Progress Implementing CIF for Powder Diffraction

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What is CIF?

Crystallographic Information File

- Developed in 1991 for exchange & archive of crystallographic *results*
- Expansion for macromolecular & powder diffraction applications complete ~1997
- Later additions: 2-D data, symmetry, modulated structures, [diffuse scattering]

What does CIF look like?

- ASCII
- “ Tags & flags” , *e.g.*

  _diffrn_radiation_wavelength 1.5418

- Tables (aka loops):

```
loop_   _atom_site_label      _atom_site_fract_x
_atom_site_fract_y    _atom_site_fract_z
O1      .4154(4)      .5699(1)      .3026(1)
C2      .5630(5)      .5087(2)      .3246(1)
C3      .5350(5)      .4920(2)      .3997(1)
```

How does CIF differ…

- Limited data structures
- Flat file (with some relational capabilities grafted on)
- Data Dictionary: Carefully thought out & machine readable data definitions

```
data_chemical_melting_point
_name
   '_chemical_melting_point'
_category        chemical
_type            numb
_enumeration_range 0.0:
_units           K
_units_detail    'kelvins'
_definition
; The temperature in kelvins
   at which a crystalline
   solid changes
   to a liquid.
;
```

Powder Diffraction CIF (pdCIF)

- Effort started in early 1990's
  - Expand CIF scope: experimental data
  - Many types of powder diffraction data:multiple ways to define data
  - Single powder project: multiple CIF blocks
    - interblock pointers
- Released on unsuspecting planet in 1997

Five years later: minimal software available

So, what's new?

- GSAS2CIF:
  - exporting Rietveld results to pdCIF
- CIF Viewer/Editor
  - browse multiblock CIFs
- pdCIF data plotter
  - designed for referee review of refinements

GSAS2CIF

- GSAS2CIF must integrate into the GSAS Rietveld package
  - (FORTRAN)
- Challenges:
  - Single-block vs. multiple block CIFs
  - Data structures depend on type of measurement
  - Facile inclusion of descriptive information

Multiple vs. Single Block CIFs

- A CIF data item can only be used once in a block (with a single value or a list of values)
  ==> only one powder diffraction data set or set of coordinates can be placed in a CIF block
- pdCIFs must contain more than one block, if more than one set of data is used or the sample contains more than one chemical species
- However: much CIF software does not [yet] handle multiple-block CIFs

Data structures

- Observables depend on type of experiment
  - *e.g.* TOF vs CW
  - averaging etc. requires 2 data tables
- Implemented:
  - Single & multiple wavelength x-ray
  - TOF & CW neutron
- Not yet addressed: energy dispersive x-ray

Challenge: Descriptive Info

"The information one <u>does not</u> supply to data analysis software is at least as important to document as anything else"

- Data & derived parameters (from Rietveld input):
  - >90% of bytes in typical pdCIF file
  - ~50% of recommended CIF data items
- So ~50% of info is manually input by user
  - Goals: maximize reuse & allow updating

