VDRIE
Data Reduction and Interactive Visualization software for Event Mode Neutron Diffraction

Dr. Ke An
Spallation Neutron Source
Oak Ridge National Laboratory
DOCUMENT AVAILABILITY

Reports produced after January 1, 1996, are generally available free via the U.S. Department of Energy (DOE) Information Bridge:

Web site: http://www.osti.gov/bridge

Reports produced before January 1, 1996, may be purchased by members of the public from the following source:

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-605-6000 (1-800-553-6847)
TDD: 703-487-4639
Fax: 703-605-6900
E-mail: info@ntis.fedworld.gov
Web site: http://www.ntis.gov/support/ordernowabout.htm

Reports are available to DOE employees, DOE contractors, Energy Technology Data Exchange (ETDE) representatives, and International Nuclear Information System (INIS) representatives from the following source:

Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831
Telephone: 865-576-8401
Fax: 865-576-5728
E-mail: reports@adonis.osti.gov
Web site: http://www.osti.gov/contact.html

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
VDRIVE-DATA REDUCTION AND INTERACTIVE VISUALIZATION SOFTWARE FOR EVENT MODE NEUTRON DIFFRACTION

Dr. Ke An

SPALLATION NEUTRON SOURCE
OAK RIDGE NATIONAL LABORATORY

© 2007–2021
Preface

VDRIVE (VULCAN Data Reduction and Interactive Visualization software) is a software package that aims at time-event neutron time of flight data reduction, visualization and analysis for engineering diffractometer – the VULCAN instrument; it includes sub programs for different data reduction purposes, sequential data analysis functions, synchronization and visualization of neutron and sample environment data, and outputs of GSAS or Fullprof data for further professional data analysis. In general it is available for event mode data reduction and analysis for TOF neutron diffractometers at spallation sources.

For the newest version of the document, it can be downloaded from the SNS data analysis computer: Applications/data analysis/VDRIVE Manual

Contact:
Dr. Ke An
kean@ornl.gov
Oak Ridge National Laboratory
Bldg 8600, MS 6475
Oak Ridge, TN 37831

Citation: when you publish your results, please cite the use of VDRIVE as:

Contents

Preface ........................................................................................................................................... i

1 Flowchart and cheat sheet .............................................................................................................. 1

2 Some Examples .............................................................................................................................. 4
  1.1 Generating your own instrument parameter files ................................................................. 4
  1.2 Single peak fit of residual strain mapping data / in-situ step loading/ heating data .............. 4
  1.3 Rietveld refinement of residual strain mapping data / in-situ step loading/heating data ....... 5
  1.4 Single peak fit of in-situ continuous loading/heating data .................................................... 5
  1.5 Rietveld refinement of in-situ continuous loading/heating data ............................................ 6
  1.6 View the detector contour ....................................................................................................... 6

3 Computer access .......................................................................................................................... 6

4 VULCAN Data ............................................................................................................................... 6
  4.1 SNS or VULCAN data folder structure ................................................................................. 6
  4.2 Instrument files location ......................................................................................................... 10
  4.3 Download/upload your data ................................................................................................. 10

5 Data reduction, visualization and analysis with VDRIVE ......................................................... 11
  5.1 Load VDRIVE in IDL ............................................................................................................. 11
  5.2 Data Reduction and Analysis Commands ................................................................................ 12
    5.2.1 VDRIVECHOP (Chop) .................................................................................................... 12
    5.2.2 VDRIVESUMGSAS (VSUM) ......................................................................................... 13
    5.2.3 VDRIVEMERGE (Merge) .............................................................................................. 13
    5.2.4 VDRIVEBIN (Vbin) ...................................................................................................... 14
    5.2.5 VDRIVEVIEW (View) .................................................................................................. 14
    5.2.6 VDRIVEFIT (VFIT) ..................................................................................................... 16
    5.2.7 VPEAK ......................................................................................................................... 18
    5.2.8 VDRIVEPoleP (Pole) .................................................................................................... 19

6 Data Analysis with GSAS ............................................................................................................. 20
  6.1 Instrument files preparation .................................................................................................... 20
    6.1.1 VULCAN instrument parameter file for GSAS ............................................................... 20
    6.1.2 Name conventions and the locations of instrument files ................................................ 21
    6.1.3 VDRIVECALI (Cali) .................................................................................................... 21
    6.1.4 VDRIVEPRM (VPRM) ................................................................................................ 21
  6.2 VDRIVESPF(VSPF) ................................................................................................................ 21
  6.3 VDRIVEGSAS(GSAS) ............................................................................................................ 23

Acknowledgement ............................................................................................................................ 25

References ......................................................................................................................................... 25

List of Figures
Figure 1 Flowchart of VDRIVE ......................................................................................................... 1
Figure 2 VDRIVE interface ............................................................................................................... 11
Figure 3 Raw histogram plots of GSAS pattern in the two banks .................................................... 15
Figure 4 2D contour and 3D surface plots generated by VDRIVEVIEW ............................................. 15
Figure 5 Plot of single peak fit in one pattern by VDRIVEFIT............................................................... 16
Figure 6 The fitting results from the VDRIVEFIT.................................................................................. 17
Figure 7 Example of the VULCAN GSAS prm file. .............................................................................. 20
1 Flowchart and cheat sheet

Figure 1 Flowchart of VDRIVE.
VDRIVE cheat sheet

Command line mode (requires IDL license on SNS server, if not available send request to linuxsupport@sns.gov and ask for releasing taken license):

Log on SNS Linux machine (http://analysis.sns.gov) or local machine in the hutch with your XCAMS account (The one with which you submit proposal). Right click mouse and open a Terminal (command line), type idl, then type @VDRIVEEX (not case sensitive for these commands anymore) for data collected since 2021 Feb.

For data collected between 2018-2020, use @VDRIVEbeta add ‘en’ to bin and chop commands, e.g. ‘vbinen’

For older legacy data, use @VDRIVE.

The different variants are due to different detector types.

