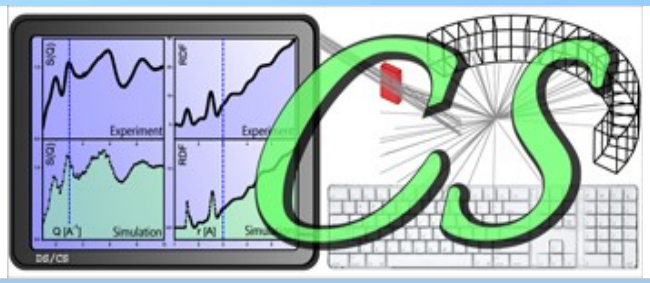


NEUTRONS FOR SCIENCE

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June 20th 2013, 9-12 am

# Data Analysis Standards

## Progress on the Mantid evaluation for reactor source instruments

# Progress on the Mantid evaluation for reactor source instruments

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- TOF:
  - IN4, 5 and 6 @ILL
  - Focus @PSI
  - MiBemol @LLB
  - TofTof @FRM-II
- SANS:
  - D33 @ILL
- Performance, functionalities/algorithms, usability
- Benchmarking with LAMP


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# IN4, 5 and 6 @ILL

- @ILL
  - “Channel number” not time bin
  - Direct conversion from channel to Energy
    - No need to know distance source-sample
  - Mantid uses time as base unit
    - Need to know:
      - distance source-sample-detector
      - Detector pixel position in space
  - All this info is in the IDF
    - Advantageous for calculation that need position in space


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# Integrating new instruments

- Can be done... all depends on the nexus format!
- Problems:
  - Different IDs with the same meaning
  - NX Types
  - Time bins not always present:
    - Necessary to find EPP and calculate TOF from E and distance


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# Focus @PSI (SINQ)

- Even easier than at the ILL:
  - Nexus file has the time bin axis
- Data array format different from ILL
  - IN5: 32-bit integer,  384 x 256 x 512
  - IN6: 32-bit integer,  337 x 1 x 1024
  - FOCUS: 32-bit integer,  375 x 1070
  - MiBemol: 32-bit floating-point,  84 x 512


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# Mibemol @LLB

- No time info:
  - Need to calculate EPP and then calculate the time binning
  - No NX_class associated with the tags


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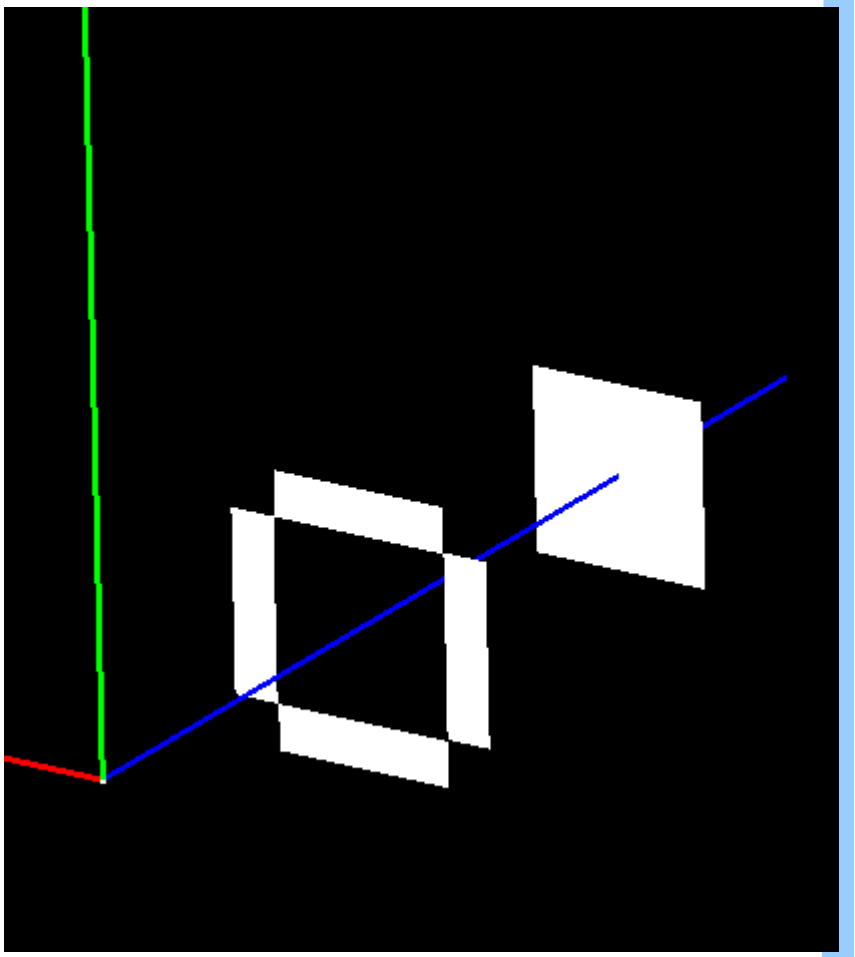
# SANS : D33

