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TOF-CT, Time-of-Flight Calibration Tool; a graphical Python application for calibration of neutron powder diffraction instruments

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TOF-CT, Time-of-Flight Calibration Tool; a graphical Python application for calibration of neutron powder diffraction instruments.

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Abstract

TOF-CT (Time-of-Flight Calibration Tool) is a standalone, GUI-based Python application designed for the calibration of neutron time-of-flight powder diffraction instruments, the principal output of which is a table of refined DIFC values for every detector pixel on a given instrument, obtained by cross correlation of observed Bragg peak positions against any user-supplied set of powder diffraction Standard peak positions. The table may be exported as a Mantid-readable DiffCal.h5 file, or an Offsets.cal file, that may be used as part of the normal Mantid powder diffraction data reduction routines. TOF-CT provides live dynamic overlays of Standard peak positions on both 2D heatmaps of the raw spectra arrays and on 1D line plots of any individual spectrum in either TOF, *d*-spacing or momentum transfer (*Q*). Changes in DIFC for any spectrum can be entered by hand in the UI's table, or refined automatically using the built-in cross correlation routine, updating the peak positions in TOF or shifting the spectra in *d*-spacing or *Q* on any open 1D or 2D plot. These features allow complete user control of the calibration workflow, enabling better understanding of measurement- or instrument-specific features in the data that potentially affect accurate and precise calibration.

1. Introduction

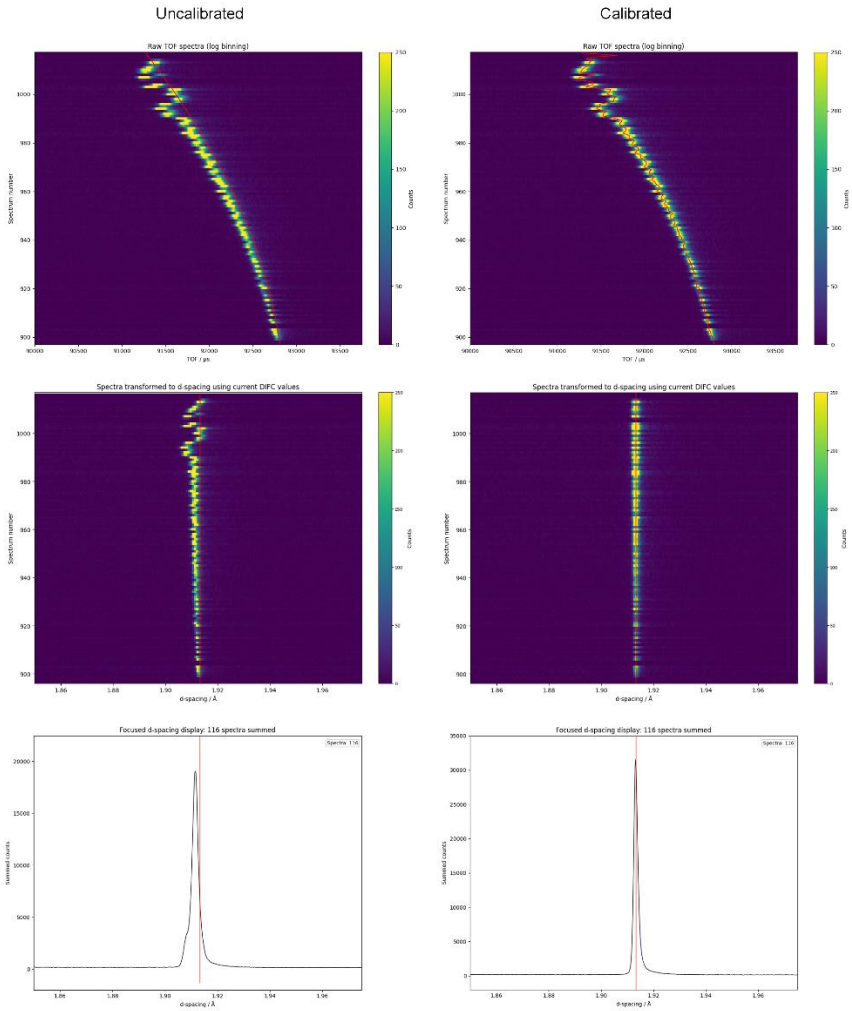
A particular advantage of the time-of-flight neutron diffraction method is the ability to capture a substantial fraction of a material's diffraction pattern in detectors at any arbitrary 2θ scattering angle around the sample position, with the caveat that there is a large gradient in resolution from low to high 2θ. This is leveraged, for example, by high-pressure beamlines, where the apertures between the anvils of common high-pressure devices are typically arranged to allow egress of the diffracted beam in a relatively narrow cone around 90° to the incident beam; detectors capturing that narrow cone of diffracted intensity nevertheless obtain a 'complete' diffraction pattern.

However, capitalizing on that advantage, considering the relatively poor counting statistics obtained in any given detector pixel, requires summation of diffraction spectra from – potentially – many hundreds or thousands of pixels comprising a detector module or bank of modules. Since pixels at one location in a detector module will normally be located at a different 2θ (and possibly a different radial distance, L2, from the sample) than other pixels in the module, a given Bragg peak from the sample will be observed at a different time-of-flight in each pixel. In order to properly sum the diffraction spectra from these pixels, they must be

transformed into another dimension where the position of the Bragg peaks is invariant with pixel location, and this will normally be *d*-spacing, although it could equally be momentum transfer (*Q*).

Proper calibration should be both precise and accurate. In this context, precise calibration means that Bragg peaks in various detector elements are as perfectly aligned in *d*-spacing (or *Q*) as can be achieved prior to summation, ensuring that the only 2θ-dependent variations in resolution affect the peak shape and that peak-shape aberrations due to misalignment are minimized (Figure 1).

Figure 1. Examples of imprecise and precise calibration of high-resolution neutron powder diffraction data collected on HRPD at the ISIS Neutron and Muon source. On the left, data from HRPD's backscattering module number 7 are shown in TOF (top left) with counts in each logarithmically binned TOF channel depicted using a colour coded heatmap. The bright yellow curve marks the strong 220 Bragg peak of the cerium oxide diffraction standard, and the solid red line indicates where that peak position is predicted to lie based on a model of the instrument's geometry. Clearly, the two deviate from one another increasing from low to high spectrum numbers (high to low 2θ in this case) and there are additional non-systematic offsets at the outer edge of the detector module. After transformation to *d*-spacing (center left) using the implicit geometry, these systematic and non-systematic offsets persist, and summation of the spectra into a 1D diffraction pattern results in an aberrant peak shape (bottom left). By contrast, when DIFC values are fitted to the standard's peak position in each spectrum (Calibrated data on the top right), transformation to *d*-spacing (center right) produces precisely aligned spectra that sum to a nice intense and sharply defined peak (bottom right).



Accurate calibration means that the aligned *d*-spacing (or *Q* values) of the peaks are correct in an absolute sense. Instrument scientists may take the view that the latter is not important, since data reduction routines transform spectra back into time-of-flight and this is the end-product delivered to the academic user for analysis. At that stage, users employ an instrument-parameter file with calibration parameters derived from fitting of a diffraction standard that should ensure accuracy. However, it is not uncommon for instruments to write end-product data in *d*-spacing for a variety of reasons, including indexing of unknown power patterns, or on-the-fly determination of pressures by reading the peak positions of a pressure marker in a high-pressure experiment. In these instances, both precision and accuracy are paramount.