*If your data is not auto reduced or you want to rebin the data use the bin command below.*

Bin data to GSAS histogram files if not binned before: (short name: vbin)

`vbin, ipts=#, runs=#, rune=# [, choprun=#]`

Chop, synchronize, and bin continuously collected data in seconds: (short name: chop)

`chop, ipts=#, runs=#, dbin=#`

View one GSAS raw pattern after binning as histogram data: (short name: view)

`view, ipts=#, runs=# [,chopruns=#, runv =#, pc=1]`

View sequential data in 2D contour and 3D surface: (short name: view)

`view, ipts= #, runs=#, rune=# [,chopruns=#] [, minv=##., maxv=##., runv=#, norm=1 , pc=1]`

Conduct GSAS single peak fit: (short name: vspf)

`vspf, ipts=#, runs=#, rune=#, runv=# [, chopruns=#] [,runr=# [,pc=1] [,norm=1] [, updatep=1] [, autofix=1] [, autopeak=1, npeaks=#]
Note: peak id file should be saved as peak.txt as the default in the binned_data folder.`

Conduct GSAS Rietveld refinement: (short name: gsas)

`gsas, ipts=#, runs=#, rune=# [,chopruns=#], runm=#`

Generate instrument parameter and instrument spectrum files (by your local contact):

`vbin, runs=#, ipts=#,tag=’V’
vppeak, ipts=# , runv=#
vprm, ipts=#, runv=#, freq= 30 (60 or 20)`
Generate instrument calibration files: (short name: cali)
cali, ipts=#, runp=#, runv=#, tag='Si', freq=20

Handy commands:
Openrecord, IPTS=12345  Open the record file
Openshare, IPTS=12345  Open the share folder
Closeplot, IPTS=12345
VDRIVEGUI mode is not updated any more. (no IDL license required, but highly recommend the command console mode):

Application/data analysis/VDRIVEGUI, or open a Terminal and type VDRIVEGUI.
In VDRIVEGUI, select VDRIVE functions in VDRIVE SUB tab to process data using the keywords above to process data.

2 Some Examples

In the examples below, the IPTS number is 1000 and the instrument parameter file is assumed to be 2000 (check instrument staff for proper instrument files for you), so make sure you have 2000-s.prm and 2000-s.gda in your “Instrument” or gda data folder.

1.1 Generating your own instrument parameter files.

Suppose a fresh calibration measurement has been done for your IPTS, you will have the 20Hz calibration powder Si run for diffraction constants, and V run for instrument spectrum. You can use a simple command to generate the instrument parameter file by the command below:

```
CALI, IPTS=1000, RUNP=1000, RUNV=1001
```

If only a change of instrument spectrum is needed due to chopper setting (e.g. 30Hz), a command below can be used to generate the specific prm file from last calibration for your IPTS.
First run VBIN to bin the V file:
```
VBIN, IPTS=1000, RUNV=1001, tag='V'
```

Then generate the prm file:
```
VPRM, IPTS=1000, RUNV=1001, freq=30
```

1.2 Single peak fit of residual strain mapping data/ in-situ step loading/heating data

Look up the runs AutoRecord.txt in the shared folder and find the correct run numbers for interest of data analysis, below suppose an IPTS 1000, with valid data from 3000 (runs, ‘s’ means ‘start’) to 4000 (run, ‘e’ means ‘end’) (missing run numbers in between is allowed), and take the 3000 as the stress free one (it can be any one in the data folder), so the data processing would be (data are now auto reduced for single runs, so you can skip the VBIN below unless you want to rebin):

```
VBIN, IPTS=1000, RUNS=3000, RUNE=4000
```

Use VIEW to look up the peaks you want to refine:

```
VIEW, IPTS=1000, RUNS=3000, RUNV=2000
```

Use VIEW to visualize the data in contour:

```
VIEW, IPTS=1000, RUNS=3000, RUNE=3200, RUNV=2000, NORM=1
```

*(runv 2000 is the instrument parameter file number under the instrument folder)*

Create a peak.txt file in the ‘binned_data’ folder (see VSPF command section for details), refine the peaks:
1.3 Rietveld refinement of residual strain mapping data/ in-situ step loading/heating data

Look up the runs summary in the shared folder and find the correct run numbers for the data analysis interest, suppose you have valid run from 3000 to 4000, (allow missing run numbers in between), and you want to take run 3000 as the stress free one (can be any one in the folder) and you have two phases in the data, so the data processing would be:

VBIN, IPTS=1000, RUNS=3000, RUNE=4000

Follow the VDRIIVEGSAS command details to prepare 3000_1.EXP
Perform the batch mode data refinement
GSAS, IPTS=1000, RUNS=3000, RUNE=4000, RUNM=3000, NPHASE=2

Look at the fitting qualities in the PDF, you may need to do it in segments for different setup data due to complication of phase transitions.

1.4 Single peak fit of in-situ continuous loading/heating data

Look up the runs summary in the shared folder and find the correct run numbers for the data analysis interest, suppose you have valid run 3000, chop the data first:

CHOP, IPTS=1000, RUNS=3000, DBIN=60, BIN=1
Suppose the data is chopped to 100 sub runs.

You can rebin the data
VBIN, IPTS=1000, CHOPRUN=3000, RUNS=1, RUNE=100

Use VIEW to look up the peaks you want to refine:

VIEW, IPTS=1000, CHOPRUN=3000, RUNS=1, RUNV=2000

Create the peak.txt file in the gda folder (see VSPF section for details), refine the peaks:
VSPF, IPTS=1000, CHOPRUN=3000, RUNS=1, RUNE=100 [,RUNR=1], RUNV=2000 [,Autofix=1]

Look at the fitting qualities in the PDF, you may need to adjust the peak positions in the peak.txt file, or use UPDATEP=1 in VSPF command.
Automatically fit a number of peaks by using the autopeak keyword:

\begin{verbatim}
VSPF, IPTS=1000, CHOPRUN=3000, RUNS=1, RUNE=100, RUNR=1, RUNV=2000, Autopeak=1, npeaks=5
\end{verbatim}

1.5 Rietveld refinement of in-situ continuous loading/heating data

Look up the runs summary in the shared folder and find the correct run numbers for the data analysis interest, and you have two phases in the data, suppose you have valid run 3000, chop the data first:

\begin{verbatim}
CHOP, IPTS=1000, RUNS=3000, DBIN=60, BIN=1
\end{verbatim}

Suppose the data is chopped to 100 sub runs.

You can rebin the data

\begin{verbatim}
VBIN, IPTS=1000, CHOPRUN=3000, RUNS=1, RUNE=100
\end{verbatim}

Follow the VDRIEGSAS command details to prepare 1_1.EXP
Perform the batch mode data refinement:

\begin{verbatim}
GSAS, IPTS=1000, CHOPRUNS=3000, RUNS=1, RUNE=100, RUNM=1, NPHASE=2
\end{verbatim}

Look at the fitting qualities in the PDF, you may need to do it in segments for different setup data due to complication of phase transitions.

1.6 View the detector contour:

\begin{verbatim}
Pixel, IPTS=1000, RUNS=1, RUNV=2000
\end{verbatim}

3 Computer access

What you need:
1 XCAMS account, the same one that you use in the IPTS system. If you do not have one follow this link to get one. (https://user.ornl.gov)

2 Once you have an XCAMS account, you can go to http://analysis.sns.gov and follow the instruction for the remote window access.

