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VDRIVE

Data Reduction and Interactive Visualization softwarE for Event Mode Neutron Diffraction

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VDRIVE-DATA REDUCTION AND INTERACTIVE VISUALIZATION SOFTWARE FOR EVENT MODE NEUTRON DIFFRACTION

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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

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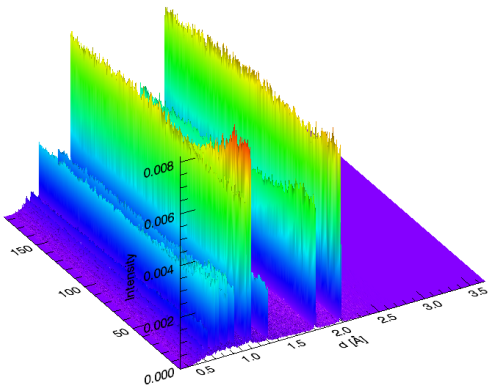

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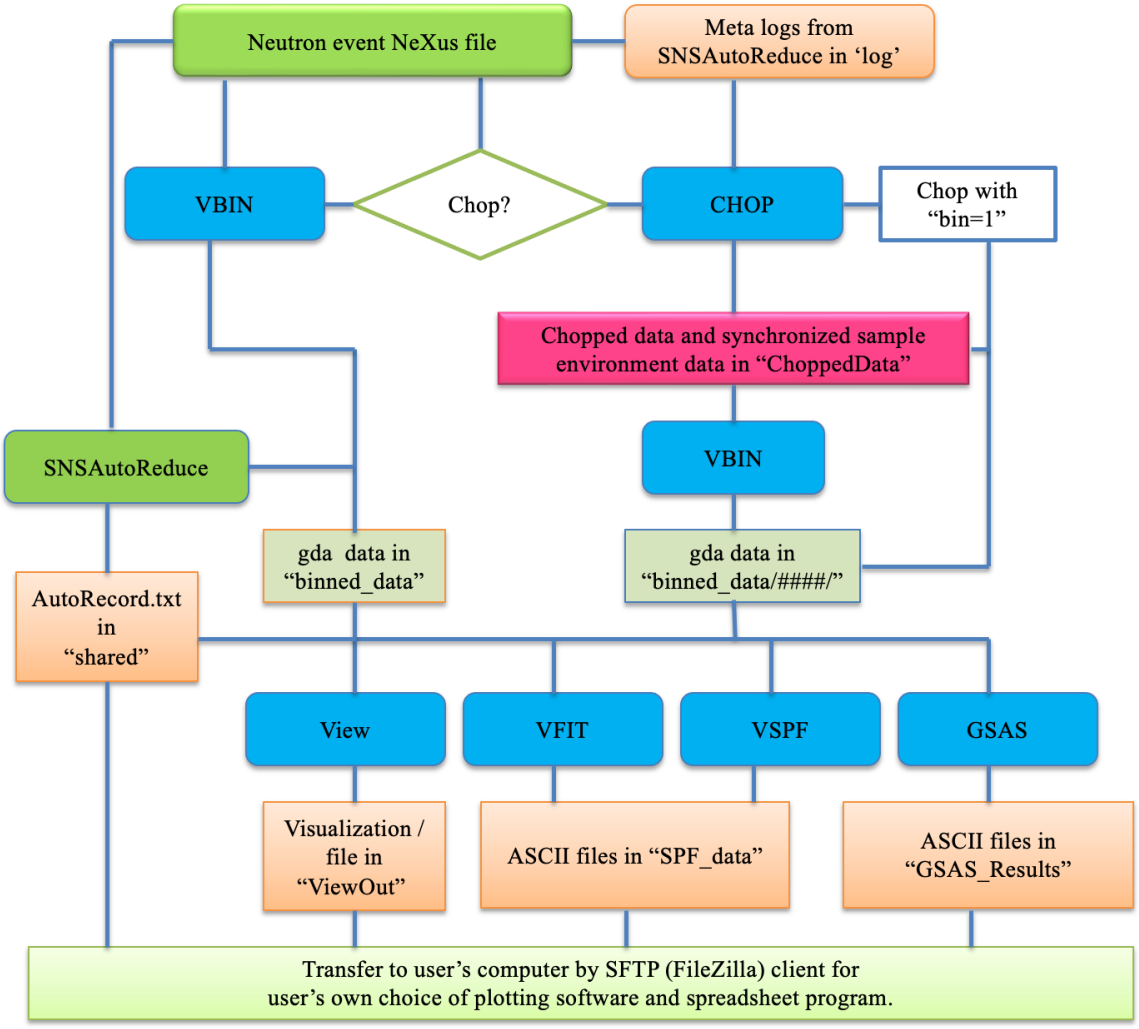

