Update from BIFROST, CSPEC

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DMSC

2023-10-26 DMSC STAP



Overview

- Dashboards
- Milestones
- Interactions
- Major risks

Update from BIFROST, CSPEC

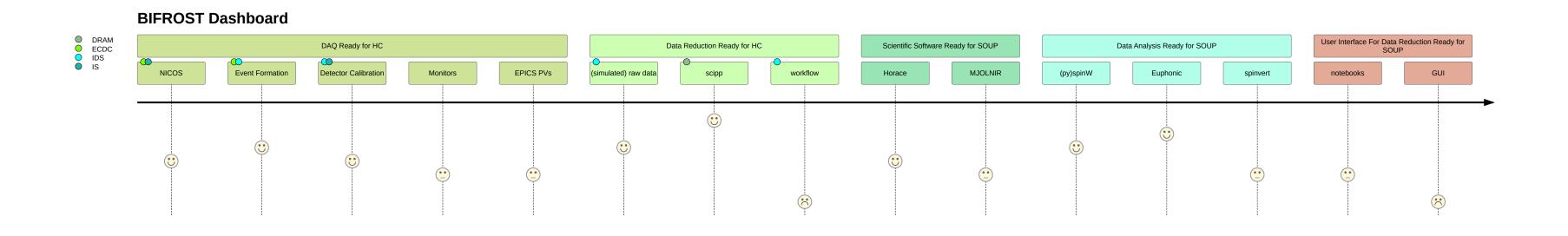
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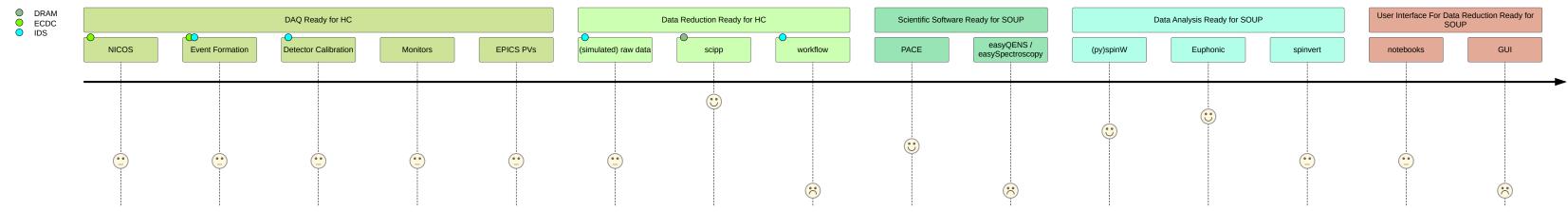
2023-10-26 DMSC STAP



Dashboards



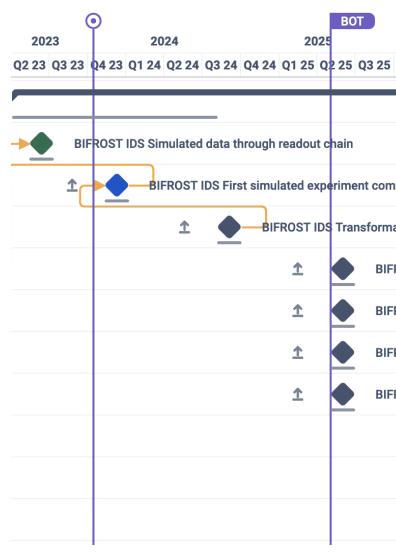
CSPEC Dashboard





Milestones

Clearly delineate the milestones for the next 6 to 18 months and provide us a status for those.



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Simulated data through readout chain

- 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 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

