Using SPEC at MHATT-CAT: Starting up, local macros, etc.

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Abstract

All SPEC installations are more or less customized. This document, currently a work in progress, lists some of the things that are specific to the SPEC installation at MHATT-CAT, Sector 7 of the Advanced Photon Source. This is not meant to be a comprehensive manual or helpfile. The online manual at http://www.certif.com and the command-line help utility are good sources of information for the standard macros and things of SPEC. This document should not be distributed beyond Sector 7.

So far this is extremely incomplete!

Starting SPEC at MHATT-CAT

Unlike epics, SPEC is a proprietary program. For a given license, only one SPEC process can be running at a given time, which, at MHATT-CAT, must be on the computer named bantu. Therefore, if you are not typing on a bantu terminal already, you must log in with a command like:

```
ssh -X bantu
```

Once on bantu, you must start the appropriate version of SPEC according to which geometry of which diffractometer you are using. The choices are:

`fourc`
: This geometry operates the Newport kappa in 7ID-C as a four-circle kappa diffractometer. The mu and nu motors must be at their zero positions. (In the latest versions of SPEC, "kappa" geometry is merely an option in fourc geometry.)

`psic`
: This geometry operates the Newport kappa in 7ID-C with all six axes. (The "psic" and "sixc" geometries of SPEC happen to be slightly different.)

`fourcD`
: This geometry operates the four-circle Huber in 7ID-D as a four-circle Eulerian diffractometer. Limit switches are not yet installed so you must be very careful when operating.

`fourcH`
: This geometry operates the six-circle Huber (momentarily stored in 7ID-B) as a four-circle diffractometer. The mu and nu axes must be at their zero positions.

`psicH`
: This geometry operates the six-circle Huber (momentarily stored in 7ID-B) with all six axes.

The basic SPEC commands

SPEC is a command-line based program. Therefore it is important to know the correct commands; fortunately, some commands will list the type of parameters needed if you enter the wrong type (or number) of parameters. Actually, most "commands" (and many variables) are actually macros and could be redefined. The writing and implementation of new macros is quite straightforward; users often write shortcut macros which are combinations of a number of commands. It is also important to note that SPEC is case-sensitive; most commands and variable names are lower-case, while certain special variables and macros are upper-case.

"Information" commands and shortcuts

`pplot`
: send the most recent scan (using cplot) to the printer with a linear y axis.

`lpplot`
: send the most recent scan (using cplot) to the printer with a logarithmic y axis.

`wu`
: where users; lists positions of all the SPEC motors in user units only, it's slightly different than the ESRF version of this macro.

`wh`
: this was redefined to show the real motors for kappa geometries as well as the pseudomotors.

`sor`
: same as `or_swap`

`ksync`
: this is a shortcut for pressing the "No encoders" button on each of the kappa motors' EPICS debug screens. It forces EPICS to update itself to the Newport MM4000 controller. (While the kappa motors do have encoders, they are not controlled by EPICS so this scheme is OK.)

`k_tab_disable`
: this is a shortcut for pressing the "Disable motor" button for the five motors of the kappa table (Y1, Y2, Y3, Xtrans, and RotAY). This should prevent the table from being accidentally moved and misaligned.

`k_tab_enable`
: this is a shortcut for pressing the "Enable motor" button for the five motors of the kappa table.

Setting things and moving things

the energy macros:
: `getE`: sets the wavelength (`LAMBDA`) based on the value of the high heatload mono's position
`moveE` *energy_in_keV*: move mono to a given energy
`Escan` *start finish intervals time [fixQ]*: scan mono (units are keV). The literal "fixQ" means hkl is kept constant during the scan.

values for kappa
: g_kappa = 49.965 degrees; this is the empirical value of the kappa tilt angle for the kappa in 7ID-C
is_kappa: flag for whether a diffractometer has (1) or does not have (0) kappa geometry

filter/attenuator

`setaz2` This is a handy macro, only available in psic geometry I think, to input the surface normal direction (or other "special direction") into SPEC. It is like `setaz` but you don't have to remember the sign conventions associated with the angles called *sigma* and *tau*. The procedure is to make your "special direction" collinear with the eta axis. That is, reflect a laser off the sample surface, adjusting chi and phi until the reflected spot doesn't move when eta is rotated. The final values of chi and phi are called their "flat" values. In setaz2, you can choose to input flat_chi and flat_phi and the macro will get the surface normal direction computed correctly.

`ummv` *mot1 pos1* [*mot2 pos2*] [*mot3 pos3*] [*mot4 pos4*]
: Like umv but moves several motors at once. It isn't implemented yet since I need to take pseudomotor/real motor issues into account (i.e., you don't want to try to move chi and kap together).

Trajectory-scan macros on the kappa

The big difference between trajectory and point-by-point scanning (the subtle difference, that is) is that in defining a point-by-point scan, you give the number of integers, while in trajectory scanning you give the number of points (i.e., one more than the number of intervals). Mark Rivers probably had a good reason for this, but it may partly reflect his preference in contrast to Gerry Swislow's. Otherwise, the macros themselves look similar.

`ton`
: read in the macros for trajectory scanning

`toff`
: read in the standard macros for point-by-point scanning

and a lot more...

Special scans

xscan's

These are from the ESRF, and are designed for efficient collection of the background intensity. They are like most regular scans except you can increase the step spacing on the ends of the scan with two extra parameters (which, if not included in your command, are the same as last time). For example, `xascan` *motor start finish intervals time* [*expansion*] [*step_ratio*]

special recip space scans

Acknowledgements/For further information

The SPEC macros described in this report were borrowed (stolen) from a variety of sources, some of which I've forgotten. Some of them were taken from, or at least inspired by, Peter Eng, Mark Rivers, Tom Trainor, Yong Chu, and Paul Lyman.

The Certified Scientific Software website has an online manual and help pages for SPEC at `http://www.certif.com/`

A collection of SPEC macros is available at `http://www.esrf.fr/computing/bliss/spec/local/`

I have written a list of basic SPEC commands and a very brief SPEC reference sheet, which can be found at `http://www.mhatt.aps.anl.gov/dohn/manuals/`