- Mantid has built in GUIs for SANS
  - They look customised for specific instruments
- IDF
- Nexus is a bit different from the others ILL instruments
-

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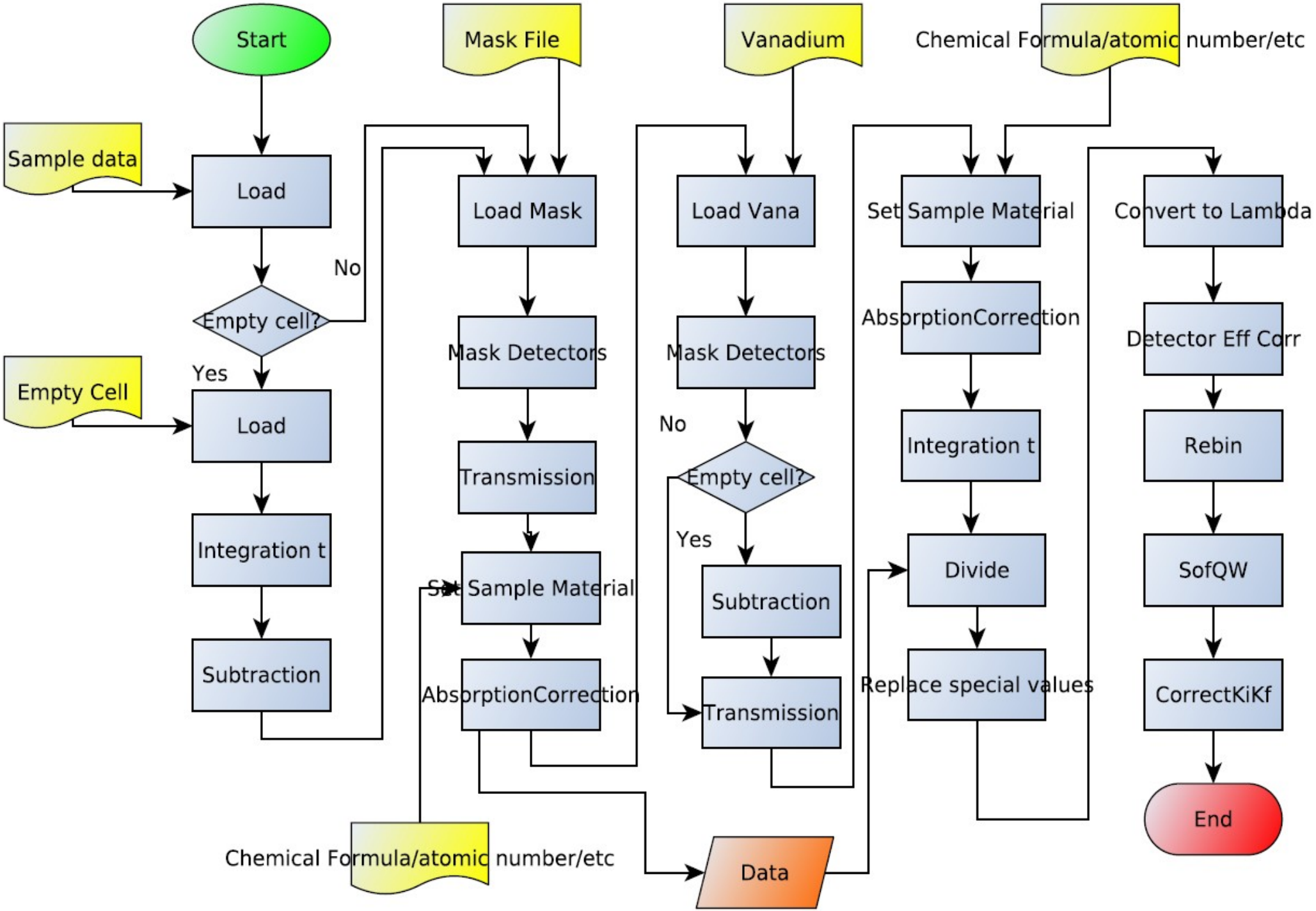
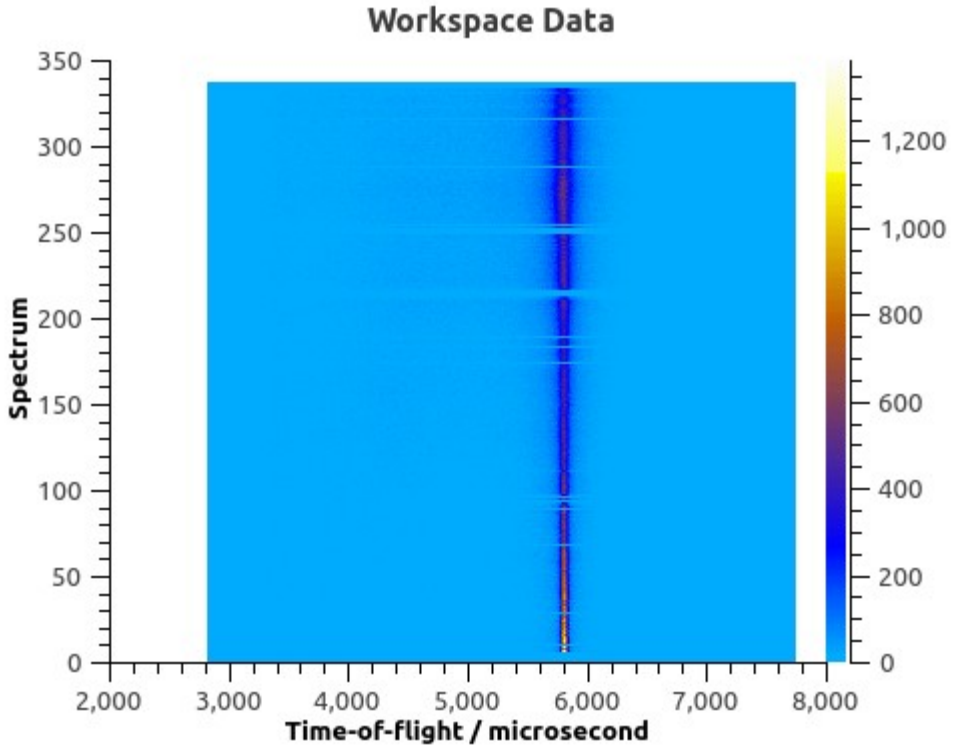
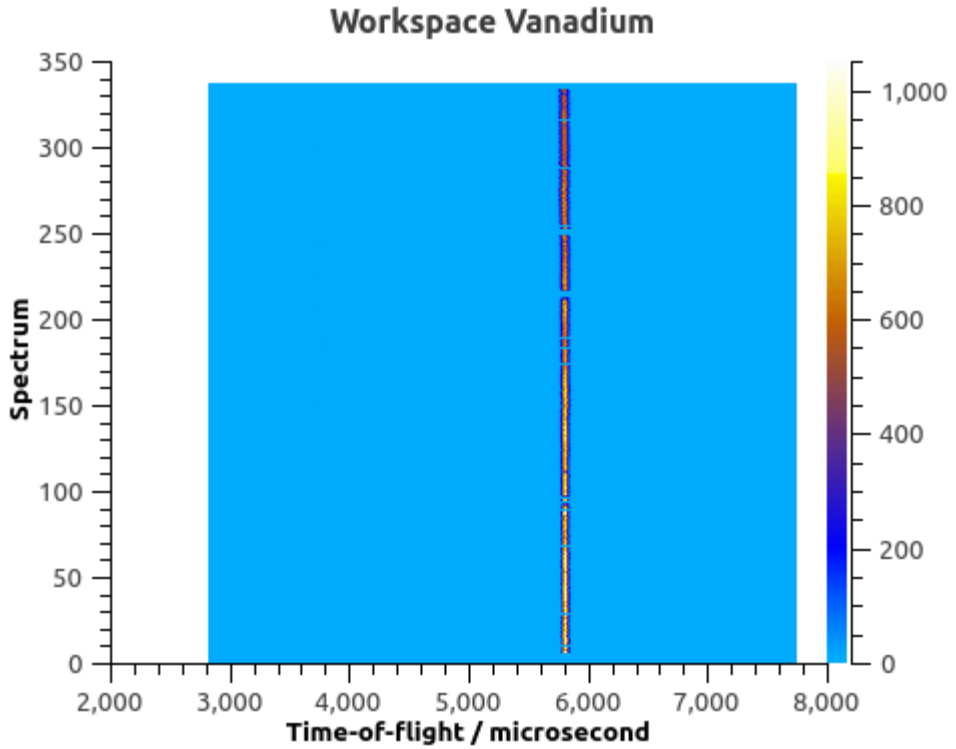