Existing calibration workflows are typically optimised for automated processing and batch reduction. In Mantid (Arnold *et al*., 2014) there are two methods: **GetDetectorOffsets** and **PDCalibration**. In the first of these, the user must select a peak in a set of spectra with a *d*-spacing that most closely matches that of the diffraction standard that has been measured. However, this is done by transforming the data in TOF to *d*-spacing using the geometry from the Instrument Definition File, which may or may not be accurate. Hence the overall accuracy of the method depends entirely on having an accurate IDF. The method requires the user to first transform data into *d*-spacing using the **ConvertUnits** algorithm, to then ensure matching bin indices across all spectra using **Rebin**, to run the **CrossCorrelate** algorithm in order to generate the cross-correlation function, and then finally to run **GetDetectorOffsets**. At this stage, the user could save an Offsets.cal file,[1] which works with the current powder reduction scripts, or preferably the offsets workspace should be converted to a list of absolute DIFC values with the **ConvertDiffCal** algorithm, which can be saved with **SaveDiffCal** and applied with **LoadDiffCal**/**ApplyDiffCal**. In principle, this method is precise but may or may not be accurate if the underlying Instrument Definition File is inaccurate.

The **PDCalibration** algorithm resembles the old **GetDetectorOffsetsMultipeaks** algorithm, which has been removed from recent versions of Mantid. This algorithm keeps the starting workspace in TOF and uses a table of absolute standard peak positions to fit the observed peaks in each spectrum and then derive DIFC values for each spectrum. The user has control over the various fit parameters used and must simply save the end result with **SaveDiffCal** and then apply the result with **LoadDiffCal**/**ApplyDiffCal**. The **PDCalibration** algorithm should be both accurate and precise.

Whilst highly capable, these workflows are quite opaque and typically present calibration results primarily as numerical tables or calibration files, with limited opportunities for interactive inspection of individual detector spectra, visualisation of calibration trends, or rapid testing of alternative fitting parameters. Understanding the origin of calibration anomalies may therefore require repeated execution of calibration algorithms interspersed with external plotting and analysis steps.

[1] Note that offsets are computed relative to the DIFC values derived from the geometry in the Instrument Definition File and require the latter to be accurate, whereas the absolute DIFC values written in a DiffCal file are entirely independent of the IDF.

The increasing complexity of modern neutron detector systems creates a need for calibration tools that combine automated fitting with direct user interaction and visual feedback. Instrument and detector scientists frequently require the ability to examine individual spectra, compare observed and predicted Bragg peak positions, investigate detector-specific calibration behaviour, visualise calibration constants across large detector arrays, and assess the physical significance of derived corrections. Such capabilities are particularly valuable during instrument commissioning, detector installation, geometry refinement and diagnostic investigations.

Modern instruments may contain many thousands, or even hundreds of thousands, of detector elements distributed over multiple detector banks. Detector geometries may evolve during instrument operation due to manufacturing tolerances, installation errors, maintenance interventions, thermal cycling or mechanical movement. Consequently, calibration often requires iterative investigation of detector-specific behaviour, identification of problematic regions, and assessment of the physical plausibility of derived corrections.

TOF-CT offers the user a graphical calibration environment for neutron time-of-flight diffraction instruments that emphasises transparency, interactivity and user control. The software provides detector-by-detector DIFC refinement using reference *d*-spacing standards while maintaining continuous visual access to the underlying data. Interactive heatmap displays, spectrum-level visualisation tools, detector geometry integration, calibration-file import/export, and physically meaningful representations of calibration corrections allow users to move seamlessly between automated fitting and detailed diagnostic investigation. The resulting workflow complements existing Mantid calibration algorithms by providing an accessible environment for calibration development, validation and instrument troubleshooting. The code is emphatically not trying to replace Mantid calibration algorithms; it is a diagnostic and exploratory environment that sits alongside them.

2. Methods

The general relationship between neutron time-of-flight (μs) and *d*-spacing (Å) is written as a quadratic equation:

$$\mathrm{TOF} = \mathrm{DIFA}\cdot d^2 + \mathrm{DIFC}\cdot d + \mathrm{T}_0 \qquad \text{Eq. 1}$$

where the constant DIFC is proportional to the neutron's total flight path according to:

$$\mathrm{DIFC} = (m_\mathrm{N} / h) \cdot (\mathrm{L1} + \mathrm{L2}) \cdot 2\sin(\theta) \qquad \text{Eq. 2}$$

L1 is the primary flight path from the source to the sample, L2 is the secondary flight path from the sample to the detector and θ is half the scattering angle, 2θ, of the detector. The terms, m_N and h are the neutron mass (1.6749275×10^{-27} kg) and Planck's constant (6.62607015×10^{-34}

kg m^2 s^{-1}), respectively. For *d*-spacings in Å, and flight paths in metres, then Equation 2 is often written simply as:

$$DIFC = 505.5568269 \cdot (L1 + L2) \cdot \sin(\theta) \qquad \text{Eq. 3}$$

The term DIFA in Eq. 1 accounts for secondary variations in flight path due to effects such as sample attenuation and finite detector thickness, and T_0 typically represents electronic timing offsets that arise in the Data Acquisition Electronics (DAE). Since these terms are usually small and, in the case of DIFA, may be sample dependent, it is appropriate to omit them from consideration for instrument detector calibration purposes, although it is entirely appropriate to determine these quantities for downstream user calibration files employed for pattern fitting and data analysis.

Consequently, the relationship used in the TOF-CT code between time-of-flight and *d*-spacings reduces to the linear equation:

$$TOF = DIFC \cdot d \qquad \text{Eq. 4}$$

Calibration of TOF diffractometers is typically performed using well-characterised reference materials such as silicon or cerium oxide, which have universally agreed lattice parameters at a given temperature, certified by recognized organisations. These will typically be American National Institute of Standards (NIST) standard reference materials (SRMs) sold as certified batches with well-determined lattice parameters, grain sizes and chemical compositions. The known *d*-spacings of these materials provide a set of reference peak positions against which DIFC may be refined. TOF-CT provides an internal set of six NIST standards (silicon, ceria, alumina, quartz, dehydrated Zeolite A and dehydrated Zeolite Y) as well as a further four commonly used diffraction standards or test samples (yttrium aluminium garnet, NACALF, iron and diamond). Between five and ten *d*-spacings of prominent peaks from these standards are tabulated in TOF-CT, although users can add to these manually, remove entries or edit the values of entries at any time.

When provided with a table of detector geometries for every pixel in the instrument (loaded as a list of L2 and 2θ values for every detector in the order in which they appear in the recorded spectra), and the primary flight path length, TOF-CT computes the Bragg peak positions of any selected diffraction standard in TOF and overlays these on the measured diffraction data as solid red lines. Users can browse a table of spectra and manually edit the DIFC values to resolve any mismatch between the observed and calculated standard peak positions. However, the most efficient way to calibrate the instrument is to carry out an automatic refinement.