Solution: Import of template files

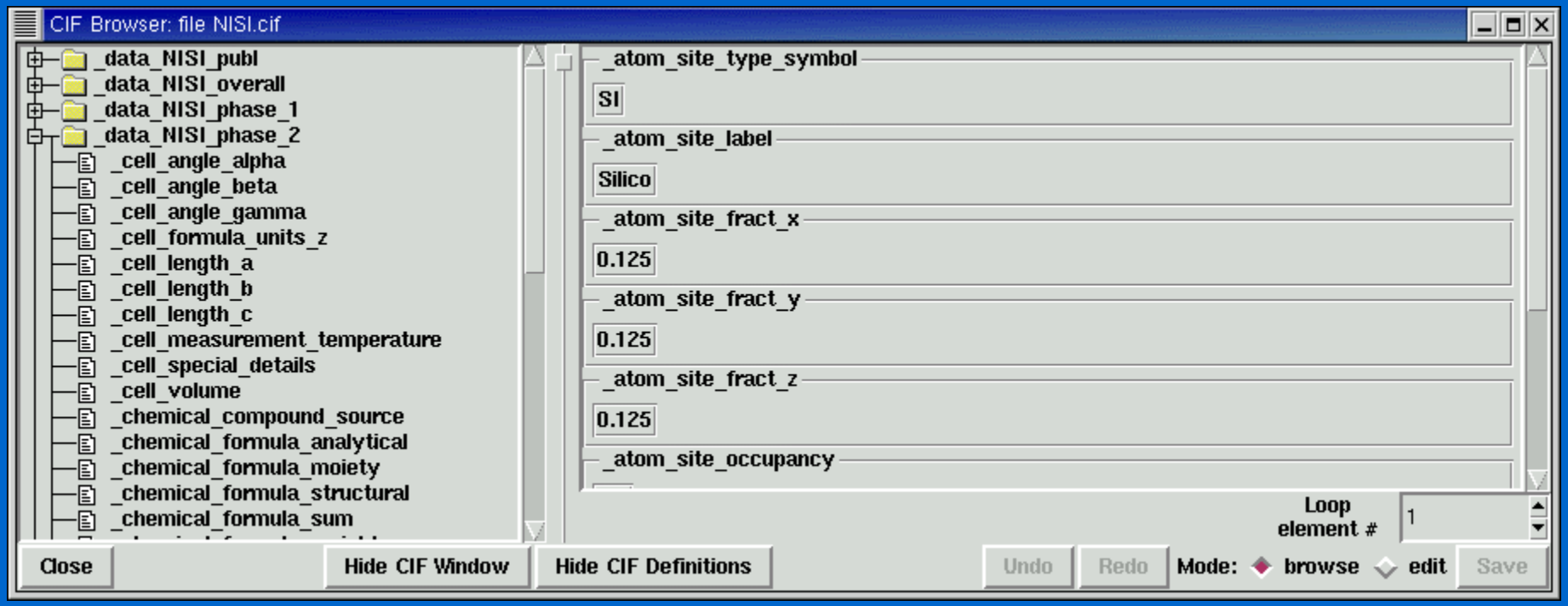
- GSAS2CIF creates template files containing descriptive CIF items
  - 3 Templates: overall info, sample/phase info & data/instrument info
  - Search name/path used to grab customized versions of files (if present) on 1st run of GSAS2CIF
- User adds info to project-specific copies of template files -- ***not to the output CIF***.
- These project-specific template files can be recycled for other projects, when appropriate

Adding info to template files...

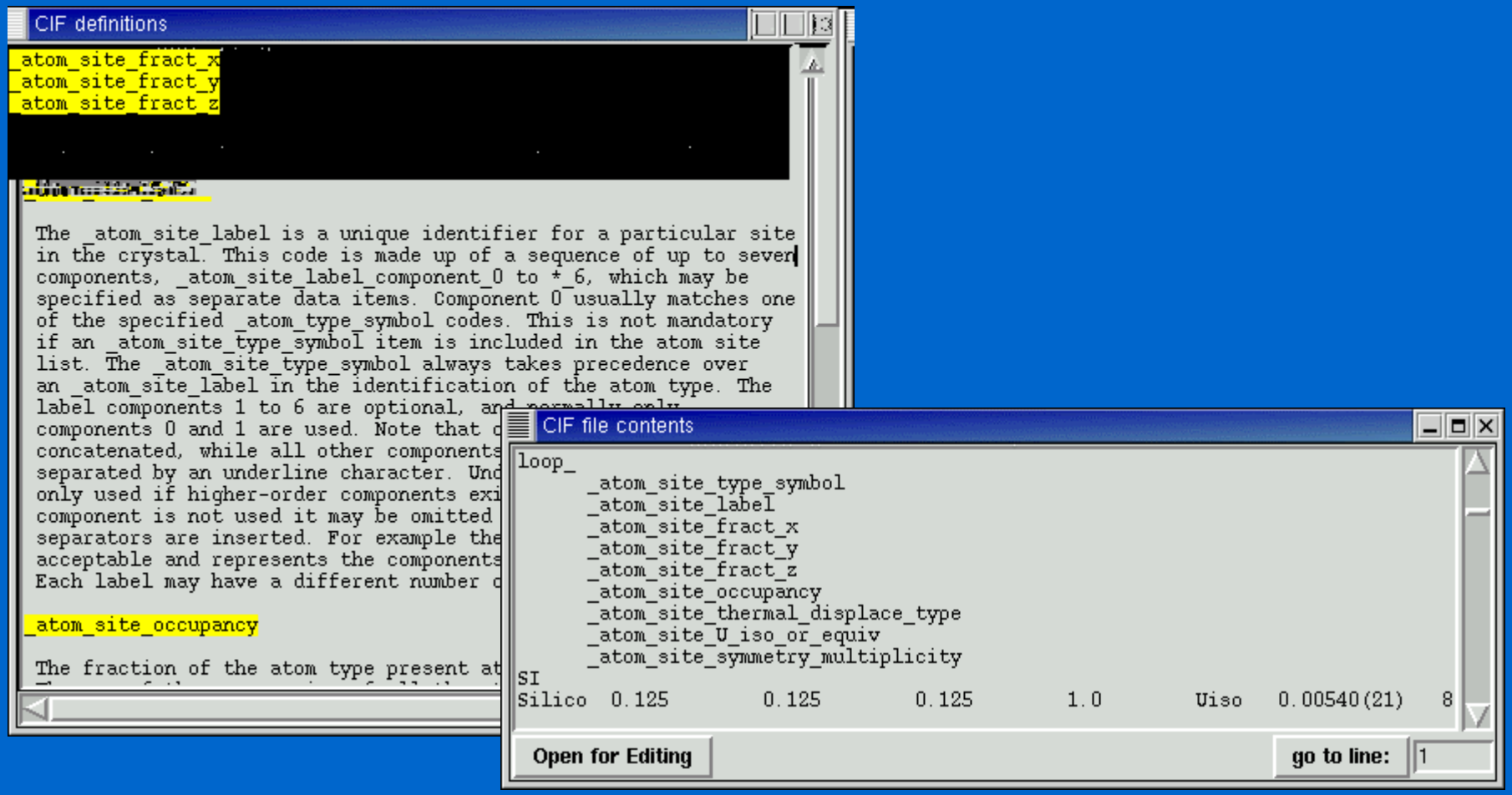
- Easy: use nice GUI-based CIF editing tool...

