

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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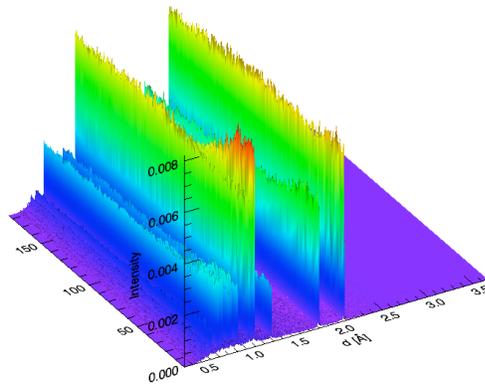
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1 Flowchart and cheat sheet

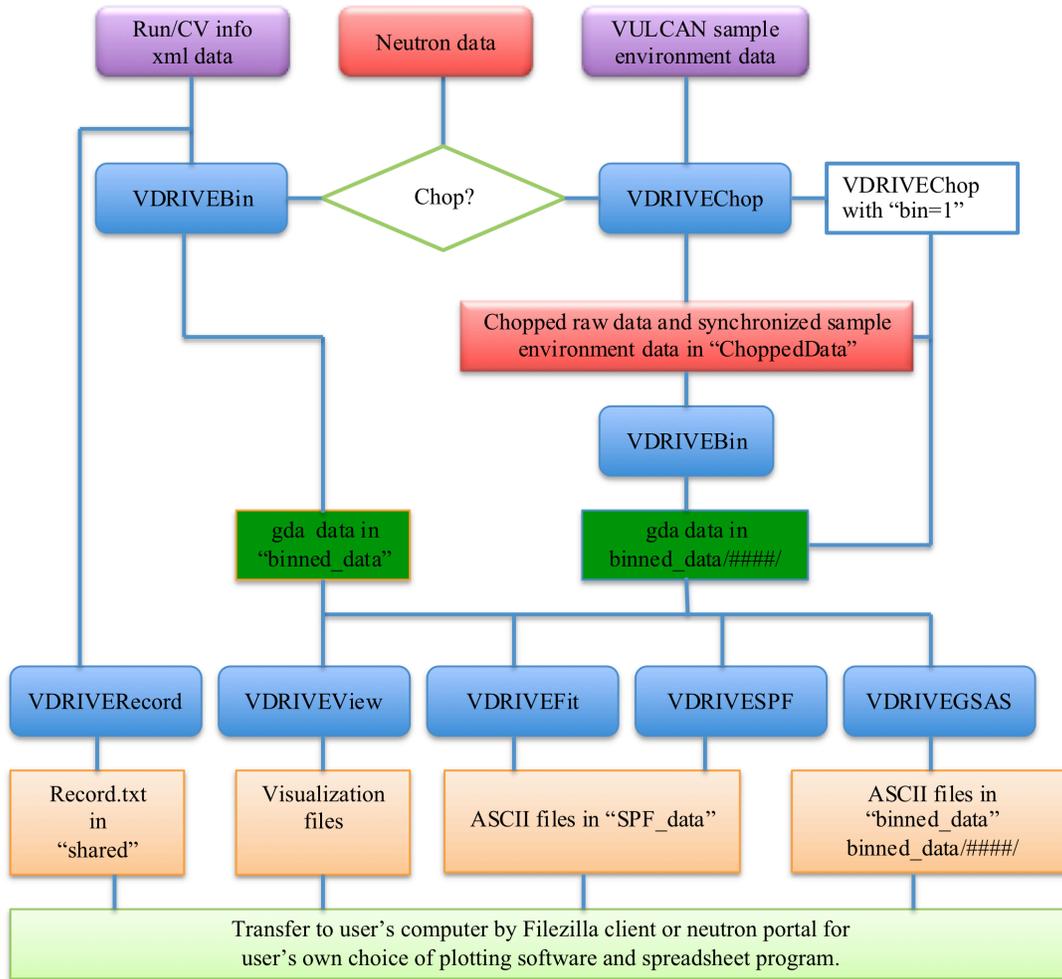


Figure 1 Flowchart of VDRIVE.

VDRIVE cheat sheet

Command line mode (requires IDL license on SNS server):

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**, type **idl** or **idld**, then type **@VDRIVE** (case sensitive for these commands).

