



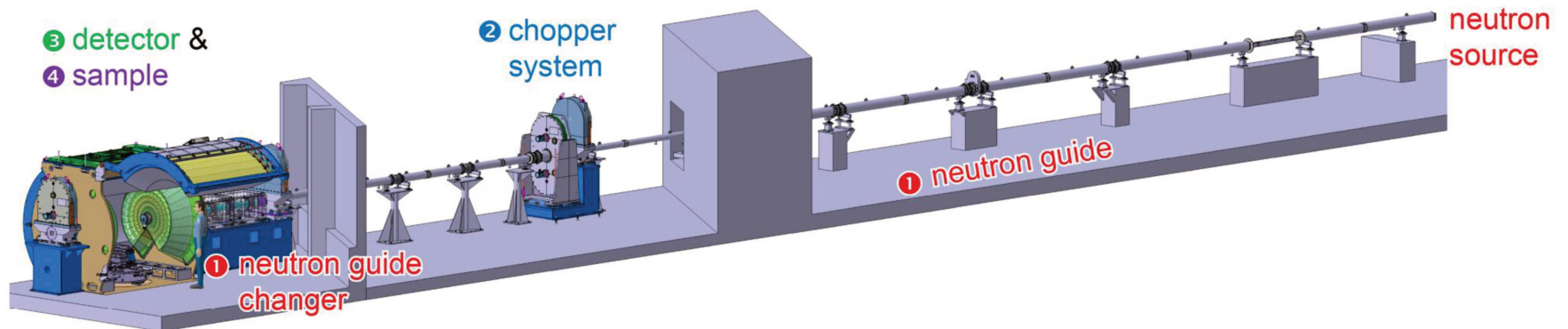
# POWTEX

High-Intensity Time-Of-Flight Neutron Diffractometer

## POWTEX-Detector @ POWGEN

Dr. Andreas Houben

# The POWTEX instrument



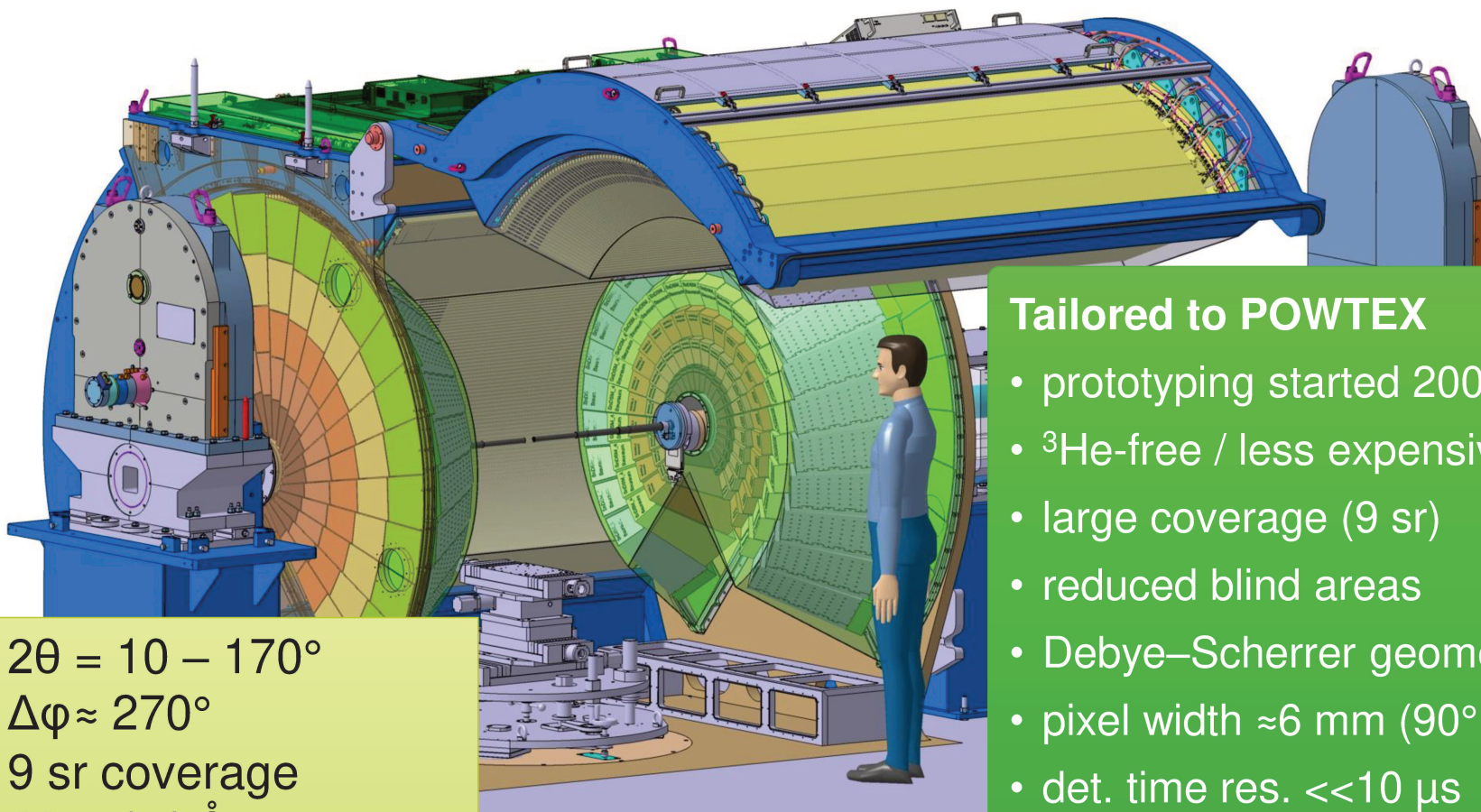
## Concept

- TOF at a continuous source
- large detector coverage, high intensity
- short measurements, small samples
- wavelength & angular dispersive
- Gaussian peak-shapes

