

Convert the GDA format to XYE format

A reduced GDA file at Vulcan contains the raw time-of-flight neutron diffraction histograms from all detector banks. The GDA format is compatible for GSAS etc.

This tip shows a quick way to normalize the raw histogram to the measured incident spectrum (by flooding on vanadium), and to save the data in XYE format as separate files for individual banks. The XYE format is compatible for TOPAS etc.

Command 1:

gsas2topas [IPTS]

It will convert all auto-reduced GDA files in the proposal number [IPTS] to XYE files. The output files are saved under /SNS/VULCAN/IPTS-[IPTS]/shared/binned_data/topas/

Command 2:

gsas2topas [IPTS] [choprun]

It will convert all GDA files in the chopped run [choprun] in the proposal number [IPTS] to XYE files (see VDRIVE manual for data chopping). The output files are saved under /SNS/VULCAN/IPTS-[IPTS]/shared/binned_data/[choprun]/topas/

Example 1: In IPTS-24680, convert all runs (from 13579 to 13600, see AutoRecord.txt for the runs summary), using vanadium file 77777-s.gda (it is found under /SNS/VULCAN/IPTS-24680/shared/Instrument/).

(a) In a terminal, use IDL to reduce the data.

```
File Edit View Search Terminal Help
[ @analysis-node17 ~]$ idl
IDL Version 8.5.1 (linux x86_64 m64). (c) 2015, Exelis Visual In
Installation number: 222151.
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IDL> @VDRIVEX
IDL> vbin, ipts=24680, runs=13579, rune=13600, runv=77777
```

(b) Open another terminal, run Command 1.

```
File Edit View Search Terminal Help
[ @analysis-node17 ~]$ gsas2topas 24680
```

The output files are saved at /SNS/VULCAN/IPTS-24680/shared/binned_data/topas/.

Example 2: In IPTS-24680, chop the run 13579 with 120 seconds time bin, which will result in 87 files, and then convert all those 87 runs (from 1 to 87) using vanadium file 77777-s.gda (it is found under /SNS/VULCAN/IPTS-24680/shared/Instrument/).

(a) In a terminal, use IDL to chop the data. (see VDRIVE manual for details)

```
File Edit View Search Terminal Help
[ @analysis-node17 ~]$ idl
IDL Version 8.5.1 (linux x86_64 m64). (c) 2015, Exelis Visual Informati
Installation number: 222151.
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IDL> @VDRIVEX
IDL> chop, ipts=24680, runs=13579, runv=77777, dbin=120
```

(b) Open another terminal, run Command 2.

```
File Edit View Search Terminal Help
[ @analysis-node17 ~]$ gsas2topas 24680 13579
```

The output files are saved at /SNS/VULCAN/IPTS-24680/shared/binned_data/13579/topas/.

The diffraction pattern of a standard Si powder for the conversion from time-of-flight to d-spacing is provided per user's request.