Introduction

The geometrical configuration (pixel positions) of the SEQ detector system needs calibration. The most obvious problem is that the detector packs consisting of short detector tubes (short packs) around the forward beam are overlapping with some normal detector packs (long packs). In this work, several calibration datasets were taken and used for geometrical calibrations.

The simplifications

- Any pack, long or short, consists of 8 tubes, and each tube contains 128 pixels.
- The tubes inside a detector pack are geometrically arranged either according to the long-pack configuration or the short-pack configuration. It means the relative positions of pixels are fixated to a pack.
- Therefore, only a calibration of a detector pack's position and orientation is necessary to fix the positions of all pixels of a detector pack in the lab coordinate system
- L1 is known

Conventions:

- Coordinate system: z along beam, y vertical up

Data

SEQUOUA, IPTS-19573.1, July 10-14, 2017

Room temperature, CCR-22 with 3-sample changer configuration, no heat shield.

C60-powder (m=?? g), in aluminum flat container 5x5cm2 plus BN-mask

Vanadium (wide, baked)

Si-powder (m=1.57 g), in cylindrical vanadium container

Run # 130248, Vanadium 5x5cm2, White beam, Ei set to 110 meV, T0=150 Hz, Attn1 in the beam, all slits 2 = 25, PC=6 C

Run # **130249-130252**, C60, White beam, Ei set to 250 meV, T0=30 Hz, no Attn in the beam, all slits 2 = 25, PC=6x4=24 C
Run # 130253-130254, C60, Ei=600 meV, F1=600 Hz, T0=150 Hz, PC=6x2=12 C
Run # 130255-130256, C60, Ei=250 meV, F1=360 Hz, T0=120 Hz, PC=6x2=12 C
Run # 130257-130258, C60, Ei=60 meV, F1=180 Hz, T0=60 Hz, PC=6x2=12 C

Run # 130259, Vanadium 5x5cm2, Ei=10 meV, F2=300 Hz, T0=30 Hz, PC=3 C
Run # **130260**, Vanadium 5x5cm2, Ei=55 meV, F2=420 Hz, T0=90 Hz, PC=3 C
Run # 130261, Vanadium 5x5cm2, Ei=160 meV, F2=600 Hz, T0=120 Hz, PC=3 C

For Si sample slits were: s2l=6, s2r=5, s2b=15, s2t=14
Run # 130262-130263, Si-powder, Ei=600 meV, F1=600 Hz, T0=150 Hz, PC=6x2=12 C
Run # 130264, Si-powder, Ei=250 meV, F1=360 Hz, T0=120 Hz, PC=6-? C – detectors/vacuum problem, run is not good

Run # 130268, Vanadium 5x5cm2, White beam, Ei set to 110 meV, T0=150 Hz, Attn1 in the beam, all slits 2 = 25, PC=6 C

For Si sample slits were: s2l=6, s2r=5, s2b=15, s2t=14
Run # 130269-130270, Si-powder, Ei=250 meV, F1=360 Hz, T0=120 Hz, PC=6x2=12 C
Run # 130271-130272, Si-powder, Ei=60 meV, F1=180 Hz, T0=60 Hz, PC=6x2=12 C
Run # **130273**-130278, Si-powder, White beam, Ei set to 250 meV, T0=30 Hz, no Attn in the beam, PC=6x6=36 C

The **bold** runs were used in this work.

Procedure

The basic principle of this work extends from detector calibration for neutron time-of-flight powder diffractometers. In calibration of a powder diffractometer, the most important quantity of interest is “DIFC”, which relates time-of-flight with d spacing in a measured diffraction pattern:

$$TOF = DIFC * d + DIFA * d^2 + TZERO \quad (1)$$

The DIFC quantity is related to instrument parameters and pixel position in first order approximation:

$$DIFC = (L1 + L2)/(\pi)\ sin(\theta) \times 0.0015882549421289758 \times 10^6$$

Here L1 is moderator-sample distance, L2 sample-pixel distance, and θ half of the scattering angle. In powder diffraction all is needed is a pixel-by-pixel calibration of the parameters in equation (1), and the L2 and the scattering angles of pixels are allowed to drift simultaneously somewhat while keeping the DIFC values nearly constant. However, in inelastic neutron scattering, we need accurate information for pixel positions, hence both L2 and θ are important. In developing the following procedure for SEQ calibration, we reuse some of the Mantid algorithms used in powder diffraction calibration.