When the automatic fitting routine is run in TOF-CT, each observed spectrum is sampled at the predicted peak positions to generate a scalar score describing the degree of agreement between the calibration standard and the measured data. The score is constructed such that

larger values indicate improved coincidence between predicted and observed Bragg peak positions. To ensure robust convergence in the presence of significant initial calibration errors, a coarse search is first performed over a user-defined fractional DIFC range centered on the starting value. The search half-width is specified as a percentage of the initial DIFC estimate. The trial DIFC producing the highest score is selected as the starting point for numerical optimisation. Following the coarse search, a one-dimensional least-squares optimisation is performed in DIFC. The objective function seeks to maximise the coincidence between predicted and observed Bragg peak positions by adjusting the DIFC value. Since only a single parameter is refined for each spectrum, the result is a computationally efficient optimisation that is readily applied to large detector arrays. To reduce sensitivity to statistical fluctuations, the observed spectra may optionally be smoothed prior to fitting using a Gaussian convolution kernel. The smoothing width is user selectable and specified in units of histogram bins. The quality of the optimisation is assessed by comparing the final score with that obtained using the initial geometric DIFC estimate. A minimum percentage improvement threshold is applied to reject unreliable fits. Spectra failing to exceed this threshold retain their original geometric DIFC values and are flagged accordingly in the results table. The resulting DIFC values are stored on a detector-by-detector basis and may subsequently be inspected, edited manually, and exported to Mantid-compatible DiffCal files or Offsets files. Because each detector is treated independently, localised calibration anomalies can be identified and investigated without imposing constraints from neighbouring detector elements.

The calibration strategy deliberately avoids explicit profile fitting of individual Bragg peaks. Instead, calibration is based on maximising the coincidence between expected and observed peak positions across the complete set of reference reflections. This approach reduces sensitivity to peak asymmetry, overlapping reflections, detector-specific line-shape variations, and low counting statistics. The resulting optimisation is computationally efficient and sufficiently robust to permit detector-by-detector calibration of large-area neutron detector systems containing many tens or hundreds of thousands of spectra.

Note that users can still manually edit DIFC values after the fit is completed, if one or more spectra have not been suitably fitted. A second round of automatic fitting can be carried out using the adjusted DIFCs as new seed values, and so on until the user is satisfied that all detector elements have been properly calibrated.

3. Implementation

TOF-CT is implemented in Python and has been tested on Python 3.13.3; the following dependencies should be installed before use: PyQt6 for the Graphical User Interface (GUI), Matplotlib for the 2D plotting, SciPy and NumPy for numerical computation, h5py to read and write Mantid-compatible NeXus and HDF5 format files writing, and Pandas for file import/export, and tabular data management.

Users can obtain the latest version of Python from www.python.org. The named dependencies may then be installed in any command window by typing, e.g.,

```
> install pip PyQt6 matplotlib numpy scipy h5py pandas
```

The TOF-CT code is available from (https://github.com/DominicFortes/TOF-CT) under an MIT License agreement.

Once the dependencies are installed, and the relevant files downloaded, navigate via the command window to the folder containing the file TOFCT.py and type

```
> python TOFCT.py
```

which will open the GUI and allow the user to load files.

What follows is a brief summary of the basic requirements to run a calibration, inspect the results and save the output. Readers should study the TOF-CT documentation supplied in the Appendix for further details on file formats and methods.

Three sources of input are required to run TOF-CT. The first is a powder diffraction dataset in NeXus format (.nxs) of any suitable material, although ideally a diffraction standard with certified lattice parameters. The second is a description of the instrument geometry, which should be a simple list of detector ID, L2 and 2θ for each detector pixel arranged in the same order in which the spectra are written in the raw data. This information is completed with the instrument's L1 value. For instruments where several detector pixels are summed together by the DAE to create a single spectrum, then an additional file describing that mapping is required. Finally, the user must choose from one of the supplied calibration standards.

The loaded diffraction data will be displayed as a heatmap on the right-hand side of the GUI, overlayed with the standard's Bragg peak positions in red, and a table beneath the display will show the detector ID (and related geometry) allocated to each spectrum, along with the computed DIFC (Figure 2).

After running a fit of DIFC, the display automatically updates and now shows that the Bragg peak positions have been well matched (Fig. 3). The table underneath the display reports the new DIFC positions and also computes offsets between the actual DIFC and the geometry-derived DIFC. Since the observed Bragg peaks may exhibit a very strong time dependence, particularly in detectors at lower 2θ, the TOF display may not be the most suitable for evaluating misfits. The user may instead open popup 2D displays in either *d*-spacing or momentum transfer, where the Bragg peak positions are d/Q invariant, and misfits are more clearly manifested.

At any time, users can examine single spectra as 1D line plots to evaluate the quality of the fit to the standard's peak positions, and optionally to characterise peak widths (displayed as an estimated FWHM), as shown in Figure 4. Furthermore, the user can sum spectra and display these as 1D line plots to evaluate the effects of the chosen calibration on the resolution of a detector module or detector bank.

Figure 2. TOF-CT screenshot after loading HRPD data from a ceria standard. Superficially, the agreement between the observed and calculated peak positions is very good. However, close examination (see, e.g., Figure 1 top left) reveals both systematic and non-systematic deviations that require calibration.

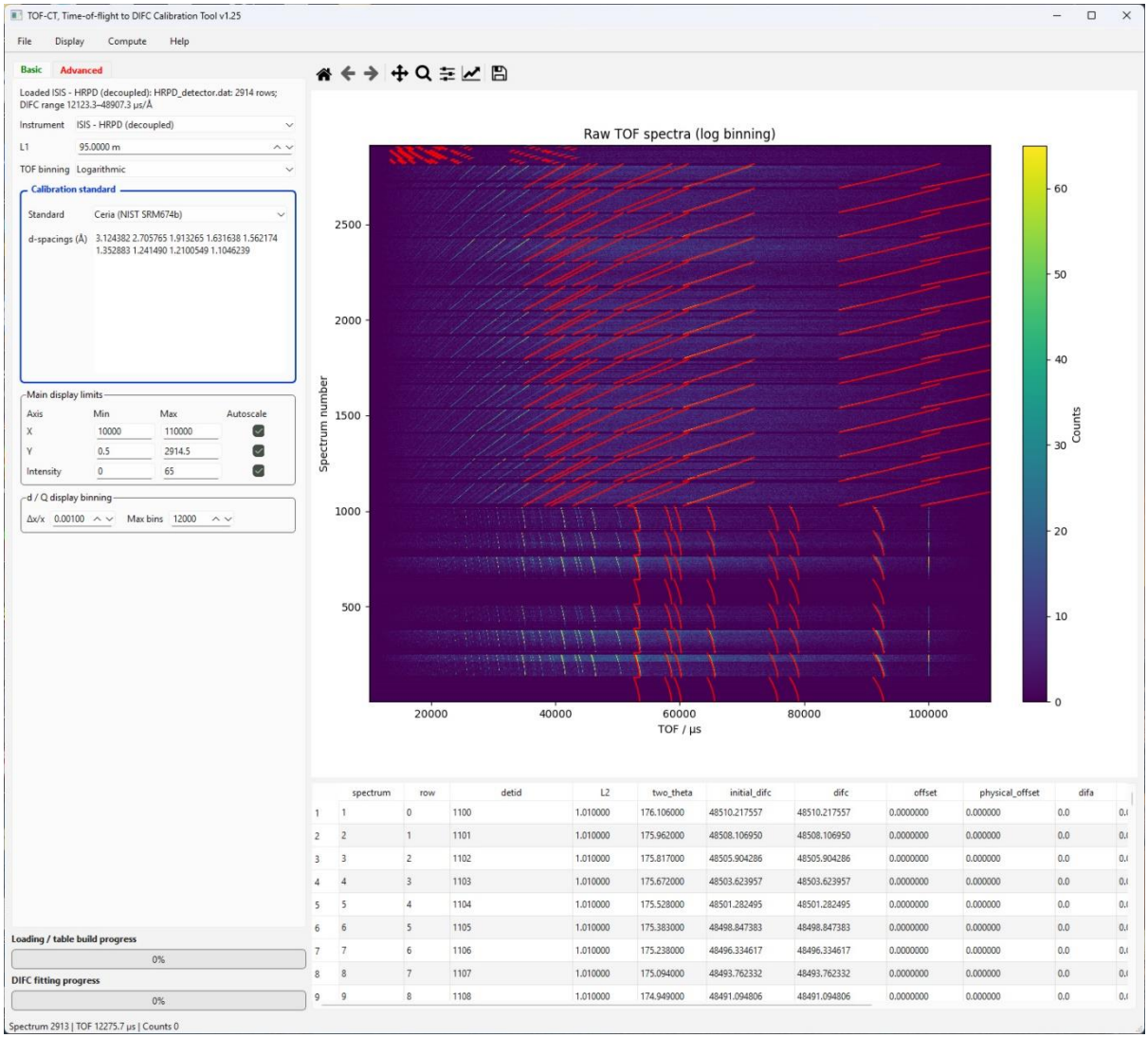


Figure 3. TOF-CT screenshot after carrying out a calibration fit, zoomed in on the fit to a single peak in HRPD's backscattering module 7. As reported in Figure 1, middle and bottom right, these calibrated data transform into d-spacing with all spectra precisely aligned and sum to give sharp 1D peaks.