Summarize, bin and view the record in one IPTS: (short name: **VLOG**)

VDRIVERecord, IPTS=####

Chop, synchronize, and bin continuously collected data: (short name: **CHOP**)

VDRIVECHOP, IPTS=####, RUNS=####, DBIN=####, BIN=1, Loadframe=1 [Furnace=1]

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

VDRIVEBIN, IPTS=####, RUNS=####, RUNE=#### [, RUNV=####, CHOPRUN=####] [,ONEBANK=1]

Note: using runv will normalize the gsas data with given instrument spectrum measured with vanadium, and use this for VDRIVESPF data analysis.

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

VDRIVEVIEW, IPTS=####, RUNS=#### [,CHOPRUN=####, RUNV=####, PCSENV=1]

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

VDRIVEVIEW, IPTS=####, RUNS=####, RUNE=#### [,CHOPRUN=####] [, MinV=#.#, MaxV=#.#, RUNV=####, NORM=1 , PCSENV=1]

Conduct Gaussian single peak fit: (short name: **VFIT**)

VDRIVEFIT, IPTS=####, RUNS=####, RUNE=#### [,CHOPRUN=####], LISTD=[#.#, #.#...], WIDTH=[#.#, #.#...], [RUNR=####], [PCSENV=1, NORM=1]

Conduct GSAS single peak fit: (short name: **VSPF**)

VDRIVESPF, IPTS=####, RUNS=####, RUNE=#### [,CHOPRUN=####], [RUNR=####], [RUNV=####], [PCSENV=1], [NORM=1]

Note: peak id file should be saved as peak.txt as the default in the binned folder.

Conduct GSAS Rietveld refinement: (short name: **GSAS**)

VDRIVEGSAS, IPTS=####, RUNS=####, RUNE=#### [,CHOPRUN=####], RUNM=#### [,BANK=[1,2]]

Generate instrument parameter and instrument spectrum files (short name **VBIN**):

VDRIVEBIN, RUNS=####, IPTS=####, TAG='V'[,ONEBANK=1]

VPEAK, IPTS=#### , RUNV=#### [,ONEBANK=1]

VDRIVEPRM, IPTS=####, RUNV=####, FREQ= 30 (60 OR 20) [,ONEBANK=1]

Generate instrument calibration files: (short name: **CALI**)

VDRIVECALI, IPTS=4744, RUNP=####, RUNV=####, TAG='Si', FREQ=20 [,ONEBANK=1]

VDRIVEGUI mode (no IDL license required):

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 Computer access

What you need:

1 XCAMS account, the same one that you used in the IPTS system. If you do not have one follow this link to get one. (<http://neutronsr.us>).

2 Request access to computer resources (<https://neutronsr.us/accounts/request.html>) select, SNS user (on-site and off-site), then select VULCAN, finally type your IPTS number in the justification.

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

3 VULCAN Data

3.1 VULCAN data folder structure

Analyzed data are stored in a shared folder that all team members have the access. If you want to use VDRIVE offline, please keep the data structure of the 'shared' folder.

[/SNS/VULCAN/IPTS-1234/shared/](#)

Under this folder you may find standard folders like below

| | |
|------------------------------|---|
| binned_data/ | GSAS file folder by created by 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. |
| Instrument/ | Instrument parameter file (*.prm) and vanadium file (*-s.gda). |
| Logs/ | Sample environment files (loadframe, furnace and others). |
| SPF_data/ | Peak fitting data created by VDRIVEFIT and VDRIVESPF . |
| Photos/ | Photos captured by the camera computer. |
| 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. |
| Record.txt | Record file generated by VDRIVERECORD . |

GSAS files are in ASCII format with three columns for each bank, and both banks data are saved in one files 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:

$$\text{Tof} = d * \text{DIFC} + d^2 * \text{DIFA} + \text{ZERO}$$

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 runnumber, proton charge (for normalization by using **pcsensv=1** keyword), and synchronized columns from sample environment files.

3.2 Instrument files location

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

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

3.3 Download/upload your data

After reduction/analysis, go to <http://neutronsr.us/portal/> and log in the portal and select the folder above and then download/upload.

A fast way is to 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.

3.4 VDRIVE offline (beta)

VDRIVE visualization and data analysis subroutines can be used offline on a pc given the same folder scheme and proper installation of other party's software. Now VDRIVE offline supports VDRIVEVIEW, VDRIVEFT, VDRIVESPF, VDRIVEGSAS. However, VDRIVERECORD, VDRIVEChop, VDRIVEBin and VDRIVECali data reduction routines are not recommended due to the raw and large data format of neutron data. Several configurations and a few of programs are needed to the successful execution of VDRIVE.