## Pioneering developments in

1. double elliptic guide
2. chopper system
3. detector development
4. multi-dimensional data analysis

# The POWTEX detector system



- $2\theta = 10 - 170^\circ$
- $\Delta\varphi \approx 270^\circ$
- 9 sr coverage
- $\Delta\lambda = 1.4 \text{ \AA}$
- Q-range:  $0.5 - 12.5 \text{ \AA}$

## Tailored to POWTEX

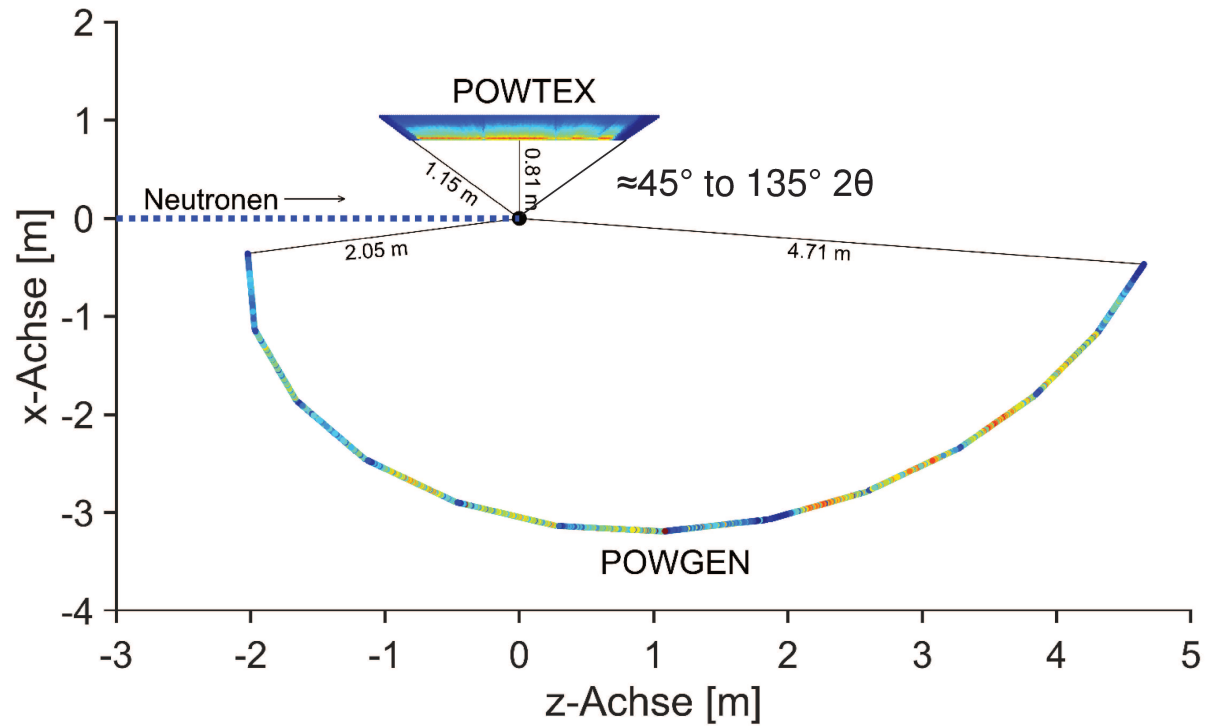
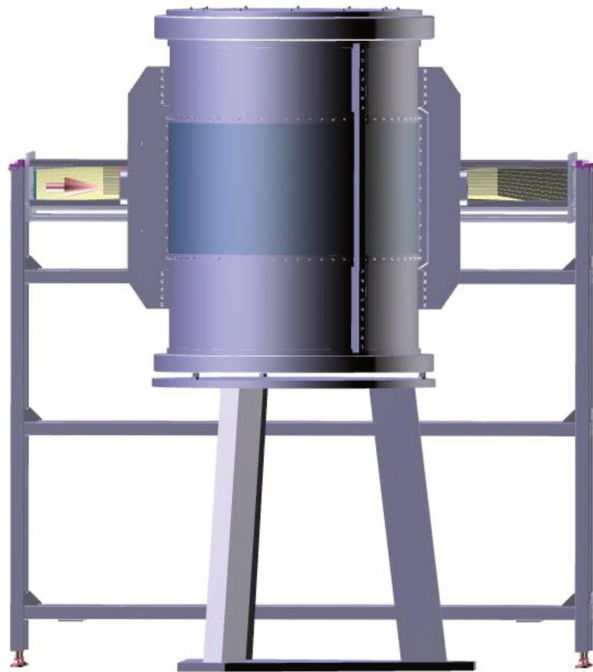
- prototyping started 2009
- $^3\text{He}$ -free / less expensive
- large coverage (9 sr)
- reduced blind areas
- Debye–Scherrer geometry
- pixel width  $\approx 6 \text{ mm}$  ( $90^\circ 2\theta$ )
- det. time res.  $\ll 10 \mu\text{s}$
- $>50\%$  efficiency at  $1.0 \text{ \AA}$



**POWGEN,  
SNS, ORNL**



# POWTEX detector – Test @ POWGEN



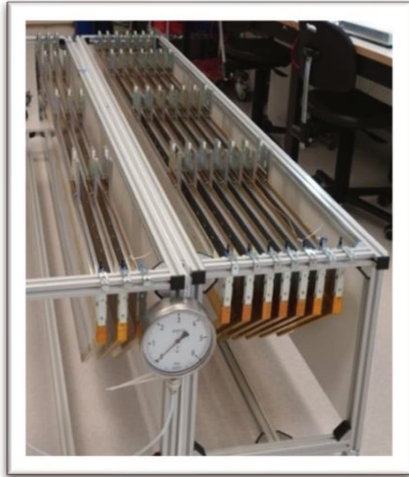
## Detector at POWGEN



Finally there... after one year of hard work, careful preparation and much bureaucracy done by many helping hands (November 2017)

# Vorhaben: Detektortest am Instrument POWGEN (SNS)

© by Jacobs, et al.



