Instrument Data Scientist for Neutron Spectroscopy

BIFROST and CSPEC
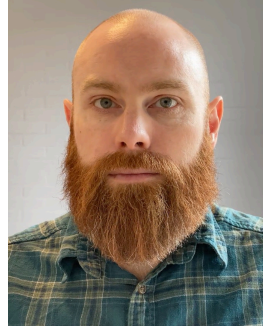
GREGORY TUCKER

2024-04-17

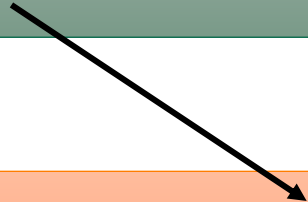# Spectroscopy instruments

Where are the (other) Instrument Data Scientists?

Tranche 1
BIFROST

Tranche 2
CSPEC

Tranche 3
CSPEC
TREX   **MIRACLES**   **VESPA**

icons created by Freepik - Flaticon

Progress for BIFROST & CSPEC

Accelerating towards commissioning

Successes / achievements

- McStas to NeXus HDF5

- Good communication through weekly meetings

Failures / setbacks

- Simon Ward (Data Analysis) left

- Student project, identifying detector failures near real-time via image recognition

- New Spectroscopy Division in Science
  - BIFROST, CSPEC, VESPA at present

- Henrik Jacobsen (Data Analysis) started
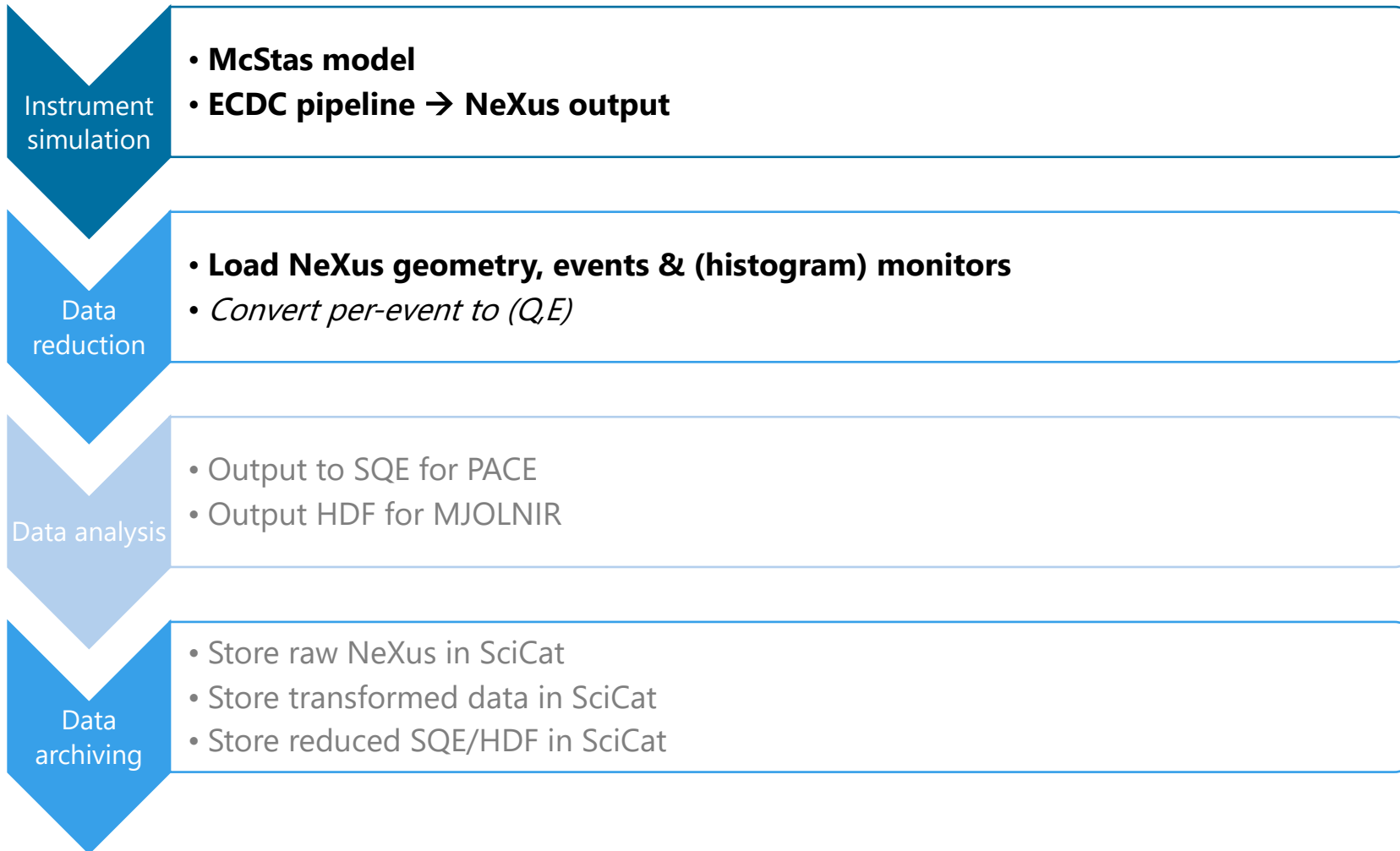
Opportunities / accelerating measures