4 VULCAN Data

4.1 SNS or VULCAN data folder structure
Analyzed data are stored in a shared folder that all team members have the access. The local machine data process is disabled due to dependency on large raw neutron event and meta data.

/SNS/VULCAN/IPTS-1234/shared/
Under this folder you may find standard folders like below
<table>
<thead>
<tr>
<th>Directory</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>autoreduce</td>
<td>auto reduced files from SNS data reduction routine. VULCAN user is recommended to use data in the binned_data folder below.</td>
</tr>
<tr>
<td>binned_data</td>
<td>GSAS file folder by created by auto reduction or VDRIVEBIN. Some analysis results may also be in the folder along with synchronized sample environment data. Results from VDRIIVESPF and VDRIVEGSAS may also store in this folder.</td>
</tr>
<tr>
<td>Pictures/Videos</td>
<td>Photos/Videos captured by the camera computer.</td>
</tr>
<tr>
<td>logs</td>
<td>Sample environment files (loadframe, furnace and others).</td>
</tr>
<tr>
<td>Instrument/</td>
<td>Instrument parameter file (<em>.prm) and vanadium file (</em>.s.gda).</td>
</tr>
<tr>
<td>ChoppedData</td>
<td>Chopped raw data by VDRIIVECHOP. Raw data need to be reduced by running VDRIIVEBIN, or selecting bin=1 when executing VDRIIVECHOP, copies of synchronized sample environment files are also in this folder.</td>
</tr>
<tr>
<td>SPF_data/</td>
<td>Peak fitting data created by VDRIIVEFIT and VDRIIVESPF.</td>
</tr>
<tr>
<td>GSAS_Results/</td>
<td>GSAS refinement results created by VDRIIVEGSAS.</td>
</tr>
<tr>
<td>Summed_GDA/</td>
<td>GSAS data merged over multiple runs created by VDRIIVESUMGSAS.</td>
</tr>
<tr>
<td>ViewOut/</td>
<td>Folder for output files when using “vout=1” keyword in VIEW.</td>
</tr>
<tr>
<td>Auto-Peak/</td>
<td>Created folder for storing peak files created by using “autopeak” keyword in VDRIIVESPF.</td>
</tr>
<tr>
<td>AutoRecord.txt</td>
<td>All Record file generated by auto reduction.</td>
</tr>
<tr>
<td>AutoRecordAlign.txt</td>
<td>Align Data (when title has prefix of ‘Align:’) Record file generated by auto reduction.</td>
</tr>
<tr>
<td>AutoRecordData.txt</td>
<td>Data Record file generated by auto reduction.</td>
</tr>
</tbody>
</table>

Result files created by VDRIIVE

/*Instrument*/
Under this folder you may find standard instrument parameter file pairs as below

123456-s.gda  The smoothen Vanadium file, you may have more than one if different instrument optics configurations are used for your IPTS. The file can be used by specifying the run number as keyword like “runv=123456” as needed in different VDRIIVE commands.

Vulcan-123456-s prm  The corresponding instrument parameters file including the calibration of the instrument. The file can be used by specifying the run number as keyword like “runv=123456” as needed in different VDRIIVE commands.

note.txt  The file contains basic information of the instrument parameter files under this folder, such as chopper or guide settings.

/*SPF_data*/
Under this folder you may find files created by VSPF as below

VDriiveSPF-1234-1-100-bk1.pdf  The snapshot of the fitting plot for each peak position fitted in VSPF. *(Runs=1 and rune=100, in chopruns=1234)*
The output file containing fitting parameters for VSPF including a copy of the synchronized sample environment data. For example, lattice d spacings in Angstrom or TOF, integrated intensity I (w/o normalization to proton charge /P, and beam spectrum /V), background (B), FWHM, and its corresponding parameters, lattice strain based on either the very first runnumber or specified run number by using “runr” keyword.

The file name can be in the format below by using collected run numbers when chopping data is not required:

VDriveSPF-1234-1-100-bk1.txt

/GSAS_Results/
Under this folder you may find files created by VDRIVEGSAS as below

VDriveGSAS-1234-1-100-bk1.pdf The snapshot of the fitting plot for each Rietveld refinement in VDRIVEGSAS. (Runs=1 and rune =100, in chopruns=1234)

VDriveGSAS-1234-1-100-atom.txt The output file containing atom fitting parameters by GSAS (the file with “_log” includes a copy of the synchronized sample environment data) given they are opted to be refined.

VDriveGSAS-1234-1-100-profile.txt The output file containing profile fitting parameters by GSAS (the file with “_log” includes a copy of the synchronized sample environment data) given they are opted to be refined. e.g. the weight fraction, scale factor, lattice parameters etc. if they are opted to be refined.

The file name can be in the format below by using collected run numbers when chopping data is not required:

VDriveGSAS-1000-1999-bk1.txt

Note: The meaning of the fitted parameters can be found in the GSAS manual.

/Summed_GDA/

12345.gda Summed GSAS data merged by VDRIVESUMGSAS.

/ViewOut/
Under this folder you may find files created by VIEW when “vout=1” is selected.

1-123456.txt Two-column data of d spacing and Intensity as seen in the VIEW plot for bank 1, first number changes to according bank.

1-totall.txt Two-column data of runnumber and total summed Intensity as seen in the VIEW plot for bank 1, first number changes to according bank.
Note: If chopped data is processed, look for those data under the folder name of chopped run number.

/ChoppedData/1234
Under this folder you may find files created by VDRIVacelop[en].

1.dat  One-column intensity data to be read by VBIN for first chopped run number. Number changes accordingly with sliced run.
choppeddatatofinfo.dat  One-column tof data to be read by VBIN for all chopped run.

1234sampleenv_chopped_mean.txt  Averaged synchronized sample environment data over the “dbin” time in VDRIVacelop command.
1234sampleenv_chopped_start.txt  Starting values of synchronized sample environment data over the “dbin” time in VDRIVacelop command.
1234sampleenv_chopped_end.txt  Ending values of synchronized sample environment data over the “dbin” time in VDRIVacelop command.

IPTS-1000-MTSLoadFrame-1234-header.txt  The header information of the sample environment data by VDRIVacelop command.

Note: If the chopped run number is 1234, for the chopped sample environment data, a copy is created in the binned_data folder/1234/.

/binned_data/1234
Under this folder you may find files created by VDRIVacelop[en].