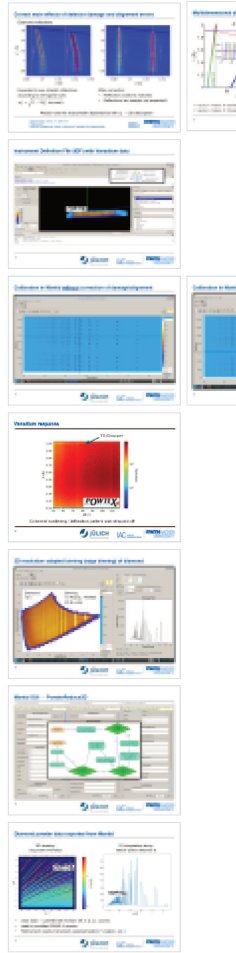
Damage:

- Deformation
- broken anodes wires
- potentially short circuit?

# Data treatment – today, still work in progress

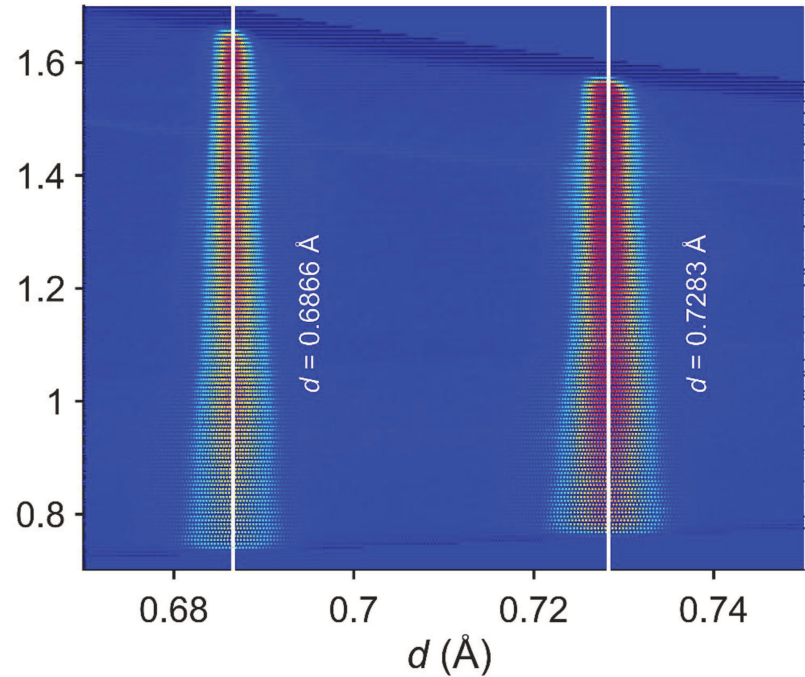
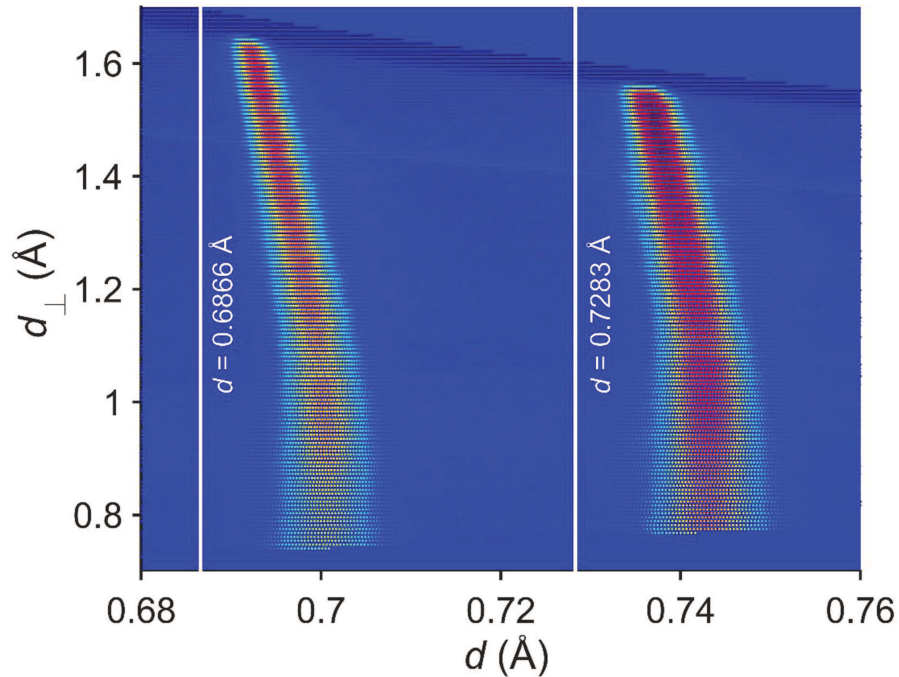


- ✓ Time slice detector raw data and merge them with meta data (sample information, absolute time-stamp, etc.) of simultaneously measured data from POWGEN → Nexus data file by G. Modzel
- ✓ Correct main effects of detector damage and alignment errors (MATLAB)
- ✓ Load Nexus files in Mantid using Instrument Definition File for test case
- ✓ Detector calibration in Mantid (CalibrateRectangularDetectors)
- ✓ Mantid routines for 2D data treatment
  - ✓ Bin2DPowderDiffraction: log- $d$ -binning, edge- $d$ -binning in  $(d, d_{\perp})$  by M. Ganeva
  - ✓ Background and Vanadium correction (similar to 1D; different parametrization)
  - ✓ SaveP2D + helper routines: cut data in  $(2\theta, \lambda)$  or  $(d, d_{\perp})$  and save ASCII data  $(2\theta, \lambda, d, d_{\perp}, \text{intensity})$
  - ✓ Finally, PowderReduceP2D → full treatment (to be submitted to Mantid soon)
- ✓ Rietveld analysis (modified version of GSAS II) or other



