BASTILLE

NEUTRONS FOR SCIENCE®

PMC June 30th 2016

BASTILLE

- Status & organisation
- Progress
- Interim organisation

Status & organisation

- New staff
  - Ian Bush – since April 18 (Tessella - only paid for days worked)
  - Verena Reimund, Antti Soininen, Gagik Vardanyan – since May 2

Status & organisation

- Training
  - Training and settling-in at ILL (May)
    - ~3 weeks
    - computers (Linux (Windows) and Mac environment setup)
  - Mantid developer training - C++ and GitHub workflow (development tools, exercises and code review)
  - Mantid user training (Python)
  - Familiarisation with LAMP for benchmarking

Status & organisation

- Ian's specific role
  - A final set of project requirement documents
  - Relevant training sessions at ILL and elsewhere
  - A document which identifies the key members of the MANTID team
  - Implement agile development techniques
  - A project report at the end of Year 1 describing the status of the project
  - A working prototype (software and documentation) for simple scanning instruments in MANTID

Status & organisation

- Organisation
  - Daily ‘stand-up’ meetings (Bastille team +)
  - Weekly ‘sprint cycle’ meetings (Bastille team + CS + scientists)
  - Fortnightly Mantid review meetings – following the whole project

Status & organisation

- Documentation
  - From

    http://intranet.ill.eu/divisions/science-ds/endurance-programme/bastille/

  - To

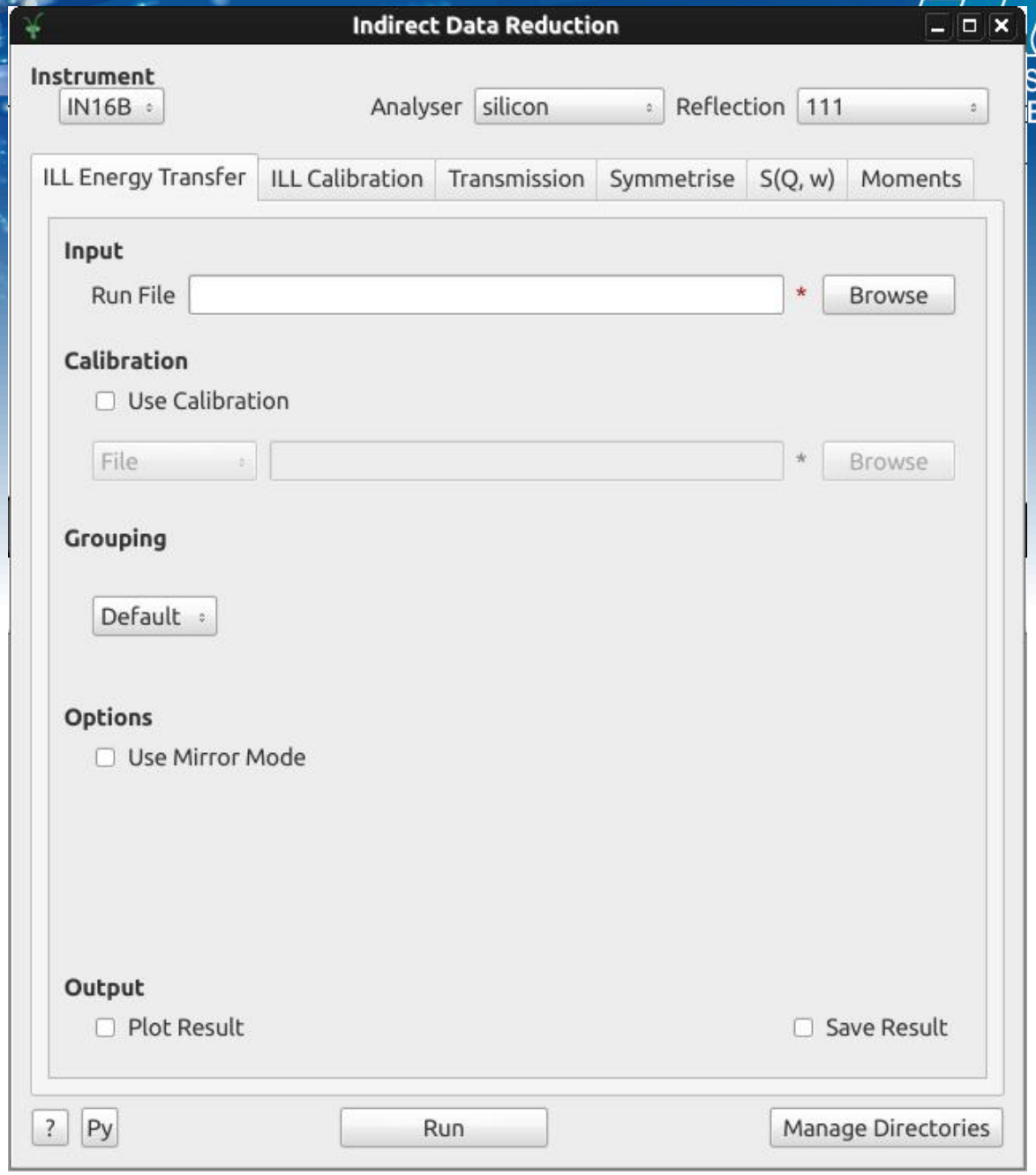
    https://github.com/mantidproject/documents/tree/master/Project-Management/ILL

    Follow Bastille here!