- Behind schedule converting NeXus events from (`relative time, pixel id`) to ($\mathbf{Q}$,E)

Threats / risks

2024-04-17

Data pipeline status

BIFROST

Instrument simulation
- **McStas model**
- **ECDC pipeline → NeXus output**

Data reduction
- **Load NeXus geometry, events & (histogram) monitors**
- *Convert per-event to (Q,E)*

Data analysis
- Output to SQE for PACE
- Output HDF for MJOLNIR

Data archiving
- Store raw NeXus in SciCat
- Store transformed data in SciCat
- Store reduced SQE/HDF in SciCat

Completed
In progress
To be done

2024-04-17

Data pipeline status

CSPEC

Instrument simulation
- *McStas model*
- **ECDC pipeline → NeXus output**

Data reduction
- **Load NeXus geometry, events & (histogram) monitors**
- Convert per-event to (Q,E)

Data analysis
- Output to SQE for PACE
- Output NXspe, MDWorkspace for Dave, Mantid, etc.

Data archiving
- Store raw NeXus in SciCat
- Store transformed data in SciCat
- Store reduced data in SciCat

Completed
In progress
To be done

2024-04-17

Major milestones
Updates to October 2023 report

✚ Simulated data through readout chain   Q2 '23

- `McStas` simulated neutrons and parameter data for BIFROST has been written to a NeXus file
    - ✚ the structure of the NeXus file may ~~not~~ match that of real instrument files
    - ✚ beam monitors produce neutron ~~events, where~~ histograms ~~are~~ as anticipated for real data files
    - ✚ information needed for transformation to (Q, E) ~~is missing, which is counter to FAIR practices~~
    - ✚ whole-instrument simulations ~~only~~ give reasonable count-rates ~~for white-beam directed at vanadium~~
- ▬ These data have not been analysed in `scipp`
- ✚ ~~Highlights need for pre-computed primary spectrometer MCPL files~~
- ✚ Completed ~~summer 2023~~

Major milestones
Updates to October 2023 report

➖ First simulated experiment complete   Q4 '23

➕ Suitable simulated samples selected with BIFROST Instrument Scientist
- Quantum Harmonic Oscillator for ($|Q|$, E)
- Single magnon for (**Q**, E)

➕ Automatic primary spectrometer MCPL generation, storage, and retrieval for new simulator scanning tool nearly ~~ready~~
           ^s
- This ~~should~~ make simulations orders of magnitude faster at cost of extra correlation

➖ ~~On track for completed simulated experiments by end of Q4.~~

➕ ~~Plan to~~ produce NeXus files via simulations with command-line interface, e.g.,

```
[user@visa]$ simulate BIFROST.instr max_ei=20 psi=1:180 a4=90:2.5:92.5 -n 1000000

  Scanning (psi, a4) over 360 points:
   pt     psi      a4     counts
  ----------------------------
    1    1.00   90.00     12345
    2    2.00   90.00     67890
  ...
  359  179.00   92.50     12345
  360  180.00   92.50     67890
  ----------------------------
  Scan saved to BIFROST_20231025_104039.nxs
```