# Correct main effects of detector damage and alignment errors

## Diamond reflections



Expected to see straight reflections according to orthogonal cuts:

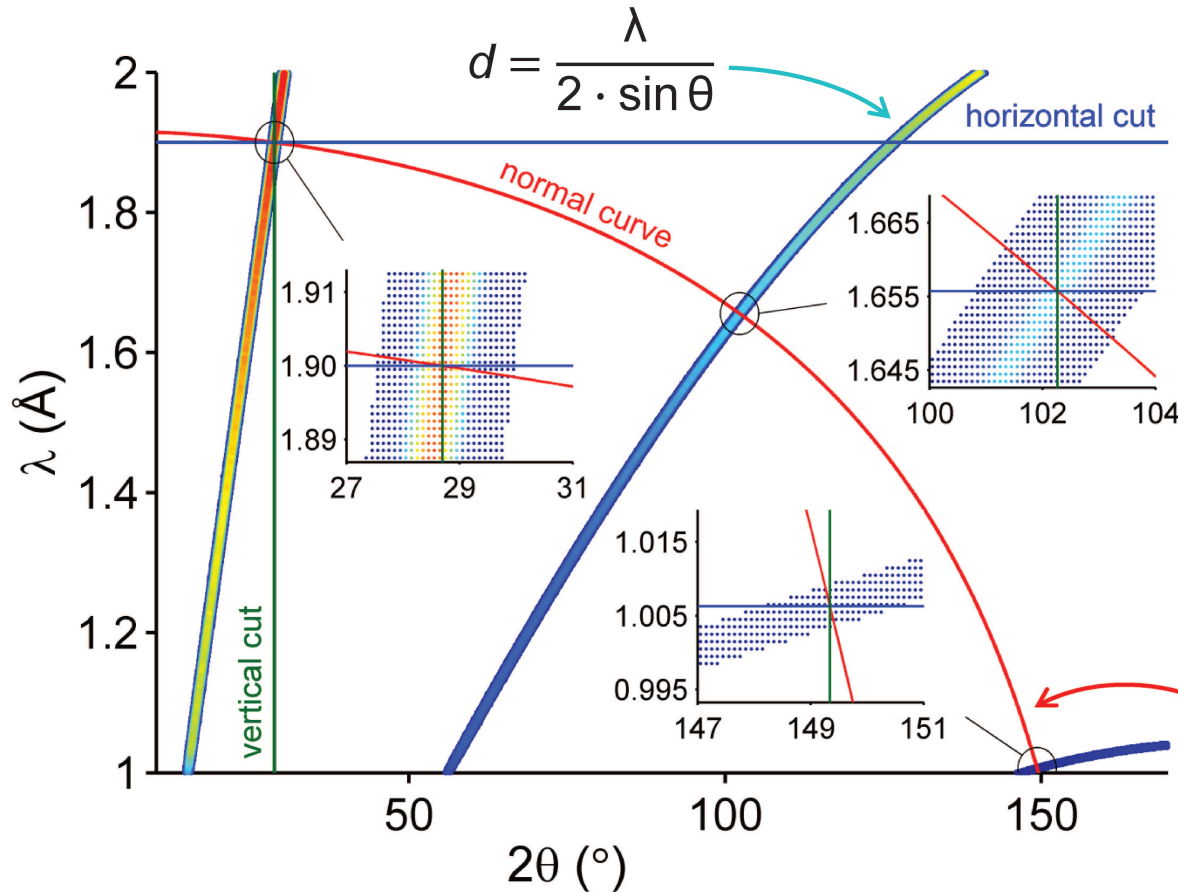
$$d_{\perp} = \sqrt{\lambda^2 - 2\lambda_K^2 \cdot \ln(\cos\theta)}$$

After correction:

- Reflection positions matches
- Reflections are straight (as expected)

Please note the shape/width dependence with  $d_{\perp} \rightarrow 2D$  description

# Multidimensional diffraction data – mathematical treatment



- Red curve derived by solving the differential equation:

$$\frac{d\lambda}{d\theta} = -\frac{1}{2 \cdot d \cdot \cos \theta}$$

- $d$  and  $d_{\perp}$  form a new orthogonal coordinate system

$$d_{\perp} = \sqrt{\lambda^2 - 2\lambda_K^2 \cdot \ln(\cos \theta)}$$

P. Jacobs, A. Houben, W. Schweika, A. L. Tchougréeff and R. Dronskowski, *J. Appl. Crystallogr.* **48** (2015), 1627–1636.

P. Jacobs, A. Houben, W. Schweika, A. L. Tchougréeff and R. Dronskowski, *J. Appl. Crystallogr.* **50** (2017), 866–875.

# Instrument Definition File (IDF) with Vanadium data

The screenshot displays the MantidPlot software interface. The main window shows a 3D visualization of a component, likely a detector or sample holder, with a color scale ranging from 0 to 5.000. The component is labeled "POWTEX". The interface includes a menu bar (File, Edit, View, Windows, Interfaces, Help), a toolbar, and a Results Log. The Results Log shows the following entries:

```
Bin2DPowderDiffraction started
Bin2DPowderDiffraction successful, Duration 27.25 seconds
Bin2DPowderDiffraction started
Bin2DPowderDiffraction successful, Duration 82 minutes 18.04 seconds
```

A diagram in the top right corner illustrates the geometry of a detector or sample holder, showing a 3D view with labeled points:

- <left-back-top-point />
- <left-front-top-point />
- <left-back-bottom-point />
- <left-front-bottom-point />
- <right-back-top-point />
- <right-front-top-point />
- <right-back-bottom-point />
- <right-front-bottom-point />

The right side of the interface shows the Workspaces panel, which lists the following workspaces:

- ./39394\_Vanadium\_0.7\_event
- ./39394\_Vanadium\_0.7\_event\_b2d
- ./39394\_Vanadium\_0.7\_event\_b2d\_edge
- Detec
- POWTEX\_cal