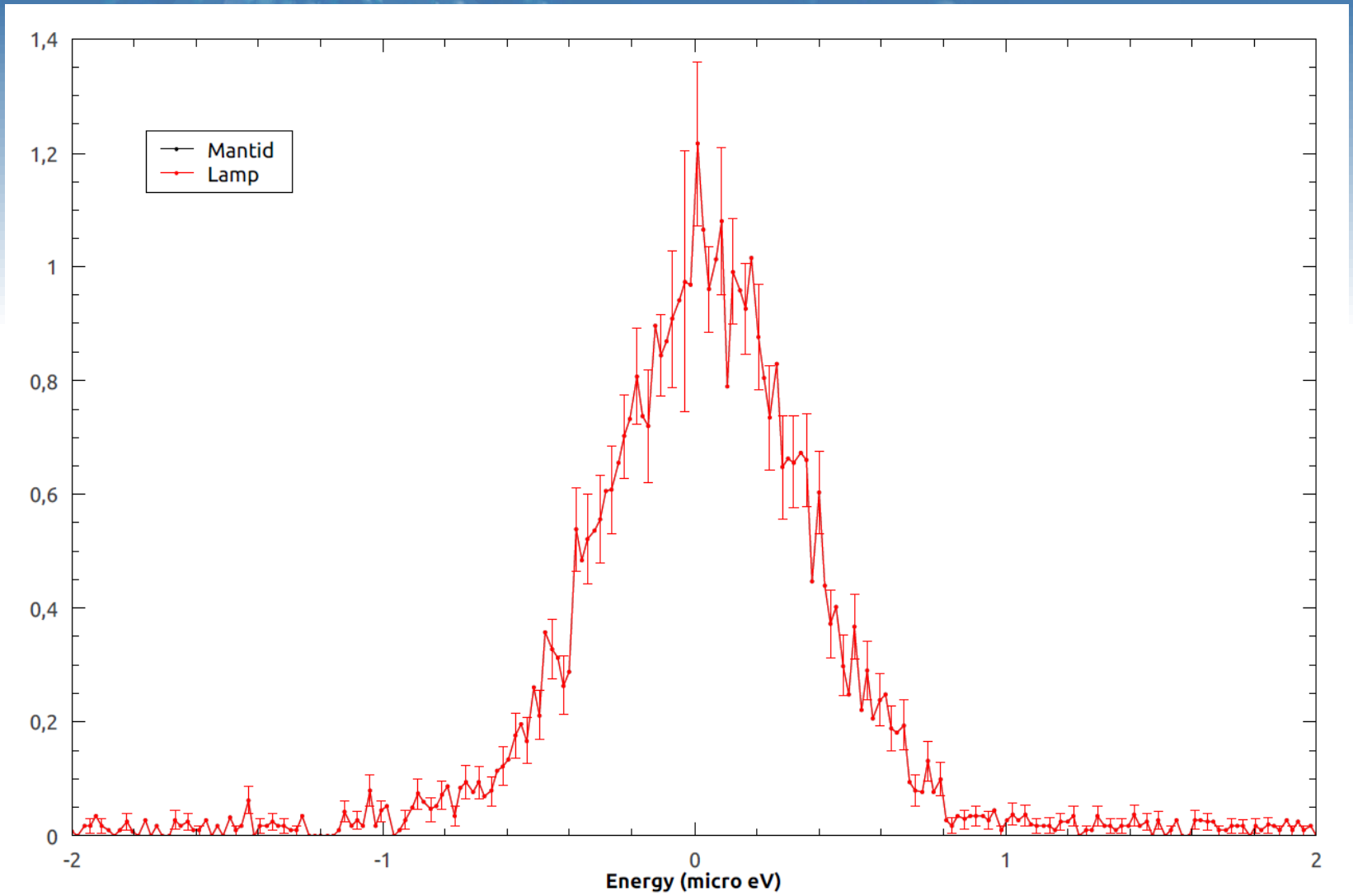
Progress

- Backscattering (Verena and Gagik)
  - Initial work in NMI3 with help Spencer Howells at ISIS
  - Graphical user interface created by SH – combines loading data, monitor normalisation, background subtraction, vanadium calibration and mirror treatment
  - Individual data reduction steps validated