On a Windows PC:

Software requirements

VDRIVEGUI.sav, download it from /SNS/VULCAN/shared/
IDL, www.exelisvis.com/idl/ (no license needed for VDRIVEGUI)

GSAS, www.ccp14.ac.uk/solution/gsas/

MikTex, <http://miktex.org>

GhostScript, <http://www.ghostscript.com/download/>

Adobe PDF Reader and MS Excel.

Folder settings

Folder paths of GSAS, MikTex, and GhostScript need manually to be set as environment paths.

Download the IPTS "shared" folder GSAS data from the analysis computer, e.g. 'c:\myvulcandata\shared'.

Execution:

Open VDRIVEGUI.sav by IDL.

Add the keyword: **UserDataDir='c:\myvulcandata\shared'** in each of the commands.

Although VDRIVE is available offline, it is recommended to use the Linux version due to the dependency of the programs settings above.

On Mac (to be constructed)

4 Data reduction, visualization and analysis with VDRIVE

4.1 Load VDRIVE in IDL

VDRIVE is based on the IDL.

| OS | License | OPEN | Type first | Then type |
|-------|---------|---------------------------|---|---------------------------------|
| Linux | Yes | Terminal | idl or idlde (case sensitive) | @VDRIVE (case sensitive) |
| Linux | No | Terminal | VDRIVEGUI | |
| Linux | No | Application/data analysis | VDRIVEGUI | |

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"

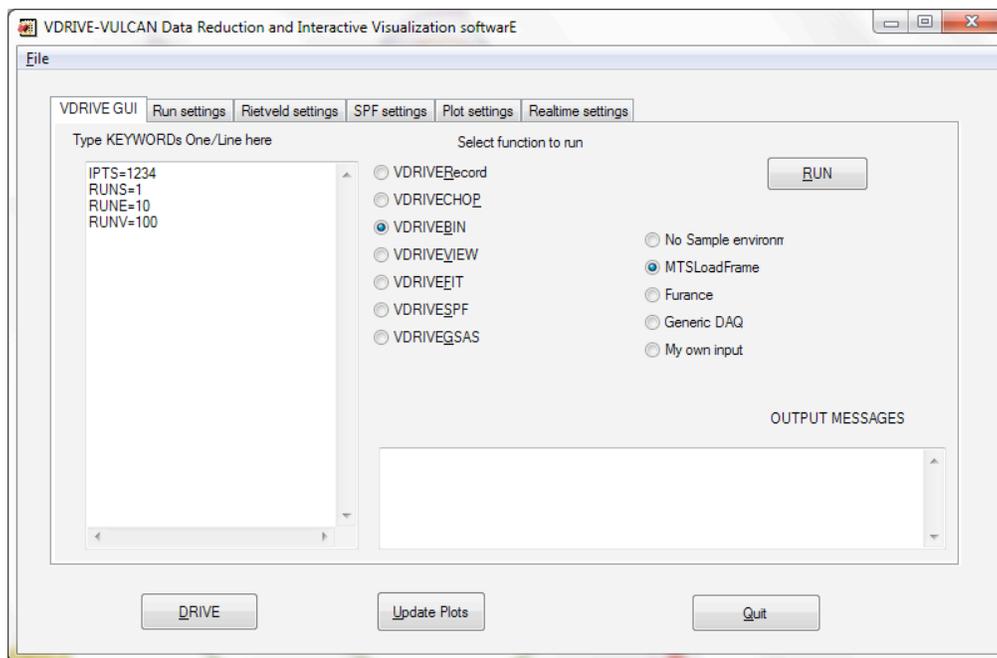


Figure 2 VDRIVE interface

4.2 Data Reduction and Analysis Commands

4.2.1 VDRIVERECORD

Purpose: Extract run info and bin data with the default **VDRIVEBIN** configuration.

Common use:

VDRIVERECORD, IPTS=1000

The information of each run will be extracted from the xml file and stored in a text file [/SNS/VULCAN/IPTS-1000/shared/Record.txt](#). New data will be binned if not done before. At the end of the execution **Record.txt** file will be opened. It is also an easy way to locate the record file.

