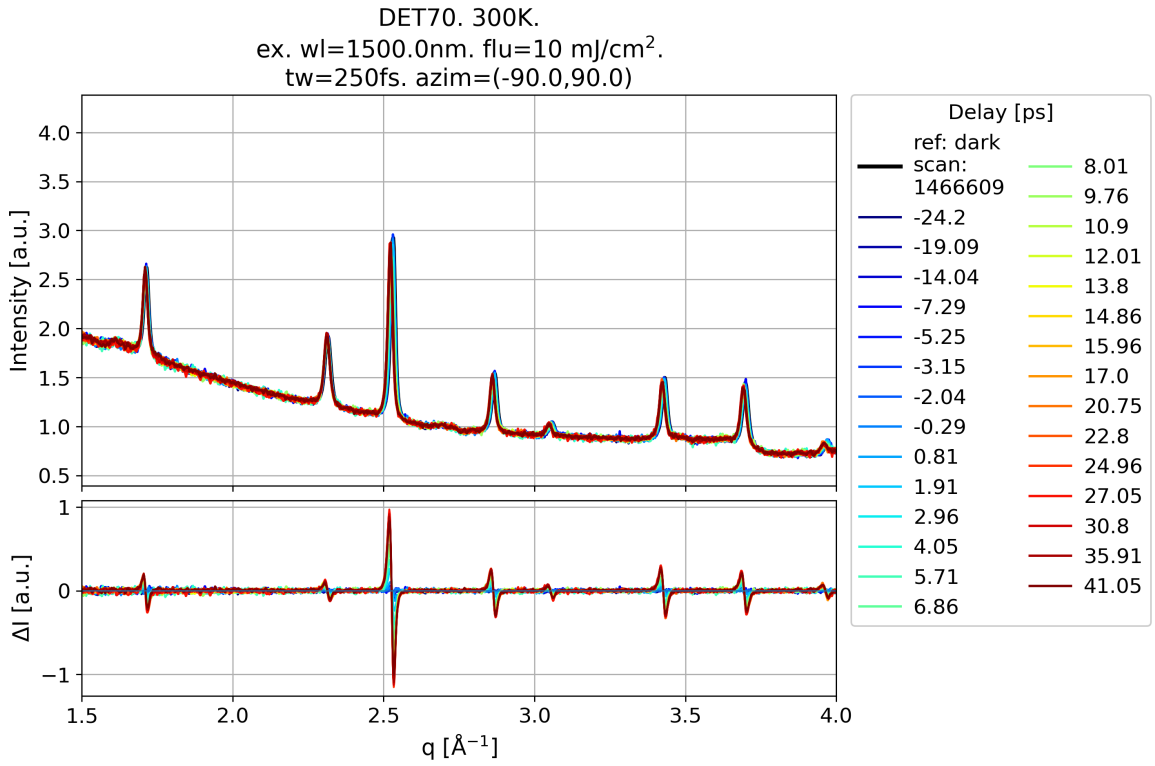

Figure 21.5: SACLA DET70 one-dimensional viewer example for the 300 K, 1500 nm delay scan. The top panel compares absolute full-azimuth patterns against dark scan 1466609, and the bottom panel shows the differences relative to the dark reference after the +9.6 ps display offset.

21.2.1.2 Differential-integral analysis for the SACLA (110) peak

The differential-analysis function integrates the signed and absolute differential response in the selected peak window. Here we use the (110) peak, $q = (2.45, 2.60)$ Å^{-1}, with the matched background window placed after the peak.

```
from pathlib import Path

from trxrdpy.analysis import differential_analysis

root = Path("/path/to/SACLA2024")
poni_path = root / "calibration/DET70_1466610.poni"
mask_path = root / "calibration/DET70_300K_mask.edf"

peak_specs = {
    "110": {"q_range": (2.45, 2.60), "bg_side": "right"},
}

df, fig = differential_analysis.plot_differential_integrals(
    sample_name="DET70",
    temperature_K=300,
    excitation_wl_nm=1500.0,
    fluence_mJ_cm2=25.0,
    time_window_fs=250,
    delays_fs="all",
    ref_type="dark",
    ref_value=1466609,
    poni_path=str(poni_path),
    mask_edf_path=str(mask_path),
    azim_window=(-90.0, 90.0),
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    peak="110",
    peak_specs=peak_specs,
    npt=1000,
    normalize_xy=True,
    q_norm_range=(2.65, 2.75),
    compute_if_missing=True,
    overwrite_xy=False,
    unit="ps",
    delay_offset_fs=9600.0,
    fluence_scale=0.4,
    show_errorbars=True,
    errorbar_scale=1.0,
    plot_abs_and_diffs=True,
    save=True,
    path_root=root,
    analysis_subdir="analysis",
)
```

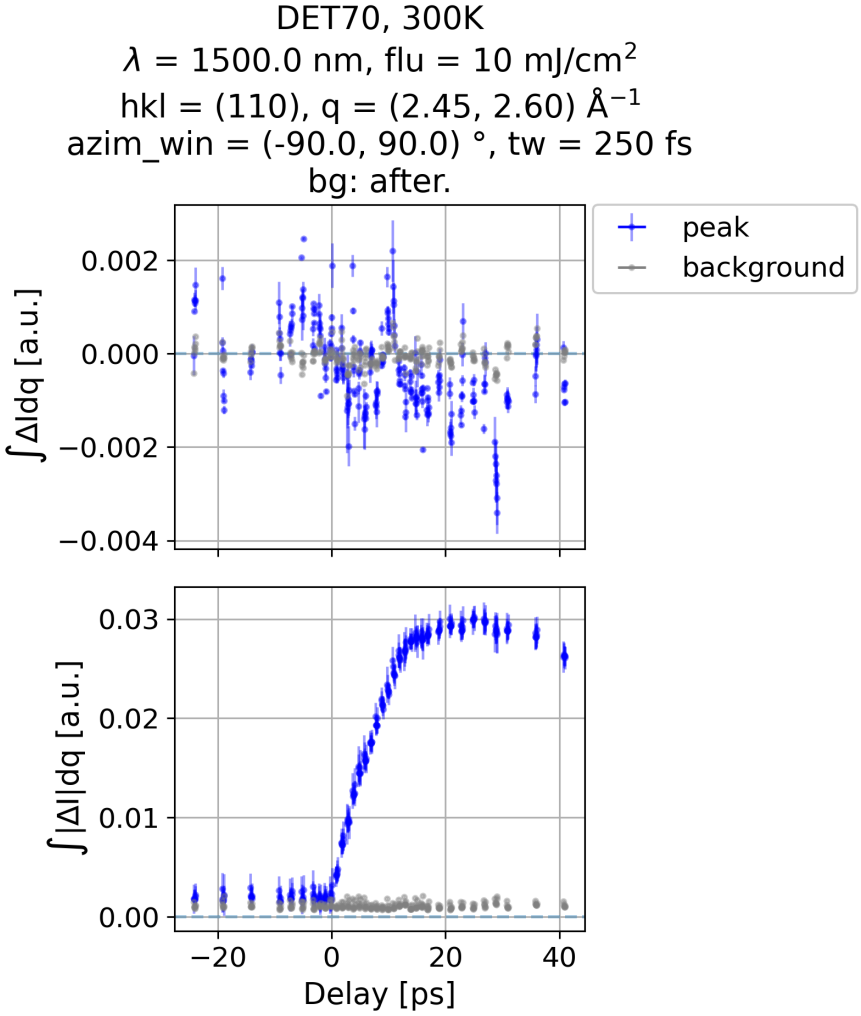

Figure 21.6: SACLA DET70 differential-integral example for the (110) peak region. The upper panel shows signed $\int \Delta I dq$, and the lower panel shows $\int |\Delta I| dq$; the gray background trace provides the error-bar estimate for the blue peak-region response.