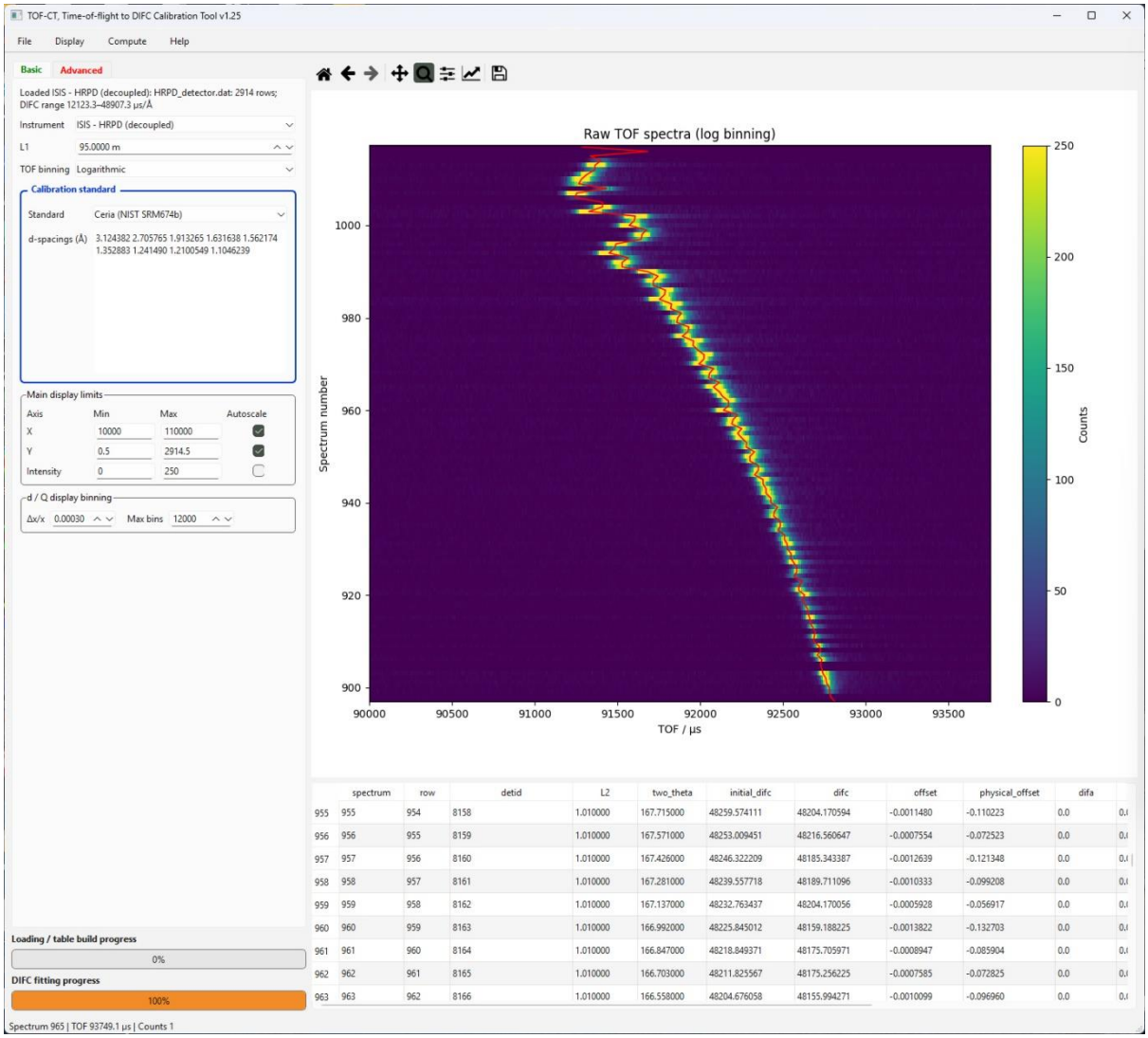
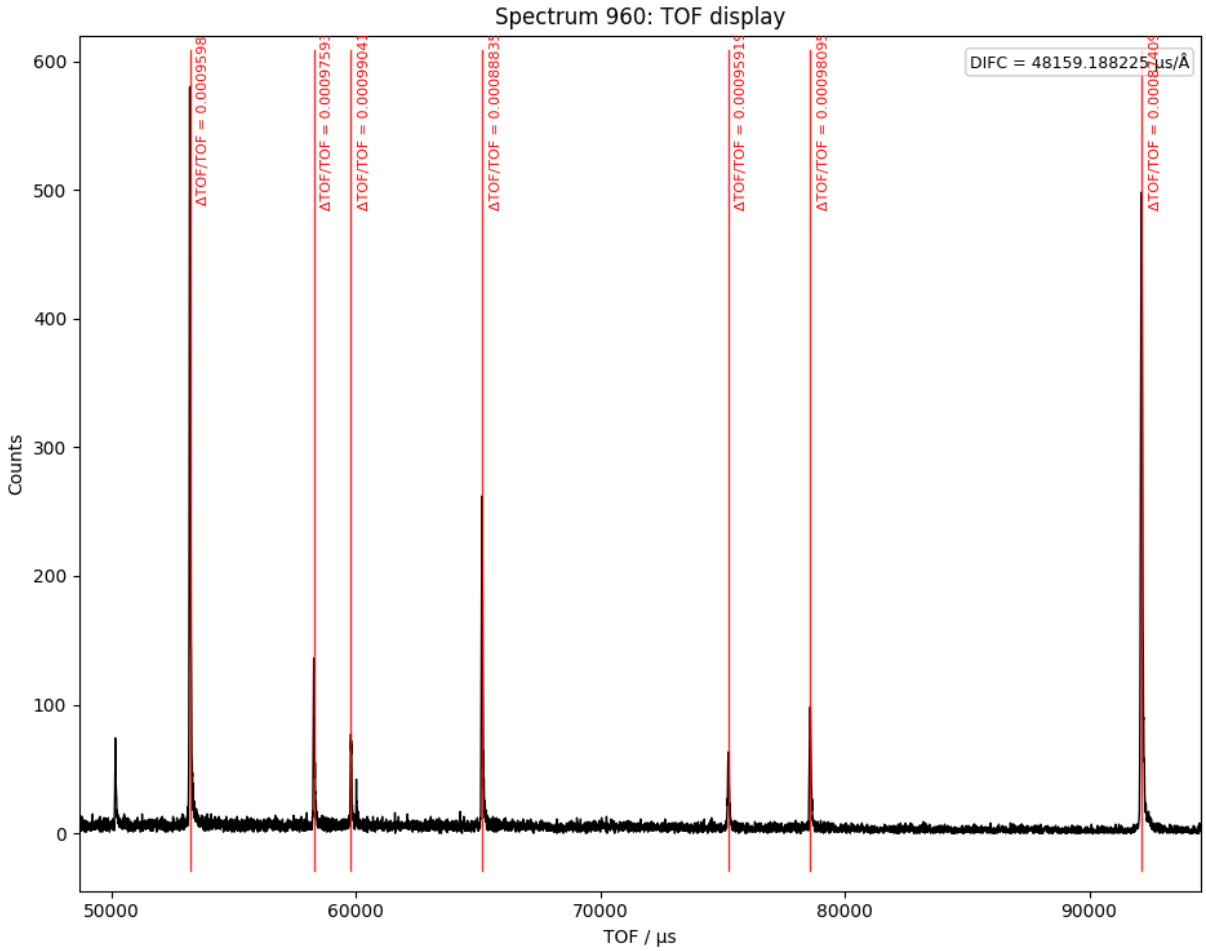