Additional keywords:

| | |
|---------------------------------|--|
| Runs=#### | Start run. |
| Rune=#### | End run. |
| RecFile='/path/file.txt' | Output records in a customized file.txt file under /path. |
| Prm='prmfile.prm' | Replace the Vulcan.prm comment line with the prmfile.prm in GSAS files when NoBin=1 is not engaged. |
| NoBin=1 | Omit binning the data. |
| NoShow=1 | Omit showing the file at the end. |
| Name='name' | With Value keyword. |
| Value=Value | With Name extract a specific variable values to the 'Value' array in current IDL workspace. |

Other keywords taken by **VDRIVEBIN**.

4.2.2 VDRIVECHOP

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

Common use:

VDRIVECHOP, IPTS=1000, RUNS=2000, dbin=60, loadframe=1, bin=1

where, **dbin** is the chop step size in seconds; **loadframe**, is set when VULCAN loadframe is used for continuous loading experiment; **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:

VDRIVECHOP, IPTS=1000, RUNS=2000, pickdata="/SNS/VULCAN/IPTS-1000/shared/picktime.txt", bin=1, loadframe=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):

```
-----
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. |
| te=###.## | End time (s) to bin. |
| 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. |
| Stroke=1 | Set stroboscopy on. |
| GSAS=1 | Plot GSAS file after binning. |
| Onelog=1 | Read sample environment parameters from one log file. |
| 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**.

4.2.3 VDRIVEMERGE

Purpose: Combine collected data. Data are combined from the runs of rest columns to the runs of the first column in the runfile.txt.

Common use:

VDRIVEMERGE, 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

4.2.4 VDRIVEBIN

Purpose: Bin collected data or chopped data by **VDRIVECHOP** to GSAS files.

Common use:

For typical mapping experiments or single run:

VDRIVEBIN, IPTS=1000, RUNS=2000, RUNE=2099