Figure 1 Simple flowchart of VDRIVE(X).

Note from the author:

The use of VDRIVE(X) commands in idl environment (think about python, or matlab etc.) is simple. It follows a uniform and simple grammar, i.e. command name, proposal number (IPTS), start run (runs), end run (rune), and plus some keywords if the default settings need to change. The VULCAN data storage structure is well defined on the analysis cluster, and by using the commands above VDRIVE(X) mainly requires user to provide measurements 'location' to be reduced or analyzed.

The VDRIVE commands evolve with the instrument 's upgrade including detectors, DAQ, new sample environments, and new measurement schemes, etc. New versions are introduced with major instrument upgrade. Some of the old keywords may obsolete without timely update in the manual. Let instrument team know if you have encountered any problem.

VDRIVE(X) 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 **@VDRIVEX** (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 and upgrade.

If your data is not automatically reduced or you want to rebin the data, use the bin command below. There is often a need of runv which is a pointer to the set of calibration files including the .prm and vanadium file under the 'Instrument' folder. Refer to instrument team for the instrument file or create one using CALI command.

Note: the software is living one because of instrument upgrades, and some of the keywords are obsoleted without being updated the manual, if you encounter any problem, let instrument team know.

Bin event 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 gda data 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, otherwise provide the full path.*

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'
vpeak, 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	Close all plots
OpenMeanlog, IPTS=12345, chopruns=1111	Open the chopped log
Openlog, IPTS=12345, runs=1000	Open the collected log
Setipts, IPTS=12345	Set the working IPTS
CurrentIPTS	Get the working IPTS
IPTSprm, IPTS=12345, runv=2000	Mark the runv in IPTS sys.

VDRIVEGUI mode is not updated or supported 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 (rune, '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:

VSPF, IPTS=1000, RUNS=3000, RUNE=4000 [, RUNR=1] , RUNV=2000 [,Autofix=1]
Automatically fit a number of peaks by using the autopeak keyword:
VSPF, IPTS=1000, RUNS=3000, RUNE=4000 [,RUNR=1], RUNV=2000, Autopeak=1, npeaks=5

Take a look at the fitting qualities from the PDF output file to see if you need to adjust the peak positions in the peak.txt file, or use UPDATEP=1 in **VSPF** command to update the peak position from previous fit.

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 runm=9999 (yes, it can be any number even not in the existing run list) as the source one (can be any existing one in the folder, but try to not use the number within your intended refinement list because it will be overwritten) and you have two phases in the data, so the data processing would be:

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

Follow the VDRIVEGSAS command details to prepare 9999_1.EXP
Perform the batch mode data refinement
GSAS, IPTS=1000, RUNS=3000, RUNE=4000, RUNM=9999, 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:
VSPF, IPTS=1000, CHOPRUN=3000, RUNS=1, RUNE=100, RUNR=1, RUNV=2000, Autopeak=1, npeaks=5

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:

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

Follow the VDRIVEGSAS command details to prepare 1_1.EXP
Perform the batch mode data refinement:
GSAS, IPTS=1000, CHOPRUNS=3000, RUNS=1, RUNE=100, RUNM=1, 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.