Major milestones

Updates to October 2023 report

Transformation workflow tested on simulated experiment data Q3 '24

- Depends strongly on the availability of simulated experiment data
- General plan in place for data transformation
    - High confidence in `scipp` tools
- Positive outlook for feasible on-time completion.
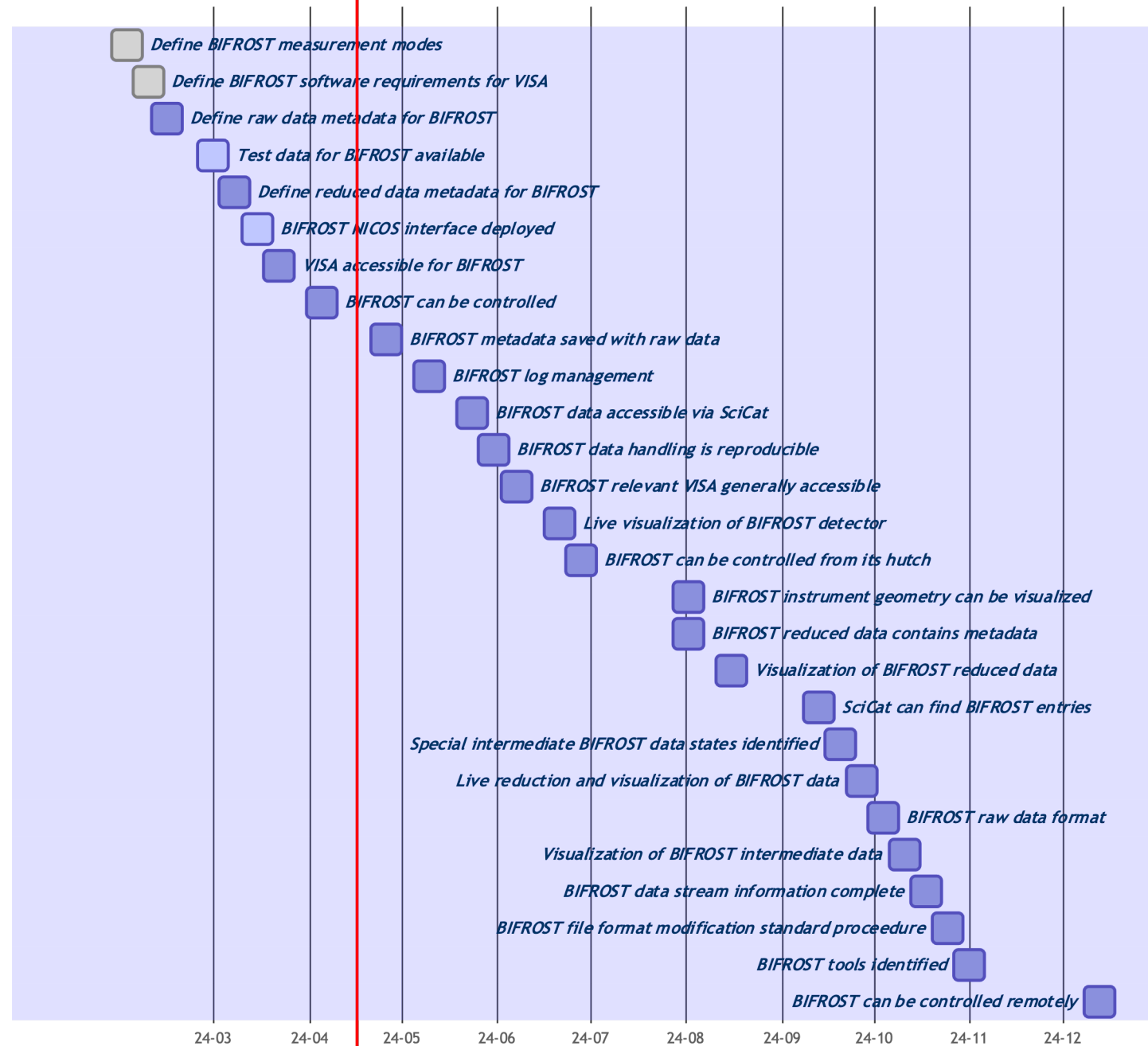
➕ In progress on S(E) data

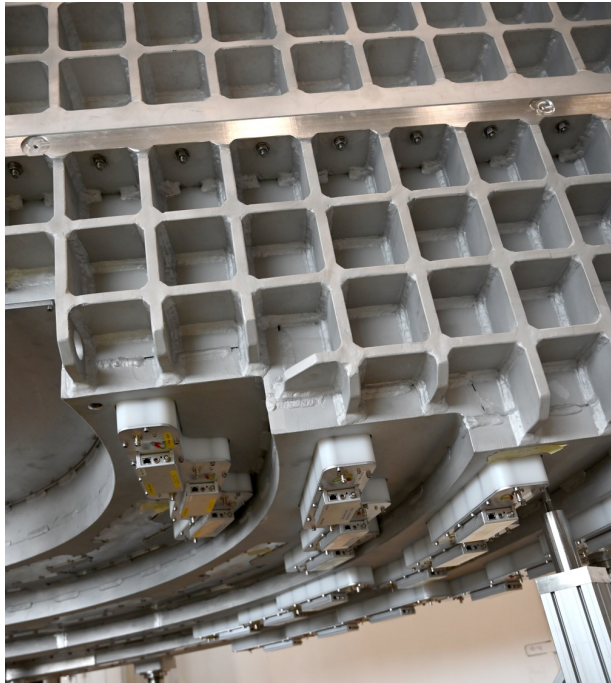➖ Delaying generation of S($\mathbf{Q}$, E) data