Start
Mask File
Vanadium
Chemical Formula/atomic number/etc
Sample data
Load
No
Empty cell?
Yes
Empty Cell
Load
Integration t
Subtraction
Load Mask
Mask Detectors
Transmission
Set Sample Material
AbsorptionCorrection
Chemical Formula/atomic number/etc
Load Vana
Mask Detectors
No
Empty cell?
Yes
Subtraction
Transmission
Data
Set Sample Material
AbsorptionCorrection
Integration t
Divide
Replace special values
Convert to Lambda
Detector Eff Corr
Rebin
SofQW
CorrectKiKf
End

# IN6 – Raw data





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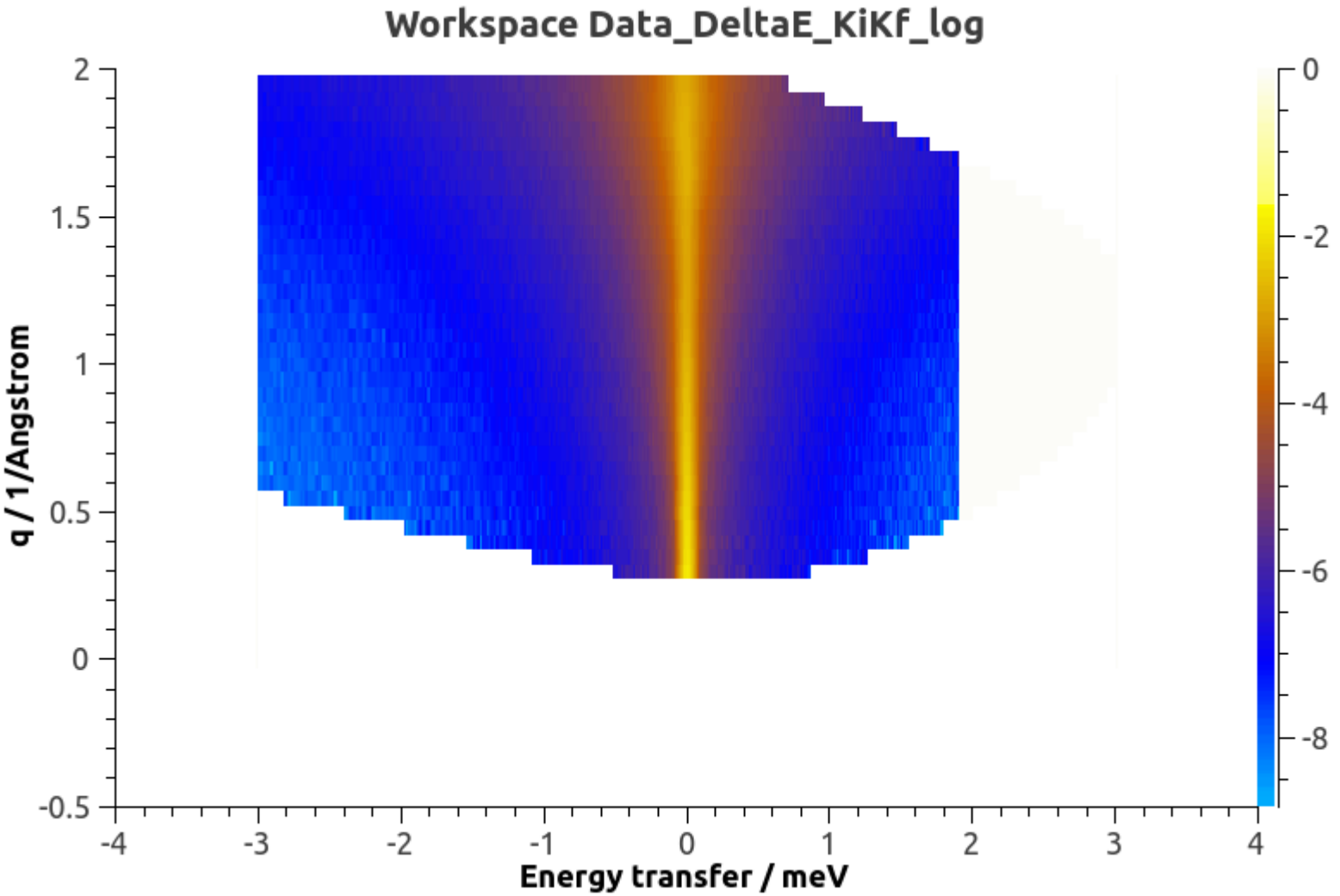
# IN6 – SofQW3