21.2.1.3 Fitting analysis for different azimuthal sectors

For the same delay scan, the fitting analysis can plot a fitted peak property for several symmetric azimuthal sectors. The example below reads the existing `phi_avg` fitting CSV and plots the (110) peak position for the full sector and the $|\Phi| = 60°, 30°, 0°$ sector groups.

```
from pathlib import Path

from trxrdpy.analysis import fitting

root = Path("/path/to/SACLA2024")
csv_path = (
    root / "analysis/DET70/temperature_300K/excitation_wl_1500nm"
    / "delay/fluence_25p0mJ/time_window_250fs"
    / "fitting/peak_fits_delay_phiavg_sum.csv"
)

out = fitting.plot_time_evolution(
    sample_name="DET70",
    temperature_K=300,
    excitation_wl_nm=1500.0,
    fluence_mJ_cm2=25.0,
    time_window_fs=250,
    peak="110",
    _property="hkl_pos",
    out_csv_name="peak_fits_delay.csv",
    unit="ps",
    group_by="azim_range_str",
    groups=["Full", 60, 30, 0],
    only_success=True,
    include_reference=True,
    as_lines=False,
    delay_offset_fs=9600.0,
    fluence_scale=0.4,
    show_baseline_sigma=True,
    baseline_sigma=1.0,
    baseline_alpha=0.18,
    baseline_mode="errorbar",
    csv_path=str(csv_path),
    phi_mode="phi_avg",
    phi_reduce="sum",
    save=True,
    path_root=root,
    analysis_subdir="analysis",
)
```

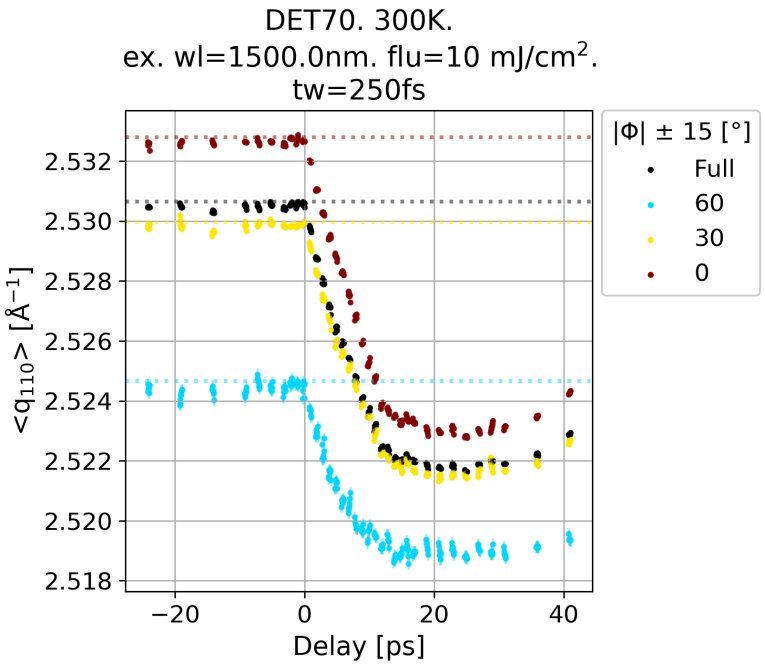

Figure 21.7: SACLA DET70 fitted (110) peak position versus delay for different symmetric azimuthal sectors. The figure is generated by the existing fitting time-evolution plotting facility using the cached `peak_fits_delay_phiavg_sum.csv` file.

21.2.1.4 Merged multi-delay fitting comparison

The multi-experiment fitting plotter can compare a merged time-resolution series with another fluence condition. In the example below, the 25 mJ cm^{-2} folder is displayed as 10 mJ cm^{-2} and combines 40 fs and 250 fs time-window CSVs. The 10 mJ cm^{-2} folder is displayed as 4 mJ cm^{-2}.

```
from pathlib import Path

from trxrdpy.analysis import fitting

root = Path("/path/to/SACLA2024")
delay_root = (
    root / "analysis/DET70/temperature_300K/excitation_wl_1500nm/delay"
)

experiments = [
    {
        "label": r"V$_2$O$_3$, 300, 1500, 10",
        "merge": [
            {
                "sample_name": "DET70",
                "temperature_K": 300,
                "excitation_wl_nm": 1500.0,
                "fluence_mJ_cm2": 25.0,
                "time_window_fs": 250,
                "ref_type": "dark",
                "ref_value": 1466609,
                "delay_offset_fs": 9600.0,
                "csv_path": str(
                    delay_root
                    / "fluence_25p0mJ/time_window_250fs"
```

```
                    / "fitting/peak_fits_delay_phiavg_sum.csv"
                ),
            },
            {
                "sample_name": "DET70",
                "temperature_K": 300,
                "excitation_wl_nm": 1500.0,
                "fluence_mJ_cm2": 25.0,
                "time_window_fs": 40,
                "ref_type": "dark",
                "ref_value": 1466610,
                "delay_offset_fs": 9600.0,
                "csv_path": str(
                    delay_root
                    / "fluence_25p0mJ/time_window_40fs"
                    / "fitting/peak_fits_delay_phiavg_sum.csv"
                ),
            },
        ],
    },
    {
        "label": r"V$_2$O$_3$, 300, 1500, 4",
        "sample_name": "DET70",
        "temperature_K": 300,
        "excitation_wl_nm": 1500.0,
        "fluence_mJ_cm2": 10.0,
        "time_window_fs": 250,
        "ref_type": "dark",
        "ref_value": 1466613,
        "delay_offset_fs": 9600.0,
        "csv_path": str(
            delay_root
            / "fluence_10p0mJ/time_window_250fs"
            / "fitting/peak_fits_delay_phiavg_sum.csv"
        ),
    },
]

result = fitting.plot_time_evolution_multi(
    experiments=experiments,
    peak="110",
    _property="hkl_pos",
    out_csv_name="peak_fits_delay.csv",
    unit="ps",
    phi_mode="phi_avg",
    phi_reduce="sum",
    phi_window="Full",
    only_success=True,
    include_reference=True,
    as_lines=False,
    show_baseline_sigma=True,
    baseline_sigma=1.0,
    baseline_mode="errorbar",
    cmap="jet_r",
    save=True,
    path_root=root,
    analysis_subdir="analysis",
)
```

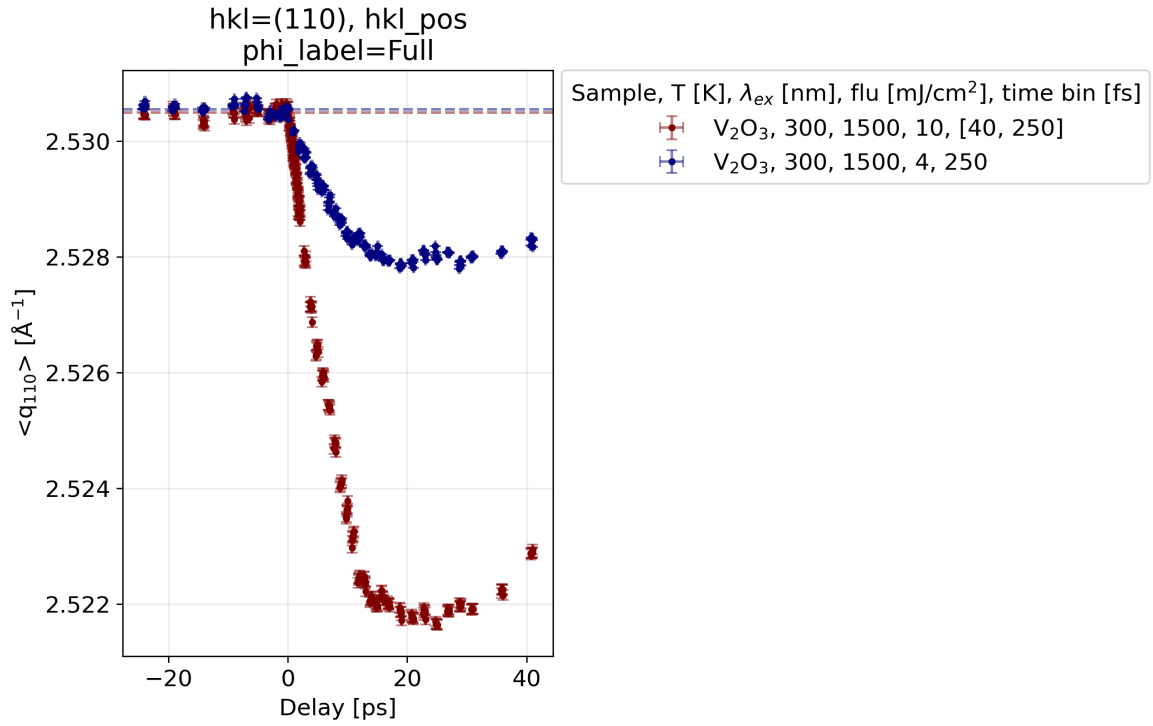

Figure 21.8: SACLA DET70 multi-delay fitting comparison for the fitted (110) position. The red series merges 40 fs and 250 fs time-window fits for the higher-fluence condition, while the blue series shows the lower-fluence 250 fs dataset.

21.2.2 SACLA fluence-scan examples from cached one-dimensional data

The SACLA fluence examples use a DET71 dataset at 300 K and 1500 nm. The single-experiment examples use the fixed-delay branch `delay_23979fs/time_window_250fs` with dark scan 1466631. A +9600 fs display offset is applied, so the fixed delay is reported as 33.6 ps. As in the SACLA delay examples, the stored fluence values are multiplied by 0.4 for display.