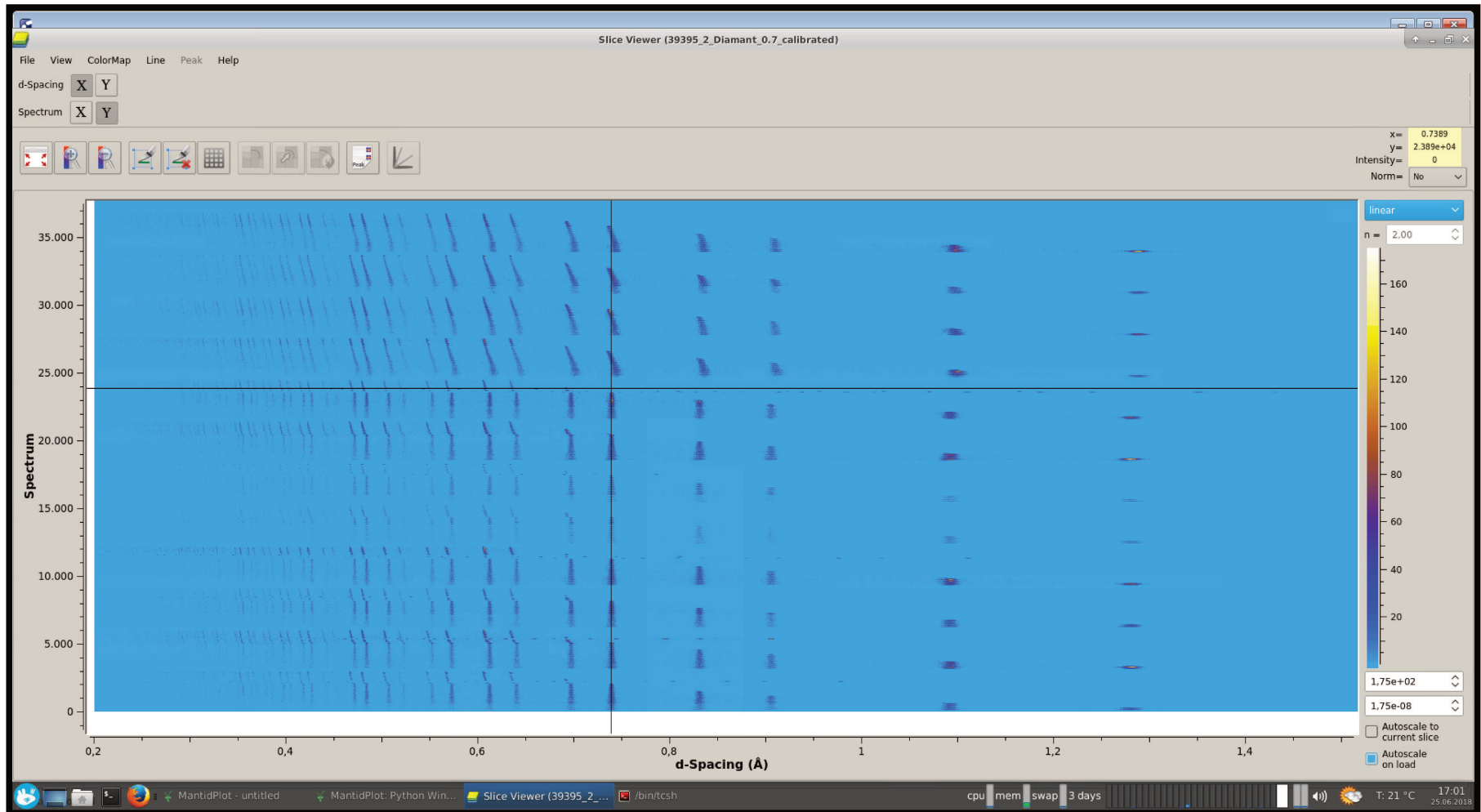
The Algorithms panel shows the following algorithms:

- Arithmetic
- CorrectionFunctions
- Crystal
- DataHandling
- Diagnostics
- Diffraction