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

For chopped files created by VDRIVECHOP:

VDRIVEBIN, 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

SKIPXML=1

FOCUS_EW=0

RUNV=5000

IParm='prmfile.prm'

FullProf=1

NoGSAS=1

PlotFlag=1

OneBank=1

NoMask=1

Tag='Si'

Focus_tof=1

BinFolder='/folder'

The logarithm bin step size of TOF and its default is 0.001.

Some parameters from xml file will be written in the GSAS files as comments, which are convenient for using **SmartsRunRep** in **SMARTSWare**.

For 6-module data binning.

Normalize data over smoothed vanadium file in **/Instrument** folder, and used for **VDRIVESPF** when normalized intensity is an output option.

Replace the **Vulcan.prm** in comment line with the customized **prmfile.prm** string in GSAS files.

Output FullProf files.

Omit GSAS files.

Plot histogram after binning.

Bin banks data to one histogram.

Bin bad pixels too.

Bin a Si calibration powder. If 'CeO2' is chosen, bin a CeO2 calibration powder. If 'V' is chosen, bin a vanadium data.

Omit time focusing.

Bin data to a specific folder.

Other variations:

VDRIVEBINP

Purpose: Bin histograms with bundled pixels. e.g. for application of single crystal patterns.

Common use:

VDRIVEBINP, IPTS=1000, RUNS=1, RUNE=100, PBinsize=8

where, **PBinsize** is the number of pixels to be bundled/binned into one histogram, and the default is 8, which means every 8 vertical pixels of each VULCAN detector module will be binned into

one histogram, thus creating 154 GSAS files for each module. Therefore it will generate lots of GSAS files.

*Note: Data is not time-focused when using **VDRIVEBINP**.*

VDRIVEBINH

Purpose: Bin 154 horizontal pixels into one individual histogram, so 7 histograms for each module, and total 42 histograms for 1 chopped data. All data will be saved as 42-bank spectrum (time focused) in one GSAS file.

VDRIVEBINV

