OAK RIDGE National Laboratory

Data and the software for Neutron Scattering at the SNS and HFIR

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ORNL is managed by UT-Battelle, LLC for the US Department of Energy

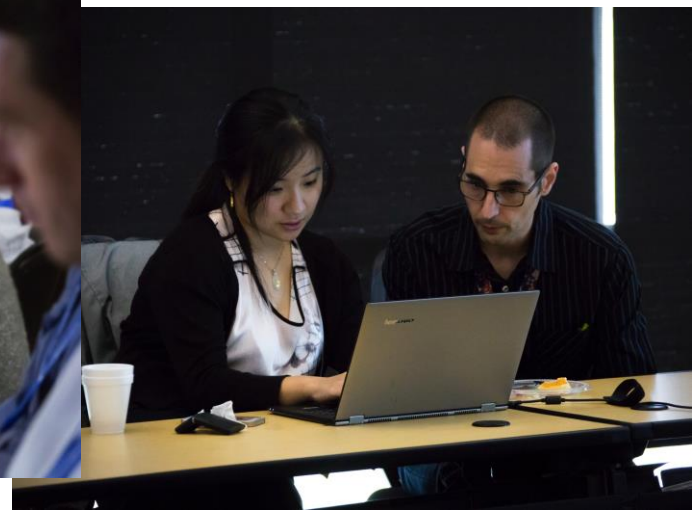
U.S. DEPARTMENT OF ENERGY

Outline

- Our Customers (Users)
- Overview of our Instruments
- Scope of Data
- Software Ecosystem
- Reduction Software
- Comparison of Models