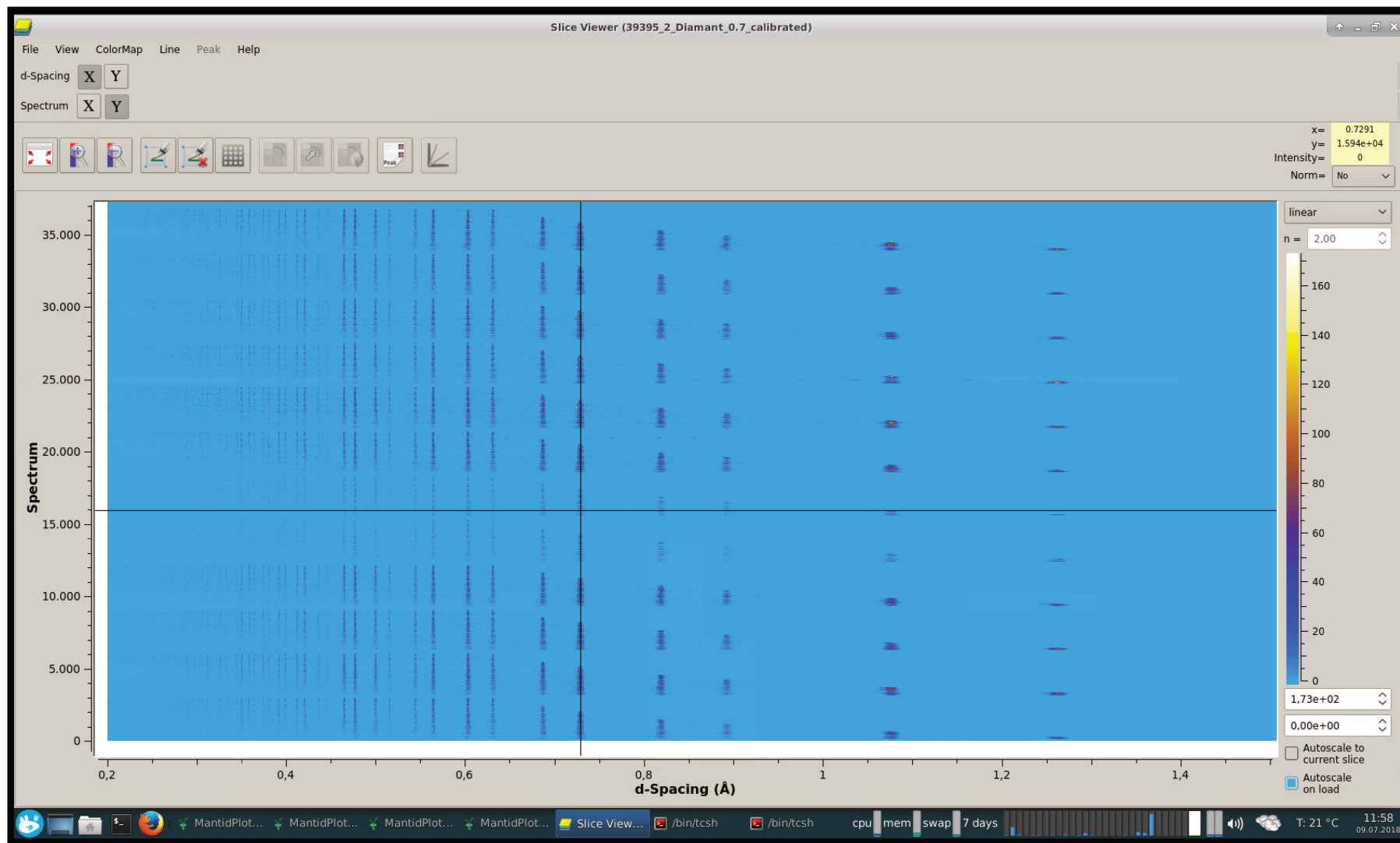
The Script Interpreter at the bottom shows the following text:

```
Script Interpreter
Introduction and overview of Python's features.
%quickref -> Quick reference.
help -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.
In [1]:
```

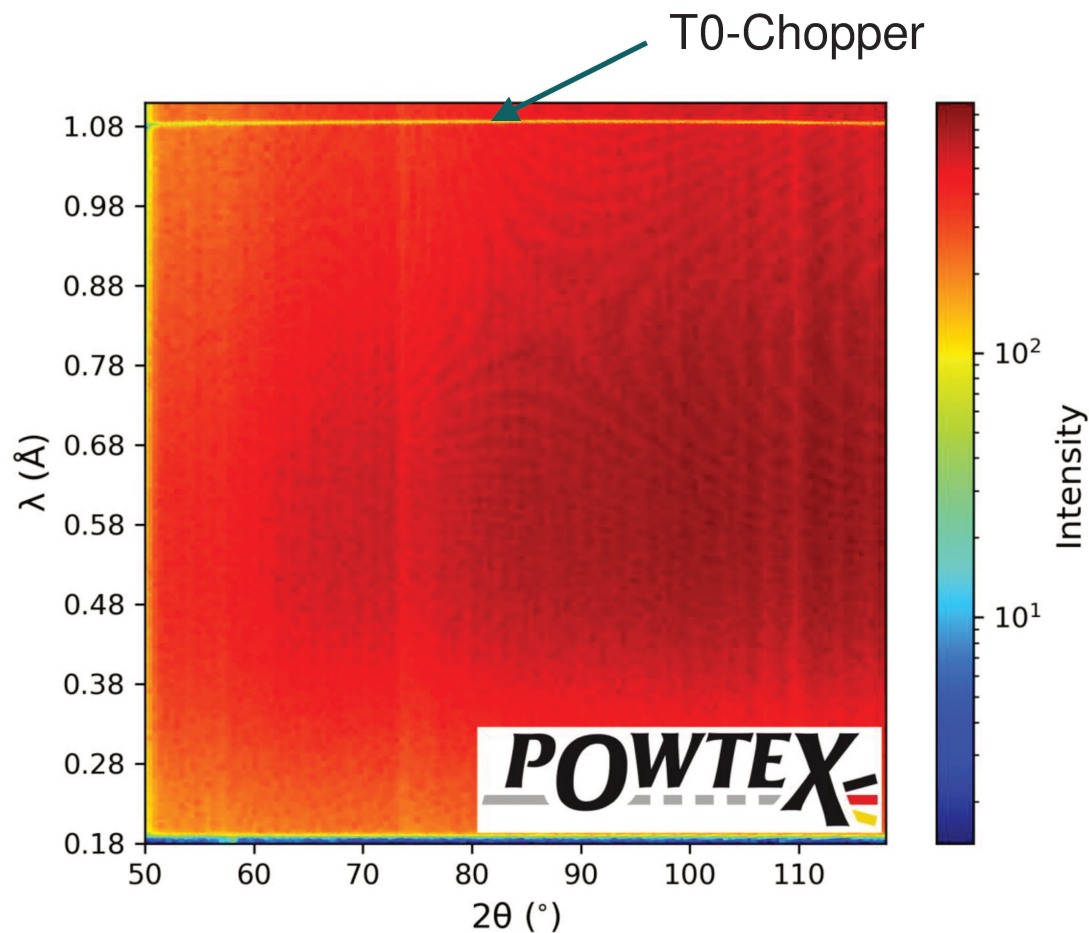
# Calibration in Mantid without correction of damage/alignment