1.6 View the detector contour:

Pixel, IPTS=1000, RUNS=1, RUNV=2000

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

autoreduce /	auto reduced files from SNS data reduction routine.VULCAN user is recommended to use data in the binned_data folder below.
binned_data/	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 **VDRIVESPF** and **VDRIVEGSAS** may also store in this folder.
Pictures/Videos	Photos/Videos captured by the camera computer.
logs/	Sample environment files (loadframe, furnace and others).
Instrument/	Instrument parameter file (*.prm) and vanadium file (*-s.gda).
ChoppedData/	Chopped raw data by **VDRIVECHOP**. Raw data need to be reduced by running **VDRIVEBIN**, or selecting bin=1 when executing **VDRIVECHOP**, copies of synchronized sample environment files are also in this folder.
SPF_data/	Peak fitting data created by **VDRIVEFIT** and **VDRIVESPF**.
GSAS_Results/	GSAS refinement results created by **VDRIVEGSAS**.
Summed_GDA /	GSAS data merged over multiple runs created by **VDRIVESUMGSAS**.
ViewOut/	Folder for output files when using "vout=1" keyword in **VIEW**.
Auto-Peak/	Created folder for storing peak files created by using "autopeak" keyword in **VDRIVESPF**.
AutoRecord.txt	All Record file generated by auto reduction.
AutoRecordAlign.txt	Align Data (when title has prefix of 'Align:') Record file generated by auto reduction.
AutoRecordData.txt	Data Record file generated by auto reduction.

Result files created by VDRIVE

/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 VDRIVE 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 VDRIVE 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

VDriveSPF-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*)
VDriveSPF-1234-1-100-bk1.txt	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-1000-1999-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 VDRIVEChop[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 VDRVEchop command.

1234sampleenv_chopped_start.txt Starting values of synchronized sample environment data over the "dbin" time in VDRVEchop command.

1234sampleenv_chopped_end.txt Ending values of synchronized sample environment data over the “dbin” time in VDRVEchop command.

IPTS-1000-MTSLoadFrame-1234-header.txt The header information of the sample environment data by VDRVECHOP 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 VDRIVEChop[en].

1.gda Gsas data of all the banks. Number changes accordingly with sliced/collected run.

1234sampleenv_chopped_mean.txt Copy if averaged synchronized sample environment data over the “dbin” time in VDRVECHOP command.

1234sampleenv_chopped_start.txt Copy of starting values of synchronized sample environment data over the “dbin” time in VDRVEchop command.

1234sampleenv_chopped_end.txt Copy of ending values of synchronized sample environment data over the “dbin” time in VDRVEchop command.

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

Tof=d*DIFC+d^2*DIFA+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(X)

5.1 Load VDRIVE(X) in IDL

VDRIVE(X) is based on the IDL.

OS	License	OPEN	Type first	Then type
Linux	Yes	Terminal	**idl** or **idlde** (case sensitive)	**@VDRIVEX or vdrivex**
Linux	No	Terminal	**VDRIVEGUI (stop updating)**	
Linux	No	Application/data analysis	**VDRIVEGUI (stop updating**	

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:

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 into bank 1 histogram.
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.
Mytofbmax=1111	max tof bin in us
Mytofbmin=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