1.gda  Gsas data of all the banks. Number changes accordingly with sliced/colllected run.
1234sampleenv_chopped_mean.txt  Copy if averaged synchronized sample environment data over the “dbin” time in VDRIVacelop command.
1234sampleenv_chopped_start.txt  Copy of starting values of synchronized sample environment data over the “dbin” time in VDRIVacelop command.
1234sampleenv_chopped_end.txt  Copy of ending values of synchronized sample environment data over the “dbin” time in VDRIVacelop command.

IPTS-1000-MTSLoadFrame-1234-header.txt  Copy the header information of the sample environment data by VDRIVacelop command.

Note: If the chopped run number is 1234, the files are found in binned_data folder/1234/.

GSAS files are in ASCII format with three columns for each bank, and both banks data are saved in one file with data structure header as a separator. The three columns are, time of flight in ms (Tof), intensity (see the file header for normalization to vanadium), square root of intensity.
The relationship between time of flight and d spacing is:

\[ T_{	ext{of}} = d \cdot \text{DIFC} + d^2 \cdot \text{DIFA} + \text{ZERO} \]

DIFC, DIFA and Zero are instrument parameters which can be found in the instrument parameter file (*.prm). (see instrument parameter file section for details).

Sample environment logs are in ASCII format with multiple columns. It has by default timestamp, time elapsed, and variables (loadframe signals, or temperatures).

Chopped sample environment files are synchronized with neutron timestamps. It has by default chopped run number, proton charge (for normalization by using `pcsenv=1` keyword), and synchronized columns from sample environment files.

4.2 Instrument files location

Processed instrument files and vanadium files are also in the VULCAN share folder.

---------------------------------------------------------------
/SNS/VULCAN/shared/Calibrationsfiles/Instrument/
  Standards/
  PRM/
  Template/
---------------------------------------------------------------

4.3 Download/upload your data

Use an SFTP client to transfer data between your own computer and the data on server. FileZilla is a free one that works across different platforms. The server is analysis.sns.gov and the port for SFTP is 22.
5 Data reduction, visualization and analysis with VDRIVE

5.1 Load VDRIVE in IDL

VDRIVE is based on the IDL.

<table>
<thead>
<tr>
<th>OS</th>
<th>License</th>
<th>OPEN</th>
<th>Type first</th>
<th>Then type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linux</td>
<td>Yes</td>
<td>Terminal</td>
<td>idl or idlde (case sensitive)</td>
<td>@VDRIVEX or vdrivex</td>
</tr>
<tr>
<td>Linux</td>
<td>No</td>
<td>Terminal</td>
<td>VDRIVEGUI (stop updating)</td>
<td></td>
</tr>
<tr>
<td>Linux</td>
<td>No</td>
<td>Application/data analysis</td>
<td>VDRIVEGUI (stop updating)</td>
<td></td>
</tr>
</tbody>
</table>

Use of VDRIVE

In the terminal command console or idl workbench command console, type VDRIVE commands to perform data reduction, data fit, and data visualization. Or with the VDRIVEGUI, choose VDRIVE SUB tab, and type parameters line by line.

Note: in the GUI, it does not support “/” in the command, should use “parameter=1” rather than “/parameter”

![Figure 2 VDRIVE interface](image-url)
5.2 Data Reduction and Analysis Commands

5.2.1 VDRIVECHOP (Chop)

**Purpose:** Chop and bin continuously measured neutron data in time sequence under changing sample environment conditions.

**Common use:**

```
CHOP, IPTS=1000, RUNS=2000, dbin=60, bin=1
```

where, `dbin` is the chop step size in seconds; `bin=1`, for binning data to GSAS file after slicing the data in time. GSAS data are stored at `/SNS/VULCAN/IPTS-1000/shared/binned_data/2000` along with the chopped sample environment files `2000sampleenv_chopped_start(mean or end).txt`.

Alternate for `loadframe=1`: `furnace=1`, or `generic=1`, when using VULCAN standard sample environment DAQ for the furnaces or others. For a customized sample environment file name, use `SampleEnv='your sample file name.txt'` (the customized sample environment file is stored in `/SNS/VULCAN/IPTS-1000/shared/logs`).

If no sample environment is chosen or `justchop=1` keyword is selected, no sample environment data synchronization will be executed.

**Other uses:**

*To chop with customized time segments:*

```
CHOP, IPTS=1000, RUNS=2000, pickdata="/SNS/VULCAN/IPTS-1000/shared/picktime.txt", bin=1, pulsetime=1
```

where `pickdata` is the file name containing several selected time segments of the neutron data with the format of below (separated by tab and unit is seconds and use pulse time):

```
--------------
1.00 10.00
20.01 30.00
40.01 50.00
...
--------------
```

**Additional keywords:**

- `Focus_EW=0`: Bin data over each detector module.
- `dt=###.##`: Time (s) between each chopped run, by default it equals `dbin`. If less than `dbin`, each run will have overlapped neutron events.
- `t0=###.##`: Time (s) offset from the start of neutron event files.
- `tend=###.##`: Time (s) offset from the end of neutron event files.
- `Ndataset=###`: Number of chopped data set. Effective when the automatically calculated data sets are more than `Ndataset`.
- `Ndbin=###`: Number of time bins per cycle for stroboscopy.
- `Ncycle=###`: Number of cycles to perform stroboscopy.
- `Strobe=1`: Set stroboscopy on.
- `GSAS=1`: Plot GSAS file after binning.
- `Onelog=1`: Read sample environment parameters from one log file.
- `Loadframe=1`: Read sample environment parameters from MTS Loadframe log file.
**Generic=1**
Read sample environment parameters from Generic log file e.g. analog inputs, voltage, current, exclusive with loadframe=1.

**Accu=1**
Accumulate data over chopped runs.

**PulseTime=1**
For **PickData**, when **PulseTime** is used in the picktime.txt file.

**AppRun=###**
Append chopped data to previously chopped data in **choprun=###**. Will not work with **Connect=1**.

**Connect=1**
Chop more than one runs and connect data after RUNS and data are saved to RUNS’s chopped data folder. Will not work with **AppRun**.

Other **VDRIVEBIN** keywords when coupled with **bin=1**.

### 5.2.2 VDRIVESUMGSAS (VSUM)

**Purpose:** Combine GSAS data. GSAS data are combined from the runs.

**Common use:**
- `VSUM, IPTS=1000, RUNFILE="/SNS/VULCAN/IPTS-1000/shared/runfile.txt"`
- `VSUM, IPTS=1000, RUNLIST=[1234,1235]`
- `VSUM, IPTS=1000, RUNS=1234, RUNE=1235`

The summed GSAS data are saved to `/SNS/VULCAN/IPTS-1000/shared/Summed_GDA/`

**Example of the tab delimited runfile.txt:**

```
1001 1002 1003 1004
1005 1006 1007
1008 1009 1010
...
```

**Additional keywords:**
- **Runv=1111** Normalize summed data over Vanadium.
- **Trans=1** Sum data to the first row runs.
- **Threeframes=1** Sum data measured by different chopper settings.