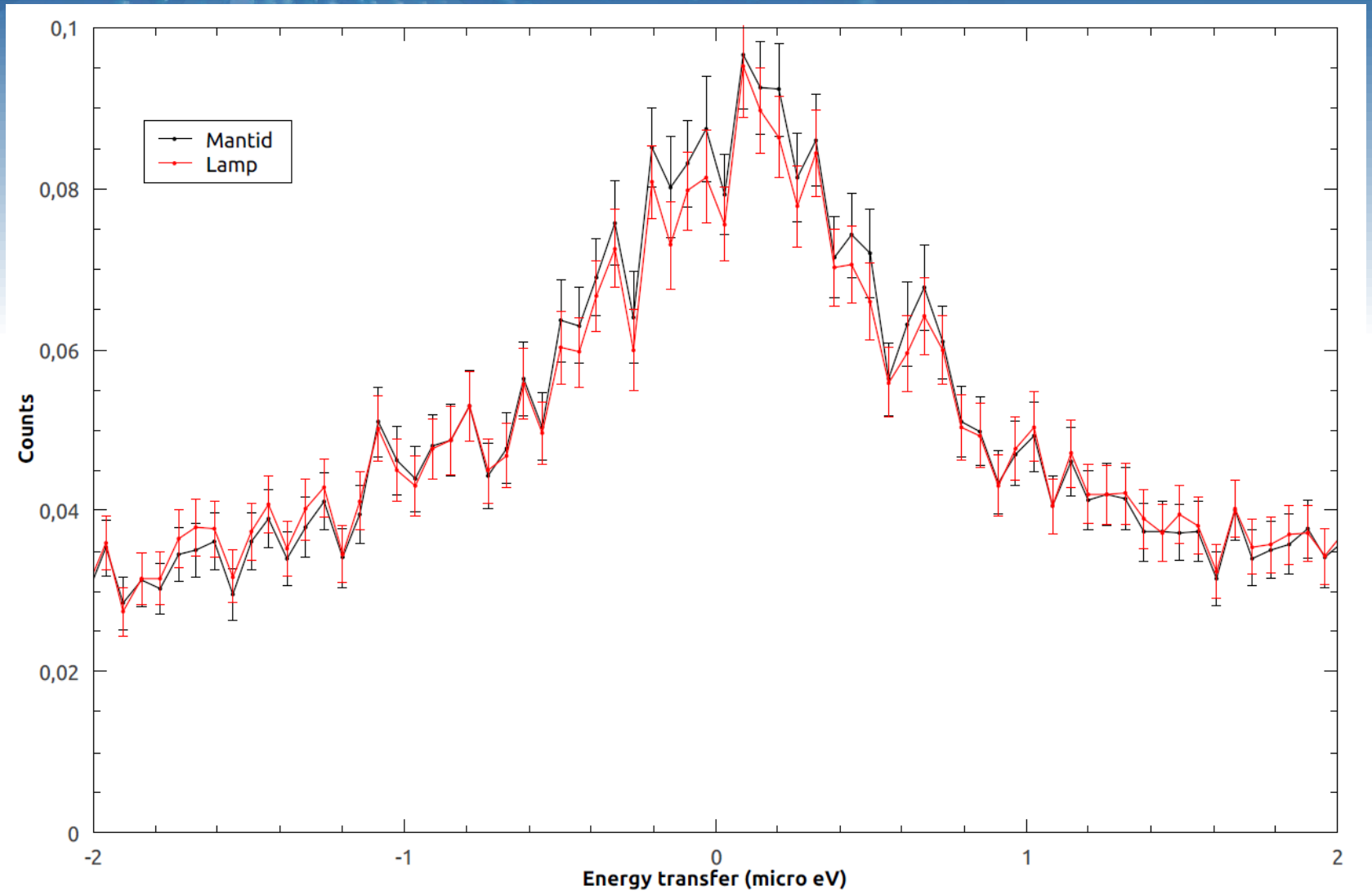
Progress


Indirect Data Reduction
Instrument
IN16B
Analyser
silicon
Reflection
111
ILL Energy Transfer
ILL Calibration
Transmission
Symmetrise
S(Q, w)
Moments
Input
Run File
Browse
Calibration
Use Calibration
File
Browse
Grouping
Default
Options
Use Mirror Mode
Output
Plot Result
Save Result
?
Py
Run
Manage Directories

Progress



Progress


Mantid
Lamp
Counts
0,1
0,08
0,06
0,04
0,02
0
-2
-1
0
1
2
Energy transfer (micro eV)