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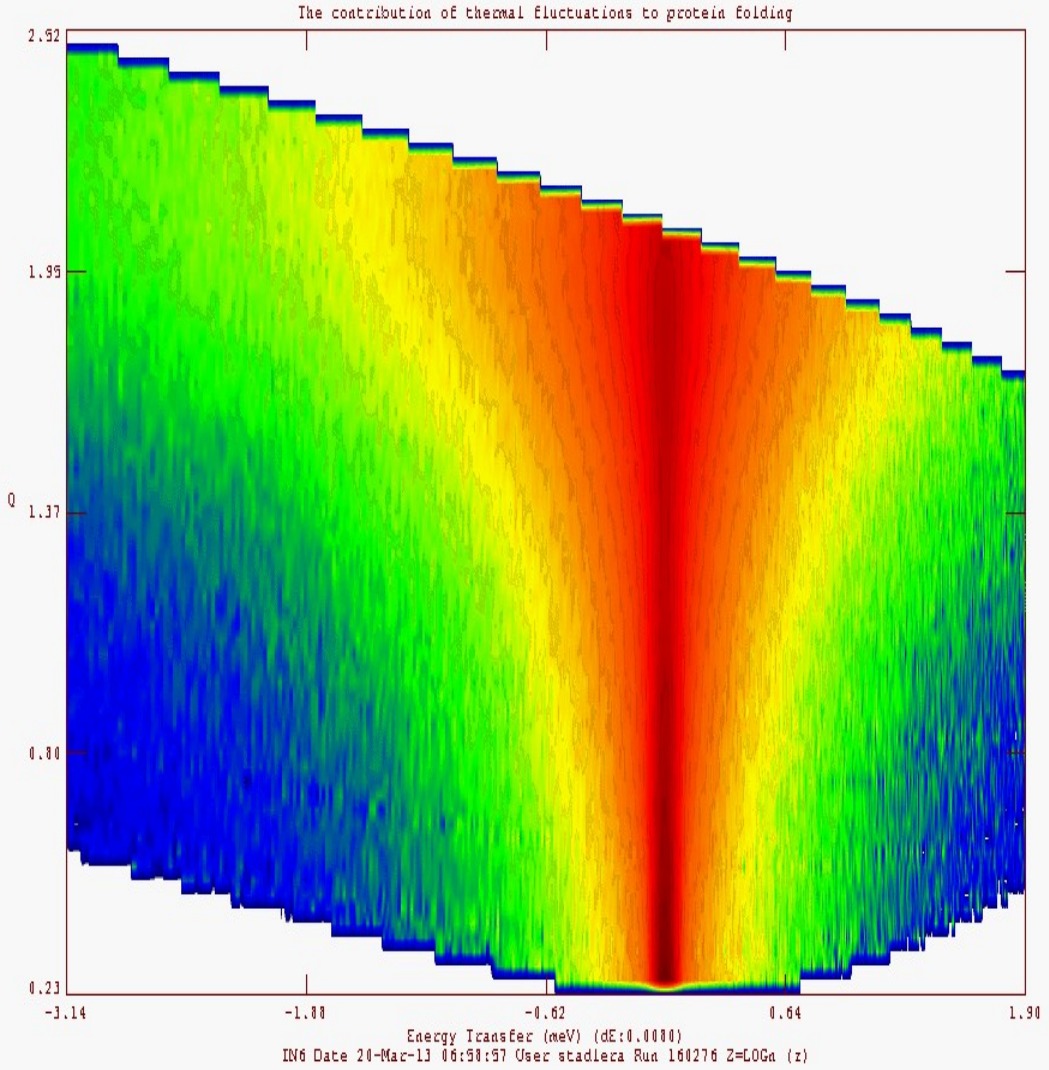