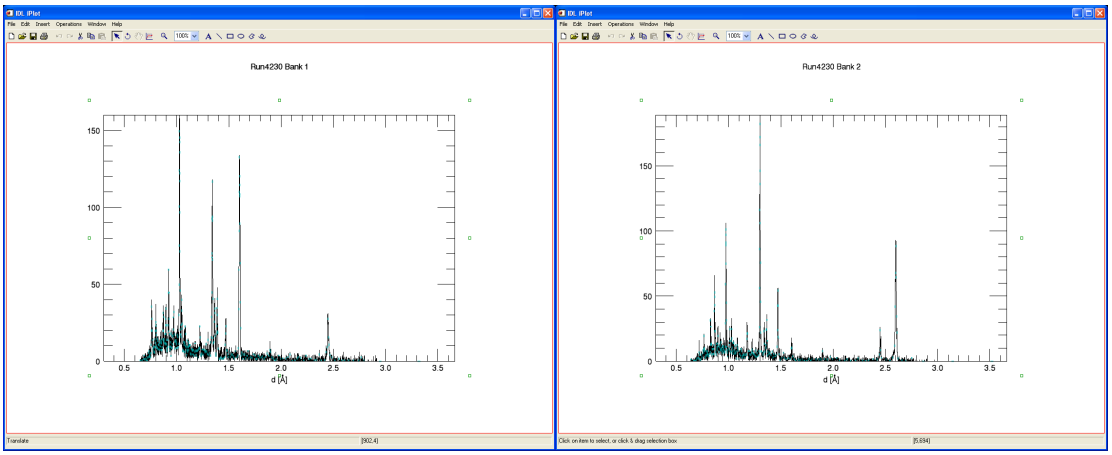

Figure 2 Raw histogram plots of GSAS pattern in the two banks.

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

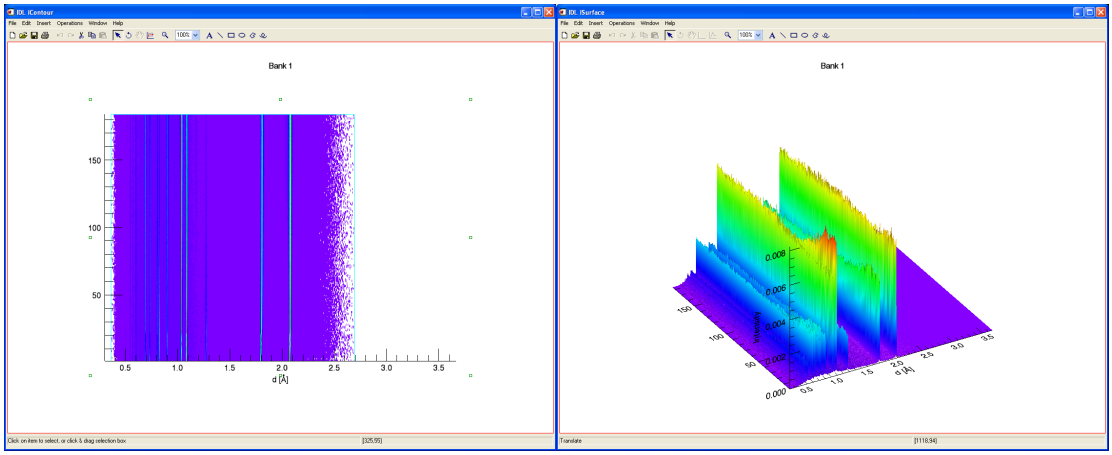

Figure 3 2D contour and 3D surface plots generated by VDRIVEVIEW.

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.
Q=1	Show x in Q.
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.
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:
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;

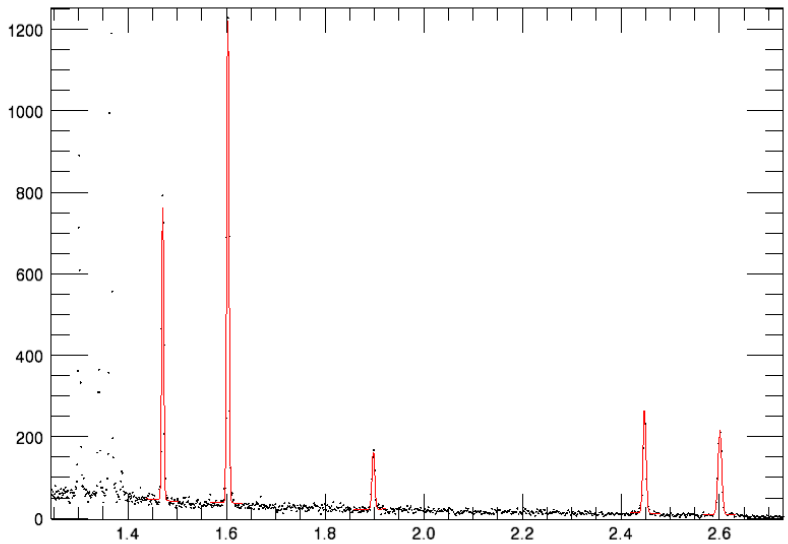

Figure 4 Plot of single peak fit in one pattern by VDRIVEFIT.