21.2.2.1 One-dimensional viewer for a SACLA fluence scan

The fluence viewer compares the fixed-delay patterns against a dark reference. The independent-variable labels in the legend use the display-scaled fluence values. The `fluence_digits` argument controls the precision of those labels without changing the delay precision used in the figure title.

```
from pathlib import Path

from trxrdpy.analysis.Spring8_SACLA import azimint as sacla_azimint

root = Path("/path/to/SACLA2024")
poni_path = root / "calibration/DET71_1466629.poni"
mask_path = root / "calibration/DET71_300K_mask.edf"

fig, axes = sacla_azimint.plot_1D_abs_and_diffs_fluence(
    sample_name="DET71",
    temperature_K=300,
    excitation_wl_nm=1500.0,
    delay_fs=23979,
    time_window_fs=250,
    fluences_mJ_cm2="all",
```

```
    ref_type="dark",
    ref_value=1466631,
    poni_path=str(poni_path),
    mask_edf_path=str(mask_path),
    azim_window=(-90.0, 90.0),
    npt=1000,
    normalize=True,
    q_norm_range=(2.65, 2.75),
    compute_if_missing=True,
    overwrite_xy=False,
    xlim=(1.5, 4.0),
    fluence_scale=0.4,
    fluence_digits=3,
    delay_offset_fs=9600.0,
    fs_or_ps="ps",
    digits=1,
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    save_plots=True,
    path_root=root,
    analysis_subdir="analysis",
)
```

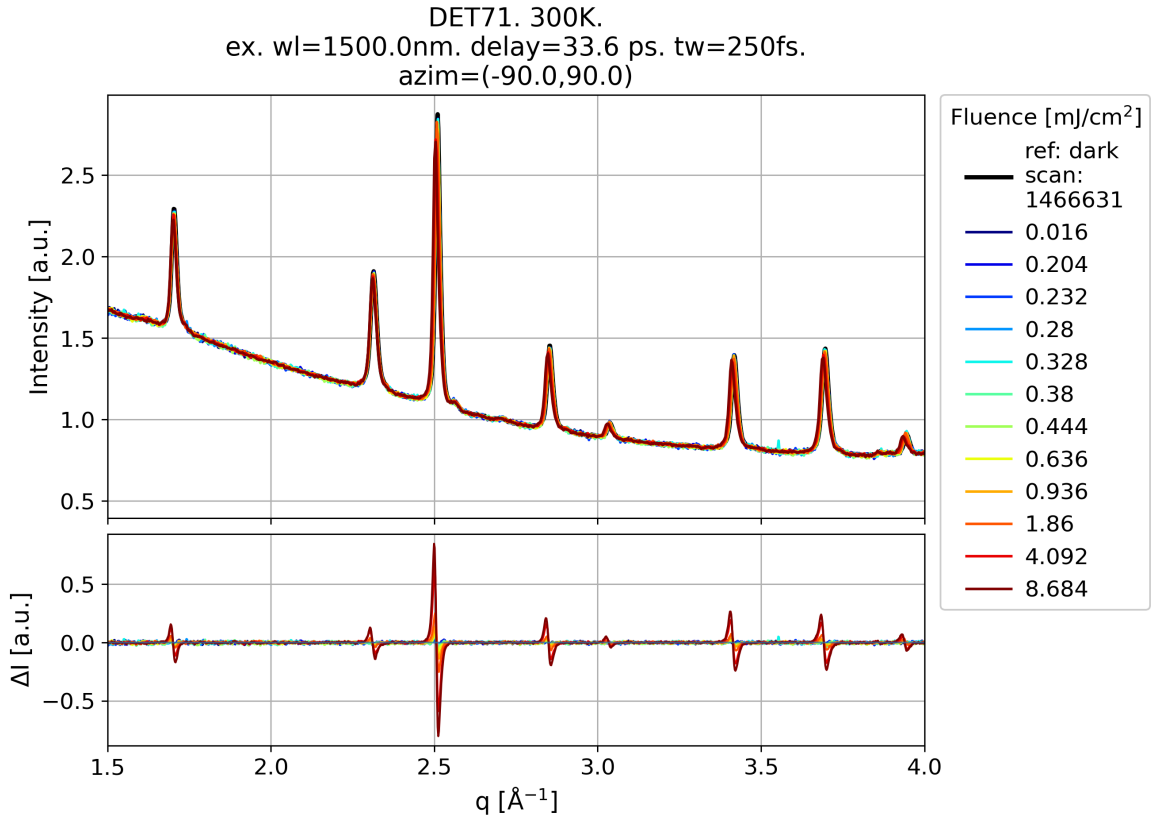

Figure 21.9: SACLA DET71 one-dimensional fluence viewer example at a displayed fixed delay of 33.6 ps. The top panel compares absolute full-azimuth patterns against dark scan 1466631, and the bottom panel shows fluence-dependent differences relative to the dark reference.

21.2.2.2 Differential-integral analysis for a SACLA fluence scan

The fluence differential analysis uses the same fixed-delay branch and dark reference. The (110) peak is integrated over $q = (2.4518, 2.55)$ Å^{-1}, with the background window placed after the peak.

```
from pathlib import Path

from trxrdpy.analysis import differential_analysis

root = Path("/path/to/SACLA2024")
poni_path = root / "calibration/DET71_1466629.poni"
mask_path = root / "calibration/DET71_300K_mask.edf"

peak_specs = {
    "110": {"q_range": (2.4518, 2.55), "bg_side": "right"},
}

df, fig = differential_analysis.plot_differential_integrals_fluence(
    sample_name="DET71",
    temperature_K=300,
    excitation_wl_nm=1500.0,
    delay_fs=23979,
    time_window_fs=250,
    fluences_mJ_cm2="all",
    ref_type="dark",
    ref_value=1466631,
    poni_path=str(poni_path),
    mask_edf_path=str(mask_path),
    azim_window=(-90.0, 90.0),
    azim_offset_deg=-90.0,
    polarization_factor=0.99,
    peak="110",
    peak_specs=peak_specs,
    npt=1000,
    normalize_xy=True,
    q_norm_range=(2.65, 2.75),
    compute_if_missing=True,
    overwrite_xy=False,
    fluence_unit="mJ/cm$^2$",
    fluence_scale=0.4,
    delay_offset_fs=9600.0,
    fs_or_ps="ps",
    digits=1,
    show_errorbars=True,
    errorbar_scale=1.0,
    plot_abs_and_diffs=True,
    save=True,
    path_root=root,
    analysis_subdir="analysis",
)
```

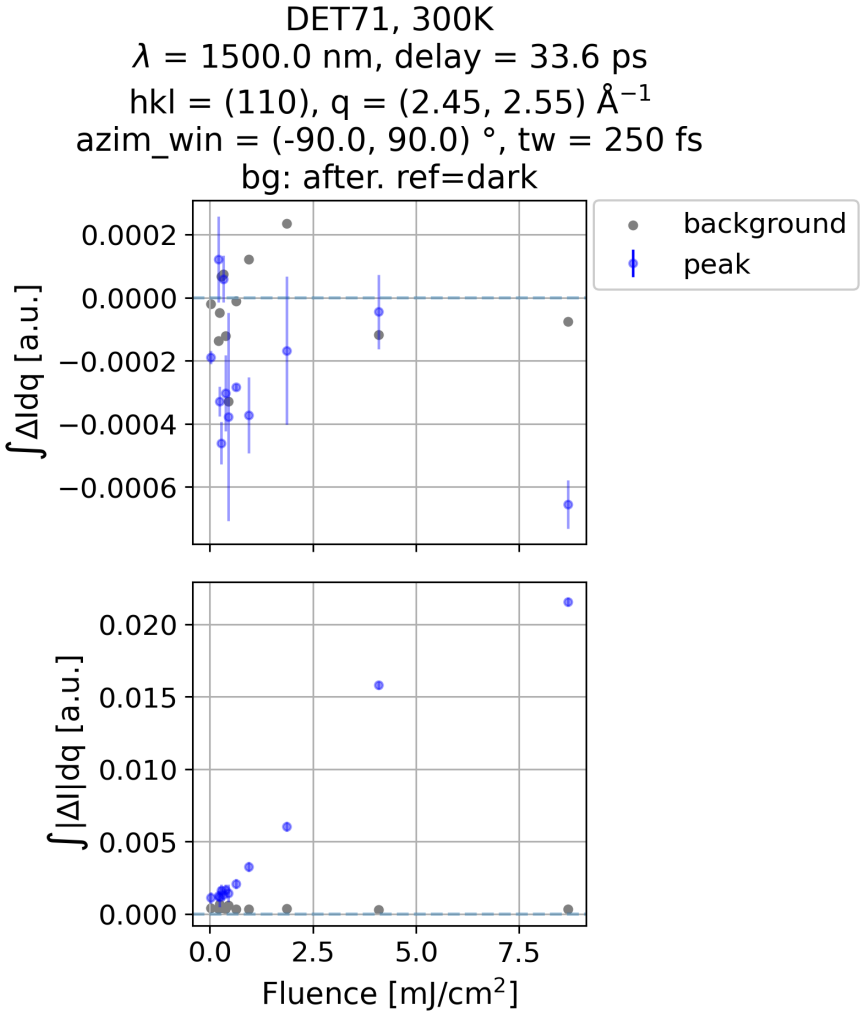

Figure 21.10: SACLA DET71 fluence-dependent differential-integral example for the (110) peak region at a displayed delay of 33.6 ps. The upper panel shows signed $\int \Delta I dq$, and the lower panel shows $\int |\Delta I| dq$.