  ...that is, if one existed
- ~2000 lines of Tcl/Tk later:
  - working CIF editor
  - Same code runs on Linux/SGI/Windows (Mac?)

CIF browser/editor



Features: view dictionary & file



pdCIF: Write-only memory?

Much-needed pdCIF app: ***plotting tool***

- Best to review results graphically -- at multiple scales

- Challenge: pdCIF has many ways data can be stored

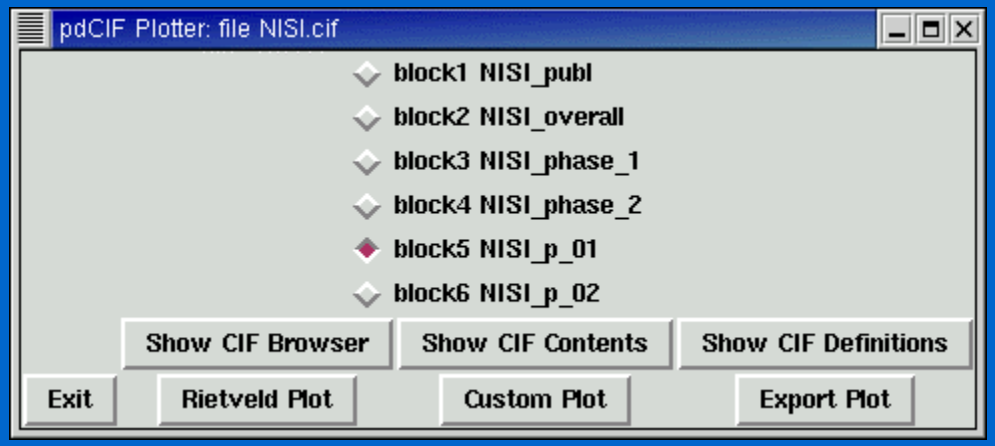
pdCIF Diffraction data items

X axis data items:

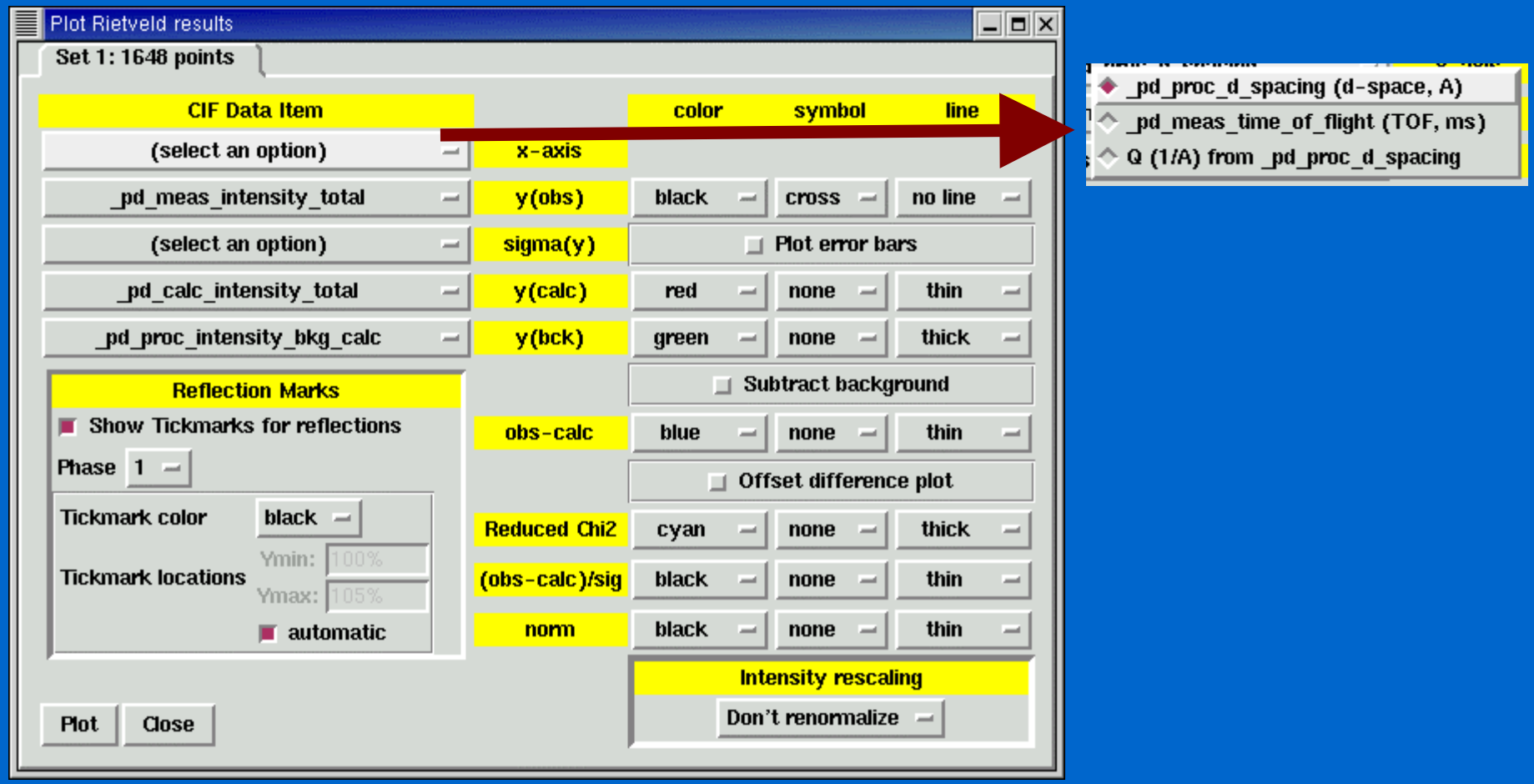
- _pd_meas_2theta_range_*
- _pd_proc_2theta_range_*
- _pd_meas_2theta_scan
- _pd_meas_time_of_flight
- _pd_proc_2theta_corrected
- _pd_proc_energy_incident
- _pd_proc_wavelength
- _pd_proc_d_spacing
- _pd_proc_recip_len_Q