Purpose: Bin 8 vertical pixels into 1 histogram, 154 histograms for each module, 154*6 GSAS files same as for **VDRIVEBINP** when **PBinsize=8**. However each GSAS file is time focused.

4.2.5 VDRIVEVIEW

Purpose: Visualize data in 2D, 3D plots.

Common use:

To view one GSAS pattern:

VDRIVEVIEW, IPTS=1000, RUNS=1, plot=1

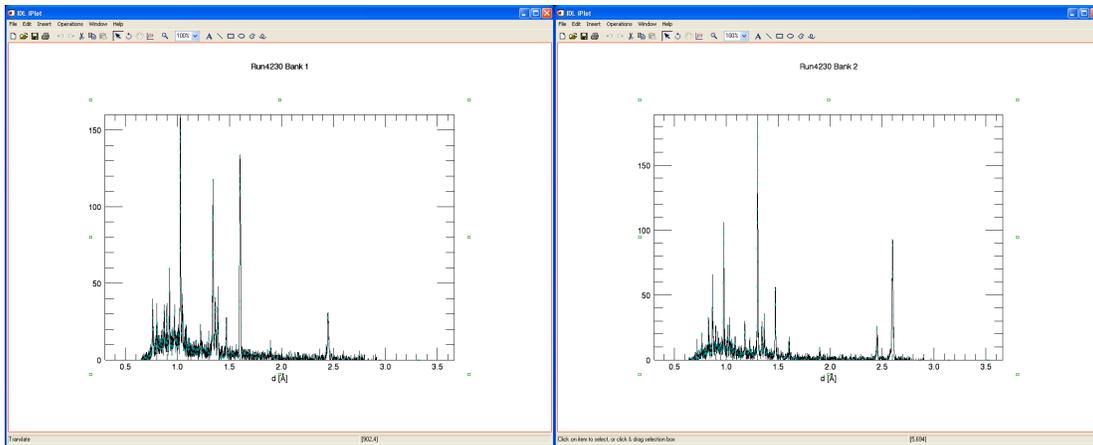


Figure 3 Raw histogram plots of GSAS pattern in the two banks.

To view sequential GSAS patterns in 2D and 3D:

VDRIVEVIEW, IPTS=1000, RUNS=1, RUNE=50

To view sequential GSAS patterns of chopped data in 2D and 3D:

VDRIVEVIEW, IPTS=1000, CHOPRUN=2000, RUNS=1, RUNE=50

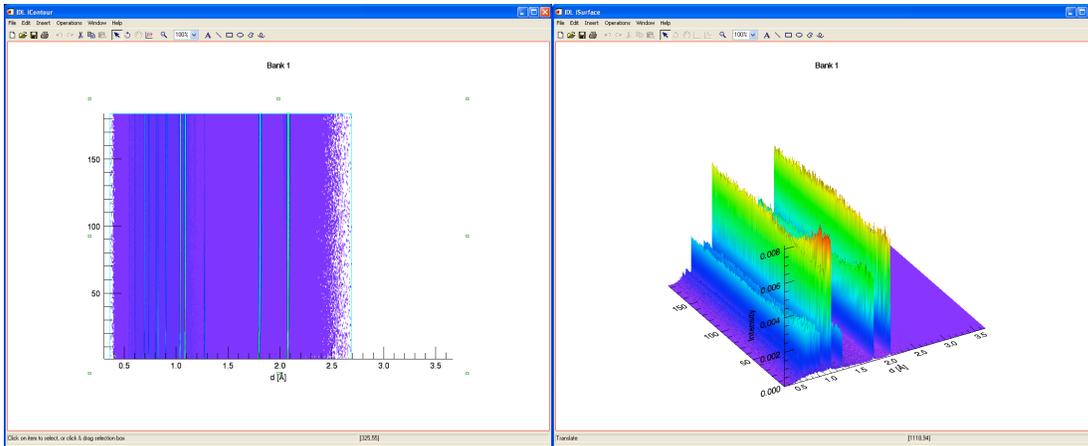


Figure 4 2D contour and 3D surface plots generated by VDRIVEVIEW.

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 proton charge from xml file 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**.

XML=1

When **Position='varialbe_name'** is set, show the value of the variable from xml file in the vertical axes.

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.

4.2.6 VDRIVEFIT

Purpose: Gaussian single peak fit and results visualization.

Common use:

For one GSAS pattern fit:

VDRIVEFIT, 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;

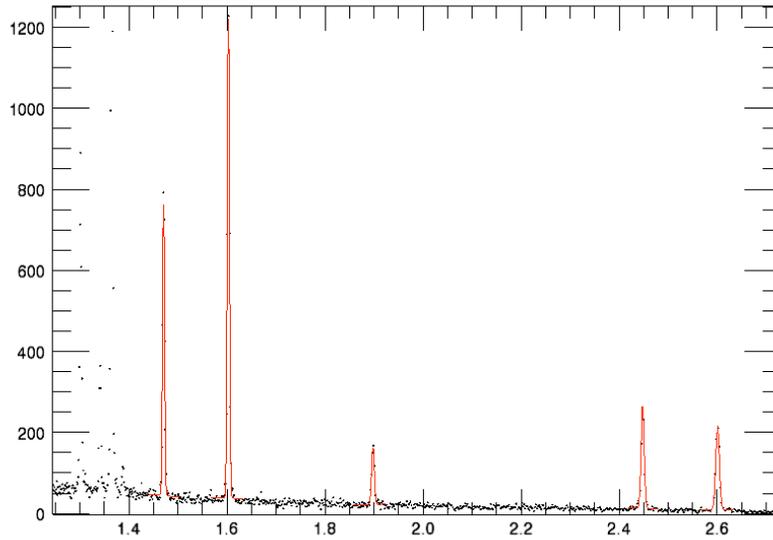


Figure 5 Plot of single peak fit in one pattern by VDRIVEFIT.

For sequential GSAS patterns fit:

VDRIVEFIT, 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

VDRIVEFIT, 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.

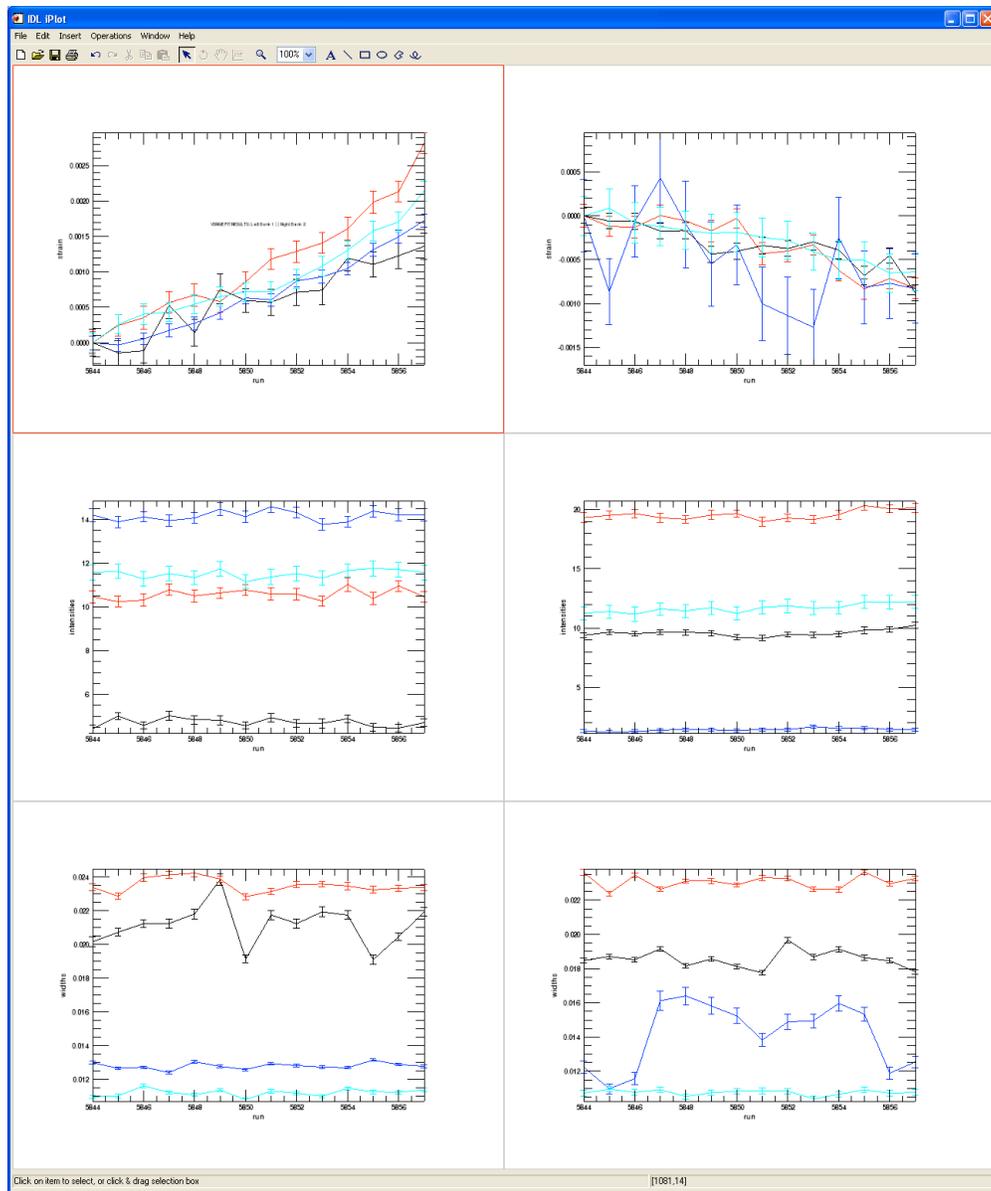


Figure 6 The fitting results from the VDRIVEFIT.

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. |

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.

4.2.7 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. |

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 Data Analysis with GSAS

5.1 Instrument files preparation

5.1.1 VULCAN instrument parameter file for GSAS