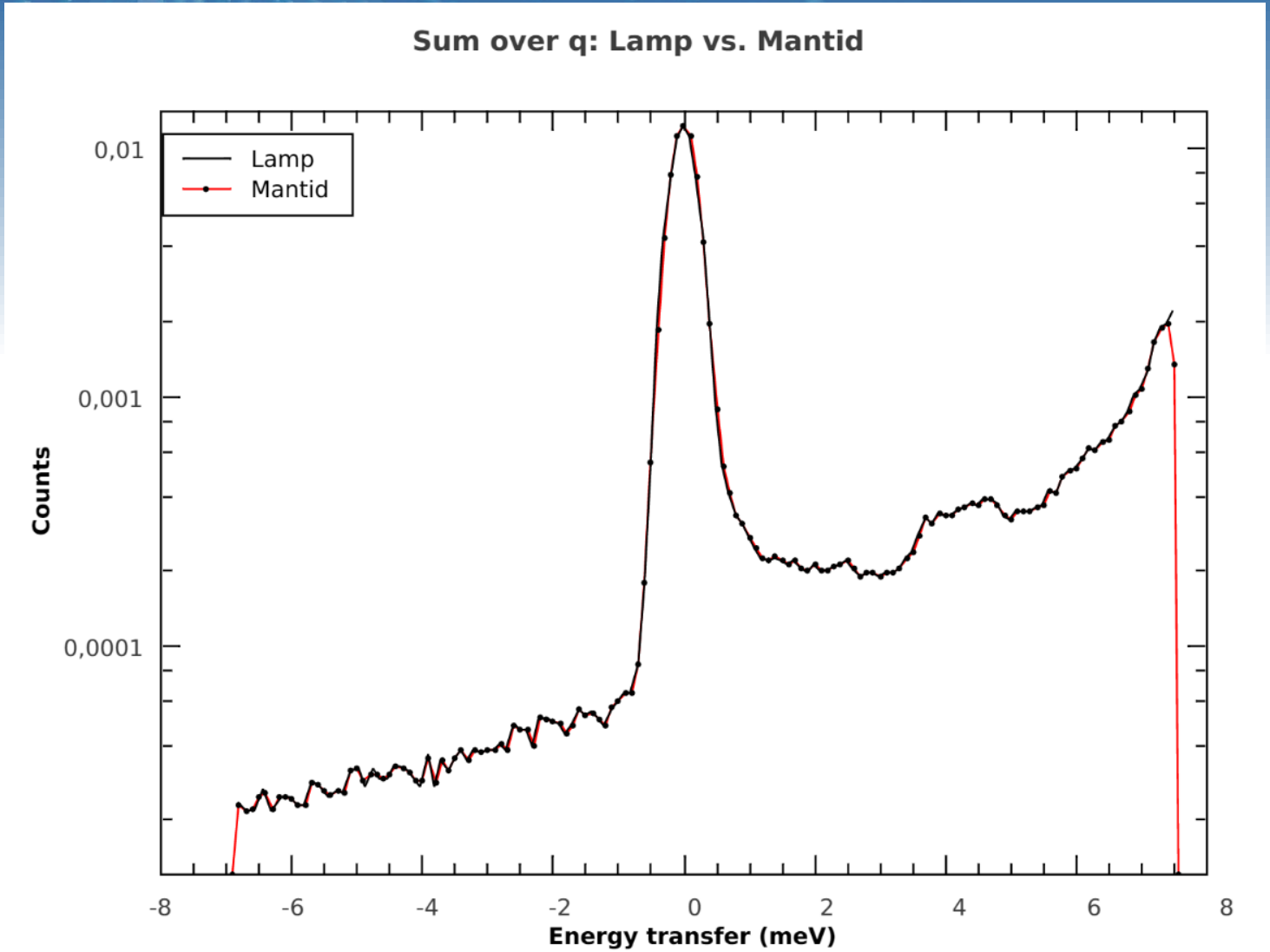
Progress

- Backscattering – to do
  - Implement mirror modes options, especially merging half data sets after fitting and aligning elastic peak positions (using vanadium data set if no elastic peak in sample data)
  - Finalise workflow and revisit GUI
  - Treat elastic scan data

