QENS software

for MLZ, ESS, and the community at large

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Scientific Computing Group

at MLZ

Built up since 2011

Mission:

- develop & maintain software
  for data reduction & analysis
  at MLZ scattering instruments

Staff:

- 5 on core budget (4 permanent)
- 1 funded by SINE2020 WP10 (2015-2018)
- 2 German in-kind contribution to ESS (2017-2020)

http://apps.jcns.fz-juelich.de
QENS experience
in our Scientific Computing Group

Joachim:
- used BS, TOF, NSE to study liquid dynamics
- commissioned & operated LS, NRSE and NBS instruments
- wrote & maintains IDA=Frida1 & Frida2

Marina:
- adapted Mantid to TOFTOF
- now working on DNS, POWTEX

excellent relations with instrument responsibles
Software practices
at SPHERES, TOFTOF, DNS

Some users have their own software
⇒reduction software must export to legacy formats

Most users do what local contact teaches them

Instrument responsibilities teach users the one software they master
Reduction software

SPHERES
- legacy

TOFTOF
- 3 legacy procedures
- slow adoption of Mantid

DNS
- legacy
- Mantid needed for forthcoming TOF mode
Analysis software

SPHERES
- Frida2

TOFTOF
- Python scripts
- Frida1 → Frida2

DNS
- legacy
- unprepared for forthcoming TOF mode
Requests by instrument responsibles

TOFTOF

- Fourier transform $\rightarrow S(q, t)$
- multi-phonon correction $\rightarrow$ DOS $g(\omega)$
- multiple scattering correction
Can we GUIfy the data analysis?

Advantages
- easier to learn
- less burden for instrument responsible
- almost indispensable for interactive 3d visualization

Problems
- how much flexibility do we need?
- how to make analysis reproducible, scriptable, communicatable?
Notebooks?

De facto standard: Jupyter

Replacement or complement for GUI?
Can we standardize & automatize data analysis?

Advantages
- more objective & reproducible
- more accessible for occasional users
- less burden for instrument responsible

Danger
- enables uneducated users to do cargo cult science
- may leave experiment underexploited
Limits of standardization

Standard analysis is good 1st-order approximation

2nd-order approximation depends on
- sample amount & geometry
- container scattering
- sample scattering & absorption
- measurement duration & strategy

Problems exacerbated by instrumental imperfections (TOF < BS ?)

Therefore we need
- huge number of different correction & fit procedures
- interactively explored in efficient expert mode
Perspective then

The easy task
  ■ automatize & GUIfy standard analysis

More difficult
  ■ assess credibility of results
  ■ help users to transit towards expert mode
If you torture the data long enough, they will confess.