21.2.2.3 Fitting analysis for different azimuthal sectors

The single-experiment fluence fitting example reads the cached `phi_avg` fitting CSV and plots the fitted (110) position for the full sector and selected symmetric $|\Phi|$ groups. The dark/reference fits are displayed as horizontal dashed lines.

```
from pathlib import Path

from trxrdpy.analysis import fitting

root = Path("/path/to/SACLA2024")

fig, ax, csv_path = fitting.plot_fluence_evolution(
    sample_name="DET71",
    temperature_K=300,
    excitation_wl_nm=1500.0,
    delay_fs=23979,
    time_window_fs=250,
    peak="110",
    _property="hkl_pos",
    unit="mJ/cm$^2$",
    out_csv_name="peak_fits_fluence.csv",
    groups=["Full", 60, 30, 0],
    phi_mode="phi_avg",
    phi_reduce="sum",
    as_lines=True,
    fluence_scale=0.4,
    fluence_offset=0.0,
    delay_offset_fs=9600.0,
    fs_or_ps="ps",
    digits=1,
    show_baseline_sigma=True,
    baseline_sigma=1.0,
    baseline_alpha=0.18,
    baseline_mode="errorbar",
    save=True,
    path_root=root,
    analysis_subdir="analysis",
)
```

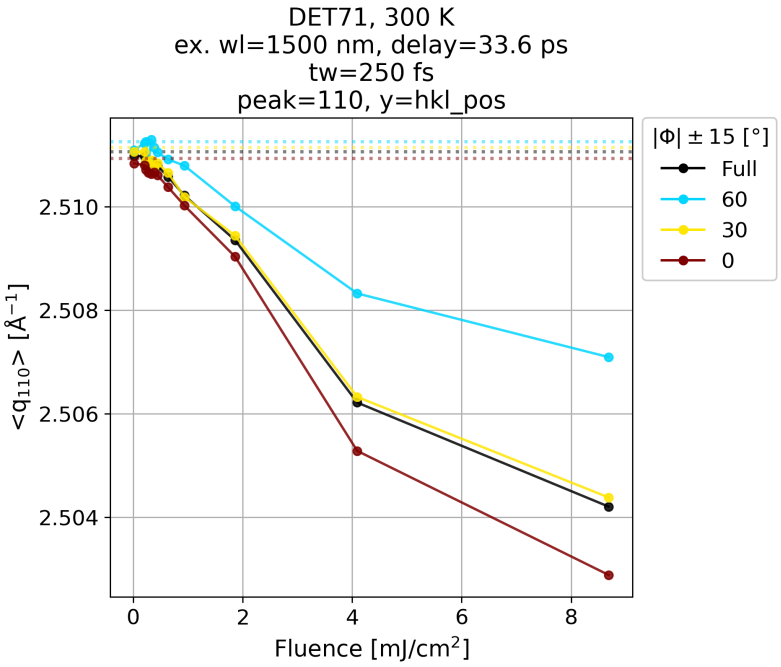

Figure 21.11: SACLA DET71 fitted (110) peak position versus fluence at a displayed delay of 33.6 ps. The plotted groups are the full $(-90°, 90°)$ range and selected `phi_avg` symmetric azimuthal sectors.

21.2.2.4 Multiple-experiment fluence fitting comparison

The multi-fluence comparison overlays two fixed-delay fluence scans. The first branch has stored delay −4042 fs and is displayed as 5.6 ps after the +9600 fs offset. The second branch has stored delay 23979 fs and is displayed as 33.6 ps. The dark/reference rows are included and plotted as horizontal dashed lines for each series.

```
from pathlib import Path

from trxrdpy.analysis import fitting

root = Path("/path/to/SACLA2024")
fluence_root = (
    root / "analysis/DET71/temperature_300K/excitation_wl_1500nm/fluence"
)

experiments = [
    {
        "label": r"(V,Cr)$_2$O$_3$, 300, 1500, 5.6, 250",
        "sample_name": "DET71",
        "temperature_K": 300,
        "excitation_wl_nm": 1500.0,
        "delay_fs": -4042,
        "time_window_fs": 250,
        "phi_mode": "phi_avg",
        "phi_reduce": "sum",
        "ref_type": "dark",
        "ref_value": 1466630,
        "fluence_scale": 0.4,
        "delay_offset_fs": 9600.0,
        "csv_path": str(
```

```
            fluence_root
            / "delay_-4042fs/time_window_250fs"
            / "fitting/peak_fits_fluence_phiavg_sum.csv"
        ),
    },
    {
        "label": r"(V,Cr)$_2$O$_3$, 300, 1500, 33.6, 250",
        "sample_name": "DET71",
        "temperature_K": 300,
        "excitation_wl_nm": 1500.0,
        "delay_fs": 23979,
        "time_window_fs": 250,
        "phi_mode": "phi_avg",
        "phi_reduce": "sum",
        "ref_type": "dark",
        "ref_value": 1466631,
        "fluence_scale": 0.4,
        "delay_offset_fs": 9600.0,
        "csv_path": str(
            fluence_root
            / "delay_23979fs/time_window_250fs"
            / "fitting/peak_fits_fluence_phiavg_sum.csv"
        ),
    },
]

fig, ax, saved_path = fitting.plot_fluence_evolution_multi(
    experiments=experiments,
    peak="110",
    prop="hkl_pos",
    group_by="azim_range_str",
    group="Full",
    fluence_unit="mJ/cm$^2$",
    fluence_scale=0.4,
    fs_or_ps="ps",
    digits=1,
    only_success=True,
    include_reference=True,
    as_lines=False,
    show_baseline_sigma=True,
    baseline_mode="errorbar",
    baseline_sigma_scale=1.0,
    show=False,
    legend_outside=True,
    save=True,
    path_root=root,
    analysis_subdir="analysis",
)
```

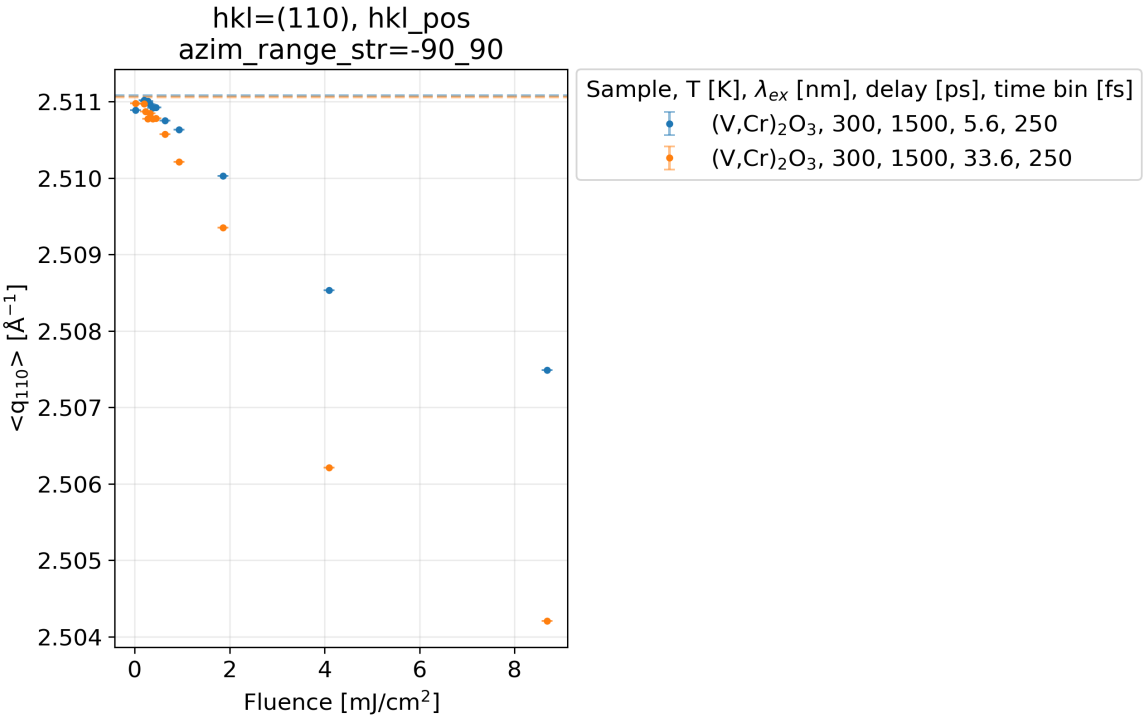

Figure 21.12: SACLA DET71 multi-experiment fluence comparison for the fitted (110) position in the full azimuthal range. The two series correspond to displayed delays of 5.6 ps and 33.6 ps, and the horizontal dashed lines show the included dark/reference fits.

Chapter 22

Analysis GUI workflows

22.1 GUI workflow map

The Analysis GUI is built around a shared `AnalysisGuiState`, a facility service, a path service, and backend services for preparation, calibration, integration, differential analysis, and fitting. The main window contains the following tabs: Session, Data Reduction, Calibration, Azimuthal Integration, 1D Viewer, Differential Analysis, and Fitting Analysis.

