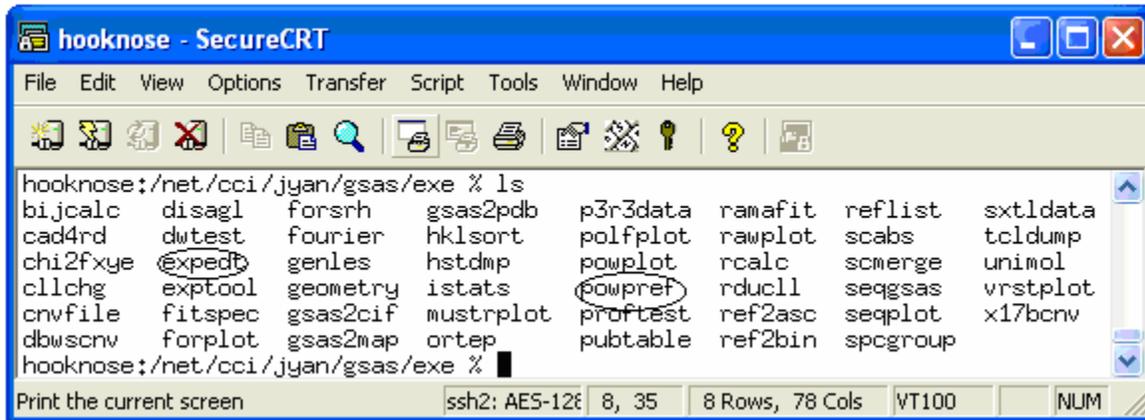


Monthly report—June, 2006

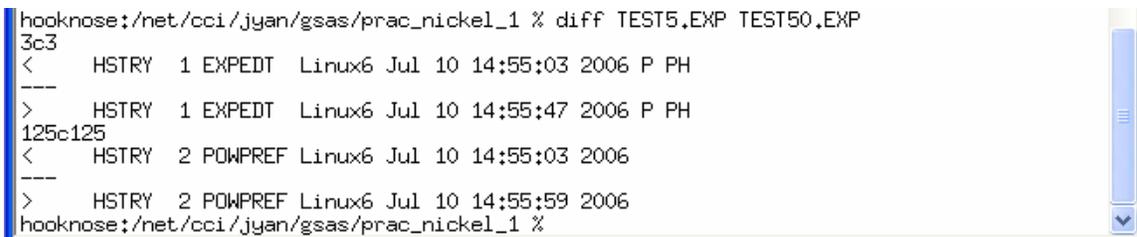
Some of my work in the past month is listed as following:

1. In the Linux system, practice of the GSAS data analysis both with shell script and without shell script was conducted, using the example data provided by GSAS manual (nickel TOF).
2. In the case of running shell script, the whole data analysis can be accomplished in the command-line interactive mode. But in the case of no shell script, I can currently complete part of input to `expedt` and then run `powpref`.



```
hooknose:/net/cci/jyan/gsas/exe % ls
bijcalc  disagl  forsrh  gsas2pdb  p3r3data  ramafit  reflist  sxtldata
cad4rd   dwtest  fourier  hkl1sort  polfplot  rawplot  scabs    tcldump
chi2fxye  expedt  genles  hstdmp    powplot   rcalc    scmerge  unimol
cllchg   exptool geometry  istats    powpref   rducll   seqgsas  vrstplot
cnvfile  fitspec  gsas2cif  mustplot  proftest  ref2asc  seqplot  x17bcnv
dbwscnv  forplot  gsas2map  ortep     pubtable  ref2bin  spcgroup
hooknose:/net/cci/jyan/gsas/exe %
```

3. For the current data analysis by both `expedt` and `powpref`, a python program was developed for automation. The experimental file from the automation python program (TEST5.EXP) was compared with the one from manually data input in command-line style (TEST50.EXP) and showed below.



```
hooknose:/net/cci/jyan/gsas/prac_nickel_1 % diff TEST5.EXP TEST50.EXP
3c3
<  HSTRY  1 EXPEDT  Linux6 Jul 10 14:55:03 2006 P PH
---
>  HSTRY  1 EXPEDT  Linux6 Jul 10 14:55:47 2006 P PH
125c125
<  HSTRY  2 POWPREF Linux6 Jul 10 14:55:03 2006
---
>  HSTRY  2 POWPREF Linux6 Jul 10 14:55:59 2006
hooknose:/net/cci/jyan/gsas/prac_nickel_1 %
```

4. The above comparison shows that both results are same except for their different running-times.

The next month work should focus on:

Continue working on the data analysis in the command-line interactive mode until the whole automation process of the GSAS data analysis is done. Then integrate the python program to the PHENIX package.