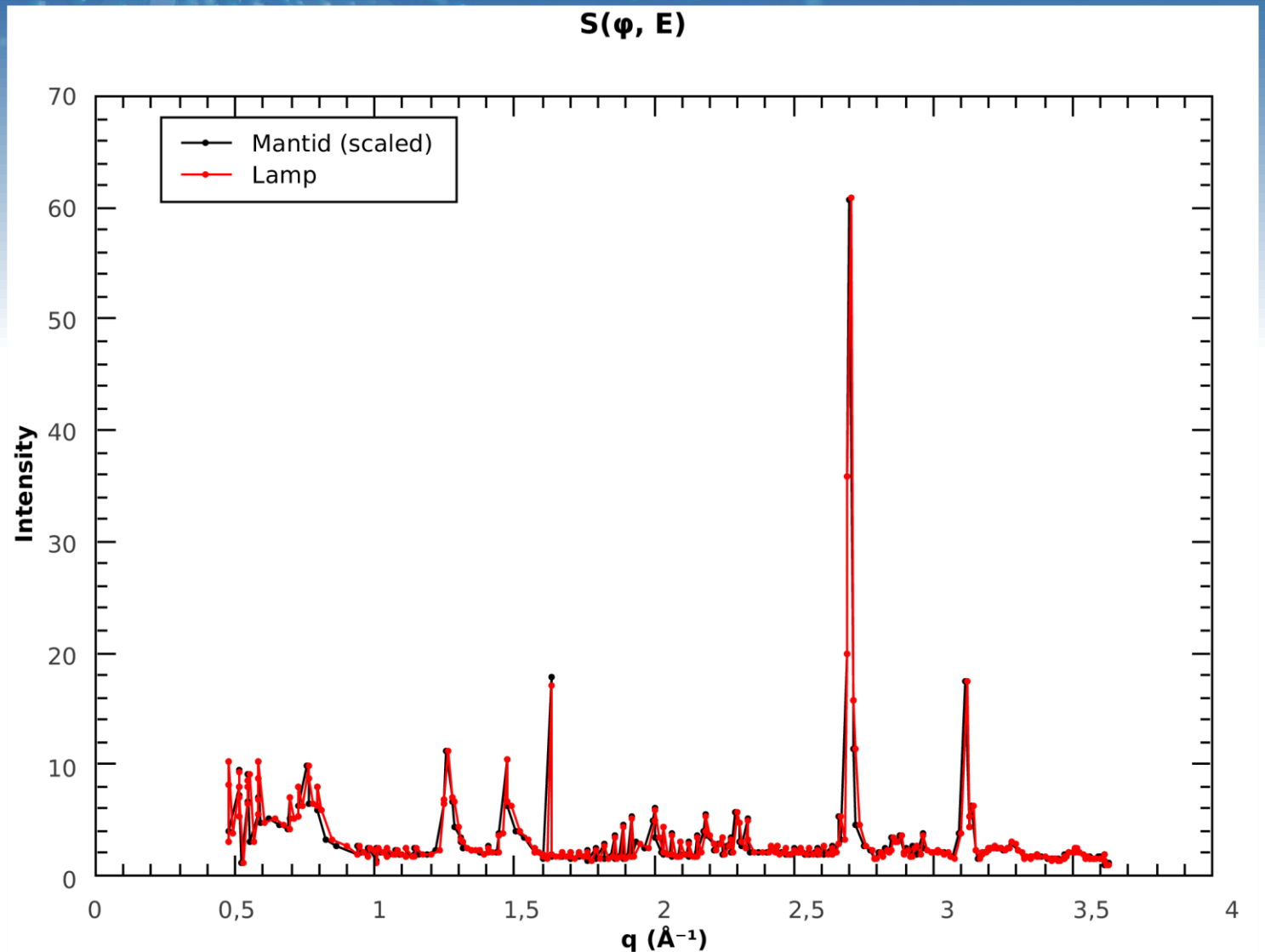
Progress

- Time-of-Flight (Antti (IN4) and Ian (IN6))
  - Initial work in NMI3 and by summer student in 2015 (on IN6 (and D33)) → discrepancies in Q and E in S(Q,E)
  - Scripts to compare data treatment
  - Q-dependence discrepancy due to detector geometry
  - E-dependence discrepancy due to detector, neutron wavelength efficiency correction