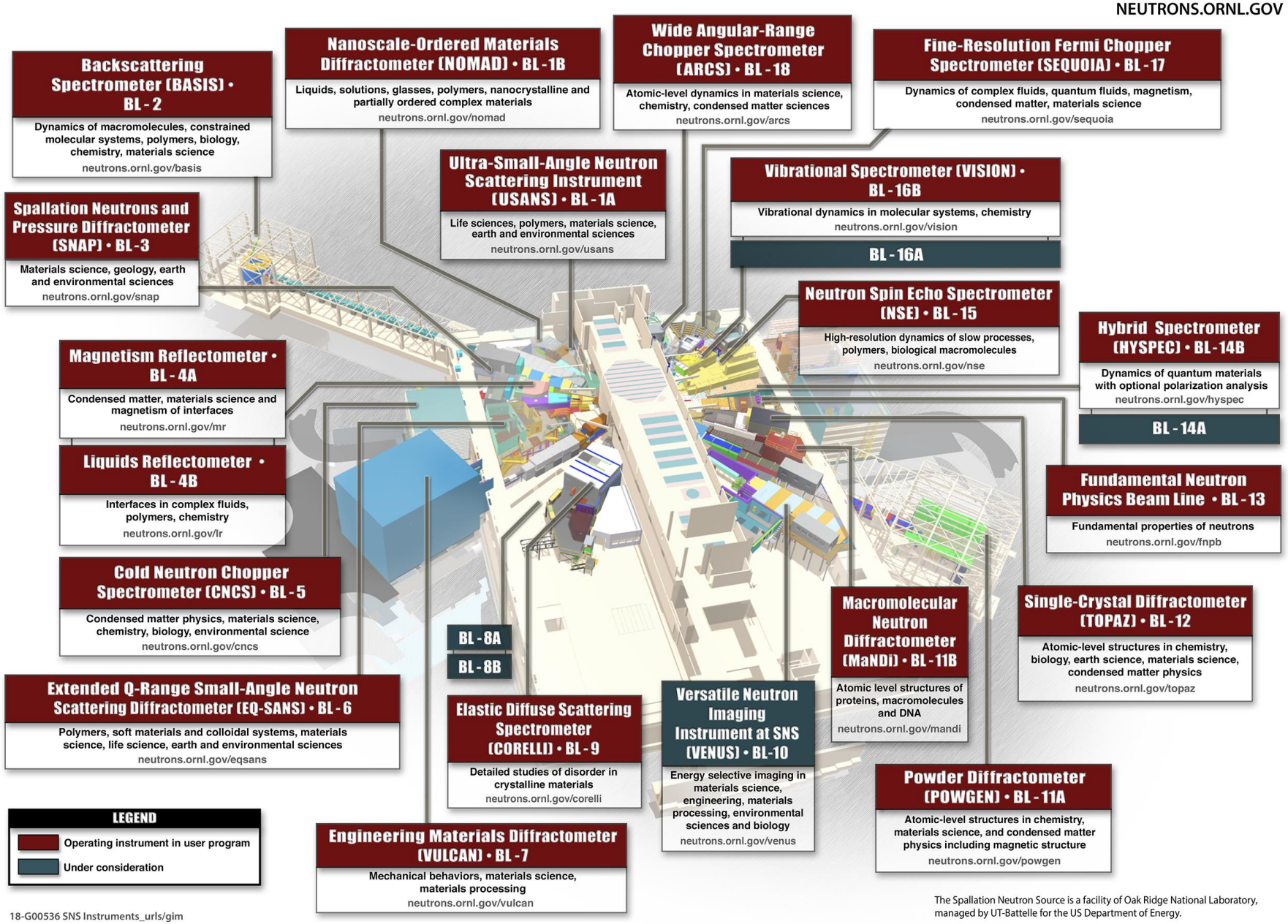
Users

- ~1000 unique users every year
- Usually groups of 2 – 5
- Broad scientific interest
  - Quantum materials, thermoelectrics, catalysts, battery materials, superconductors, polymers, macro molecules, bio fuels, engineering, materials, and many more.