The practical tab order is:

1. session and path setup;
2. data reduction;
3. calibration;
4. azimuthal integration and viewer;
5. differential analysis;
6. fitting analysis; and
7. export and reproducibility recording.

The map separates raw-data reduction from final-pattern production. Data Reduction owns facility metadata, representative detector-image production, and, where supported, single-shot 1D cache production. Calibration still requires a representative detector image. After calibration, Azimuthal Integration creates the final `xy_files` by integrating representative dark, delay, or fluence images, or by aggregating the compatible single-shot 1D files currently available.

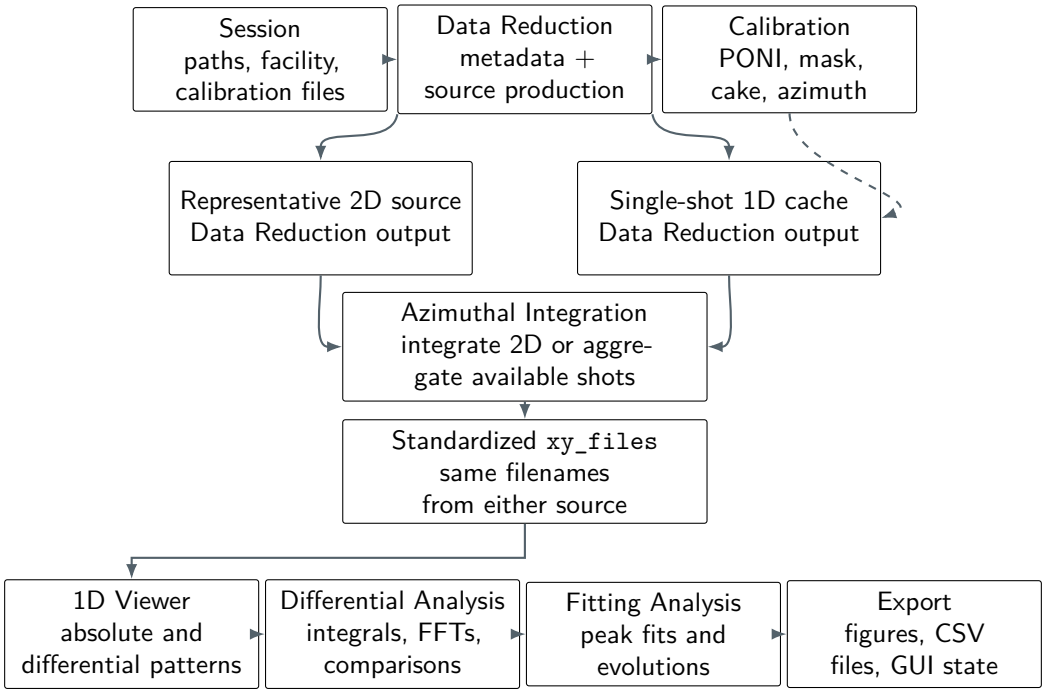

Figure 22.1: Analysis GUI workflow with both final-pattern sources. Data Reduction creates or locates metadata and the representative detector image required for calibration. Where supported, the calibrated geometry is then reused in Data Reduction to publish a single-shot one-dimensional cache progressively. Azimuthal Integration consumes either representative two-dimensional images or the compatible completed shot files and writes the same final `xy_files`.

22.2 Session and facility setup

The Session tab establishes the state used by the rest of the GUI. It selects the facility, experiment root, raw and analysis subdirectories, optional FemtoMAX ping-reference configuration, PONI path, mask path, azimuthal offset, and polarization factor. These values are not cosmetic. They determine which backend module is called and where files are read or written.

Fill the Session tab before running any analysis action. Changing the facility or analysis root after generating files can make later tabs point to a different dataset than expected. For careful work, save the GUI state after the paths and detector settings are finalized.

A saved GUI state can be restored either with *Load GUI State...* or by dropping a saved `xrdpy_gui_state.json` file into the GUI-state path field and pressing *Load Path*. After loading, the field is updated to the resolved JSON path so the active state file is visible.

22.3 Data Reduction tab

The Data Reduction tab is the GUI route into facility-specific preparation. For FemtoMAX it exposes metadata creation, ping-reference handling, averaged-image export, and single-shot 1D production. For ID09 it exposes delay selection and final-image creation. For SACLA it exposes the metadata-HDF5-driven single-shot controls alongside the facility-dependent representative-image workflow. Every long-running reduction action exposed by the GUI runs in a nonmodal worker with live output, so the main window and its other analysis tabs remain responsive. Task dialogs display measured tqdm progress where available and a busy indicator during preparation without a known total. FemtoMAX representative-image export and single-shot production have separately

visible parallel controls; the GUI defaults to the safer `spawn` method while still loading saved states that explicitly selected another method. During FemtoMAX shot production, *Stop safely* ends work at an HDF5-batch boundary and a later overwrite-disabled launch resumes missing files. SACLA production remains scheduler-oriented for large datasets and uses the packaged PBS array sender rather than local multiprocessing around `stpy`.

For FemtoMAX scans that need explicitly assigned timing, enter a mapping in *Scan delay overrides* and select *Override delay unit*. For example, `{167300: 200, 167301: 200, 167302: 500}` with `ns` assigns those scans to 200, 200, and 500 ns. Include these scans in the main scan selection; unlisted scans continue to use the normal ping controls. Blank or `None` means no override. Unit conversion must yield whole femtoseconds; finer values are rejected rather than silently rounded. The controls apply to timing diagnostics, metadata creation, and automatic metadata creation during 2D export. They are disabled for dark scans. After metadata creation, single-shot production uses the stored selection directly. See Section 16.1.1 for selection precedence, fluence constraints, and regeneration requirements.

The mapping and unit are included in saved GUI states. Loading a state written before these controls existed clears any current overrides and restores the default `ns` input unit, without altering the saved experimental metadata.

Check the output of this tab before moving on. At minimum, identify the metadata file and the representative dark or calibration image used to validate geometry. If the representative-image route will be used for final patterns, also identify the delay or fluence images that were created. If the single-shot route will be used instead, complete calibration first, return to Data Reduction, and start *Produce Single-Shot 1D Patterns*. Final delay, fluence, or dark two-dimensional image production can then be bypassed.

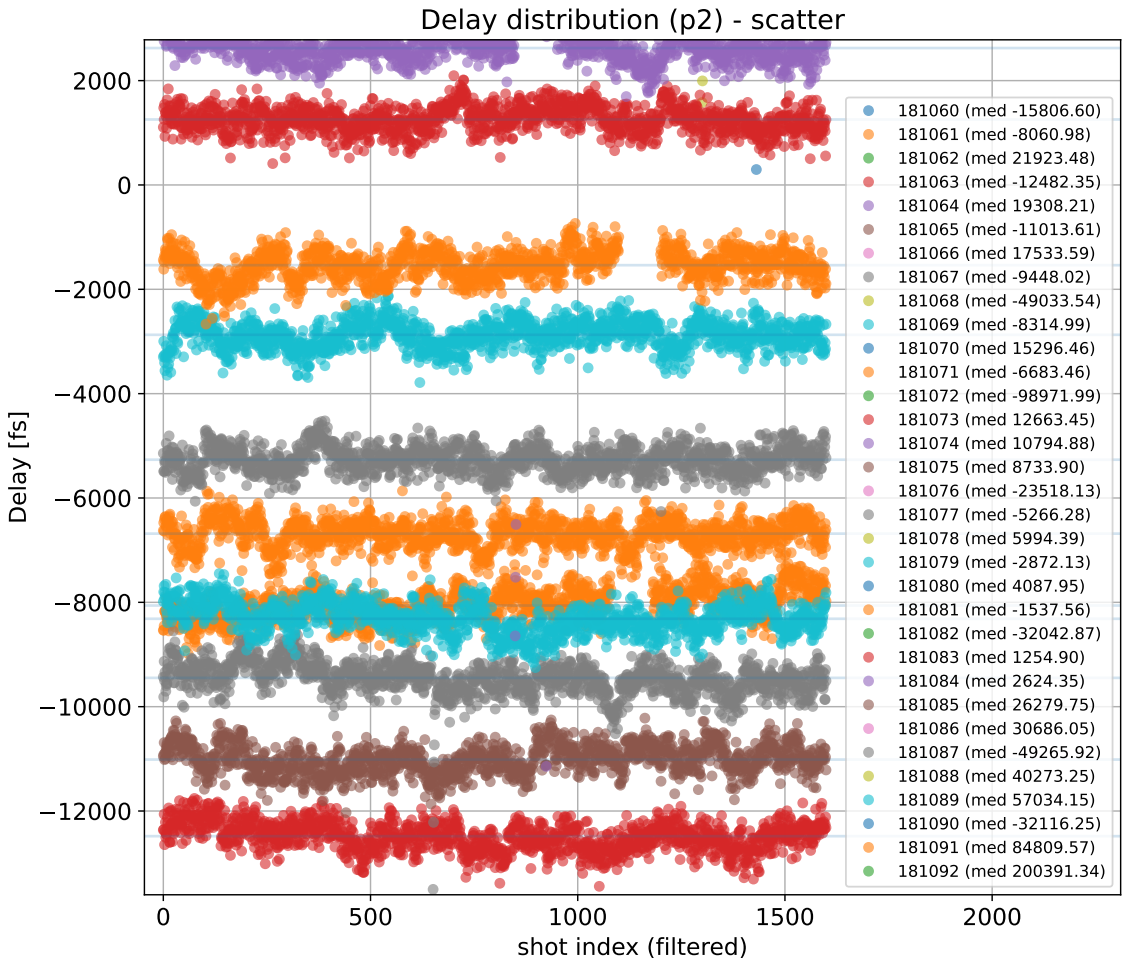

Figure 22.2: Analysis GUI preparation output example: FemtoMAX timing distribution inspected before delay-bin image production.