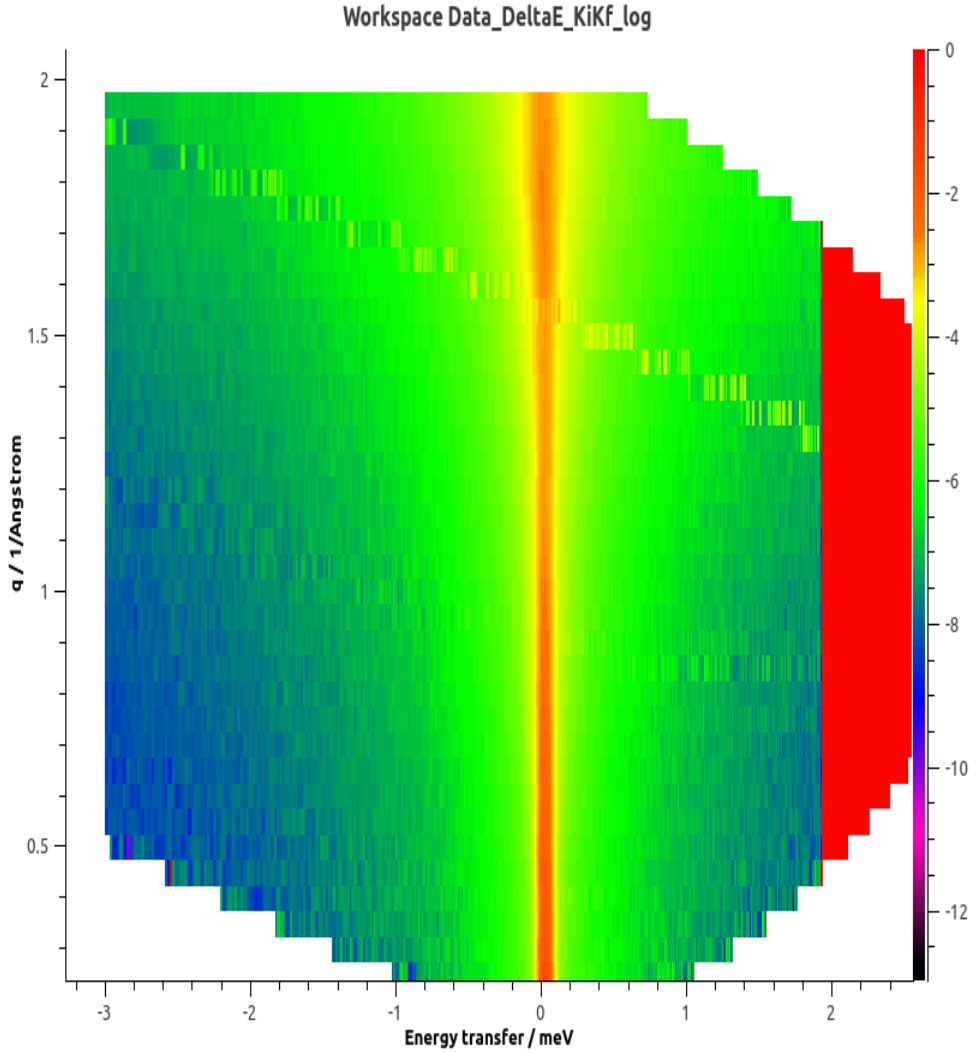
# Mantid vs Lamp: SofQW