# Calibration in Mantid after correction of damage/alignment

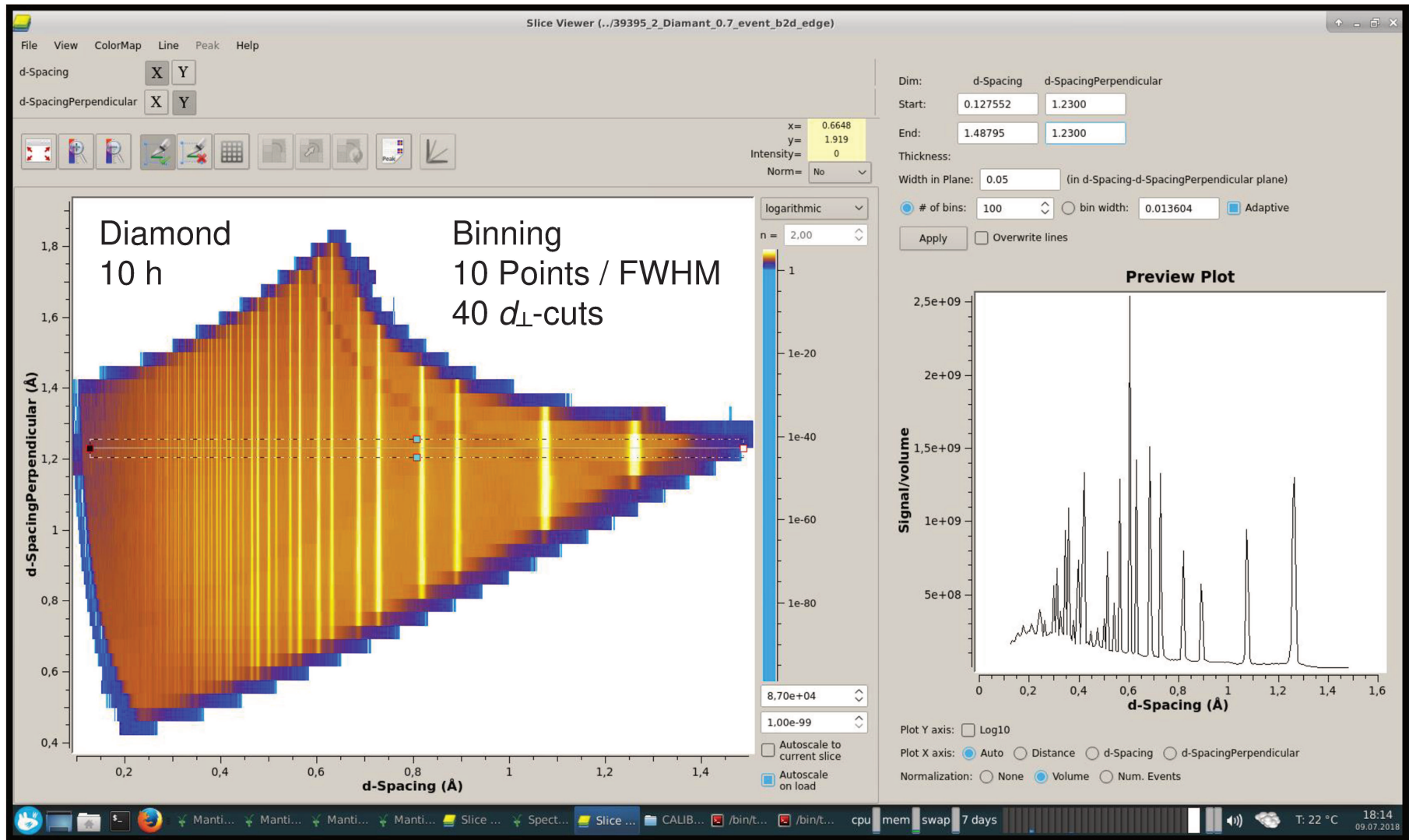


# Vanadium response



Coherent scattering / diffraction pattern was stripped off

# 2D resolution adapted binning (edge binning) of diamond



# Mantid GUI → PowderReduce2D

The screenshot displays the Mantid GUI for PowderReduce2D, showing three instances of the input dialog. A central flowchart outlines the processing workflow:

```

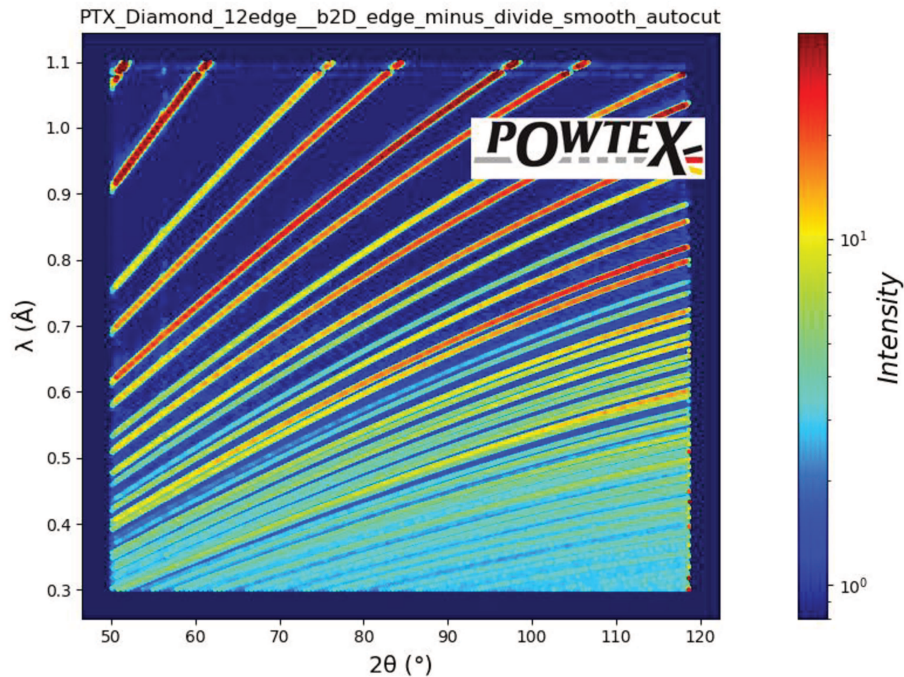
    graph TD
      SD([SampleData]) --> PSR[Process Sample Run  
(see workflow diagram)]
      PSR --> IS1{Is container run  
specified?}
      IS1 -- Yes --> PCR[Process Container Run  
(see workflow diagram)]
      IS1 -- No --> IS2{Is Vanadium run  
specified?}
      PCR --> SCR[Subtract Container Run  
from Sample Run  
using Minus v1.]
      SCR --> IS2
      IS2 -- Yes --> PVR[Process Vanadium Run  
(see workflow diagram)]
      IS2 -- No --> IS1
      PVR --> DSR[Divide Sample Run  
by Vanadium Run  
using Divide v1.]
      DSR --> IS3{Does data have to  
be positive?}
      IS3 -- Yes --> RN[ResetNegatives v1]
      IS3 -- No --> CR[Create p2d File]
      RN --> CR
      CR --> OP2([OutputP2dFile])
  