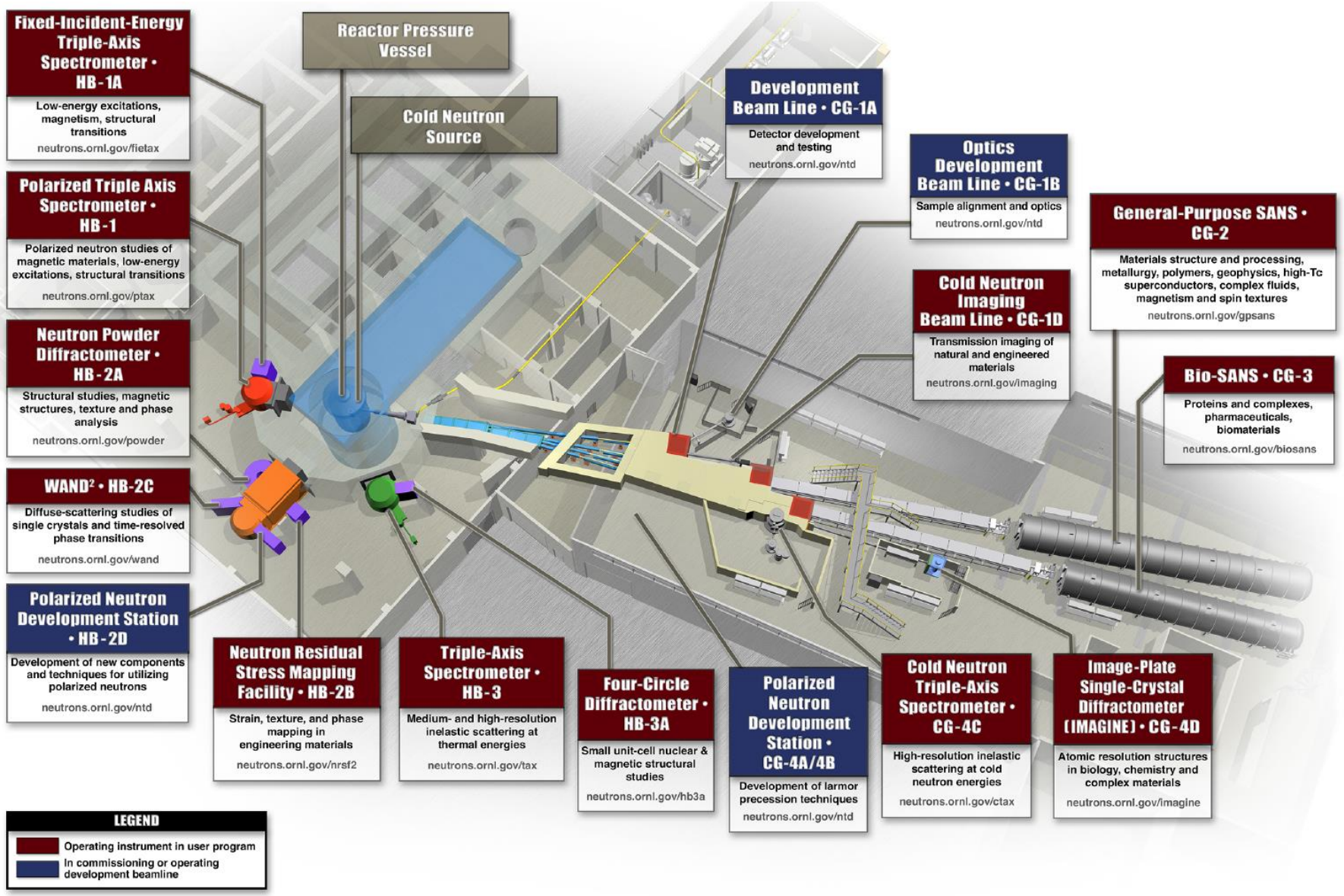
Spallation Neutron Source instruments

- 18 Instruments
  - In User Program
  - For studying materials
- Pulsed; 60 Hz; 1.4MW
- Operates ~ 200 days per year
- experiment changes ~ 1 - 5 days per instrument

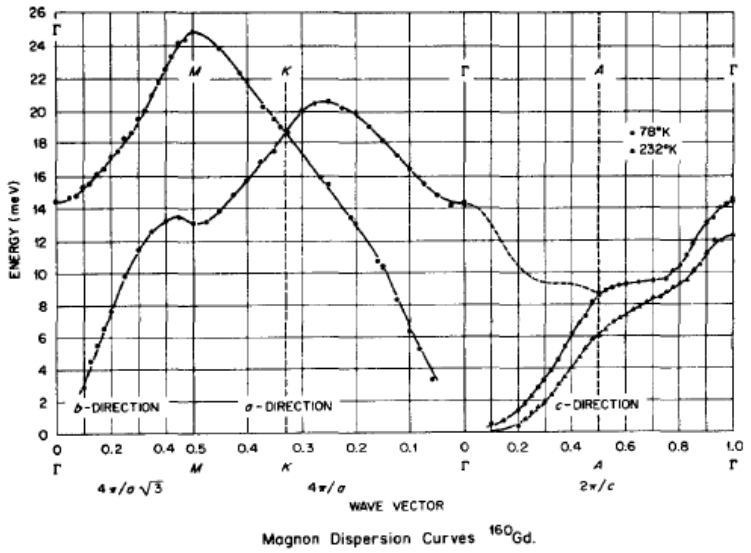


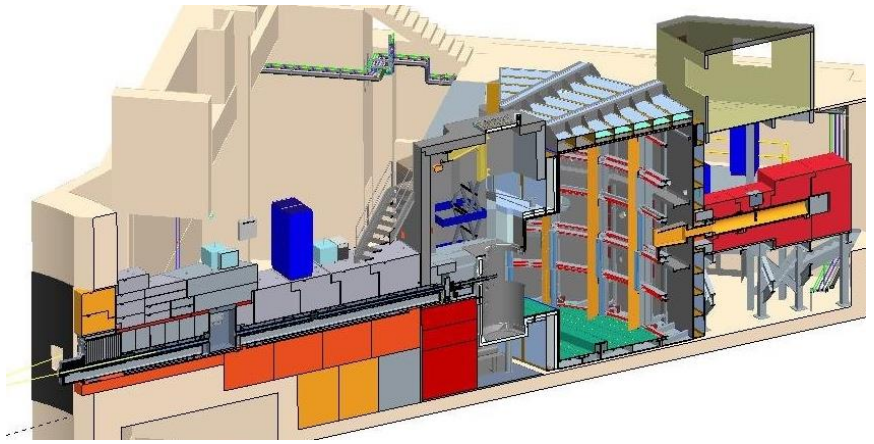
High Flux Isotope Reactor Instruments

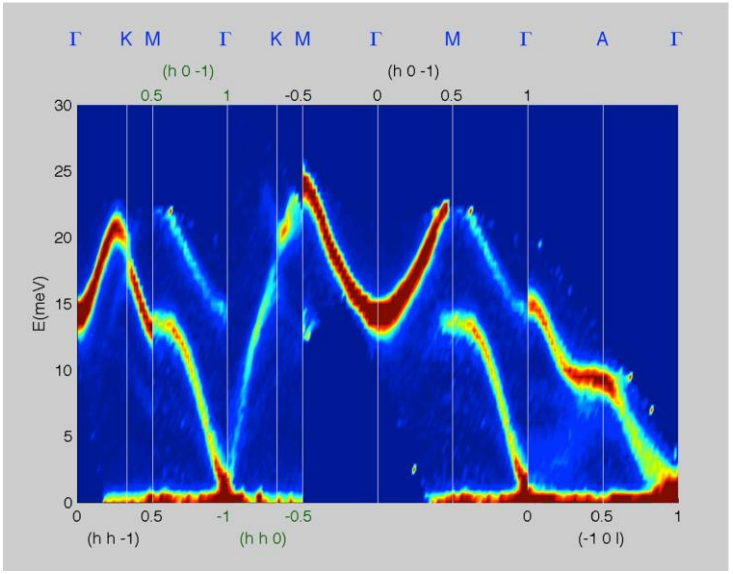
- 12 Instruments
  - In User Program
  - Materials studies
- Continuous 85 MW
- Operates 7, 24 day cycles
- Experiment changes every ~ 1 - 5 days per instrument