Y axis - Observed

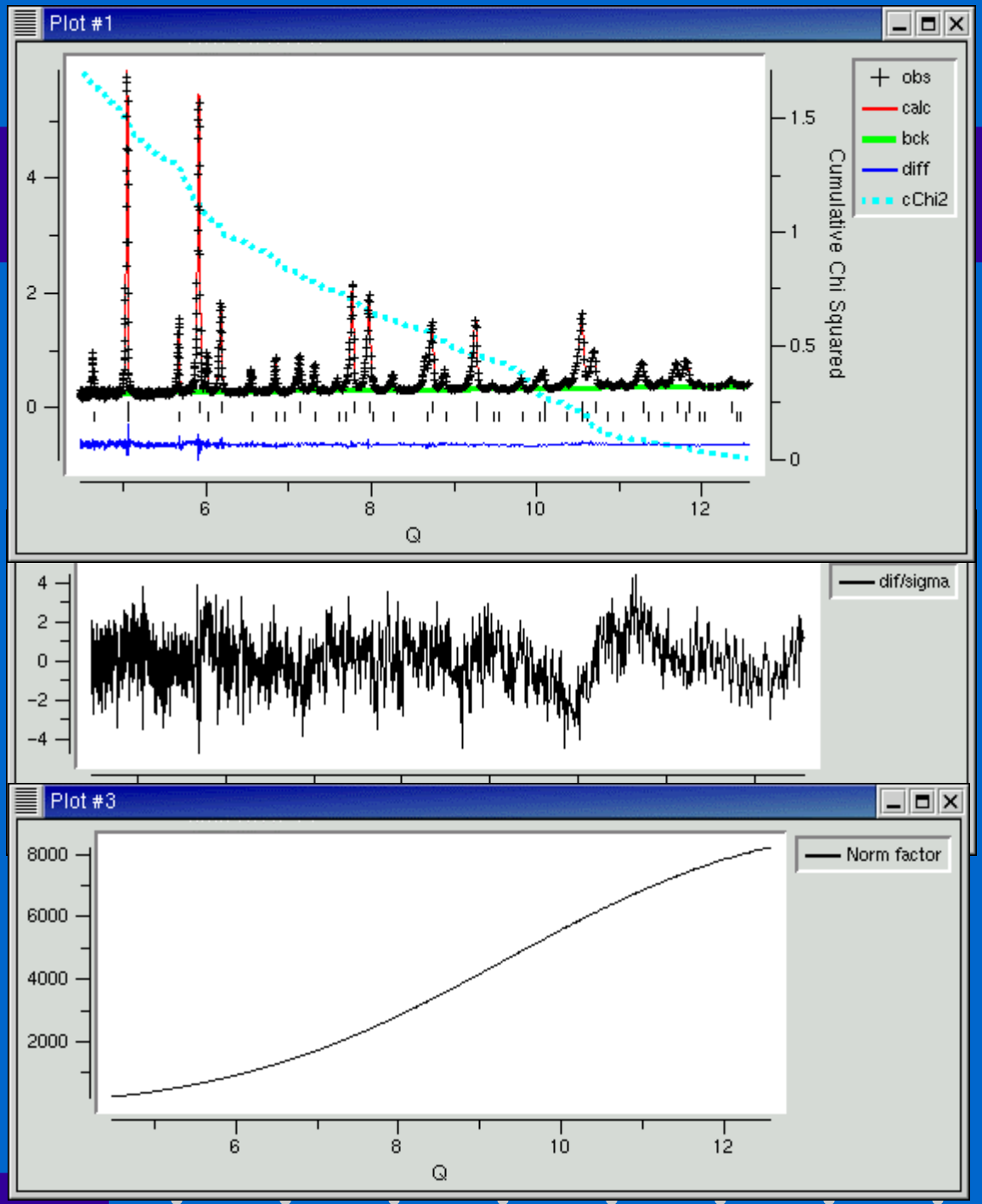
- _pd_meas_counts_total
- _pd_meas_intensity_total
- _pd_proc_intensity_net
- _pd_proc_intensity_total



Select Plot Option



Some Plots


Plot #1
obs
calc
bck
diff
cChi2
Cumulative Chi Squared
Q
dif/sigma
Plot #3
Norm factor
Q

Software Status

- GSAS2CIF: included in 10/02 GSAS release
  - Rough draft of *J. Appl. Cryst.* paper complete
  - Web code documentation
- CIF editor: code available on request
  - Paper in preparation
- pdCIF Plotter: code on request
  - Paper to be started soon

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WWW Links

- CIF:
  - http://www.iucr.org/iucr-top/cif/ (*UK*)
  - http://iucr.sdsc.edu/iucr-top/cif/ (*US mirror*)
- GSAS2CIF
  - http://www.ncnr.nist.gov/xtal/software/expgui/gsas2cif.html
- CIFEDIT and pdCIFPLOT
  - http://www.ncnr.nist.gov/xtal/software/cif (*in development*)