22.4 Calibration and Azimuthal Integration tabs

The Calibration tab wraps detector/cake plotting, calibration `xy` creation, calibration peak fitting, q-band cake azimuthal-distribution analysis, caked pattern plotting, and property-versus-azimuth visualization. The controls map directly to calibration arguments: scan selector, azimuthal edges, full-range inclusion, q range, normalization range, mask usage, azimuthal offset, polarization factor, q-band/background selectors, phi-window selectors, and save options.

The Azimuthal Integration tab computes standardized `xy` files for dark, delay, or fluence datasets. For FemtoMAX and SACLA, *Final 1D source* selects either *Representative 2D images*, which remains the default, or *Single-shot 1D patterns*. Selecting the single-shot source reveals the metadata-HDF5 field and, for SACLA, the preprocessing settings required to validate cache compatibility. For FemtoMAX the metadata path is optional in both Data Reduction and Azimuthal Integration: when blank, it is resolved from the experiment fields and standardized analysis location. The normal dark, delay, or fluence action then builds or refreshes final `xy_files` from the compatible completed shot files currently available. Its Runtime Options provide *parallel processing* and *Parallel workers*; parallel operation is enabled by default with four workers for either supported source. These controls are hidden for ID09, whose `pytxs` raw-scan reduction remains a separate workflow.

Single-shot cache production itself lives in Data Reduction. Its PONI and detector-mask paths come from the canonical controls in Session and are not repeated in the production panel. The panel exposes the azimuthal offset, polarization correction, azimuthal edges, full-range choice, radial grid, metadata path, and SACLA compatibility fields. The remaining shared settings stay synchronized with Session, Calibration, and Azimuthal Integration. The panel also exposes the final-pattern normalization choice and q normalization range, synchronized with Azimuthal Integration and the downstream analysis windows; these two settings are intentionally applied only after the available shot patterns have been averaged. FemtoMAX production and final aggregation run in independent nonmodal workers, while the SACLA action submits its PBS array and returns control to the GUI. A user can switch tabs and refresh final patterns without interrupting either production route. Concurrent task dialogs route progress independently, and atomic publication prevents aggregation from reading a partially written shot file.

The source mode, synchronized geometry and compatibility fields, polarization and normalization controls, final-integration parallel settings, Data Reduction overwrite choice, FemtoMAX frame-batch, worker-task, and multiprocessing settings, and SACLA preprocessing fields are included in saved GUI states. States written before this reorganization are migrated automatically: former Pattern-tab production values are restored into Data Reduction, PONI or mask paths formerly stored in Data Reduction are promoted into Session, formerly shared FemtoMAX parallel values seed the dedicated single-shot controls, historical metadata-widget aliases are mapped to the current experiment editors, and sample, temperature, excitation, fluence, time-window, and ID09 metadata values remain available. A state without final-integration parallel fields retains the current enabled, four-worker defaults. The default final source remains *Representative 2D images* when no source was saved. Single-shot controls are hidden for ID09 because that pipeline does not provide this mode.

The 1D Viewer tab loads or computes patterns and plots absolute and differential views. Its regenerated XY pattern uses the *Number of q points* setting from Azimuthal Integration. ID09 synthetic fluence scans reuse the integrated source q grid. Use these two tabs together: creation makes the cache explicit, and the viewer checks whether the resulting patterns are scientifically usable.

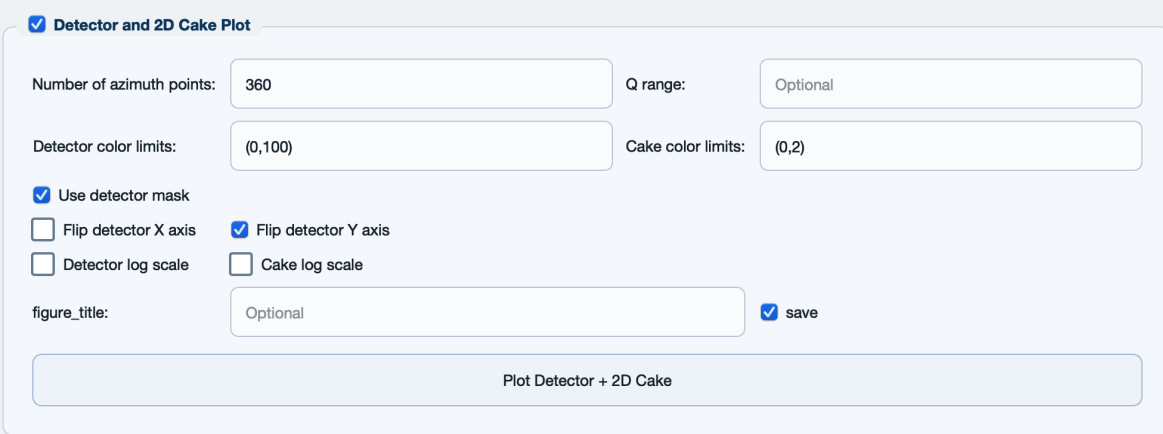

Figure 22.3: Analysis GUI calibration controls for detector/cake plotting. The same panel controls detector-axis inversion, mask use, detector and cake color limits, q range, azimuthal binning, and save behavior.

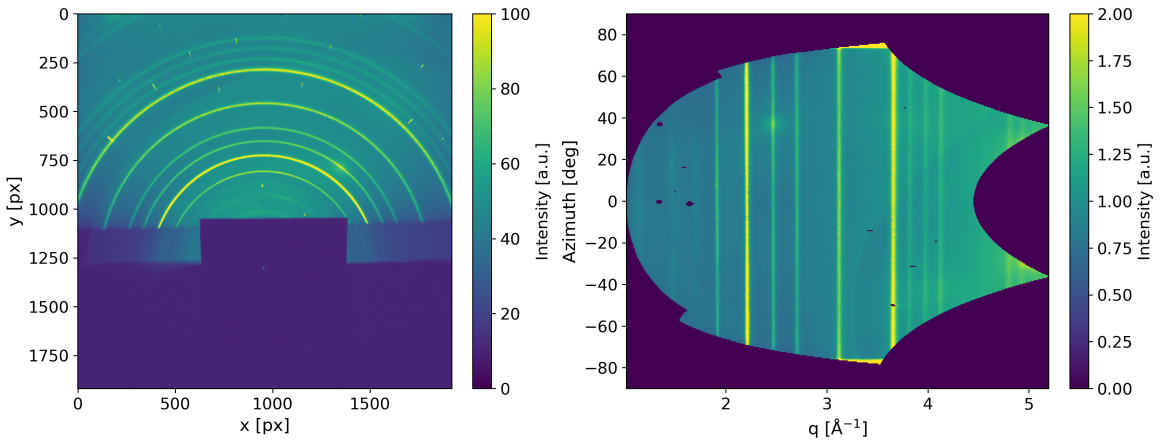

Figure 22.4: Analysis GUI calibration output example: detector image and 2D cake diagnostic produced before one-dimensional integration.