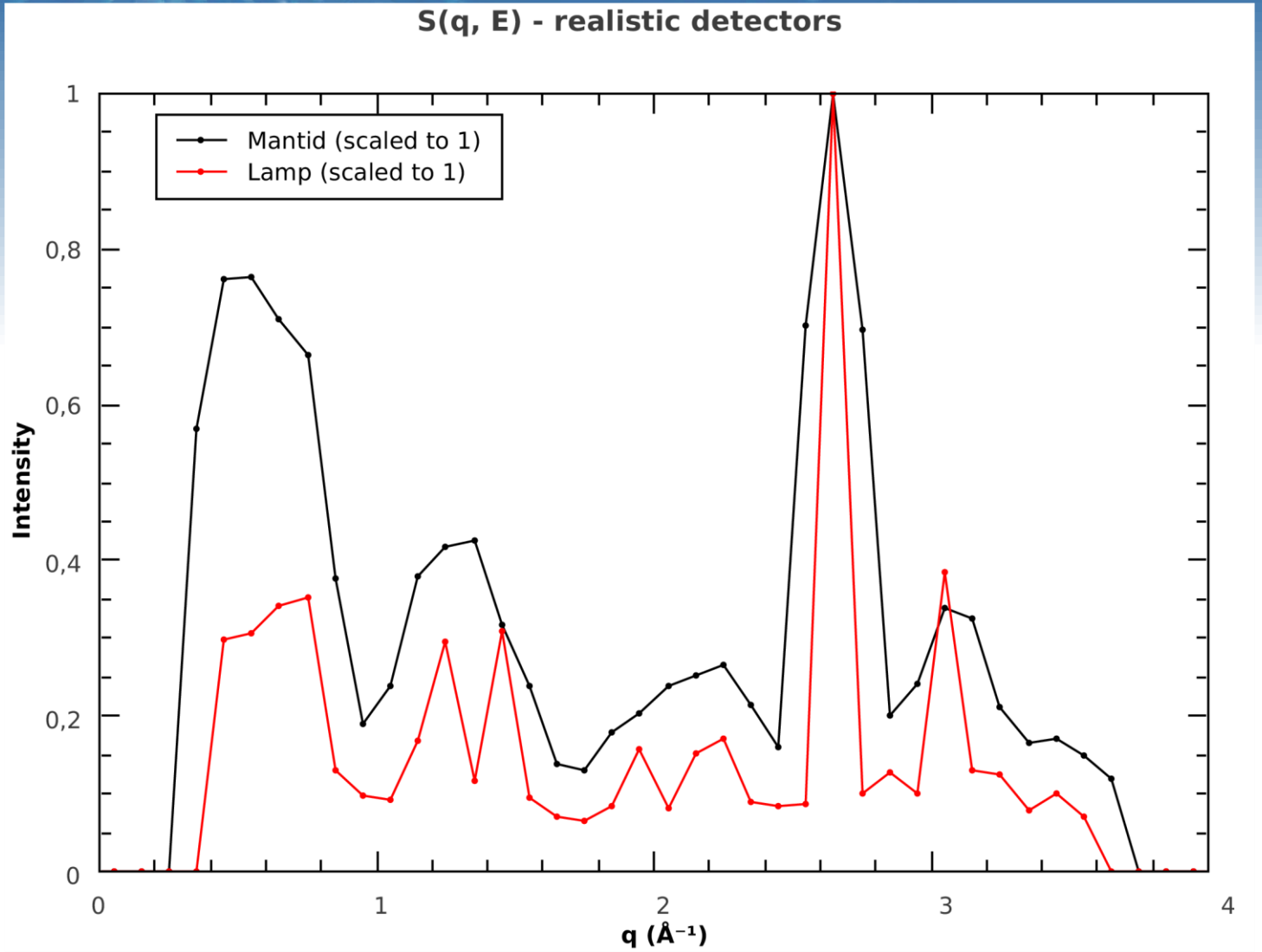
Progress


Sum over q: Lamp vs. Mantid
Lamp
Mantid
0,01
0,001
0,0001
Counts
-8
-6
-4
-2
0
2
4
6
8
Energy transfer (meV)