### 5.2.3 VDRIVEMERGE (Merge)

**Purpose:** Combine collected event data (not work with new nED data anymore). Data are combined from the runs of rest columns to the runs of the first column in the runfile.txt.

**Common use:**
- `MERGE, IPTS=1000, RUNFILE="/SNS/VULCAN/IPTS-1000/shared/runfile.txt", CHOPRUN=2`

The combined data are saved to `/SNS/VULCAN/IPTS-1000/shared/chopped_data/2/`

To bin the data combined by **VDRIVEMERGE**:
- `VDRIVEBIN, IPTS=1000, CHOPRUN=2`

GSAS files are stored in `/SNS/VULCAN/IPTS-1000/shared/binned_data/2/`
Example of the tab delimited runfile.txt:

irement------------------------
1001 1002 1003 1004
1005 1006 1007
1008 1009 1010
…

Additional keywords:
NONE

5.2.4 VDRIVEBIN (Vbin)
Purpose: Bin collected data or chopped data by VDRIVECHOP to GSAS files.
Common use:
For typical mapping experiments or single run:
VBIN, IPTS=1000, RUNS=2000, RUNE=2099

GSAS files are stored in /SNS/VULCAN/IPTS-1000/shared/binned_data/

For chopped files created by VDRIVECHOP:
VBIN, IPTS=1000, CHOPRUN=2000, RUNS=1, RUNE=100

GSAS files are stored in /SNS/VULCAN/IPTS-1000/shared/binned_data/2000/

Additional keywords:
BINW=0.005 The logarithm bin step size of TOF and its default is 0.001.
FOCUS_EW=0 For 7-module data binning.
RUNV=5000 Normalize data over smoothed vanadium file in /Instrument folder, and used for VDRIVEFit when normalized intensity is an output option, for VDRIVESPF, NORMALIZE=0 should be taken.
Runb=5001 Correct data by background file, use with NORMALIZE=1
IParm='prmfile.prm' Replace the Vulcan.prm in comment line with the customized prmfile.prm string in GSAS files.
FullProf=1 Output FullProf files.
NoGSAS=1 Omit GSAS files.
PlotFlag=1 Plot histogram after binning.
Merge_EW=1 Bin east and west banks data to one histogram. Bank 3 number will become 2.
NoMask=1 Bin bad pixels too.
Tag='Si' Bin a Si calibration powder. If ‘CeO2’ is chosen, bin a CeO2 calibration powder. If ‘V’ is chosen, bin a vanadium data.
Mytofmax=1111 max tof bin in us
Mytofmin=1111 min tof bin in us

5.2.5 VDRIVEVIEW (View)
Purpose: Visualize data in 2D, 3D plots.
Common use:
To view one GSAS pattern:
VIEW, IPTS=1000, RUNS=1, plot=1

Figure 3 Raw histogram plots of GSAS pattern in the two banks.

To view sequential GSAS patterns in 2D and 3D:
VIEW, IPTS=1000, RUNS=1, RUNE=50

To view sequential GSAS patterns of chopped data in 2D and 3D:
VIEW, IPTS=1000, CHOPRUN=2000, RUNS=1, RUNE=50

Figure 4 2D contour and 3D surface plots generated by VDRIVEVIEW.

Additional keywords:
- **RUNV=5000** Normalize GSAS pattern with instrument spectrum by the vanadium pattern.
- **TOTALCOUNTS=1** Normalize with total counts of each bank.
- **PCSENV=1** For chopped data, normalize chopped data with proton charge (beam charge).
- **MinV=0.7, MaxV=2.7** Define the display range in d space.
- **Position=1, SENV=5** Show the 6th variable (starting from 0) as the vertical axis in the contour and surface plots. Can be any Nth column in the chopped sample environment files.
Norm=1 Normalize to proton charge of single run measurement (differs from PCSENV for chopped runs).
Tof=1 Show x in time of flight.
Angle=1 Show x in 2 theta angle.
Q=1 Show x in Q.
Lambda=1 Show x in wavelength.
PlotGSAS=1 Show individual GSAS pattern.
ClearPlot=1 Reset plotted windows by previous execution of VDRIVEVIEW.
SameScale=1 Show two banks data in same scale.
Merge=1 Show two banks data in one window.
Log=1 Plot intensity in logarithm.
DIFC=[16370,16372] Manually input DIFCs of the two banks.
Summed=1 View summed GSAS data in Summed_GDA folder.

5.2.6 VDRIVEFIT (VFIT)

**Purpose:** Gaussian function single peak fit and results visualization.

**Common use:**
*Note: use VDRIVESPF whenever possible.*

*For one GSAS pattern fit:*

\[
\text{VFIT, IPTS=1000, RUNS=1, listd=[2.60,2.45,1.89,1.6,1.47], width=[0.035, 0.03, 0.03, 0.03, 0.03], plot=1}
\]

where, listd is the list of initial guess of the peak position, width is the data range of the peak in d-space for each peak, can be one value for all peaks, or an array of values for each peak;

![Figure 5 Plot of single peak fit in one pattern by VDRIVEFIT.](image)

*For sequential GSAS patterns fit:*
VFIT, IPTS=1000, RUNS=1, RUNE=50, RUNR=1, listd=[2.04, 1.76, 1.243, 1.06], width=[0.03,0.03,0.03,0.02], UpdateP=1

or for chopped GSAS patterns fit
VFIT, IPTS=1000, ChopRun=2000, RUNS=1, RUNE=50, RUNR=1, listd=[2.04, 1.76, 1.243, 1.06], width=[0.03,0.03,0.03,0.02], UpdateP=1

where RUNR is the strain reference run, otherwise, d-space will be the only output; UpdateP=1, peak center of previous run will be used as the guess of current run.

Figure 6 The fitting results from the VDRIVEFIT.