Q2 '23



First simulated experiment complete

- 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
 - 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
```

Q4 '23



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.



Interactions

A discussion of interaction with the instrument teams is also helpful.

BIFROST

- Instrument Scientist visits DMSC regularly
- Interaction with ICEB members, e.g., through Danscatt

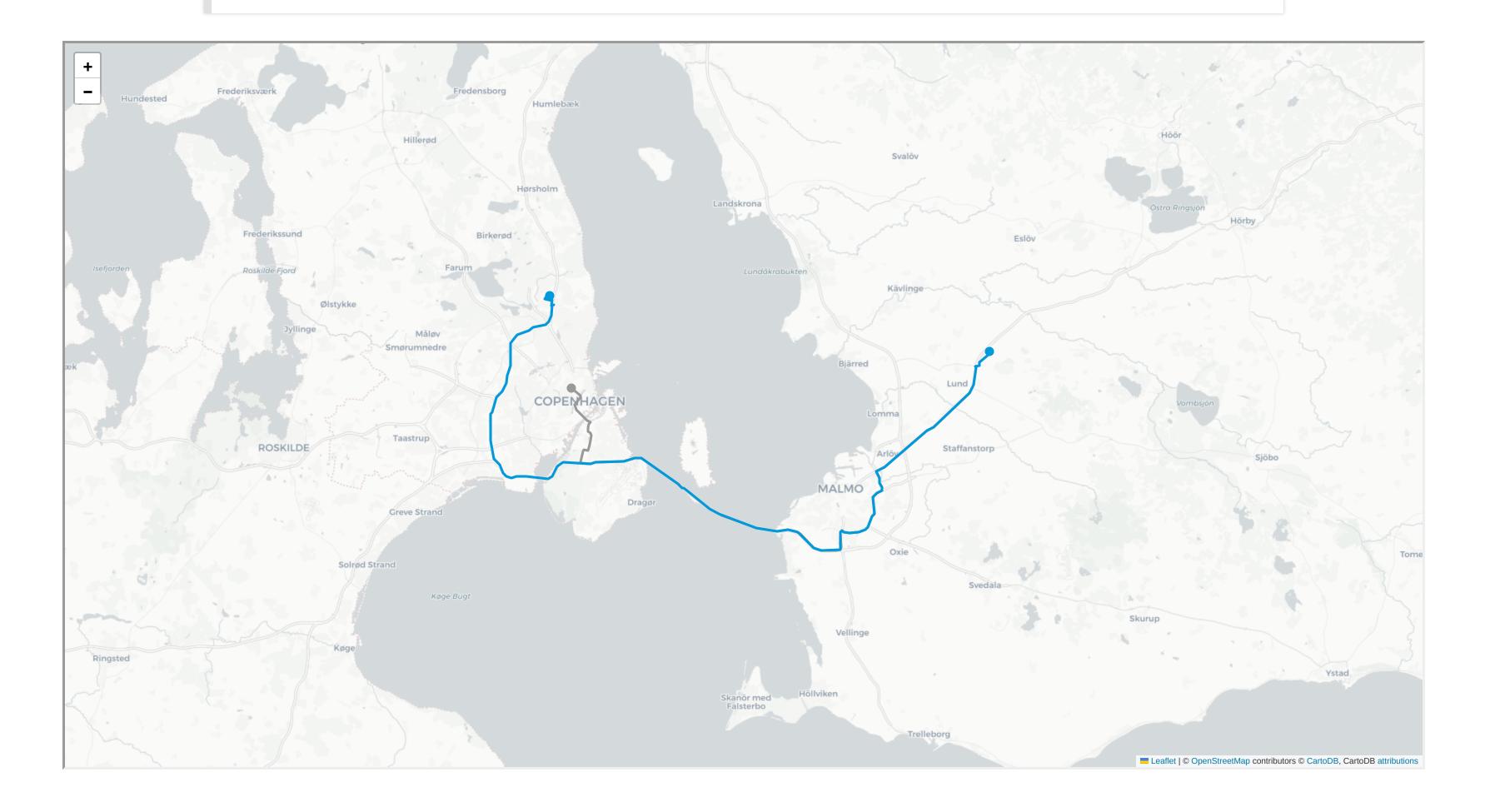
CSPEC

- Instrument Scientist on maternity leave
 - Regular meetings before & anticipated to resume early next year



Major risks

Finally, a summary of major risks, "What keeps you awake at night?" should be provided.





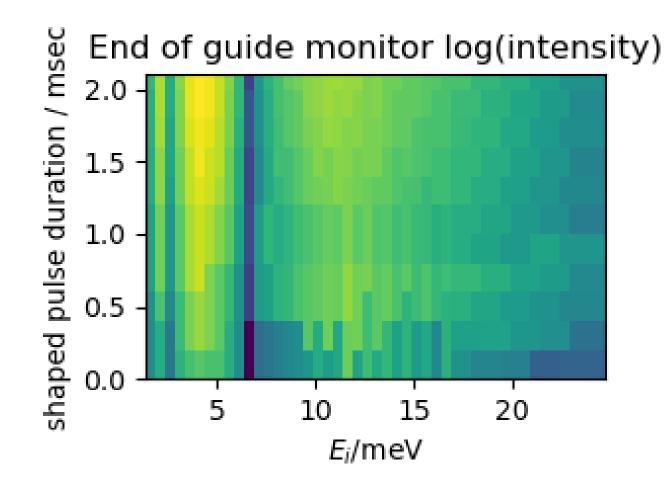
Technical discussions

Technical discussions, though interesting, should be limited.