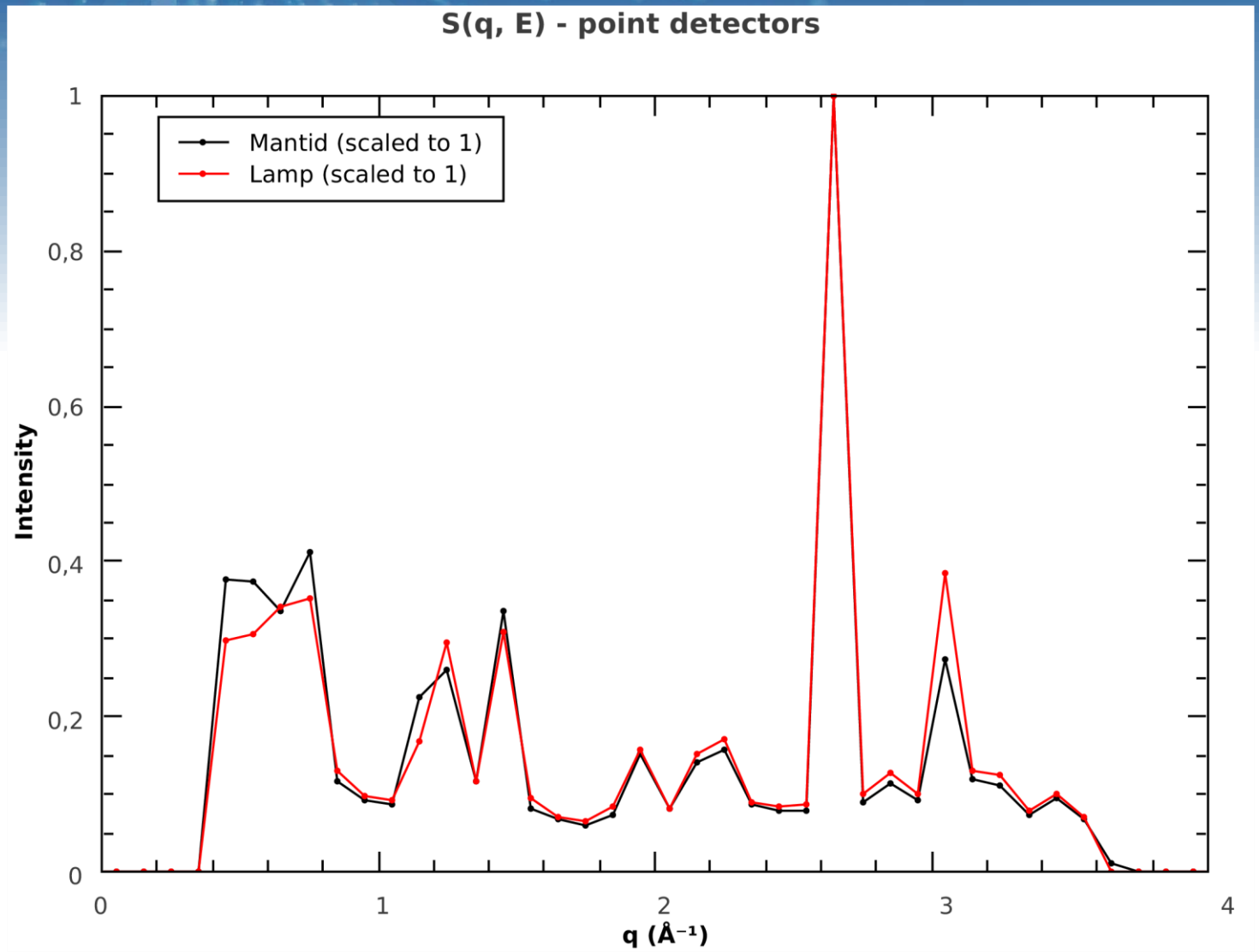
Progress


S(φ, E)
Mantid (scaled)
Lamp
Intensity
q (Å⁻¹)
0
10
20
30
40
50
60
70
0
0,5
1
1,5
2
2,5
3
3,5
4