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.

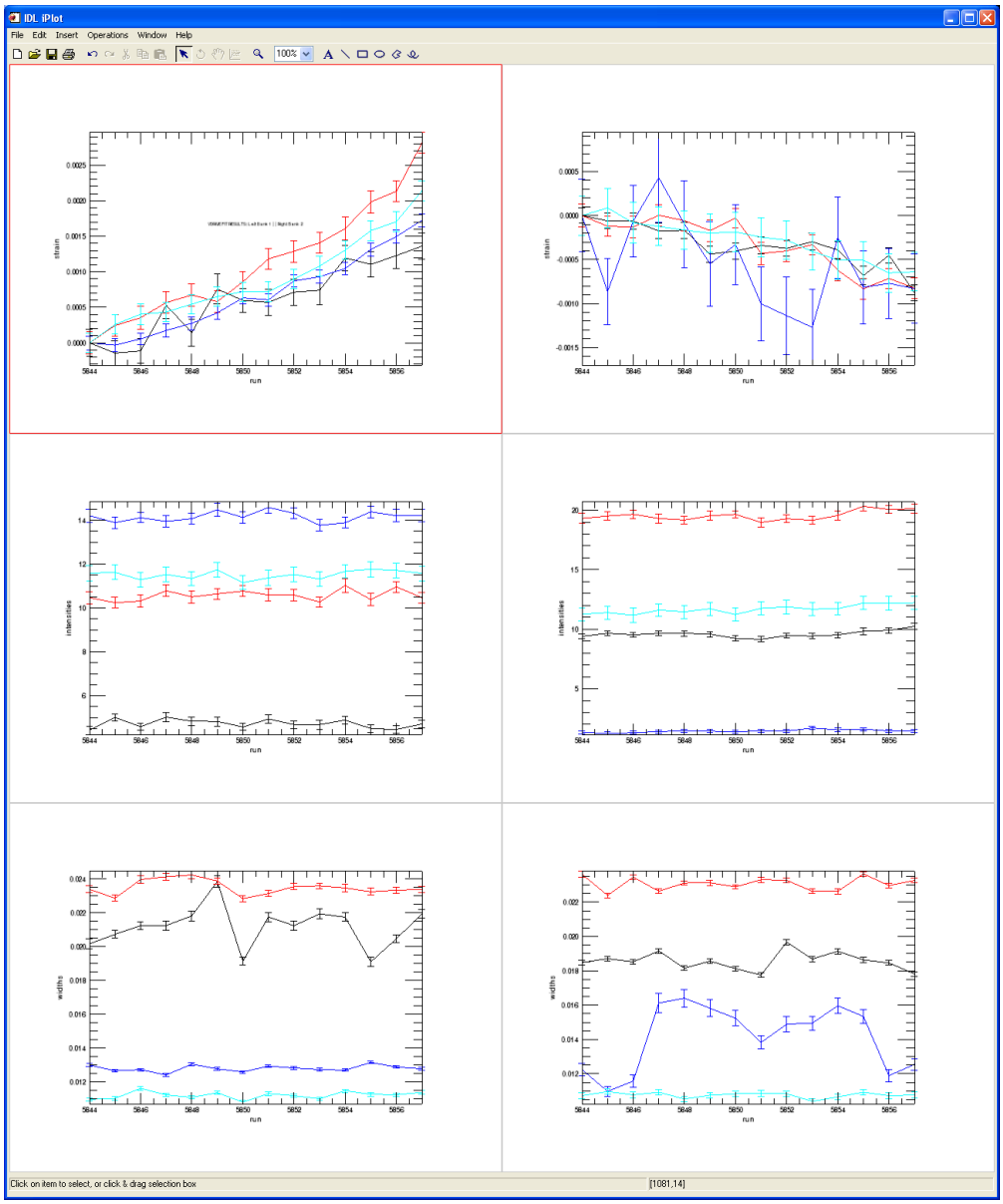

Figure 5 The fitting results from the VDRIVEFIT.