The following is an outline of the calibration procedure:

- Use white beam powder data (Si/C60) to obtain DIFC
    - Compute initial DIFC from nominal geometrical info of det packs using Mantid
    - Obtain I(d) spectrum for each pixel using the initial geo info of det packs
    - For each pixel, fit I(d) to peaks and compare them to standard d spacing values of the crystal, and calculate the calibrated DIFC
- Use V powder data to obtain L2
    - Use Mantid to compute Ei and emission time
    - For each pixel, compute tof of the elastic peak, then determine L2
- Use DIFC+L2 of all pixels in a pack (excluding bad fits etc) to optimize the position (x,z) and orientation of this pack (y). This is done with the scipy optimization routine. The position and orientation of the pack is varied using in a range +/-30cm (x,z) and +/-2 degrees (y) around the initial values and the best match to the calibrated DIFC+L2 values is found in optimization.
- Check the calibration by
    - Visualize the det system in mantid
    - Compute and compare I(d) spectra of a pack before and after calibration

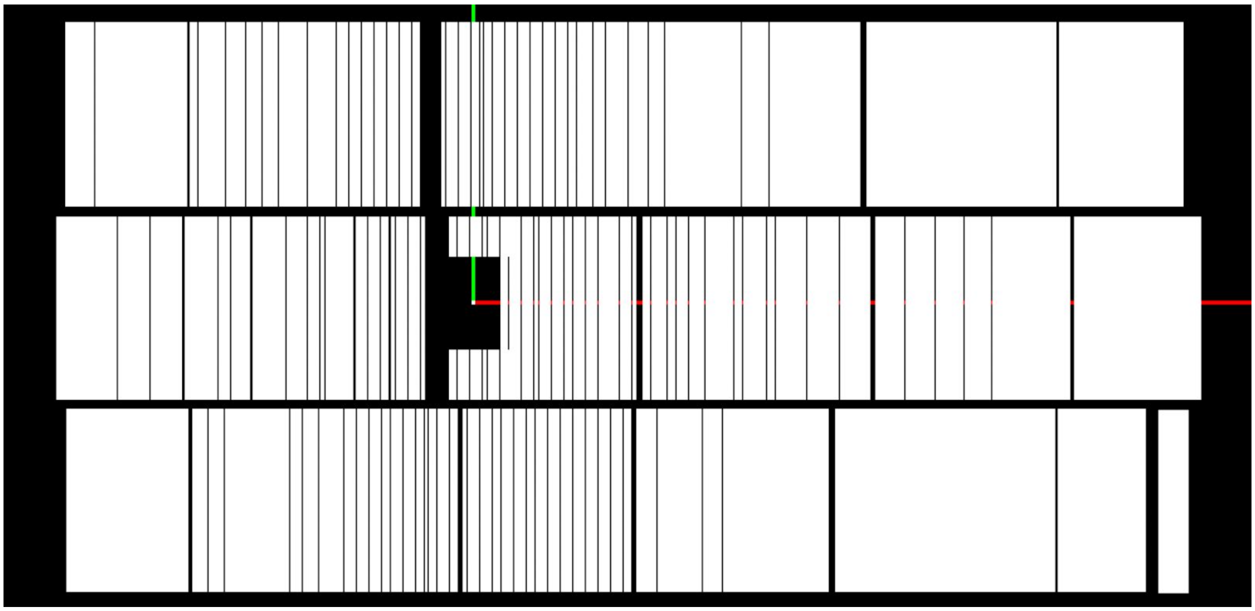
Notes

- The original positions of the short packs were very wrong. We made a guess and put them to reasonable positions
- The short packs are around forward beam. They have very small scattering angles. Hence the C60 data with large d values is used for short packs, while the Si data is used for long packs.
- C60 datasets are huge. Had to load them in small pieces.