```
D:\UserData\IPITS-4342\Instrument\Vulcan-6887-s.prm - Notepad++
File Edit Search View Encoding Language Settings Macro Run TextFX Plugins Window ?
Vulcan-6887-s.prm
1 30hz HI customized 3x15x2mm slit
2 ID Si Standard Run 6886 Vanadium 6887, 30hz HI center=2.0, band=2.88
3 INS BANK 2
4 INS FPATH1 43.754
5 INS HTYPE PNTR
6 INS NSPEC 6
7 INS 1 ICONE 16364.280 -0.2200 0.0000 0.000 0 0.000
8 INS 1 IRAD 0
9 INS 1BNKPAR 1.5000 -90.00 0.00 .00000 .3000 1 1
10 INS 1I HEAD No title
11 INS 1I ITYP 10 6.5000 42.0000 42432
12 INS 1INAME Vulcan
13 INS 1PRCF1 3 21 0.00050
14 INS 1PRCF11 1.0 0.0601700 0.00203650 0.000000E+000
15 INS 1PRCF12 612.000000 0.000000E+000 0.000000E+000 4.040000
16 INS 1PRCF13 0.000000E+000 0.000000E+000 0.000000E+000 0.000000E+000
17 INS 1PRCF14 0.000000E+000 0.000000E+000 0.000000E+000 0.000000E+000
18 INS 1PRCF15 0.000000E+000 0.000000E+000 0.000000E+000 0.000000E+000
19 INS 1PRCF16 0.000000E+000
20 INS 2 ICONE 16368.300 -0.870 0.0000 0.000 0 0.000
21 INS 2 IRAD 0
22 INS 2BNKPAR 1.5000 90.00 0.00 .00000 .3000 1 1
23 INS 2I HEAD No title
24 INS 2I ITYP 10 6.5000 42.0000 40348
25 INS 2INAME Vulcan
26 INS 2PRCF1 3 21 0.00050
27 INS 2PRCF11 1.0 0.0615814 0.00873451 0.000000E+000
28 INS 2PRCF12 612.100000 0.000000E+000 0.000000E+000 5.100000
29 INS 2PRCF13 0.000000E+000 0.000000E+000 0.000000E+000 0.000000E+000
30 INS 2PRCF14 0.000000E+000 0.000000E+000 0.000000E+000 0.000000E+000
31 INS 2PRCF15 0.000000E+000 0.000000E+000 0.000000E+000 0.000000E+000
32 INS 2PRCF16 0.000000E+000
33 INS 1 MFIL 6887-s.gda
34 INS 2 MFIL 6887-s.gda
35
Normal text file length: 2788 lines: 35 Ln: 7 Col: 2 Sel: 0 Dos/Windows ANSI INS
```

Figure 7 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.

5.1.2 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.

5.1.3 VDRIVECALI

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

Common use:

[VDRIVECALI, 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.

5.1.4 VDRIVEPRM

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

Common use:

[VDRIVEPRM, 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](#).

5.2 VDRIVESPF

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

Common use:

For typical mapping experiments:

[VDRIVESPF, IPTS=1000, RUNS=1, RUNE=100, RUNR=1, RUNV=5000\[, Normalize=1\]](#)

For sequential GSAS files of chopped run:

VDRIVESPF, 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:

```
-----  
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=1 | Normalize to Vanadium file (with runv). |

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.

5.3 VDRIVEGSAS

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

Common use:

For typical runs:

VDRIVEGSAS, IPTS=1000, RUNS=1, RUNE=100, RUNM=1, BANK=1

For GSAS files from chopped data:

VDRIVEGSAS, 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.
- 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, 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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