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.
Sho=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 /SNS/VULCAN/shared/Calibrationsfiles/Instrument/Standards/.

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

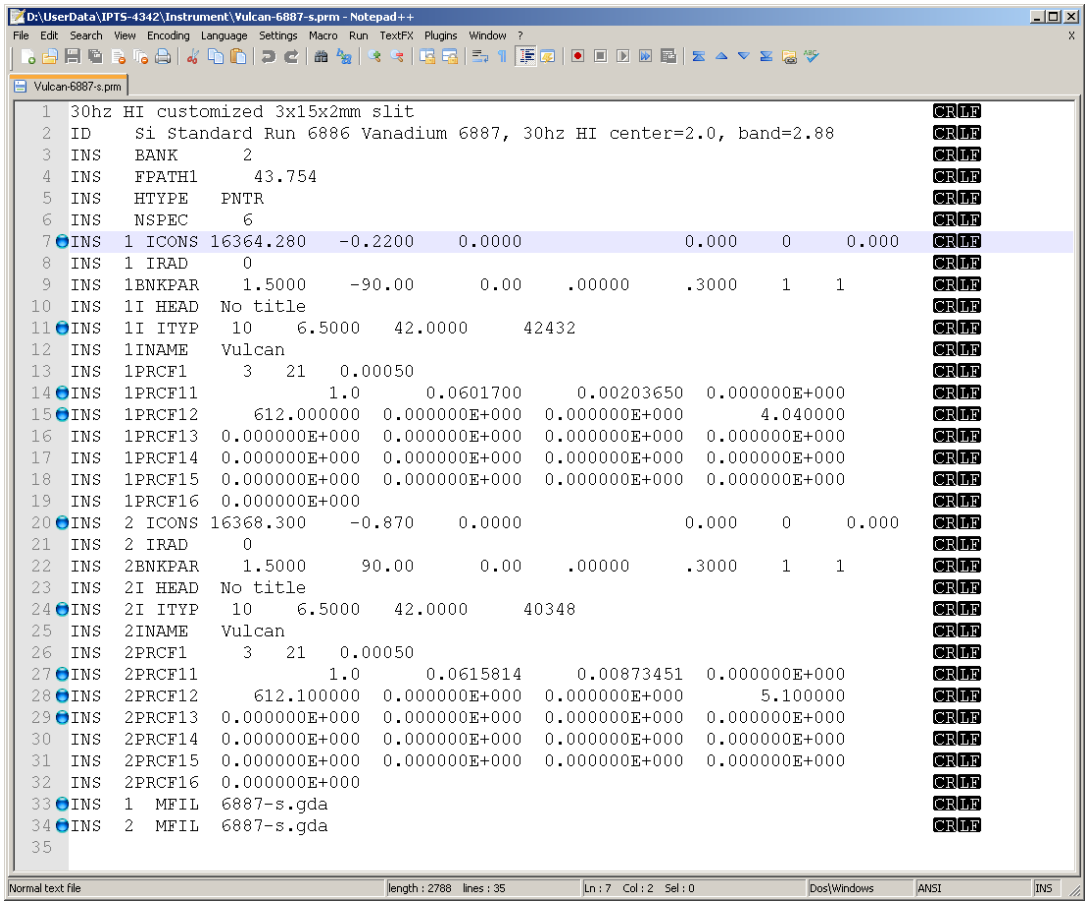

Figure 6 Example of the VULCAN GSAS prm file.

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 VDRIVESPF(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:

```
------------------------------------------------------------------
$bk     name  number              pos          range
1       110   1          2.02692       0.0300000

$1      310   1         0.906467       0.0250000

$2      110   1          2.02692       0.0300000

$2      200   1          1.43325       0.0300000

2       211   1          1.17024       0.0200000

$2      220   1          1.01346       0.0300000
------------------------------------------------------------------
```

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.
UpdataP=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.
Normalization=0	Not normalize to Vanadium file (with runv) for data already normalized by VDRIVEBIN.
AutoPeak=1	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" .
NPeaks=#	Specify number of peaks to search in Autopeak option.
AutoFix=1	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.