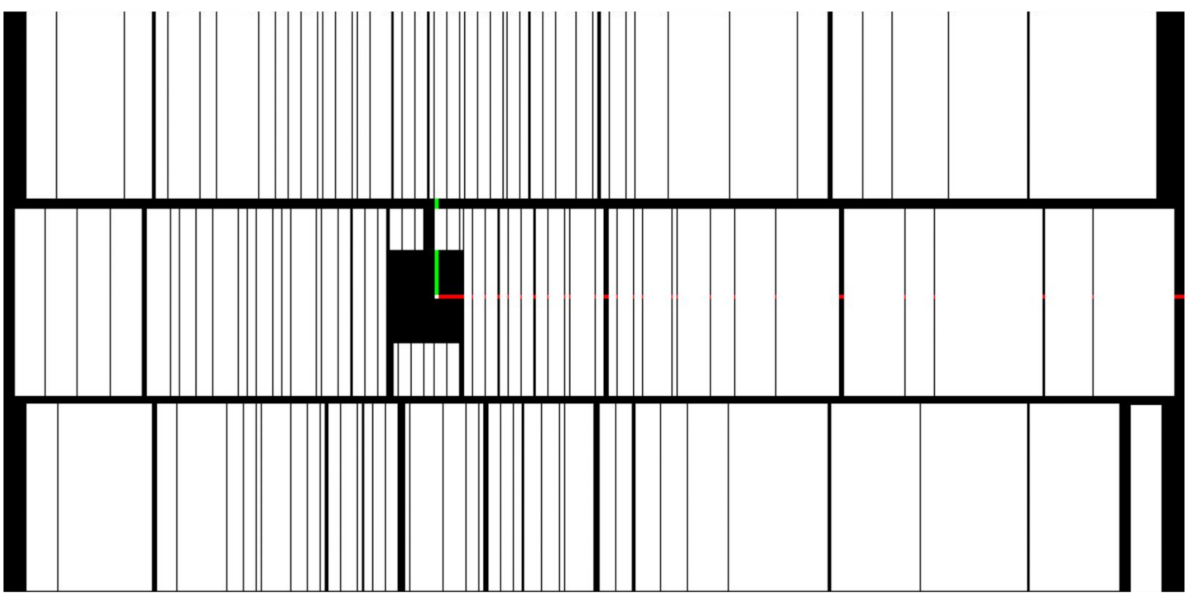
Results

Detector View

Original

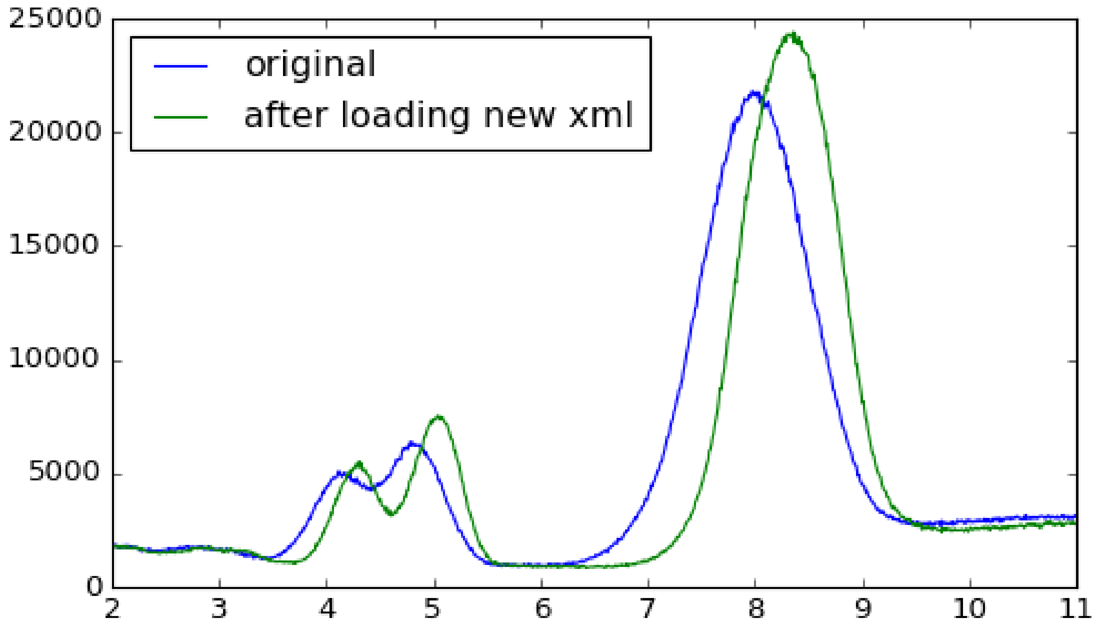


Calibrated