Figure 4. Example single spectrum display with the overlay of the standard's peak positions and optional display of estimated FWHM. TOF-CT enables single-spectrum displays in TOF, *d*-spacing and *Q*, and permits summation in *d*-spacing or *Q*.



Once the calibration is complete, the user can save the entire results table as a comma-separated variables (CSV) file for processing elsewhere, or else the per-detector DIFC values can be exported as a DiffCal.h5 file, or the per-detector offsets exported as an Offsets.cal file. Both of the latter two files can be used interchangeably (at the time of writing) by Mantid during the standard powder diffraction data reduction routines (namely the **ApplyDiffCal** algorithm). Note that for the Offsets.cal file to work correctly, the geometry used by TOF-CT to determine the offsets must match precisely the geometry of the Instrument Definition File used by Mantid.

References

Arnold, O., Bilheux, J. C., Borreguero, J. M., Buts, A., Campbell, S. I., Chapon, L., ... & Zikovsky, J. (2014). Mantid—Data analysis and visualization package for neutron scattering and μ SR experiments. *Nuclear instruments and methods in physics research section a: accelerators, spectrometers, detectors and associated equipment*, *764*, 156-166.

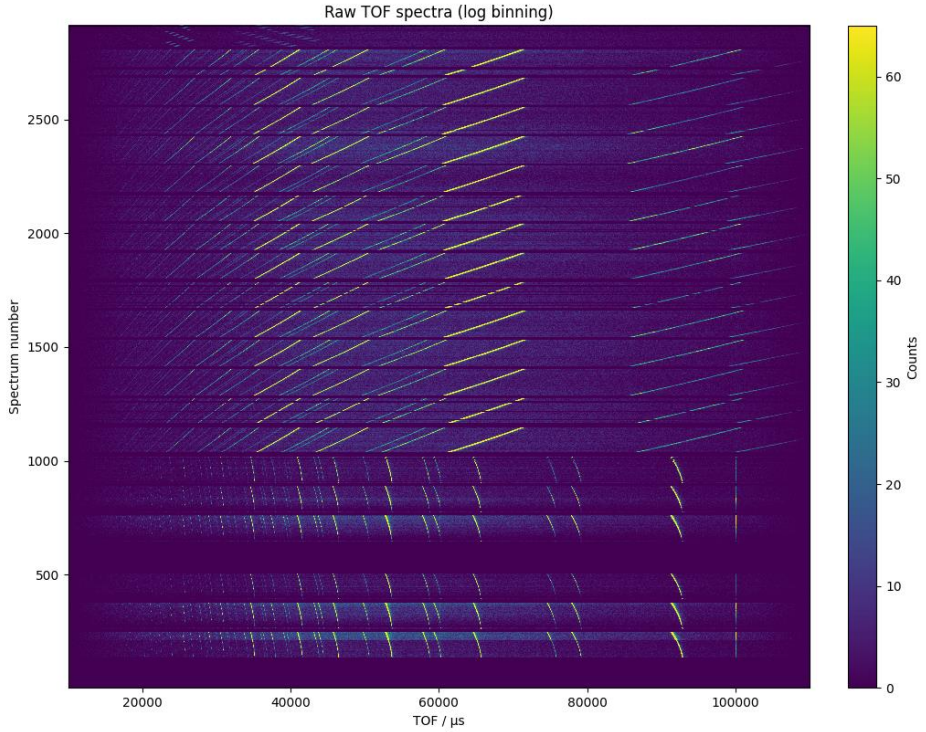
APPENDIX

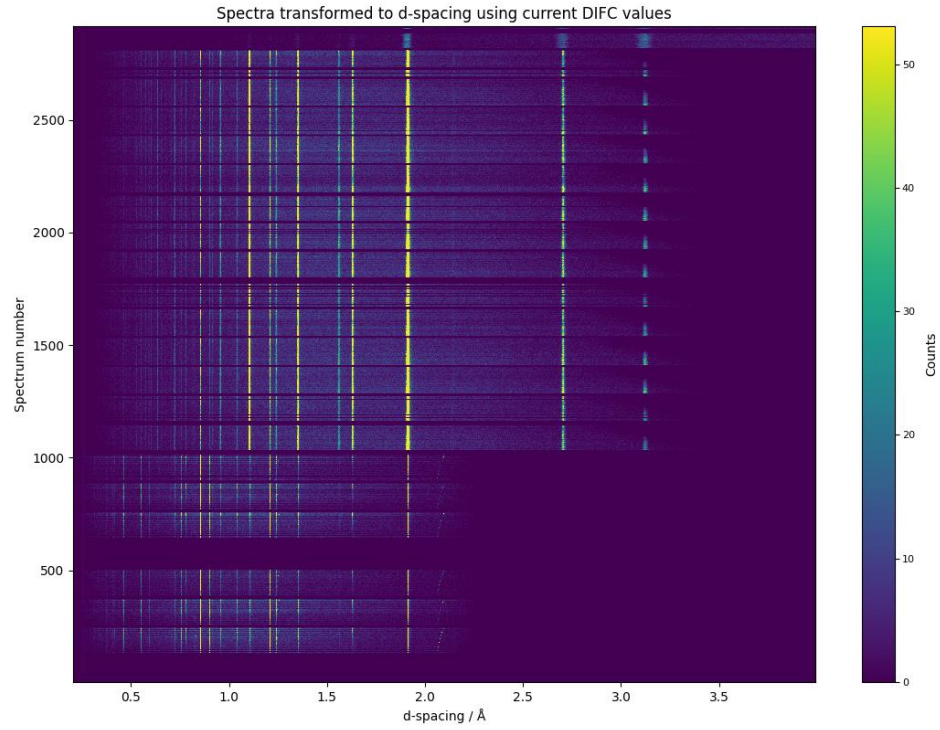
TOF-CT DOCUMENTATION AND USER GUIDE

Time-of-Flight - DIFC Calibration Tool Documentation

Table of Contents

Time-of-Flight - DIFC Calibration Tool Documentation





1. Introduction

TOF-CT (Time-of-Flight - DIFC Calibration Tool) is a Python-based graphical application designed for accurate and precise calibration of time-of-flight neutron diffraction instruments. TOF-CT's principal function is to fit the Bragg peak positions in a stack of raw diffraction spectra to peaks positions from a user-defined powder diffraction standard, typically one with lattice parameters certified by the National Institute of Standards (NIST, USA). The application allows visualisation of spectra as 2D Heat maps both in the original TOF units and transformed into either *d*-spacing or momentum transfer (*Q*). It further allows plotting of individual spectra as 1D line plots and summation (or time focussing) of multiple spectra also as 1D line plots.

