SHARP tutorial (by Priscila Giuseppe)

Presently the SHARP is only installed in the computer MX2C

A. SAD using iodide

1. Copy the files **file.mtz** (SCALA or HKL2000 outputs) and **file.res** (SHELX ouput) to the directory:
   /progs/sharp/users/usermx2/sharpfiles/datafiles

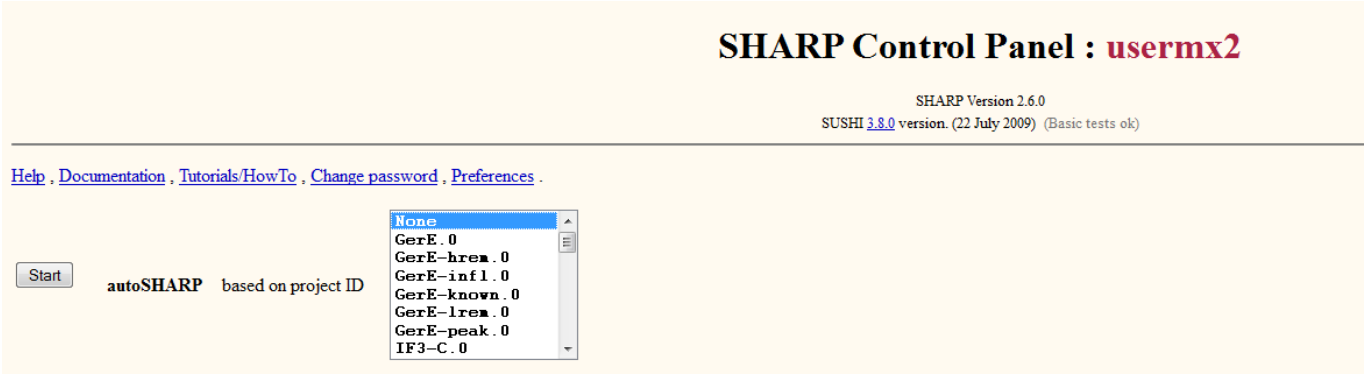
2. Rename **file.mtz** to **file.data.mtz**:
   >mv file.mtz file.data.mtz

3. Rename **file.res** to **file.hatom**:
   >mv file.res file.hatom

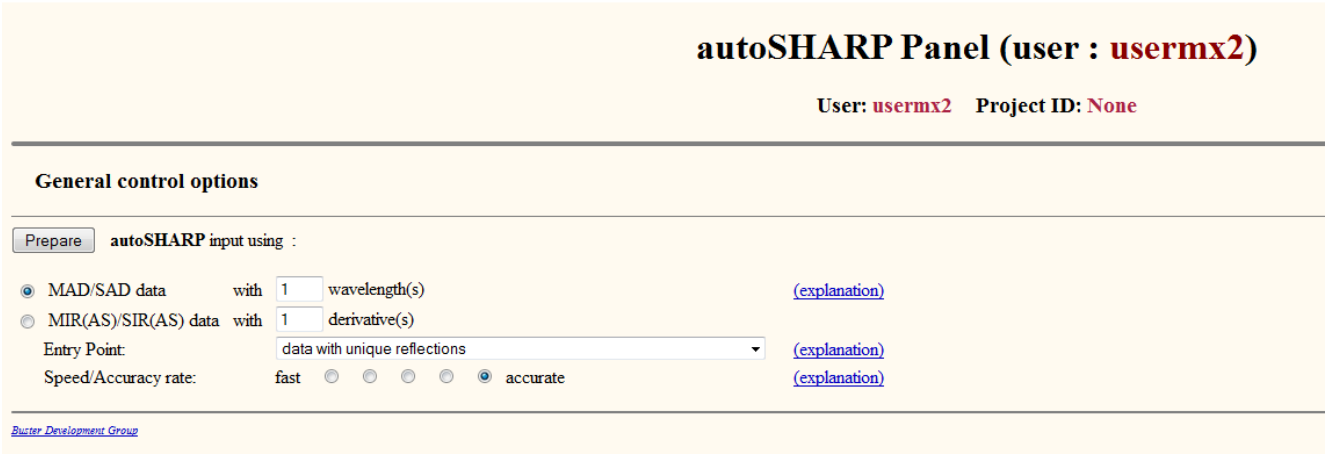
4. Edit the file **file.hatom**:
   >nedit file.hatom
   Delete the header and the two last columns.
   Change I001 1 *to* ATOM I (or ATOM Se – when using SeMet)

5. Open SHARP:
   > type **sharp** in the terminal
   The web browser will open automatically.
   Login: usermx2
   Password: usermx2

click START autoSHARP based on project id **none**



choose MAD/SAD data with 1 wavelength



6. Set the parameters:
   - Project identifier (use a short name. ex: SAD_NaIx2)
   - at G site editor, show, inverted hand (if indicated as the best hand by SHELXE)
   - Number of expected sites per monomer <4>
   - Run density modification
   - HA sites <none> (let SHARP find the sites)
   - Wavelength (w1) <1.427>
   - To find f´ and f´´ of iodide, type crossec in a terminal. Then type:

     ATOM I <ENTER>

     N WAV 1 1.427 <ENTER>

     END <ENTER>
   - Copy the values at SHARP window.
   - datafile.sca

B. SIRAS using iodide:

Before start, be aware that identifiers were appended to column labels at the input files nat.mtz, der1.mtz:

When run SCALA, choose the option <identifier to append to column labels>

nat (for native data)

I1 (for derivative data 1)

After performing the steps A1 to A4...

5. Open SHARP:

- type *sharp* in the terminal

The web browser will open automatically

- click START autoSHARP

> choose SIRAS

> choose the option merged and unscaled

> set the parameters as in step A6

OBS:

- To see the output map at coot, manually open the file test_eden_solvflat.mtz and choose FBshasol and PHBshasol.
- When running SAD using SeMet sites, set the occupancy for each Se site as those estimated by SHELX and set the Bvalue to 50, set max. resolution as the max resolution of the data (defined at the scaling step).
- In case of error due to the absence of the Isym column, scale the data selecting the option (old truncate) in SCALA
- If you are in other computer connected to the network you can open the SHARP using the web browser by typing:

  http://mx2c-linux:8080

  - Login:usermx2
  - Password:usermx2

  Note that the input files need to be in the folders cited at the item 1 of this tutorial, before start running SHARP

  The output files can be found in the directory:

  /progs/sharp/users/usermx2/sharpfiles/logfiles/

  Or, using the browser, in the link results at the Control Panel.