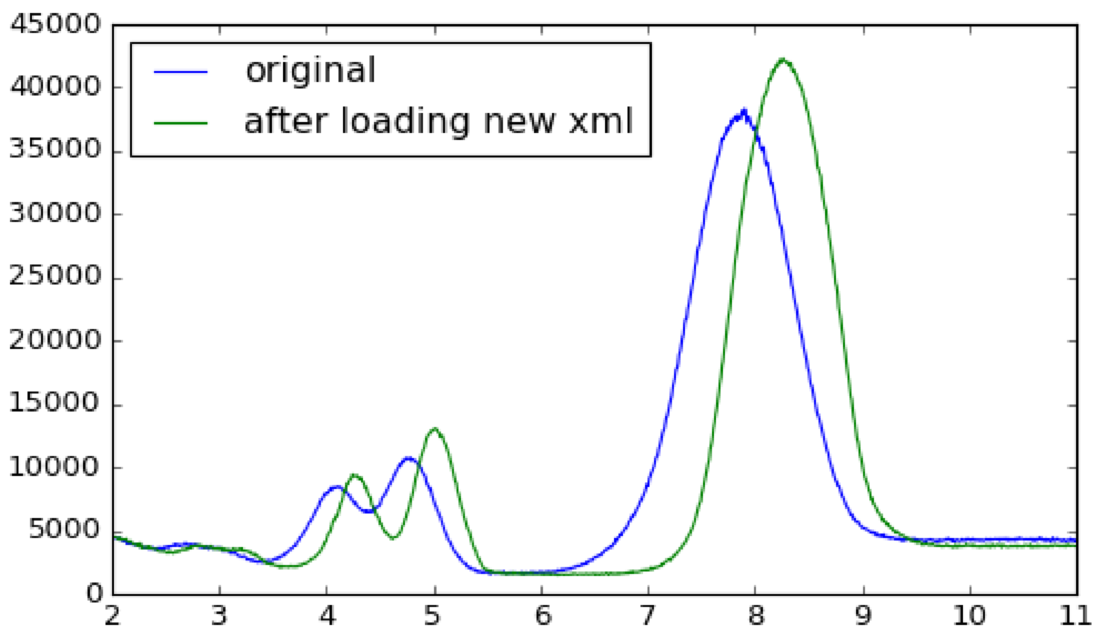


Short packs

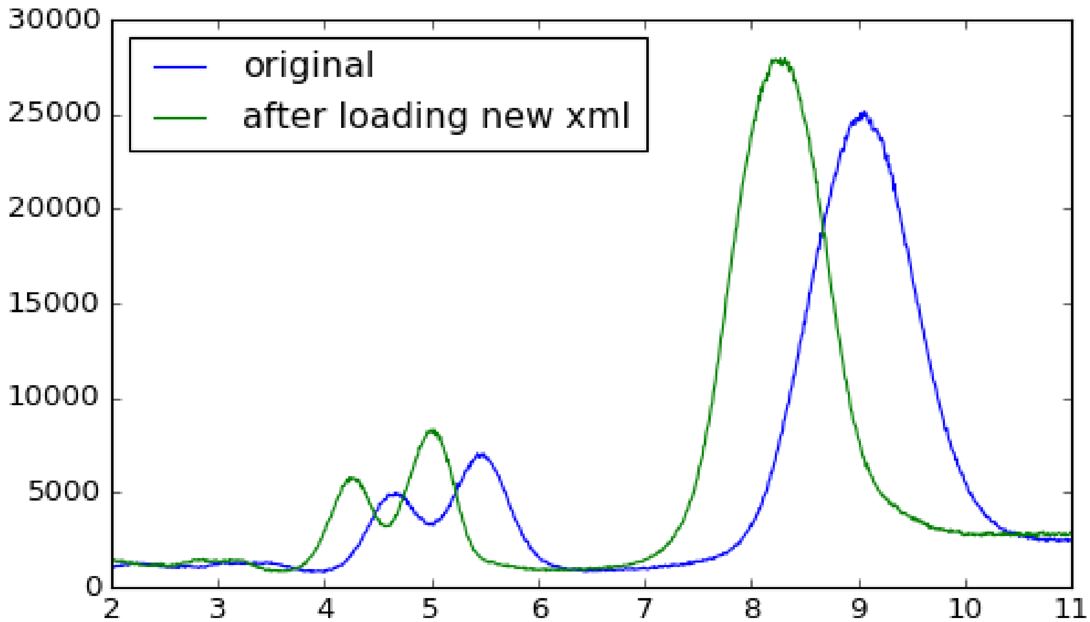
C25T, C60



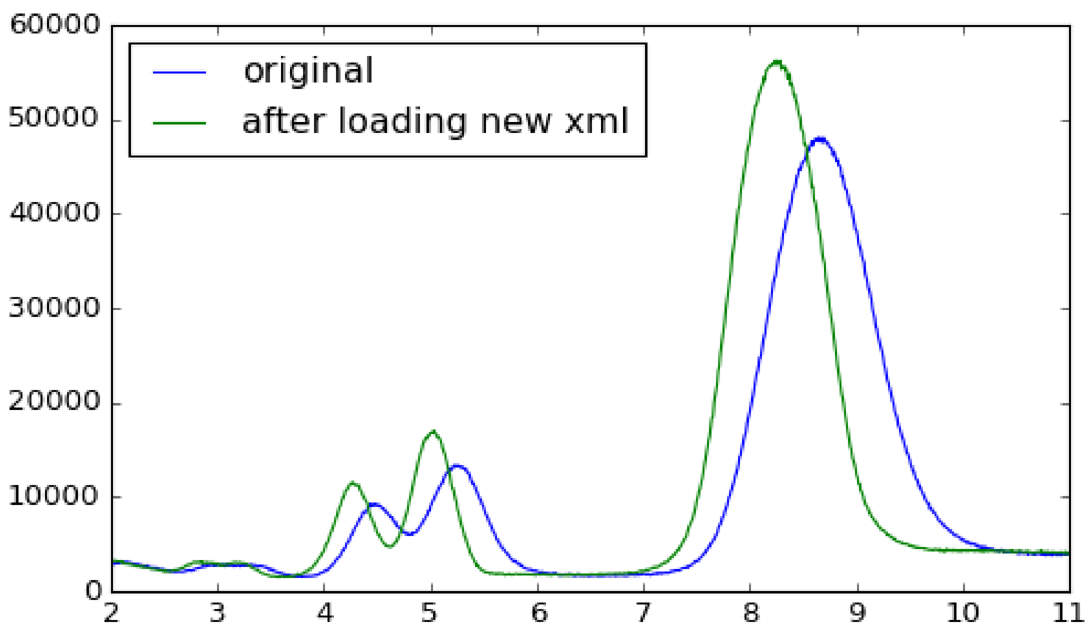