The crucial differences from Mantid's calibration, alignment and focussing algorithms are as follows: (1) The positions of the peaks from the standards are overlaid on the 1D and 2D plots for direct visual comparison; (2) The results of fitting DIFC are presented in an editable table, where users can manually alter the calibration constant and observe dynamic updates of the result on any open 1D or 2D plot.

The final calibration table can be exported as files suitable for use by Mantid's powder diffraction data reduction scripts. This documentation provides a comprehensive guide to installing and using TOF-CT.

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2. Installation

To install and run TOF-CT, follow these steps:

- Ensure Python is Installed:
  - TOF-CT has been tested on **Python 3.13.3**. Download & install Python from python.org.
  - Verify the installation by running: `> python --version`
- Install Dependencies:
  - Install the required Python packages using pip (see Section 3)
- Download TOF-CT Source Code (https://github.com/DominicFortes/TOF-CT):
  - Save the provided Python modules (TOF_CT.py, instruments.py, standards.py, help.py, and the Instruments folder) in a single directory.
- Run TOF_CT:
  - Navigate to the directory containing the TOF_CT modules and run:

    ```
    > python TOF_CT.py
    ```

  - The application GUI will launch, displaying the main window with a plot area on the right and a control panel on the left.

3. Dependencies

TOF-CT requires the following Python packages, which can be installed via pip:

Package	Purpose
PyQt6	GUI framework for the application
Matplotlib	Plotting and visualisation
NumPy	Numerical data handling
SciPy	Numerical data handling
h5Py	Reading and writing Mantid-compatible NeXus and HDF5 format files
Pandas	File import/export, and tabular data management.

To install these dependencies, run:

```
> install pip PyQt6 matplotlib numpy scipy h5py pandas
```

---

4. Getting started

TOF-CT requires the following sources of input:

- Raw diffraction data
- A description of the instrument geometry
- Optionally, a table that describes coupling of detector elements into single raw spectra
- A choice of powder diffraction standard

TOF-CT only supports loading of diffraction data in the form of raw Mantid-format NeXus files (.nxs). The application supports both linearly and logarithmically binned data.

Instrument geometry may be loaded as an IBEX/DAE style detector.dat file, provided the file contains an accurate representation of each detector's secondary flightpath (L2) in metres and scattering angle (2θ) in degrees. Alternatively, a simple text file listing the detector ID, L2 and 2θ associated with each spectrum in the raw data file may be used. Examples are provided in the Instruments folder.

Detector coupling can be loaded using IBEX/DAE style spectra.dat files.

4.1 Single NeXus File Loading

- From the menu bar, select **File > Load NXS**.
- In the file dialogue, choose a single data file (e.g., HRPD80982.nxs).
- The raw spectra are displayed as a heat map in the right-hand part of the GUI.

Note that instruments with 10s to 100s of thousands of spectra will take time to load and subsequent display actions will generally be sluggish (See section 9).

4.2 Multiple NeXus File Loading

It is not uncommon for instruments to collect data in multiple short runs that are later summed, instead of one long measurement. As long as each run is binned identically, then TOF-CT offers the capability to select multiple NeXus files and sum them internally.

- Select **File > Load multiple NXS runs.**
- In the file dialogue, use SHIFT or CTRL to select multiple NeXus files or a range of files.
- The raw spectra are summed together and displayed as a heat map in the right-hand part of the GUI.

Note that multiple file loading also offers the unique capability to load data from two different standards simultaneously and have them merged into a single dataset for calibration. This could be of value for instruments with detectors extending to low 2θ, where peaks from common diffraction standards like silicon or ceria may not be well represented. This requires building a bespoke table of standard peak positions (see section 4.5).

4.3 Loading instrument geometry

TOF-CT has been built and tested on eleven ISIS instruments that acquire neutron TOF diffraction data: ENGIN-X, GEM, HRPD (pre-upgrade), IMAT, INES, OSIRIS, PEARL, POLARIS, SANDALS, SXD, and WISH. Consequently, geometry files for these instruments are supplied with the installation and can be selected from the dropdown menu on the **Basic** parameters tab of the UI. This action automatically loads the available detector table, any spectra table, and sets the length of the primary flight path. For some instruments, a preferred calibration standard is also set.

If the required instrument is not listed, then the detector geometry must be loaded.

- Select **File > Load ISIS detector table.**

- In the file dialogue, choose the relevant file (e.g., HRPD_detector.dat).
- TOF-CT prompts the user to specify if any detectors are coupled; click 'No' or see section 4.4.
- Manually set the length of the instrument's primary flight path, L1 in metres, on the **Basic** parameters tab.

Users can add new instruments to the dropdown by editing the instruments.py file and ensuring the relevant detector.dat and any spectra.dat files are placed in the Instruments folder.

Ease of fitting DIFC benefits from an accurate input instrument geometry. However, if you plan to use the Offsets.cal file output instead of the DIffCal.h5 output, then the input geometry **must match perfectly** to the Mantid Instrument Definition File.

To aid in construction of accurate input geometry files, a Python script is provided with the installation, "export_mantid_geometry.py", which should be loaded and run from within a Mantid scripting window. After editing the file paths (lines 30-31) and executing the script, Mantid will read in the requested IDF and then write a CSV file with all of the information necessary (and a bit more besides) to allow construction of an accurate detector.dat file.

Once loaded, the geometric information, and derived calibration constants are written in a table underneath the main display. For instruments with a large number of pixels, this table takes some time to build, and a progress bar is used to indicate when the table will be complete.

4.4 Loading spectra tables

It is common for pixels to be 'coupled' such that data from multiple detector elements are combined by the Data Acquisition Electronics and written into a single spectrum. In order to work with such data, TOF-CT must be aware of the additional mapping layer between detector IDs and spectrum number, and this is provided in the most straightforward fashion by using the same spectra tables as the DAE employs in the first place.

For the instruments on which TOF-CT has been tested and where coupling is used (HRPD and WISH), there are discrete options in the Instrument selection menu that ensure the correct tables are loaded. These tables are provided in the Instruments folder.

If your instrument is not represented and you are loading geometry manually, you will be prompted on loading the detector tables (section 4.3) to specify if any detectors are coupled. If the answer is 'Yes', a file dialogue will open automatically allowing the user to select the required spectra tables.

If the user clicks 'No' by mistake and still wishes to load a spectra table, then this can be done from the main menu.

- Select **File > Load spectra table for coupled detectors**

TOF-CT provides a popup information box indicating the spread of L2 and 2θ between the coupled detectors. Ideally, to avoid degrading resolution, these values should be very small. If large difference in L2 and/or 2θ are reported then the user should check the loaded spectra table for errors in the first instance.

The table underneath the main display will now show a list of detector IDs for each spectrum instead of a singular value.

4.5 Selecting a diffraction standard

Users can select from one of ten different crystalline materials in the dropdown menu on the **Basic** parameters tab, most of which are NIST standard reference materials.