This program can search peaks based on statics:

VFIT, IPTS=1000, RUNS=1, RUNE=50, RUNR=1, npeaks=8, UpdateP=1
Additional keywords:

- **Bterm=1** Background parameter. Default is 1 for flat background, 2 is for linear background.
- **Bank=[1,2]** Choose specific bank data to fit.
- **Norm=1** Normalize the integrated intensity to total counts.
- **Voigt=1** Peak shape function option. Default peak shape is Gaussian, if Voigt=1, VDRIVEFIT will use the asymmetric Voigt function (Note: Voigt function has 2 more parameters than Gaussian function, so if the peak intensity is low, the fit may not converge).
- **NoErrorBar=1** Omit the error bars in plots.
- **Position=1, SENV=5** Show the 6th variable (starting from 0) as the vertical axis in the contour and surface plots. Can be any Nth column in the chopped sample environment files.
- **Log=1** Take logarithm of the intensity and then perform the fit.
- **Pcsenv=1** Normalize the intensity by the proton charge in the chopped sample environment file.
- **Show=1** Show the fitting results in the command console.
- **Showbad=1** Show the bad fitting results in plots.
- **Npeaks=1** Set number of highest peaks (raw data) to be detected and conduct fitting by the program itself.
- **AutoPeak=1** Output the fit result (only with one run fitting) to a peak txt file for VSPF input.

Peak positions, intensities, peak widths and strains of each peak are stored in ASCII files RUNS_1.txt and RUNS_2.txt under /SNS/VULCAN/IPTS-####/shared/SPF_data. Results should be checked. Usually if there are some exotic points, it means either the statistics of these data are poor, or some initial parameters such as peak position or width should be adjusted. If peaks are too close, initial values of original position and width are important. This command is not recommended for overlapping peaks fitting.

### 5.2.7 VPEAK

**Purpose:** Process vanadium diffraction peak and data noise.

**Common use:**

VPEAK, IPTS=1000, RUNV=5000

**Additional keyword:**

- **Nsmooth =51** The number of points to be used in the boxcar smoothing algorithm, the bigger the smoother.
- **OneBank=1** When all banks’ data are binned as one bank data.
- **Shift=1** When the chopper center is shift to large lambda aggressively.

The smoothed data is named as ####-s.gda and located at /SNS/VULCAN/IPTS-1000/shared/Instrument as well as a copy in the VULCAN shared folder
5.2.8 VDRIVEPoleP (Pole)

**Purpose:** Process single peak data texture measurement and output pole figure data.

**Common use:**

```
VDRIVEPoleP, IPTS=1000, RUNS=1, RUNE=120, bina=1, focus_ew=0
```

**Additional keyword:**

- **Involume=1**
  - When the sample is a thin and long bar measured. If the sample fully embraces the 5x5x5mm³ gauge volume, no need to use this keyword.

- **Std4590=1**
  - When the measurement uses standard rotation of Omega or VROT from 45 to 90 degrees.

- **rotation=value of angle**
  - Specify a value of angle in degree to rotate the plot, default is -90.

- **bina=1**
  - Bin the data with overlaps in pole/Q space, and plot will be generated if the binning is successful.

A detailed instruction of generating texture pole figure can be found in Appendix.
6 Data Analysis with GSAS

6.1 Instrument files preparation

6.1.1 VULCAN instrument parameter file for GSAS

Contents of instrument (*.prm) file

Basically the prm file contains 2 parts:

1) **Instrument spectrum for normalization**

Lines with keyword “ITYP” and “MFIL” are related to instrument spectrum file by vanadium. In the ITYP line, “10” means the normalization method is using vanadium pattern directly, “6.5” and “42” are the valid data range in TOF ms. The MFIL lines specify the vanadium file that is used.

2) **Instrument calibration and peak profile information**

Lines with keyword “ICONS” and “PRCF” are related to the calibration information of the instrument. In the ICONS line, DIFC, DIFA and Zero are given. In the PRCF line, the peak profile parameters are given. These values should be obtained by fitting the pattern of a standard sample e.g. Si.
More information of the instrument parameter files can be found in the GSAS manual.

If needed, instrument files can be created/updated by refining the standard data Si every cycle along with the smoothed vanadium data. Or one can look for one instrument file that has the same configuration (guide, chopper, lambda center, lambda width, and sample environment) from /SNS/VULCAN/shared/Calibrationfiles/Instrument/PRM. The files are updated usually once in a cycle.

### 6.1.2 Name conventions and the locations of instrument files

VULCAN GSAS instrument files are named according to the vanadium run number, such as **Vulcan-5000-s.prm**, where 5000 is the vanadium run number, and “-s” means the vanadium pattern has been smoothed by VPEAK.

For each user project, the instrument files, including the prm file and the smoothed vanadium data, should be stored in the IPTS folder /SNS/VULCAN/IPTS-####/shared/Instrument. The template prm files are in the folder /SNS/VULCAN/shared/Calibrationfiles/PRM/Template.

Note: User may have more than one instrument prm files depending on the configurations used in the experiment.

### 6.1.3 VDRIVECALI (Cali)

**Purpose:** Generate instrument calibration files from Si and vanadium measurements.

**Common use:**

```
CALI, IPTS=4744, RUNP=12474, RUNV=12475, TAG='Si', Freq=20
```

This example is based on high intensity (HI) 20Hz chopper setting Si powder measurement **RUNP=12474**, and the corresponding vanadium measurement **RUNV=12735**. Instrument parameter file **Vulcan-12735-s.prm** will be created in /SNS/VULCAN/shared/Calibrationfiles/Instrument/PRM/ and also the template instrument file **Vulcan-template-HI.prm** is created or updated under /SNS/VULCAN/shared/Calibrationfiles/Instrument/Template.

**Additional keywords:**

- **OneBank=1**
  
  For one bank calibration when two banks data are binned as one. The files will be saved in `/1bk` under those instrument folders.

### 6.1.4 VDRIVEPRM (VPRM)

**Purpose:** Generate user specific instrument files from calibration (template) files.

**Common use:**

```
VPRM, IPTS=1000, RUNV=5000, FREQ=20 (or 30, 60), ONEBANK=1
```

**Vulcan-5000-s.prm** and **5000-s.gda** will be created in /SNS/VULCAN/IPTS-1000/shared/Instrument.

### 6.2 VDRIEVSPF(VSPF)

**Purpose:** Use GSAS for single peak fit including overlapping peaks.

**Common use:**

*For typical mapping experiments:*

```
VSPF, IPTS=1000, RUNS=1, RUNE=100, RUNR=1, RUNV=5000
```
For sequential GSAS files of chopped run:

**VSPF, IPTS=1000, CHOPRUN=2000, RUNS=1, RUNE=100, RUNR=1, RUNV=5000, PCSENV=1**

**Required files:** Peak ID file (peak.txt), instrument parameter file (*.prm), and instrument spectrum file by vanadium (*.s.gda). *.prm and *.s.gda should be under the instrument folder. The peak ID file is recommended to be named as `peak.txt` under the (chopped) GSAS data folder.