C25B, C60



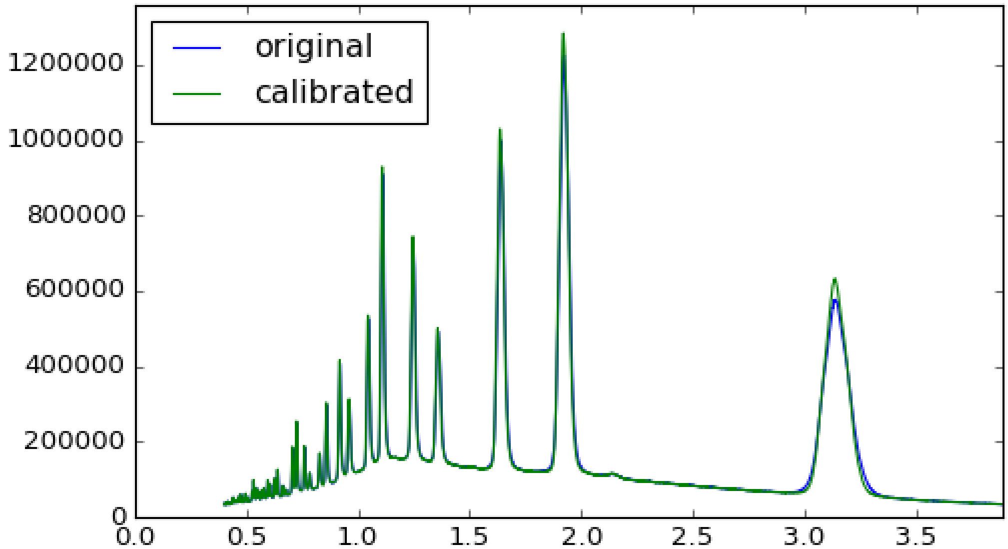
C26T, C60

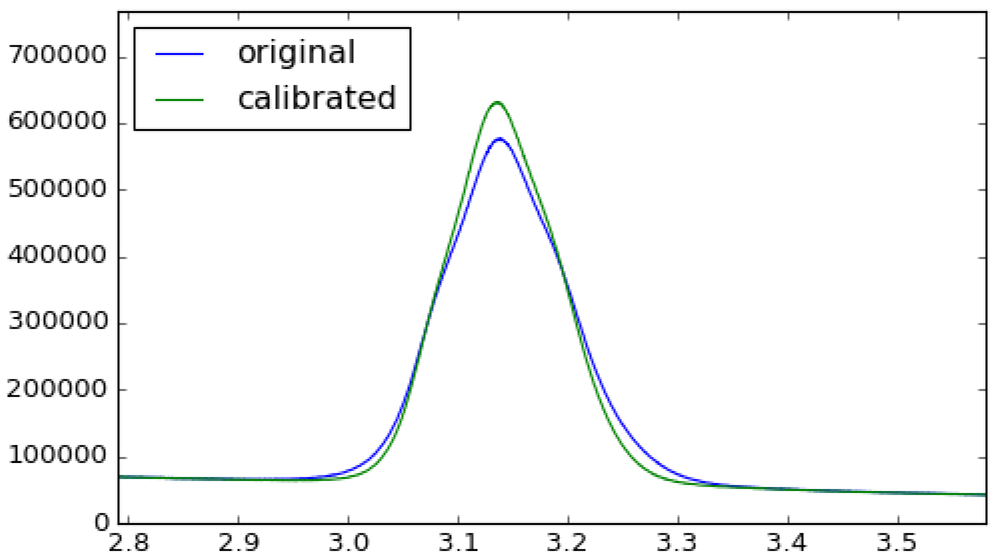


C26B. C60

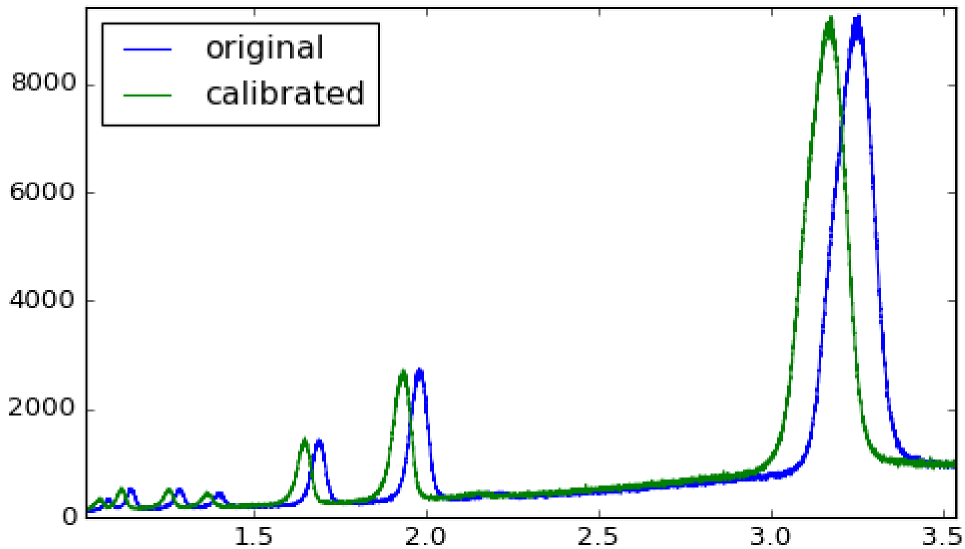


All packs. Silicon data





Pack 26. Silicon data



Known problems

- In DIFC calculation, Tzero (emission time) is not considered