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).
VDriveSPF-2000-1-50-bk1.log	Refinement histories.

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=9999, BANK=1

For GSAS files from chopped data:
GSAS, IPTS=1000, CHOPRUN=2000, RUNS=1, RUNE=100, RUNM=9999, 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 9999, **VDRIVEGSAS** needs GSAS EXP files 9999_1.EXP and 9999_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='runlistfile.txt'	Fit runs in a text file, one run per line.
Title='Title'	Title for all GSAS refinement.
Samerunm=1	Use the same source runm for all GSAS refinement
Extractlist=1	Extract data from lst file only, use after manually refining individual runs.

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.
VDriveGSAS-2000-1-50-bk1.log	Refinement histories.

Create a source run for VDRVIEGSAS
Open Terminal
Type *expgui*
Direct to your "binned_folder" then type *####_1.EXP*,(#### can be any number even not exist in the current runlist, which is recommended) 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*.

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References

1. A.C. Larson and R.B. Von Dreele, "General Structure Analysis System (GSAS)", Los Alamos National Laboratory Report LAUR 86-748 (2000).
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.*

peak.txt

$bk	Pkid	Npk	pos	range
1	111B1	1	2.34	0.03
1	200B1	1	2.02	0.03
#1	220B1	1	1.43	0.03
#1	311B1	1	1.22	0.03
#1	222B1	1	1.16	0.03
#1	400B1	1	1.01	0.03
#1	331B1	1	0.93	0.025
#1	420B1	1	0.90	0.025
2	111B2	1	2.34	0.03
2	200B2	1	2.03	0.03
#2	220B2	1	1.43	0.03
#2	311B2	1	1.22	0.03
#2	222B2	1	1.16	0.03
#2	400B2	1	1.01	0.03
#2	331B2	1	0.93	0.025
#2	420B2	1	0.90	0.025
3	111B3	1	2.34	0.03
3	200B3	1	2.02	0.03
#1	220B1	1	1.43	0.03
#1	311B1	1	1.22	0.03
#1	222B1	1	1.16	0.03
#1	400B1	1	1.01	0.03
#1	331B1	1	0.93	0.025
#1	420B1	1	0.90	0.025

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 B1=0, B2=-90

187487	IPTS-25434	Sample 5	B1=0, B2=-90	b'
187488	IPTS-25434	Sample 5	B1=0, B2=-90	b'
187489	IPTS-25434	Sample 5	B1=0, B2=-90	b'

4 Find the last run with B1=45, B2=-45

187604	IPTS-25434	Sample 5	B1=45, B2=-45	l
187605	IPTS-25434	Sample 5	B1=45, B2=-45	l
187606	IPTS-25434	Sample 5	B1=45, B2=-45	l

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

```
IDL> vdrivebinen, ipts=25434, runs=187487, rune=187606, focus_ew=0
```

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

```
IDL> vspf, ipts=25434, runs=187487, rune=187606,runv=187154
```

Double check the fitting quality for peaks showing, and adjust the input peak values in the peak.txt file, 'update=1' is not recommended as in certain angle, for a strong textured sample, peaks would be missing.

7 Run VDRIVEPOLEP to process the data for pole figures

vdrivepolep, ipts=25434, runs=187487, rune=187606, involume=1, focus_ew=0 [,std4590=1]

The use of "involume=1" is when you have a thin and long bar measured. If the sample is large enough contains fully the 5x5x5mm^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.