Schedule

Spectroscopy Ready For Hot Commissioning milestones

Done
In Progress
To Do

Define BIFROST measurement modes
Define BIFROST software requirements for VISA
Define raw data metadata for BIFROST
Test data for BIFROST available
Define reduced data metadata for BIFROST
BIFROST NICOS interface deployed
VISA accessible for BIFROST
BIFROST can be controlled
BIFROST metadata saved with raw data
BIFROST log management
BIFROST data accessible via SciCat
BIFROST data handling is reproducible
BIFROST relevant VISA generally accessible
Live visualization of BIFROST detector
BIFROST can be controlled from its hutch
BIFROST instrument geometry can be visualized
BIFROST reduced data contains metadata
Visualization of BIFROST reduced data
SciCat can find BIFROST entries
Special intermediate BIFROST data states identified
Live reduction and visualization of BIFROST data
BIFROST raw data format
Visualization of BIFROST intermediate data
BIFROST data stream information complete
BIFROST file format modification standard proceedure
BIFROST tools identified
BIFROST can be controlled remotely

24-03   24-04   24-05   24-06   24-07   24-08   24-09   24-10   24-11   24-12
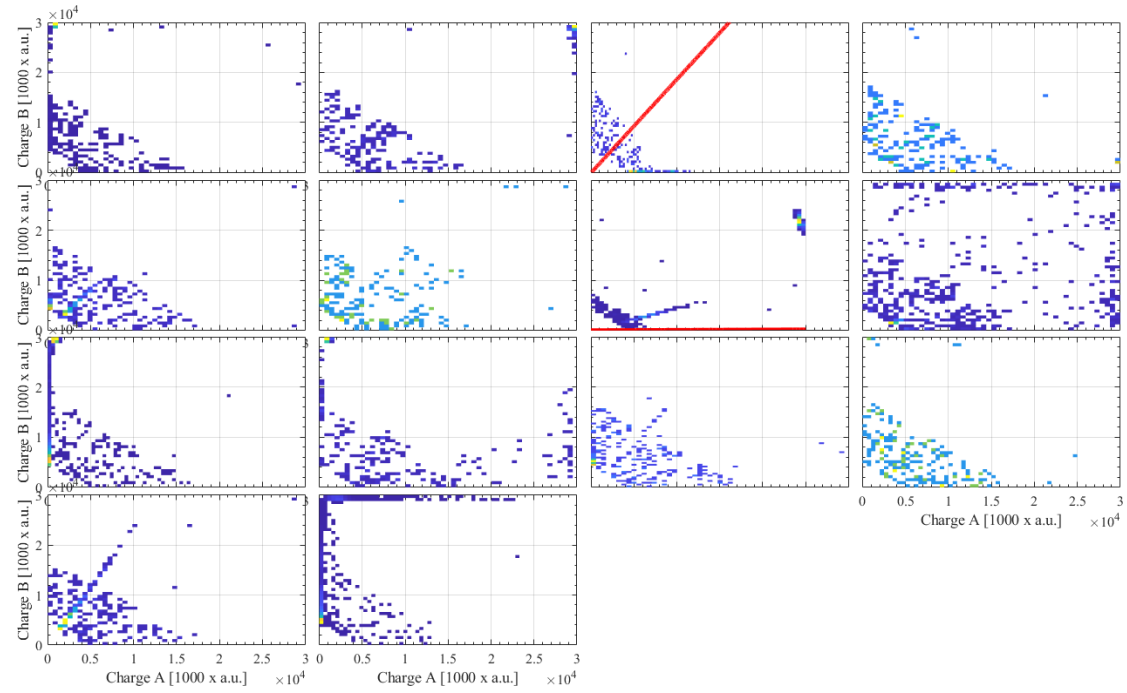
2024-04-17

Concluding remarks

BIFROST is coming together

Detectors mounted to the tank

Cosmic neutrons detected in E01

Opportunity to exercise the whole data collection and curation pathway soon