QENS software

for MLZ, ESS, and the community at large

Joachim Wuttke, MLZ Scientific Computing Group, Garching, Germany

MLZ is a cooperation between

JÜLICH
FORSCHUNGSZENTRUM

Helmholtz-Zentrum
Geesthacht
Zentrum für Material- und Küstenforschung

TUM
Technische Universität München

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)

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 responsibles 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 $\rightarrow$ 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 acessible 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 intrumental 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