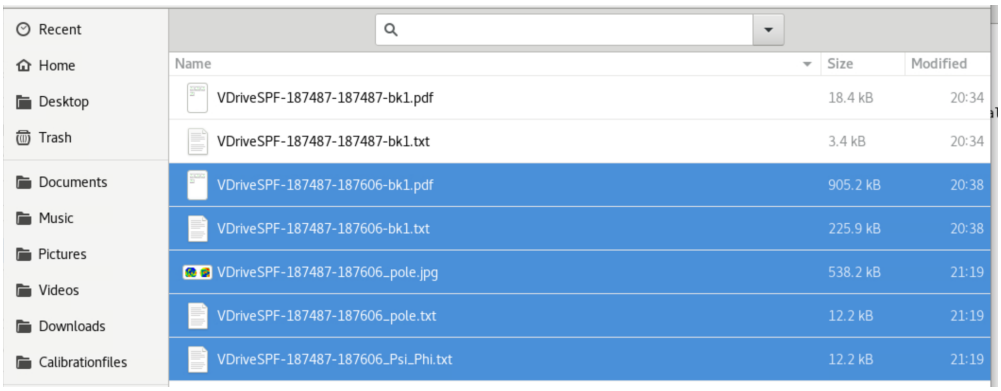
This command will simply output 120 records after coordinates transformation and intensity normalization. At this point the output data as measured can be plotted in plotting software.

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.

vderivepolep, ipts=25434, runs=187487, rune=187606, involume=1, focus_ew=0, bina=1 [,std4590=1]

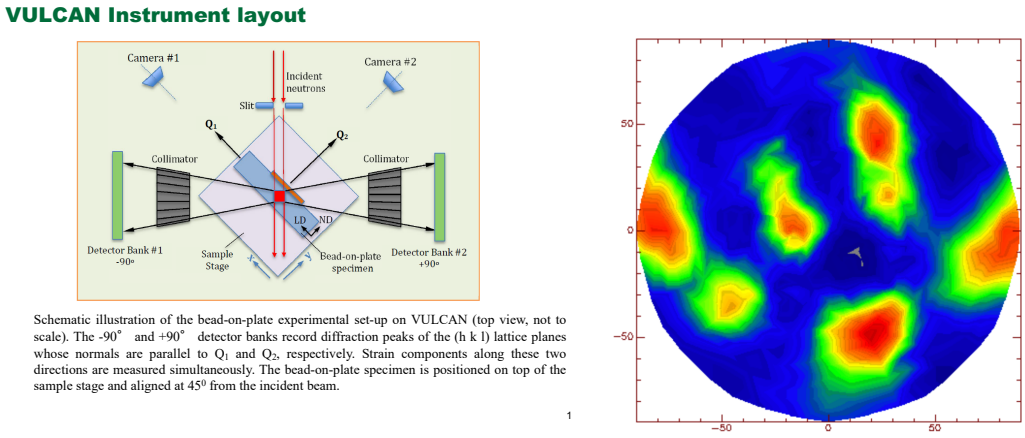
Finally, the file outputs are

```
pole data is saved in: /SNS/VULCAN/IPTS-25434/shared/SPF_data/VDriveSPF-187487-187606_pole.txt
Sample Psi and Phi data is saved in: /SNS/VULCAN/IPTS-25434/shared/SPF_data/VDriveSPF-187487-187606_Psi_Phi.txt
a copy of the pole jpg is saved in: /SNS/VULCAN/IPTS-25434/shared/SPF_data/VDriveSPF-187487-187606_pole.jpg
```



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.



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

187487	IPTS-25434	Sample 5	B1=0, B2=-90	b'
187488	IPTS-25434	Sample 5	B1=0, B2=-90	b'
187489	IPTS-25434	Sample 5	B1=0, B2=-90	b'

3 Find the last run with B1=45, B2=-45

187604	IPTS-25434	Sample 5	B1=45, B2=-45	
187605	IPTS-25434	Sample 5	B1=45, B2=-45	
187606	IPTS-25434	Sample 5	B1=45, B2=-45	

4.Holistic binning, fitting, pole data, processing and plotting.

Texture, ipts=26807, runs=firstrun, rune=lastrun, runv=texturevanadiumrun, listd=[peakposition1, peakposition2,…], width=[width1, widht2,…], /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.