Running the primary and seconary spectrometer simulations separately

run BIFROST.instr order=14 ei=1.7:0.5:24.7 t=0.0001:0.0002:0.002248 --split-at=split_at -m -n 10000



- Cached minimum-particle-count MCPL files
 - slow to generate fast to reuse
- This 517-point mesh scan of expected (E_i , t) parameter space takes 135 seconds the first time and ~50 seconds when repeated
 - strong intensity variation with *E_i* is likely a failure of the simulation, but needs further investigation

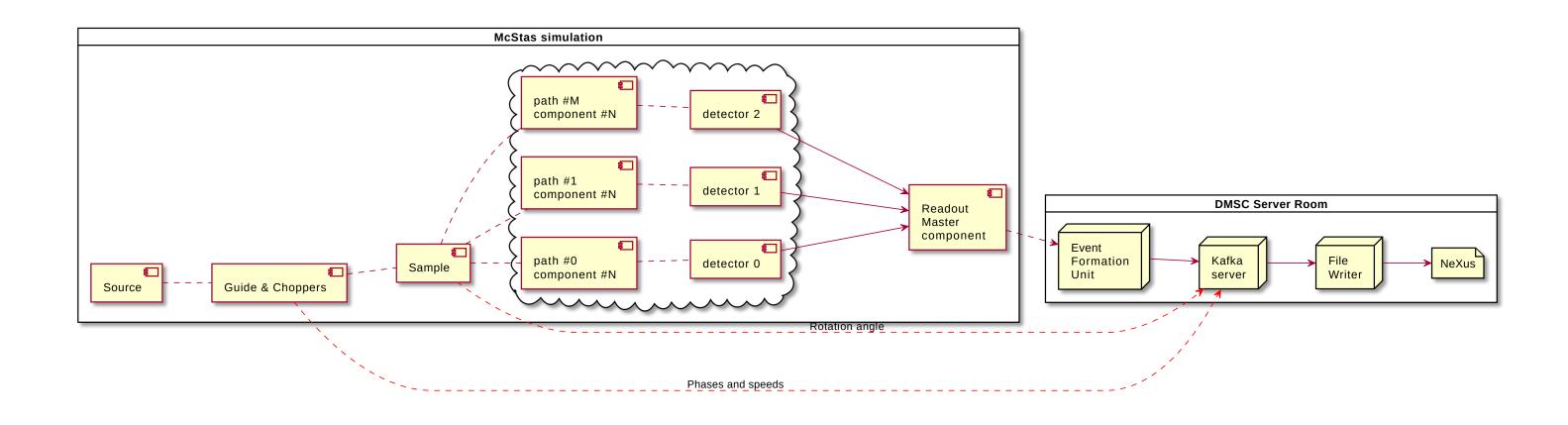
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BIFROST simulations

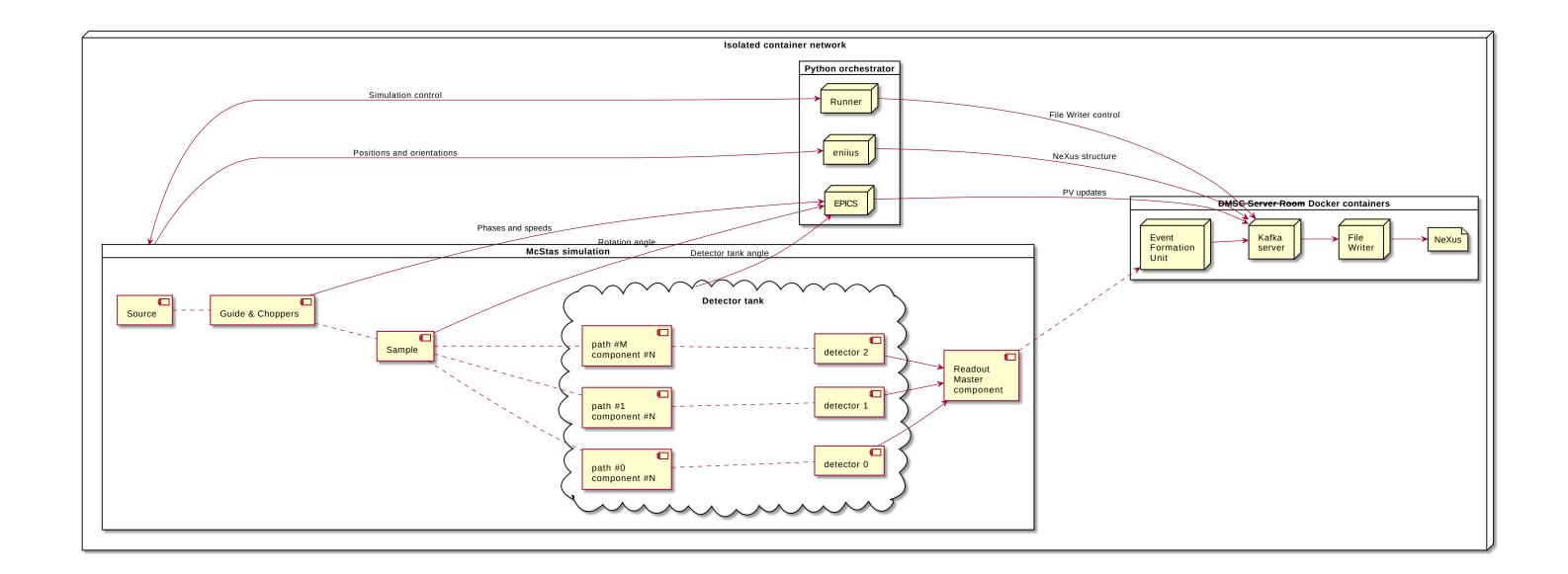
Reminder

- BIFROST is the first CAMEA Time-of-Flight spectrometer
- Need realistic data to test workflows
 - data transformation
 - instrument calibration





Implementation (simplified)





Questions?