The certified standards are:

- Silicon, SRM640e
- Ceria, SRM647b
- Alumina, SRM676a
- Quartz, SRM1878b
- Zeolite A (dried), NIST8851
- Zeolite Y (dried), NIST8850

A number of additional materials that are not NIST SRMs are also provided, since these are used commonly, either by instrument scientists or detector development scientists. The lattice parameters for these items are derived from the most recent ICSD entries:

- YAG ($Y_3Al_5O_{12}$)
- NACALF ($Na_2Ca_3Al_2F_{14}$)
- Iron
- Diamond

For each of the supplied standards, TOF-CT has a list of *d*-spacings for five or more strong Bragg peaks. When a standard is selected, the list of *d*-spacings is displayed in the box below the dropdown menu.

The list of *d*-spacings can be edited directly in the box, to either add or remove peaks or to change the *d*-spacing values.

Users can add their own standards to the dropdown by editing the file standards.py.

As soon as a standard is selected, the positions of the Bragg peaks in TOF are drawn on the main heatmap display as solid red lines. Provided the geometry supplied is accurate, then these curves should align closely with the measured Bragg peaks.

Bragg peak positions are marked automatically on any other open 1D or 2D display and update automatically if the standard is changed or any other parameter is altered (e.g., L1, DIFC etc).

To turn off the Bragg peaks, select 'None' from the Calibration standards dropdown.

If data from a mixture of standard are measured (or created by merging two data files), users can edit the *d*-spacings of a given standard to add the extra peaks or create their own bespoke standard in the standards.py file.

4.6 Loading previous calibrations

Instrument scientists will rarely be calibrating an instrument from scratch and will instead have a previous calibration that simply needs honing.

Previous calibrations in Mantid's HDF5 format (e.g., DiffCal.h5) can be loaded from the main menu:

- Select **File > Load DiffCal.h5 calibration**
- In the file dialogue, choose the relevant file (e.g., HRPD_DiffCal.h5).

The new list of DIFC value populate the 'difc' column of the table underneath the main display, overwriting any prior values, and updating the calculated offsets. If the differences are significant, then shifts in the red Bragg peak curves from the calibration standard will also be perceived.

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5. Data plots

TOF-CT supports two plot types: 1D line plot (single spectra or focussed spectra) and 2D heat maps. These plots are updated automatically when data or settings change.

The Matplotlib toolbar on any 1D or 2D plot allows zooming, scrolling, formatting and saving of the displayed image. The time-of-flight (or *d*-spacing or *Q*), spectrum number and binned counts under the tooltip are reported in the plot header (top right), and at the bottom left of the GUI window.

5.1 Heat Maps

- Heat maps display data as a 2D image, with TOF, *d*-spacing or *Q* as the x-axis parameter, *y* as the spectrum number, and Heat (or colour) representing intensity or raw neutron counts.
- The main GUI display only shows the raw data in TOF.
- Unless Calibration standard = None is selected, the heatmaps always display the positions of the standard's Bragg peaks as solid red lines.
- Use **Display > Show d-spacing heatmap** or **Display > Show momentum transfer (Q) heatmap** to transform the full spectra stack into *d*-spacing or *Q* in separate popup Matplotlib displays.

5.2 Single spectrum line Plots

- Individual spectra can be drawn as line plots (including the calibration standards overlays) in either TOF, *d*-spacing or *Q* using the three **Display > Show single spectrum** options.
- The user is prompted to enter a spectrum number.
- The individual spectrum appears in a separate popup Matplotlib display.
- Unless Calibration standard = None is selected, the 1D plots always display the positions of the standard's Bragg peaks as solid red lines.
- The menu bar of the single spectrum plot has one option – **Analysis** – which computes and displays the estimated resolution of peaks in proximity to the marked standard peaks. Note that TOF-CT does NOT do peak fitting; theses values are derived from observed maxima alone and are therefore quite inaccurate for noisy spectra. Use focussed spectra plots (5.3) to improve counting statistics and obtain more accurate resolution values.

5.3 Focussed spectra line plots

- Spectra may be summed to improve statistics and show the effect of different calibrations on peak shapes from a complete module or complete detector bank.
- Use **Display > Focus spectra in d**, or **Display > Focus spectra in Q**.
- The user is prompted to enter a list and/or range of spectra to sum.
- The focussed data appear in a separate popup Matplotlib display.
- Unless Calibration standard = None is selected, the 1D plots always display the positions of the standard's Bragg peaks as solid red lines.
- The menu bar of the focussed spectra plot has one option – **Analysis** – which computes and displays the estimated resolution of peaks in proximity to the marked standard peaks. Note that TOF-CT does NOT do peak fitting; theses values are derived from observed maxima alone and are therefore quite inaccurate for noisy data.

6. Formatting Plots

TOF-CT offers a few basic formatting options from the Display menu and the Basic parameters tab. Some other formatting options are available via the native Matplotlib toolbars.

6.1 Changing colour maps

The default colour map is viridis, which is the most widely used and perceptually uniform colour map intended for legibility by individuals with common colour vision impairments, and which is also well suited to monochrome printing. However, the user can select a range of alternative colour maps:

- Use **Display > Format NXS heatmap > Select colour map.**
- Alternatively, use the "*Edit axis, curve and image parameters*" button on the Matplotlib toolbar.

6.2 Scales, limits and binning

On the 2D heatmaps, users can toggle between a linear and a logarithmic brightness scale

- Use **Display > Format NXS heatmap > Log brightness scale**
- Use **Display > Format NXS heatmap > Linear brightness scale**

The Matplotlib *zoom*, *pan* and *reset* buttons allow dynamic changes of display limits. The user can also set the limits of the main TOF display manually from the **Basic** parameters tab by entering values in the **Main display limits** box.

The *d*-spacing and *Q* heatmaps are logarithmically binned to ensure accurate representation of peaks over a wide range of d-spacing or momentum transfer. The *d*-spacing display uses zoom-dependent binning and culling of spectra to ensure rapid and smooth display of data even from instruments with 10s or 100s of thousands of spectra. The binning becomes finer (up to the limit specified in the Δx/x spinner of the **d / Q display binning** box) as the zoom level is increased, and the spectra culling is reduced.

If users, particular of high-resolution instruments, find the binning limit too coarse, this should be manually adjusted downwards.

Note that this binning is purely for display purposes, the underlying data is not rebinned.

6.3 Formatting line styles

Whilst the default line style for the calibration standard's Bragg peak positions is a solid red line, this can be altered from the main menu:

- Use **Display > Format Bragg peak curves.**
- Select from Colour, Line Weight and Line Style to suit.

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7. Fitting DIFC

7.1 Automatic settings

In principle, with well counted data in every pixel and an accurate instrument geometry, TOF-CT will have no problem with fitting DIFC to every spectrum using the built-in settings.

- From the menu bar, select **Compute > Fit DIFC to observed peaks**
- The applied Bragg peaks will disappear while the fitting takes place. An orange progress bar indicates the status of the fitting. For instruments with 10s or 100s of thousands of pixels, this will take a few minutes.
- After fitting is complete, the main TOF display (and any other open displays) will update with revised Bragg peaks and the new DIFC values will populate the results table.
- Examine the quality of the fit closely on the TOF display and optionally open a *d*-spacing or *Q* heatmap to better appreciate the quality of the alignment for all spectra.
- If the results are satisfactory then proceed directly to file export (section 8).

Note that spectra where the fitting failed, either because those spectra are empty or the data are too poor, will be coloured in red on the results table.

7.2 Manual adjustment

The first manual intervention should be to adjust the fitting parameters.

- Click on to the **Advanced** parameters tab.

- Adjust the DIFC search half width upwards; this is by far the most common reason for failing to capture a spectrum's DIFC value correctly. Try adjusting the default value from 1 % to 2 % in the first instance and then widen the band as required.