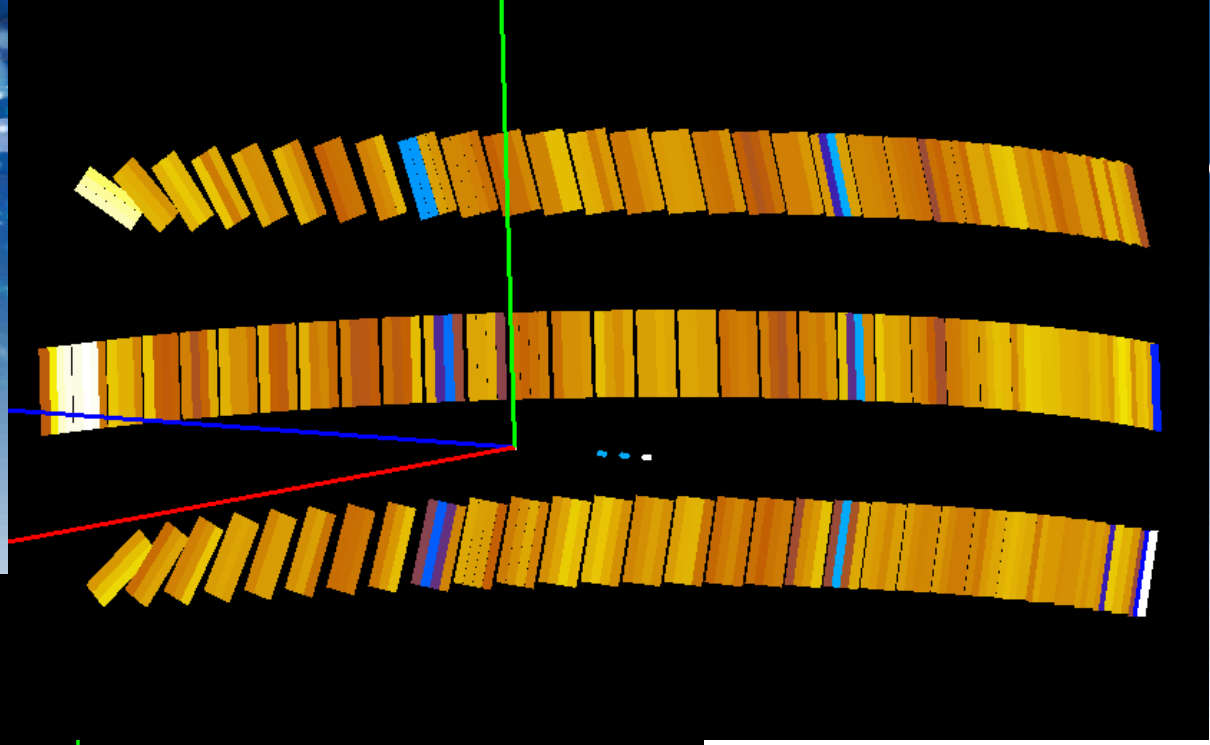
Progress

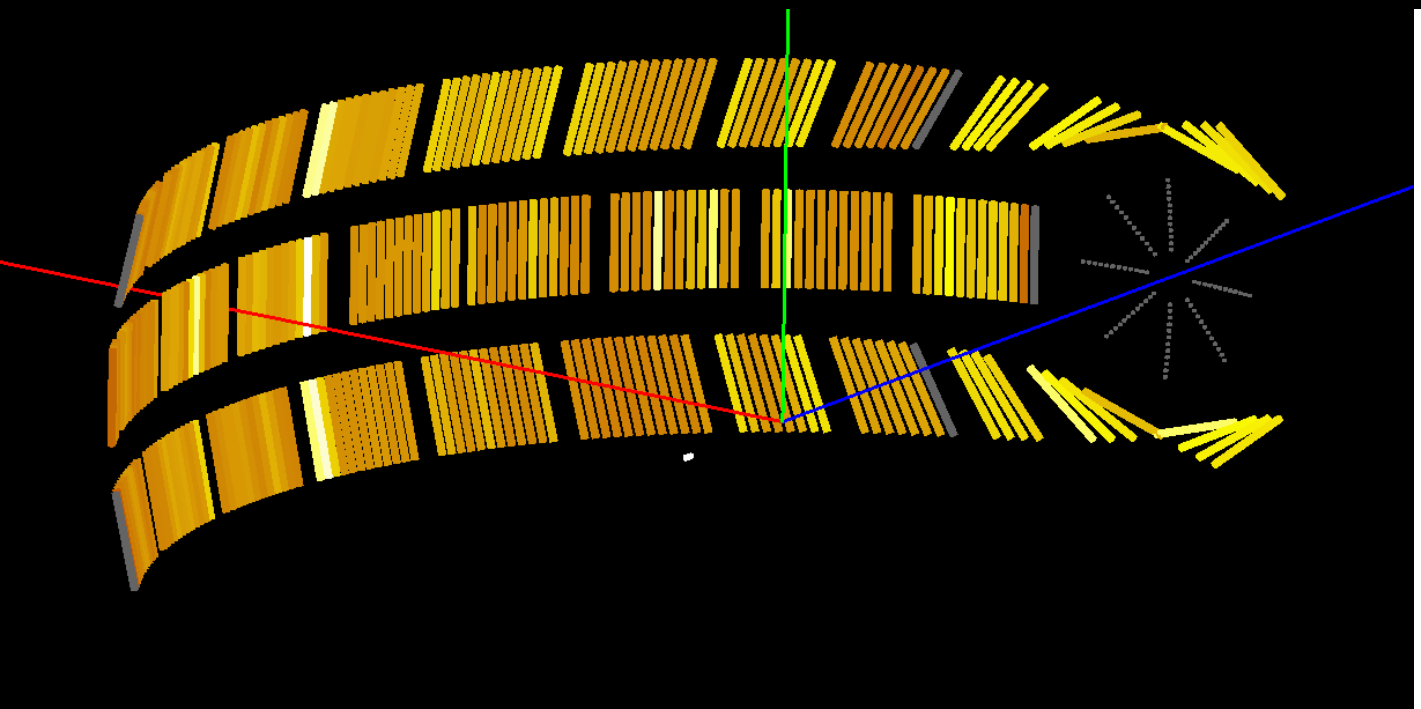

S(q, E) - realistic detectors
Mantid (scaled to 1)
Lamp (scaled to 1)
Intensity
q (Å⁻¹)
0
0,2
0,4
0,6
0,8
1
0
1
2
3
4

Progress


S(q, E) - point detectors
Mantid (scaled to 1)
Lamp (scaled to 1)
Intensity
q (Å⁻¹)
0
0,2
0,4
0,6
0,8
1
0
1
2
3
4

Progress





Progress

- Time-of-Flight – to do
  - Validate IDF's – choose point detectors OR full detector geometry
  - Finalise data reduction workflows with inst scientists – adapt DGSReduction GUI
  - Provide all outputs: S(Q,w), GDOS (S(phi,E) or S(Q,E)), susceptibility,…
  - IN5 – full 3D data treatment (exists) and/or reduction to 2D for powders/liquids as in LAMP

Progress

- Other, related work
  - Compiling Mantid on Mac
  - Multiple file load for IN16
    - Using Mantid core functionality instead of IN16 specific with Python scripts
  - Export/import Lamp/Mantid for benchmarking

Future progress

- September → Presentation of Backscattering & TOF to spectroscopy group – deploy and support software
- Scanning instruments – Ian
- Discuss, choose and start work on next techniques (SANS,…)
- Verena, Ian, Antti, Gagik working individually

BASTILLE – Interim organisation

- Technical project leader - Ian Bush
- Scientific project leader (until recruitment of new group leader)
  - Techniques: TOF, BS, SANS, REF,…
  - Attend daily meetings and give scientific input
  - Lead weekly meetings with Ian
  - Ensure efficient interaction with scientists
  - Report to PMC
- Propose Miguel Gonzalez