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# Performance

- Longest tasks in Mantid:
  - Convert units
    - There's a X-axis per spectra!
    - Not a common time bin for all spectra
  - SofQW
    1. Centre
    2. Parallelepiped
    3. Parallelepiped / Fractional data
- Lamp:
  - E.g. for IN5:
    - File read: 15sec
    - Instrument tranformation (detector mask...): < 0.5sec
    - Convert to energy: < 0.5 sec
    - SofQW: 1min (maximum)


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# Performance

- From raw data to SofQW (SofQW3)
- Xeon 8 core, 16Gb Ram, SSD drive:
  - IN4 and IN6 : ~10 sec
  - IN5 (512 time channels):
    - Raw file: 98304 spectra:
      - 384 * 256 * 512 * 4B  = 192 MB
      - In Mantid:
        - 98304 * 512 * 8B  * 3 =  1.152 GB
          - Mantid goes from ~200MB to 1.4GB of memory
    - ~ **13** mins (SofQW3 successful, Duration 723.29 seconds )

| Process Name | User | Virtual Memory | % CPU | ID | Memory ▾ | Priority |
|---|---|---|---|---|---|---|
| MantidPlot | leal | 13.1 GiB | 0 | 14737 | 11.7 GiB | Normal |


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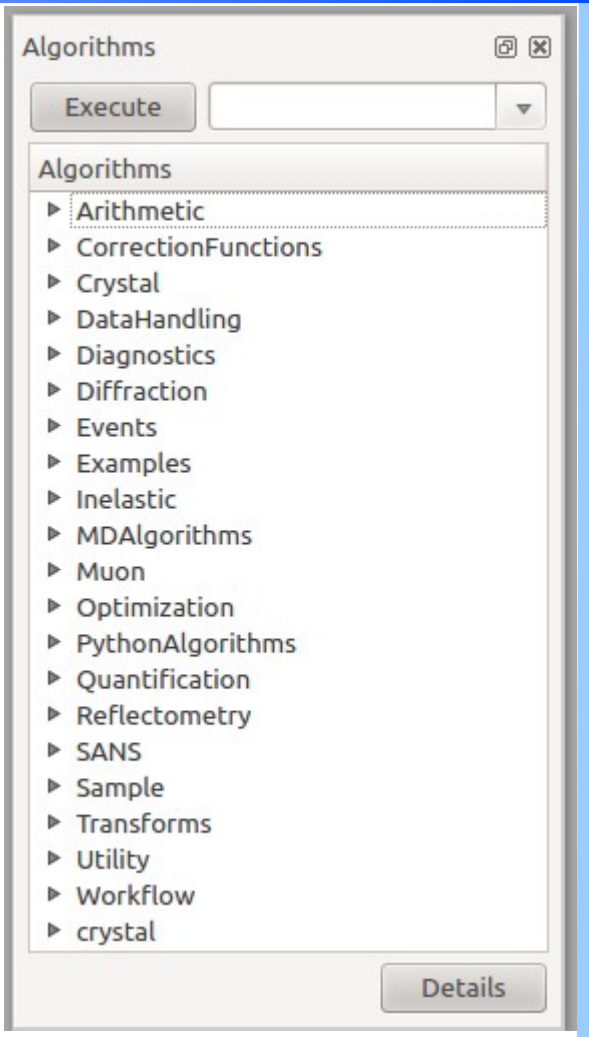
# Mantid Functionalities / Algorithms