An example of the `peak.txt` file is below:

```
<table>
<thead>
<tr>
<th>$bk</th>
<th>name number</th>
<th>pos</th>
<th>range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>110 1</td>
<td>2.02692</td>
<td>0.03000</td>
</tr>
<tr>
<td>$1</td>
<td>310 1</td>
<td>0.90647</td>
<td>0.02500</td>
</tr>
<tr>
<td>$2</td>
<td>110 1</td>
<td>2.02692</td>
<td>0.03000</td>
</tr>
<tr>
<td>$2</td>
<td>200 1</td>
<td>1.43325</td>
<td>0.03000</td>
</tr>
<tr>
<td>2</td>
<td>211 1</td>
<td>1.17024</td>
<td>0.02000</td>
</tr>
<tr>
<td>$2</td>
<td>220 1</td>
<td>1.01346</td>
<td>0.03000</td>
</tr>
</tbody>
</table>
```

The names of the columns are:
Bank ID, name of the peak, number of peaks, estimated peak position (in d), estimated peak range (in d). $ sign is for comment line.

For overlapped peaks, which are too close to perform single peak fit, alternate the first peak column value for the purpose of fitting and outputting the corresponding results. An example is given below:

```
$ Fit the first peak
1    peak1 2    2.02345 2.03456 0.04
$ Fit the second peak
1    peak2 2    2.03456 2.02345 0.04
```

**Additional keywords:**
- `peakFile='peak.txt'`: For customized peak ID file name other than the default one.
- `Runfile='file.txt'`: Fit runs in a text file, one run per line.
- `UpdateP=1`: Take previous run as the peak parameters guess for current run.
- `prmFile='prmfile.prm'`: Use different prm file.
- `myRefine='Refine.txt'`: Use a customized refinement steps in a macro file.
- `NoErrorBar=1`: Omit the error bars in plots.
- `UserDataDir='folder'`: Direct the data in a specific folder.
- `Plotdata=0`: Omit the plots.
- `Showbad=1`: Show bad refinement results in the plots.
- `Pcsenv=1`: Spectrum divided by proton charge, not with `monitor`.
- `Monitor=1`: Spectrum divided by monitor 2, not with `pcsenv`. 

22
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normalization=0</td>
<td>Not normalize to Vanadium file (with runv) for data already normalized by VDRIVEBIN.</td>
</tr>
<tr>
<td>AutoPeak=1</td>
<td>With the keyword below to automatically search for number of peaks from the order of high to low intensity and allow user to fit the data with the found peaks; not with “peakfile” .</td>
</tr>
<tr>
<td>NOPeaks=#</td>
<td>Specify number of peaks to search in Autopeak option.</td>
</tr>
<tr>
<td>AutoFix=1</td>
<td>When a fitting fails due to a miss input of the initial peak position, this command enable the program to automatically adjust the input value over small step ( dtweack=0.001, ) over a total number of iterations ( ntweack=200) to fit the data.</td>
</tr>
</tbody>
</table>

Result file list:
- VDriveSPF-2000-1-50-bk1.txt  Peak positions, widths, intensities, and strains (in refinement folder as well as a copy in SPF_data folder).
- VDriveSPF-2000-1-50-bk1.pdf  Fitting plots for quality check (in refinement folder as well as a copy in SPF_data folder).

6.3 VDRIVEGSAS(GSAS)

**Purpose:** Use GSAS for Rietveld Refinement based on a source run.

**Common use:**
* For typical runs:
  GSAS, IPTS=1000, RUNS=1, RUNE=100, RUNM=1, BANK=1
* For GSAS files from chopped data:
  GSAS, IPTS=1000, CHOPRUN=2000, RUNS=1, RUNE=100, RUNM=1, BANK=1

**Required files:** Instrument parameter file (*.prm), instrument spectrum file by vanadium (*.s.gda) and a source run (RUNM) which has been refined well by GSAS are required and stored the GSAS data folder before the execution of this command. The source files will define the refinement scheme of Rietveld refinement in GSAS. If the source RUNM is 1, VDRIVEGSAS needs GSAS EXP files 1_1.EXP and 1_2.EXP for bank 1 and 2, respectively.

**Additional keywords:**
- Nphase=2  Number of phases in the GSAS data.
- UserDataDir='folder'  Direct the data in a specific folder.
- Runfile='listfile.txt'  Fit runs in a text file, one run per line.
- Title='Title'  Title for all GSAS refinement.

Result file list:
- VDriveGSAS-2000-1-50-bk1.txt  Lattice parameters, strains.
- VDriveGSAS-2000-1-50-bk1.pdf  Refinement plots for quality check
- VDriveGSAS-2000-1-50-bk1-atom.txt  Atom occupancies if turned on.
- VDriveGSAS-2000-1-50-bk1-profile.txt  Peak profile parameters.

Create a source run for VDRVIEGSAS
Open Terminal
Type `expgui`
Direct to your “binned_folder” then type `####_1.EXP`, then click “Create” button
Type a string for the exp file title.
Click “Add Phase”
Select the way to add new phase (either by previous EXP file, or CIF file)
Point to the file containing crystal phase information
Click “Continue”
Modify the atom name properly and click “Add Atoms”
In “Powder” tab, click “Add New Histogram”
In Data file, click “Select”
In Instrument file, click “Select” (better copy the instrument files to the binned_data folder)
Follow the GSAS manual to perform a good refinement of the data.

Perform same way to generate source run for bank 2 by simply change `####_1.EXP` to `####_2.EXP`. 
Acknowledgement

The computer and software supports from Harley Skorpenske, Ling Yang, Jean C. Bilheux, John Quigley, Kyle Anderson, and Jason Hodges are acknowledged. The Spallation Neutron Source is a user facility at Oak Ridge National Laboratory sponsored by the Office of Basic Energy Science, the Office of Science, the Department of Energy, USA. Oak Ridge National Laboratory is managed by UT-Battelle, LLC, for the U.S. Dept. of Energy under contract DE-AC05-00OR22725.

References

2. IDL, http://www.exelisvis.com/

Appendix

Texture pole figure instruction on VULCAN

9.22.20 (for data collected before 2021 Feb)

For texture data collected after 2021 Feb, see next instruction.