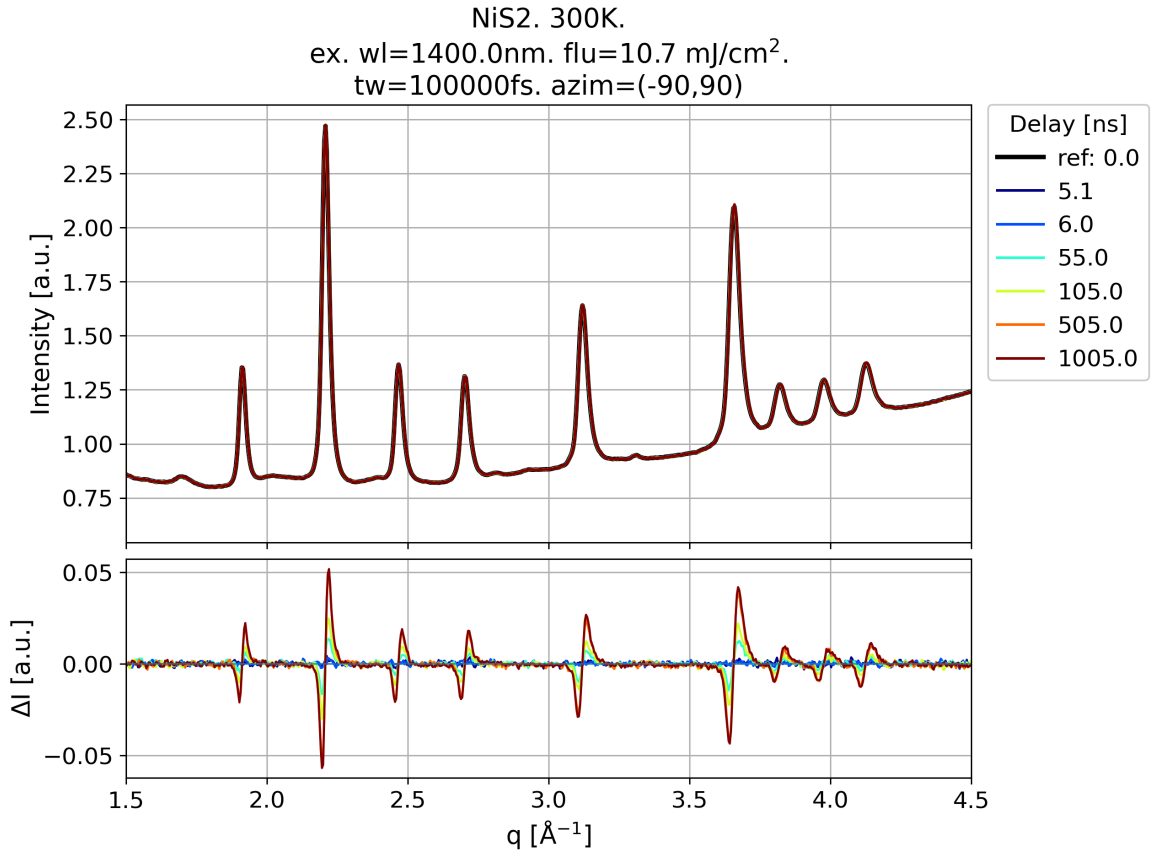

Figure 22.5: Analysis GUI 1D Viewer output example: absolute delay patterns and their differential traces after cached `xy` files have been selected or generated.

22.5 Differential and fitting tabs

The Differential Analysis tab collects peak/background definitions and reference settings before plotting integrals, FFTs, or multi-experiment comparisons. The Fitting Analysis tab collects peak specifications, azimuthal windows, reference settings, and output choices before calling the fitting backend. Both tabs depend on the pattern cache and detector settings established earlier.

For fitted-property evolution, choose absolute values, *Normalize (0–1)*, or *Relative variation (%)*. The latter two boxes are mutually exclusive. Single-experiment references come from the series controls; multi-experiment entries carry their own references. Each multi-experiment entry may also override the shared azimuthal selection with *Full*, a center angle, or a sector interval. Multi-fluence plots additionally offer an optional Matplotlib colormap. These choices are retained in GUI states.

Do not use the GUI as a black box. After a differential or fit plot is produced, record the peak specification, reference choice, azimuthal window, q normalization range, and output CSV path. Those values are the bridge from interactive exploration to reproducible analysis.

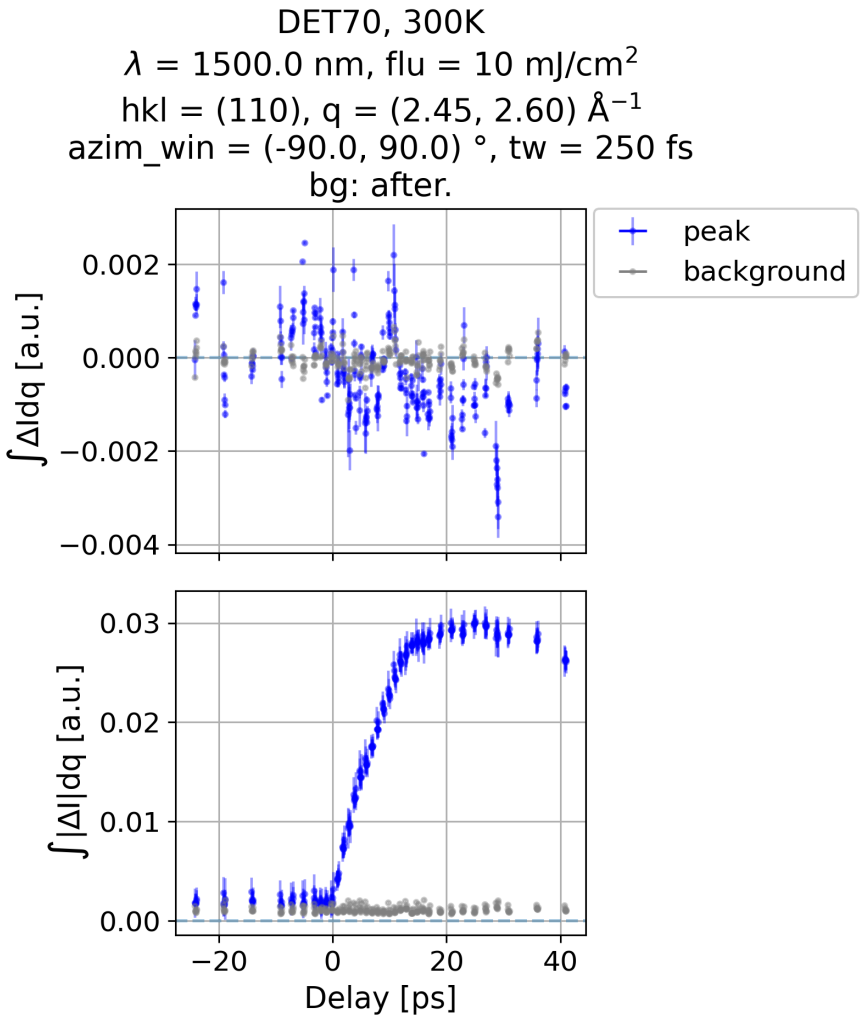

Figure 22.6: Analysis GUI Differential Analysis output example: signed and absolute differential integrals for a selected peak/background definition.

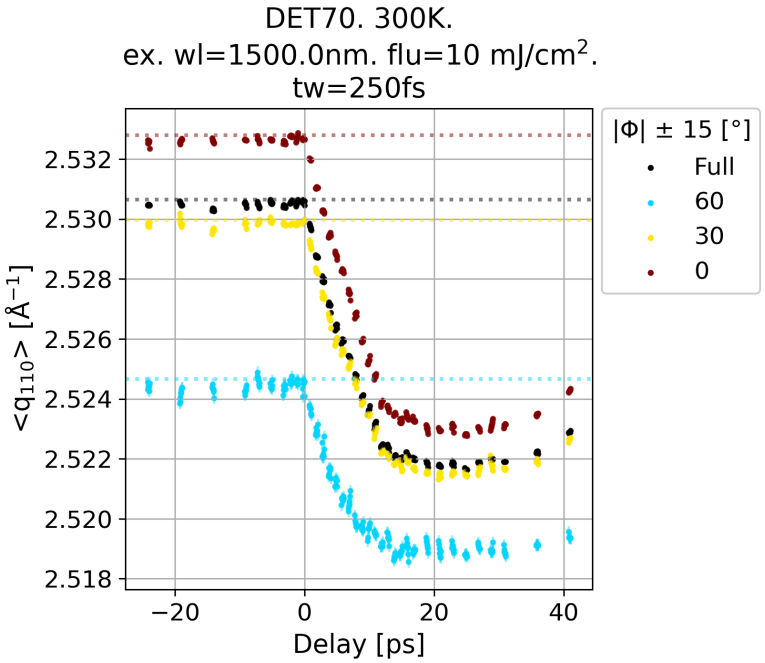

Figure 22.7: Analysis GUI Fitting Analysis output example: fitted peak position versus delay for several azimuthal sectors.

Chapter 23

Analysis API reference and troubleshooting

23.1 User-facing API map

The Analysis API is large. This manual documents the user-facing surface needed for real workflows and avoids turning internal helpers into public commitments. Internal utilities appear only when they define path naming, conventions, or important validation behavior.

Module	Documentation role
`trxrdpy.analysis.calibration`	User-facing calibration, cake diagnostics, q-band cake azimuthal-distribution analysis, calibration fitting, and pattern comparison.
`trxrdpy.analysis.MaxIV_FemtoMAX`	FemtoMAX metadata, representative-image reduction, single-shot production and aggregation, and facility wrappers.
`trxrdpy.analysis.ESRF_ID09`	ID09 raw-data reduction, delay handling, integration, and plotting.
`trxrdpy.analysis.Spring8_SACLA`	SACLA metadata, dark/background processing, representative-image reduction, PBS single-shot production, aggregation, and integration exposure.
`trxrdpy.analysis.fitting`	Delay and fluence peak fitting, fit overlays, and evolution plots.
`trxrdpy.analysis.differential_analysis`	Differential traces, FFTs, and multi-experiment comparison.
`trxrdpy.analysis.gui`	Graphical workflow controller for the same backend operations.