- Several scientific techniques:
  - Direct Inelastic
  - Indirect Inelastic
  - SANS
  - Diffraction
  - Muon Analysis
- There's an algorithm for everything and anything...
  - http://www.mantidproject.org/Category:Algorithms
  - 532 in total
  - The steps may be different from the usual procedures
  -





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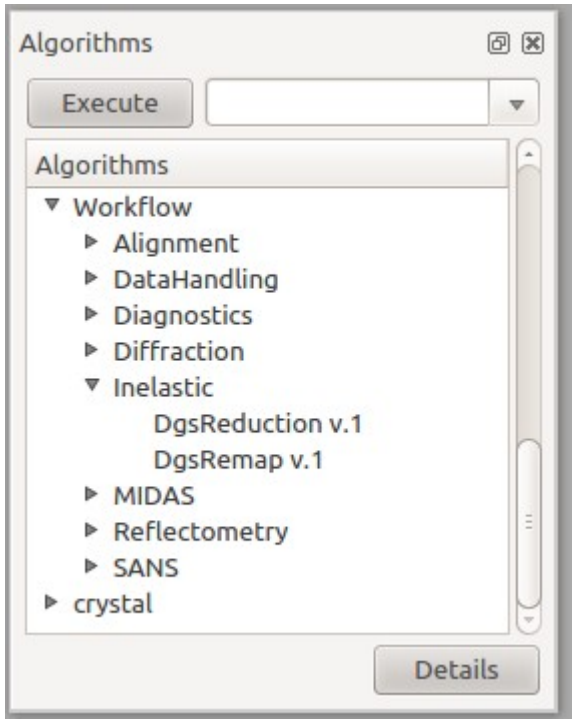
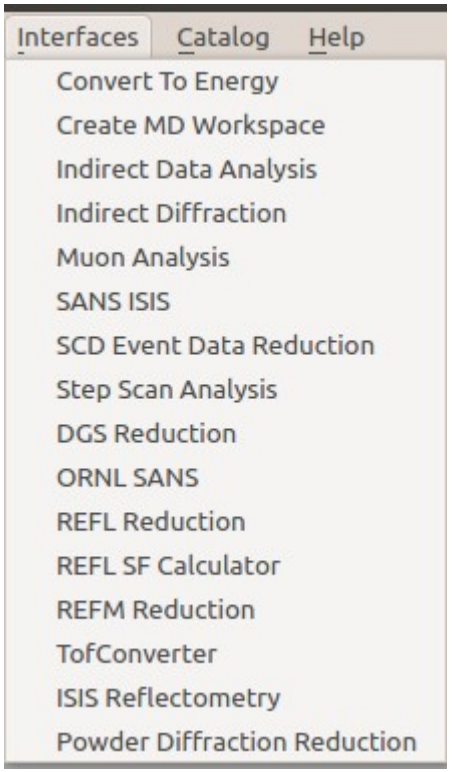
# Usability

- Python scripting is a plus for scientists / “Geeks”
- Several instrument specific GUIs
- GUI for fitting
- Instrument view
- Plotting facilities





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Questions?

THE END