1. load VDRIVE

idl, @vdrivebeta

2. Create peak.txt file for fitting of 6 modules/detectors and save in the binned_data folder

For cubic system first 4 peaks are good start. Note here: no underscore should be used in peak id. For FCC you can just choose a few first peaks, and fit same peaks in six banks.

```
<table>
<thead>
<tr>
<th>l</th>
<th>Phid</th>
<th>Npk</th>
<th>pos</th>
<th>range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>11181</td>
<td>1</td>
<td>2.34</td>
<td>0.03</td>
</tr>
<tr>
<td>1</td>
<td>20001</td>
<td>1</td>
<td>2.02</td>
<td>0.03</td>
</tr>
<tr>
<td>#1</td>
<td>22801</td>
<td>1</td>
<td>1.43</td>
<td>0.03</td>
</tr>
<tr>
<td>#1</td>
<td>31181</td>
<td>1</td>
<td>1.22</td>
<td>0.03</td>
</tr>
<tr>
<td>#1</td>
<td>22281</td>
<td>1</td>
<td>1.16</td>
<td>0.03</td>
</tr>
<tr>
<td>#1</td>
<td>40001</td>
<td>1</td>
<td>1.01</td>
<td>0.03</td>
</tr>
<tr>
<td>#1</td>
<td>33181</td>
<td>1</td>
<td>0.93</td>
<td>0.025</td>
</tr>
<tr>
<td>#1</td>
<td>42001</td>
<td>1</td>
<td>0.90</td>
<td>0.025</td>
</tr>
<tr>
<td>2</td>
<td>11182</td>
<td>1</td>
<td>2.34</td>
<td>0.03</td>
</tr>
<tr>
<td>2</td>
<td>20002</td>
<td>1</td>
<td>2.03</td>
<td>0.03</td>
</tr>
<tr>
<td>#2</td>
<td>22802</td>
<td>1</td>
<td>1.43</td>
<td>0.03</td>
</tr>
<tr>
<td>#2</td>
<td>31182</td>
<td>1</td>
<td>1.22</td>
<td>0.03</td>
</tr>
<tr>
<td>#2</td>
<td>22282</td>
<td>1</td>
<td>1.16</td>
<td>0.03</td>
</tr>
<tr>
<td>#2</td>
<td>40002</td>
<td>1</td>
<td>1.01</td>
<td>0.03</td>
</tr>
<tr>
<td>#2</td>
<td>33182</td>
<td>1</td>
<td>0.93</td>
<td>0.025</td>
</tr>
<tr>
<td>#2</td>
<td>42002</td>
<td>1</td>
<td>0.90</td>
<td>0.025</td>
</tr>
<tr>
<td>3</td>
<td>11183</td>
<td>1</td>
<td>2.34</td>
<td>0.03</td>
</tr>
<tr>
<td>3</td>
<td>20003</td>
<td>1</td>
<td>2.02</td>
<td>0.03</td>
</tr>
<tr>
<td>#1</td>
<td>22803</td>
<td>1</td>
<td>1.43</td>
<td>0.03</td>
</tr>
<tr>
<td>#1</td>
<td>31183</td>
<td>1</td>
<td>1.22</td>
<td>0.03</td>
</tr>
<tr>
<td>#1</td>
<td>22283</td>
<td>1</td>
<td>1.16</td>
<td>0.03</td>
</tr>
<tr>
<td>#1</td>
<td>40001</td>
<td>1</td>
<td>1.01</td>
<td>0.03</td>
</tr>
<tr>
<td>#1</td>
<td>33183</td>
<td>1</td>
<td>0.93</td>
<td>0.025</td>
</tr>
<tr>
<td>#1</td>
<td>42003</td>
<td>1</td>
<td>0.90</td>
<td>0.025</td>
</tr>
</tbody>
</table>
```

We used standard rotation process to measure texture data, i.e. rotate vertical axis 45 degrees by 5 degree/step, and rotate horizontal axis by 360 degrees by 30 degree/step. The total measurements are 120 runs.
3 For a specific sample, find the first run with $B_1=0$, $B_2=-90$

4 Find the last run with $B_1=45$, $B_2=-45$

5 Rebin the 120 data runs into individual banks by using the keyword focus_ew=0 in VBINEN

6 Do the single peak fitting with VSPF as usual except that the runv needs to contain 7-bank calibration, ask instrument staff if it is not available

7 Run VDRIVEPOLEP to process the data for pole figures

The use of “involume=1” is when you have a thin and long bar measured. If the sample is large enough contains fully the $5x5x5\text{mm}^3$ gauge volume, or the sample is a small cube and fully buried within the gauge volume, no need to use “involume=1”.

Use “std4590=1” when the measurement is conducted by standard rotation of Omega or vertical rotation axis from 45 degree to 90 degree.

This command will simply output 120 records after coordinates transformation and intensity normalization. At this point the output data as measured can be plotted in plotting software.

Below is recommended to run with “bina=1” for binning the data with overlaps in pole/Q space, and plot will be generated if the binning is successful.

Finally, the file outputs are
A quick view of the pole figure of the fitted peak is shown, and the files are saved in the SPF_data folder.*_pole.txt is the data of *_pole.jpg file. Use *_Psi_Phi.txt to plot pole figure in other plotting software, such as OriginPro.

When using bina=1, a pole plot is generated as shown by the example below.

**VULCAN Instrument layout**

Instrument layout and an example pole figure from the fitted data.

In the pole figure’s polar coordinates, the radial coordinate is linked to Psi (or omega of the instrument), and the angular coordinate is linked to Phi (or HROT of the instrument motor). With relative to the sample mount starting as above, Q1/LD is at the center of the pole middle (pointing out), Q2/ND at 0 degree, and Q3/TD (perpendicular to the paper in the instrument plot) is at -90 degree.

Currently the plotted pole figure is rotated about -90 degree from the measurement. You can adjust it back by using “rotation=0” in the VDRIVEPOLEP command. This can also be used to slightly adjust the offset of the rotation by specifying an angle in degree. When using “bina=1”, adjusting rotation with this keyword may produce error in area binning. You can tweak it to avoid it.

**New Texture pole figure instruction on VULCAN (beta)**

For data collected after 2021 Feb
1. load VDRIVE
   idl, @vdrivex

2. For a specific sample, find the first run with B1=0, B2=−90
   ![](image1)

3. Find the last run with B1=45, B2=−45
   ![](image2)

4. Holistic binning, fitting, pole data, processing and plotting.
   Texture, ipts=26807, runs=firstrun, rune=lastrun, runv=texturevanadiumrun,
   listd=[peakposition1, peakposition2,…], width=[width1, width2,…], /autopeak

   Note: number of elements in listd and width should be equal. They are initial estimate and
   autopeak will refine them spit out a peak data for vdrivespf. Check on the file to decide to
   continue the process or not.

   You can then play with vdrivepolep command to change the different parameters as the
   prior instruction.