Many instruments have strong time-invariant artefacts their data due to prompt radiation from the source. Where these are sufficiently strong and overlap with Bragg peaks from the calibration standard, then they can interfere with the fitting. The time channels containing the artefacts should be masked.

- Click on to the **Advanced** parameters tab.
- Enter start and end TOF values for the range to be masked
- Use the button "*Add masked TOF range*" to create more than one masking region.
- The mask(s) are shown on the displays as black rectangular overlays; the underlying spectra are not edited.

The ultimate level of manual adjustment is to edit DIFC values by hand in the table underneath the main display. For any given spectrum deemed to have been improperly fitted, the user can type a new value in the "difc" column, press 'enter' and have the displays update automatically. Edited cells are coloured a light amber colour.

For low resolution and poorly counted spectra, or spectra with artefacts, this level of manual adjustment may be essential, although it typically only occurs when the underlying instrument geometry is inaccurate or the prior calibration is inaccurate.

Editing DIFC values by hand benefits from inspection of single spectra line plots as well as TOF and *d*-spacing (or *Q*) heatmaps.

Once these manual adjustments have been made, the user can run the DIFC fitting again using the new values as input for the fit.

- From the menu bar, select **Compute > Fit DIFC using current table as seeds.**

This should resolve any outstanding misfit spectra and provide a calibration suitable for export. Manually edited cells will now be coloured pale green if the revised fit was successful or remain amber if the fitting score improvement was below the threshold set on the **Advanced** parameter tab.

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8. Saving results

The two main calibration file types used by Mantid are tables of offsets (i.e., relative changes in DIFC with respect to the Instrument Definition File's geometry, in the form of a .cal) file or an absolute table of DIFC values in the form of a DiffCal.h5 file. At the time of writing, the preferred option for use with the ConvertUnits algorithm is the DiffCal file, while must be loaded and/or applied using the LoadDiffCal / ApplyDiffCal algorithms.

TOF-CT will write either of these file types:

8.1 Exporting DiffCal.h5 files

- Use **File > Save results to DiffCal.h5**.
- Check in Mantid by using ApplyDiffCal on any given workspace, followed by ConvertUnits to transform a workspace into *d*-spacing (or *Q*) and confirm precise alignment of all spectra.

8.2 Exporting Offsets.cal files

- Use **File > Save results to Offsets.cal**
- This writes an older format offsets/grouping file, but with all detectors selected (select = 1) and sharing a common grouping (group = 1); the user should edit these in a text editor as appropriate.
- In older versions of Mantid, check the offsets file using the AlignDetectors algorithm. In newer versions of Mantid, ApplyDiffCal can still be used to apply the offsets to a workspace, followed by ConvertUnits.

8.2 Exporting CSV files

- Use **File > Save results to CSV**
- This writes the entire contents of the results table, including the detector geometry to a comma-separated variables file, that can be opened in any spreadsheet applications.
- This allows users to troubleshoot issues, easily use the data in other applications (for example plotting and fitting DIFC to find translations and/or rotations of the detector modules that better fit the observed calibration contstants).
- CSV files that have been saved for offline editing can also be re-imported via **File > Import Edited CSV**

9. Troubleshooting

Common problems

Nothing is happening

Large instruments with 10s to 100s of thousands of spectra will incur significant delays in loading or carrying out certain operations, and the application may appear to be 'doing nothing'.

For guidance, the times (in seconds) taken to carry out certain actions for different ISIS instruments are shown in the table below.

Instrument	No' spectra	Loading[1]	Apply Tables[2]	Fit DIFC[3]
POLARIS	3008	2	0.8	4
GEM	7290	2.5	1.4	8
SXD	45100	4	4.3	45
WISH	194565	38	46	560

[1]Time taken for the spectra to load and be displayed. For reference, WISH data take 54s to load in Mantid.

[2]Time taken for tables to load, compute initial DIFC, compute Bragg peaks and display

[3]Time taken to fit all spectra, recompute Bragg peaks and display. Note that for WISH, there is a period of 2m 30s where nothing appears to be happening prior to the start of the fit, and a further 2m 20 after the fit is completed to display the results. The fit itself takes 4m 30s.

No red Bragg peak curves appear
→ check that an instrument is selected or a detector table is loaded
→ check that a standard is selected

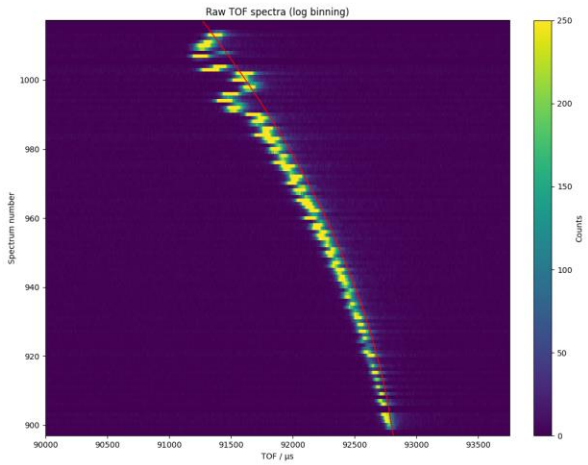
All Bragg peak curves are displaced from observed intensity maxima
→ incorrect standard is selected
→ incorrect instrument is selected (or wrong detector / spectra tables loaded)
→ incorrect L1 is set

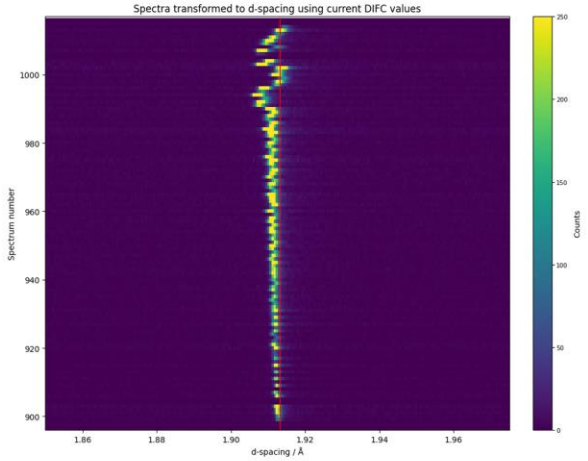
Failed spectra fitting
→ search half-width tool small - increase the width
→ insufficient counts in spectrum
→ detector shadowed
→ prompt pulse interference - time channel masking needed

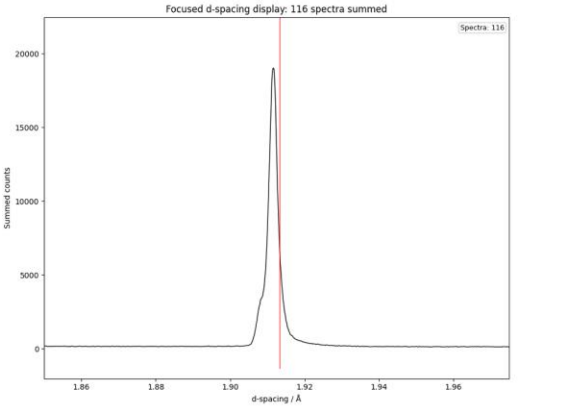
Calibration imports incorrectly in Mantid
→ detector IDs do not match IDF
→ detector table ordering differs from workspace ordering

Examples of uncalibrated and calibrated data from HRPD backscattering module 7 (cerium oxide), before and after spectra alignment, showing the systematic difference from observations due to inaccurate IDF geometry, and likely physical artefacts on the outer edge of the module – all corrected after calibration. The effects on the peak shape for the focussed spectra are shown at the bottom.

Uncalibrated







Calibrated