23.2 Common analysis failures

Most analysis failures fall into one of a few categories. The error message usually points to a missing file or invalid selector, but the root cause is often an earlier mismatch in paths, calibration, or reference choice.

- missing or inconsistent raw-data paths;
- scan tags that do not match cached outputs;
- wrong PONI or detector mask;
- inverted detector axes or azimuthal offset mistakes;
- empty integrations caused by q or azimuthal limits;
- empty q bands or background bands in cake azimuthal-distribution analysis;
- incomplete or incompatible single-shot caches caused by mismatched metadata, geometry,

masks, radial grids, polarization, or azimuthal settings;
- failed peak fits caused by poor initial windows or baseline choices;
- inconsistent reference delay or fluence choices; and
- GUI/backend environment mismatches.

When a failure occurs, debug in pipeline order. First confirm that the raw files exist and that the path configuration points to them. Then confirm that facility data reduction produced the metadata and representative detector image required for calibration. Confirm that the PONI and mask load correctly and produce a sensible cake, and that q bands, background bands, and azimuthal limits intersect the computed cake grid. For the representative-image route, verify that the requested dark, delay, or fluence images exist. For the single-shot route, verify that the metadata HDF5 and cache describe the same experiment, that compatible completed files exist for every requested azimuthal window, and that the cache fingerprint matches the current integration settings. Finally confirm that the standard final `xy` files correspond to the selected source and settings. Only after those checks is differential-analysis or fitting code the likely source of the problem.

23.3 Publication checklist

Before publishing an analysis result, record the facility, scan/run identifiers, raw and analysis paths, calibration file, mask file, polarization factor, azimuthal windows, q ranges, normalization method, final-pattern source, reference choice, fitting windows, q-band/background definitions for cake azimuthal-distribution analysis, software version, and output filenames. For a single-shot result, also record the metadata HDF5 path, cache path, integration fingerprint inputs, worker or scheduler chunking, and whether the reported refresh used a partial or complete cache.

For time-resolved work, also record the delay units, time-zero offset, time-window width, timing-reference source, and whether invalid shots were rejected. For fluence work, record the fluence units, fixed delay, excitation wavelength, and how fluence values were assigned to scans. For multi-experiment comparisons, record whether traces were plotted on an absolute scale or normalized for comparison.

For software releases, publish the compiled `XRDpy_manual.pdf` together with the package version. The local source figures and experimental folders used to build the examples are not required in the source distribution when the released PDF is included.

Part III

Shared reference and appendices

Chapter 24

Project and contribution information

Project record

Use the package version, repository URL, Zenodo DOI, and saved analysis or simulation parameters when citing or reproducing results made with XRDpy.

24.1 Versioning and compatibility

Record the installed XRDpy package version with every simulation or analysis result. A saved figure should be traceable to a script, GUI state, parameter file, or CSV table that includes the package version and the relevant experimental or simulated geometry.

24.2 Reporting issues

Useful issue reports include the operating system, Python version, package version, installation route, minimal script or GUI state, complete error message, and the smallest input file needed to reproduce the behavior. For analysis issues, include the facility, path layout, PONI file, mask file, selected scan or delay, final-pattern source, and whether cached `xy` files were reused. Single-shot reports should also include the metadata-HDF5 provenance, cache fingerprint mismatch text when present, and the production/aggregation worker or PBS settings.

24.3 Citation, license, and acknowledgments

The project repository and Zenodo concept DOI are listed in the front matter. Version-specific Zenodo records should be used when a publication depends on a specific release. The package is distributed under the Creative Commons Attribution 4.0 International license.

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Chapter A

Glossary

Bragg condition Geometrical condition under which elastic scattering from lattice planes is constructive.

CIF Crystallographic Information File containing structured crystallographic metadata.

Direct lattice Real-space periodic basis of the crystal.

Ewald sphere Reciprocal-space construction representing elastic-scattering solutions at fixed wavelength.

HKL Miller-index triplet (h, k, l) identifying a reciprocal-lattice vector or lattice-plane family.

PONI Point of normal incidence in pyFAI detector geometry; also the calibration-file format used to store that geometry.

Representative image Averaged two-dimensional detector image used for calibration and, in the default final-pattern route, for condition-resolved azimuthal integration.

Reciprocal lattice Fourier-space lattice used to represent diffraction vectors.

q Magnitude of the scattering vector, expressed here in Å^{-1}.

Single-shot 1D cache Separate resumable collection of frame-resolved one-dimensional patterns, with scan/run and shot/tag identity, used as an optional aggregation source at FemtoMAX and SACLA.

Two theta Angle between incident and diffracted beam directions.

Chapter B

Package map

Module	Responsibility
`trxrdpy.simulation.utils`	Unit conversion, rotation matrices, and homogeneous transforms.
`trxrdpy.simulation.cif`	CIF parsing and validation.
`trxrdpy.simulation.sample`	Lattice, reflections, Bragg checks, and powder intensities.
`trxrdpy.simulation.poni`	PONI parsing and normalization.
`trxrdpy.simulation.attenuation`	Offline Henke optical constants, material attenuation, and grazing-incidence depth.
`trxrdpy.simulation.attenuation_plot`	Attenuation plotting and CSV/HDF5 exchange.
`trxrdpy.simulation.detector`	Area-detector geometry and lab grid.
`trxrdpy.simulation.geometry`	Motors, motor chains, and paired geometries.
`trxrdpy.simulation.diffractometers`	Predefined geometry factories and serialization.
`trxrdpy.simulation.experiment`	Combined experiment calculations and plots.
`trxrdpy.simulation.polycrystalline`	High-level 1D, 2D, and 3D powder workflows.
`trxrdpy.simulation.detector_coverage`	Detector q limit and laboratory-azimuth coverage of powder rings.
`trxrdpy.simulation.intensity_view`	Relative structure factors, polarization, detector images, and display noise.
`trxrdpy.simulation.powder_preparation`	Automatic CIF/lattice reflection families shared with the powder GUI.
`trxrdpy.simulation.single_crystal`	High-level single-crystal simulation, scans, and targeting.
`trxrdpy.simulation.single_crystal_scan`	2D/3D detector-view scan axes and interactive navigation.
`trxrdpy.simulation.orientation_fit`	Measured-Bragg projects, pose inheritance, candidate refinement, diagnostics, and JSON persistence.
`trxrdpy.simulation.reciprocal_scan`	Compact reciprocal configuration scans and on-demand plotting.
`trxrdpy.simulation.mapping_slices`	Computed extra-parameter Bragg mapping slices.
`trxrdpy.simulation.results`	Portable numerical simulation results and HDF5 save/load/replot.
`trxrdpy.simulation.plot`	Simulation visualization functions.
`trxrdpy.simulation.gui`	Qt graphical simulation workflows.
`trxrdpy.analysis.common`	Shared paths, integration helpers, plotting, calibration, fitting, and differential-analysis utilities.
`trxrdpy.analysis._shared_2d`	Representative-image azimuthal integration and final-pattern caching.
`trxrdpy.analysis.MaxIV_FemtoMAX.datared`	FemtoMAX timing-reference handling, metadata selection, and representative-image reduction.
`trxrdpy.analysis.MaxIV_FemtoMAX.single_shot_azimint`	FemtoMAX frame-resolved integration, resumable cache production, compatibility validation, and aggregation.

`trxrdpy.analysis.ESRF_ID09`	ID09 image-based raw-data reduction, delay handling, integration, and plotting.
`trxrdpy.analysis.Spring8_SACLA.datared`	SACLA run/tag metadata, dark/background processing, and representative-image reduction.
`trxrdpy.analysis.Spring8_SACLA.single_shot_azimint`	SACLA run/tag single-shot integration, cache compatibility, chunking, and aggregation.
`trxrdpy.analysis.calibration`	Calibration, detector/cake diagnostics, and q-band azimuthal-distribution analysis.
`trxrdpy.analysis.differential_analysis`	Differential traces, FFTs, and multi-experiment comparisons.
`trxrdpy.analysis.fitting`	Delay/fluence peak fitting, overlays, and evolution plots.
`trxrdpy.analysis.gui`	Qt session, Data Reduction, Calibration, Azimuthal Integration, Viewer, Differential, and Fitting workflows.

Chapter C

Citation and license

If XRDpy contributes to academic work, cite the Zenodo record corresponding to the version used. The concept DOI for all versions is https://doi.org/10.5281/zenodo.18634909. Version-specific citation metadata is available from Zenodo.

The project is distributed under the Creative Commons Attribution 4.0 International license (CC BY 4.0). The repository's `LICENSE` file records the SPDX identifier and links to the official legal code.