```

The GUI interface includes the following sections:

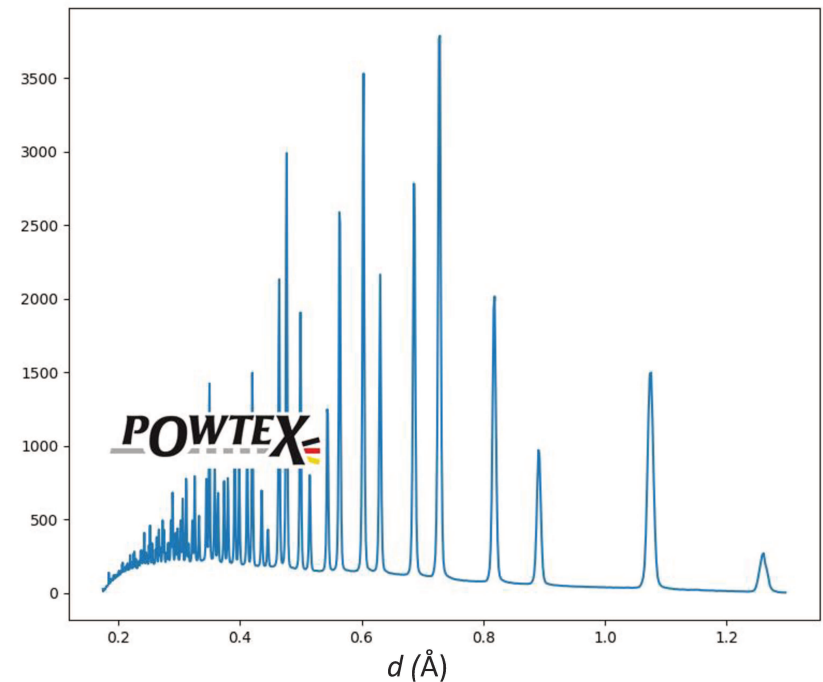
- Input and Output Files:** Fields for SampleData, VanaData, EmptyData, CalFile, BinEdgesFile, and OutputFile.
- Data Ranges:** Sliders for TwoThetaMin, TwoThetaMax, WavelengthCenter, LambdaMin, LambdaMax, DMin, DMax, DpMin, and DpMax.
- FilterBadPulses:** LowerCutoff field.
- RemovePromptPulse:** Section for prompt pulse removal.
- FindDetectorsPar:** ParFile and OutputParTable fields.
- ResetNegatives:** AddMinimum checkbox and ResetValue field.
- 3DPowderDiffraction:** Normalization and background options.
- StripVanadiumPeaks:** Peak stripping options.
- FFTSmooth:** Smoothing parameters.

# Diamond powder data exported from Mantid

2D drawing  
(log scale intensity)

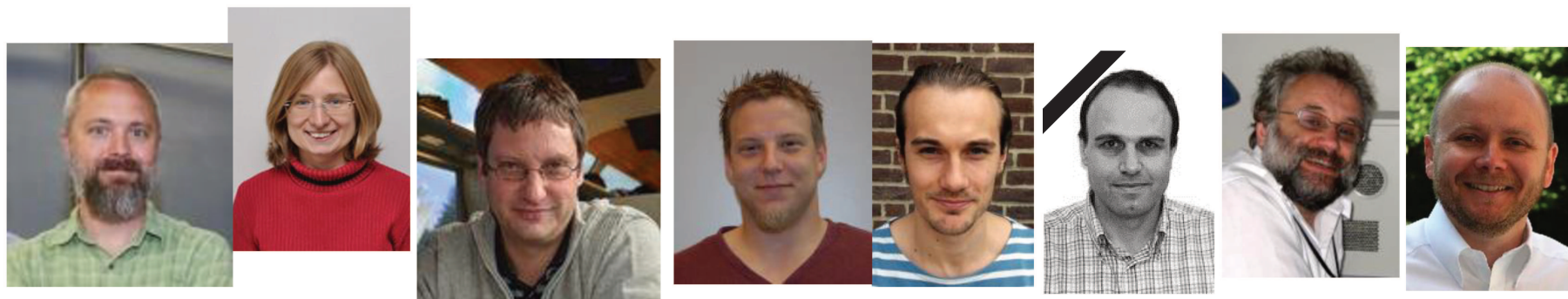


1D integration along  
lattice space distance  $d$



- User data → p2d-file with format:  $2\theta$ ,  $\lambda$ ,  $d$ ,  $d_{\perp}$ , counts
- read by modified GSAS II version
- Refinement needs instrument parametrization (\*.instprm, etc.)

# Thanks to everybody involved (including those without picture!)



# Thank you for your attention!

---



Bundesministerium  
für Bildung  
und Forschung

Bundesministerium für Bildung und Forschung (BMBF)



Projekträger DESY



Forschungszentrum Jülich



Jülich Centre for Neutron Science



Forschungsneutronenquelle  
Heinz Maier-Leibnitz (FRM II)



SwissNeutronics



CDT GmbH