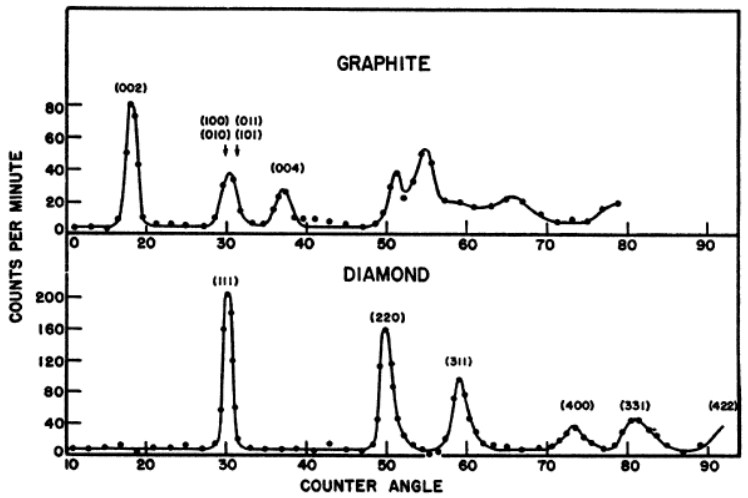


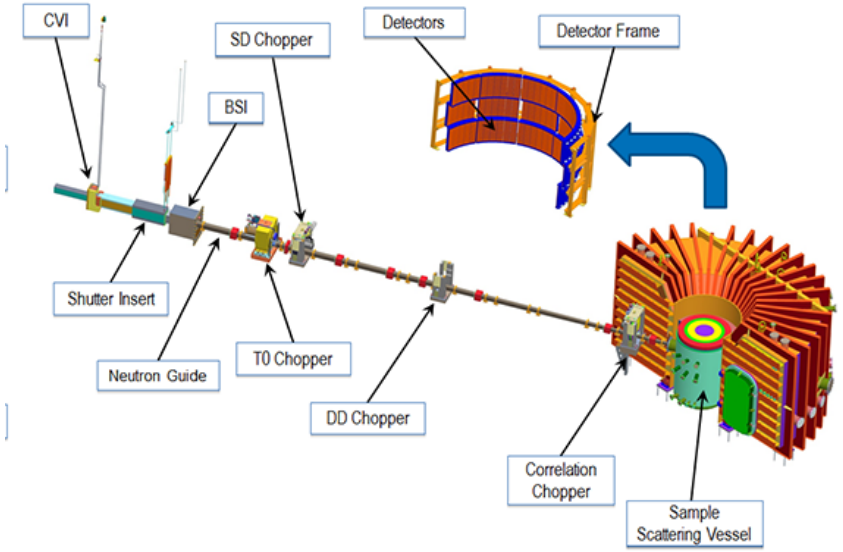
Neutron data has expanded in size and complexity

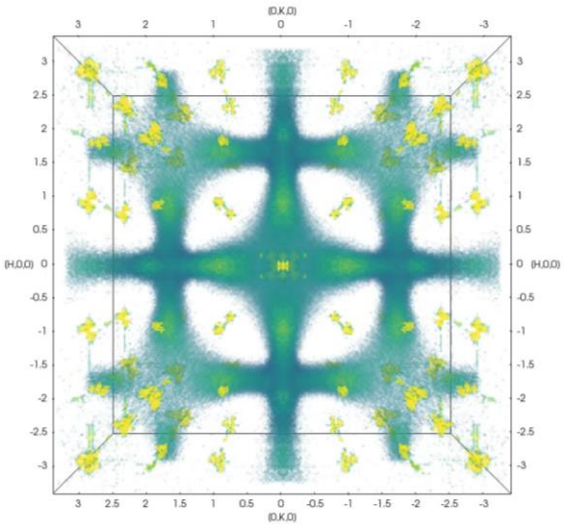










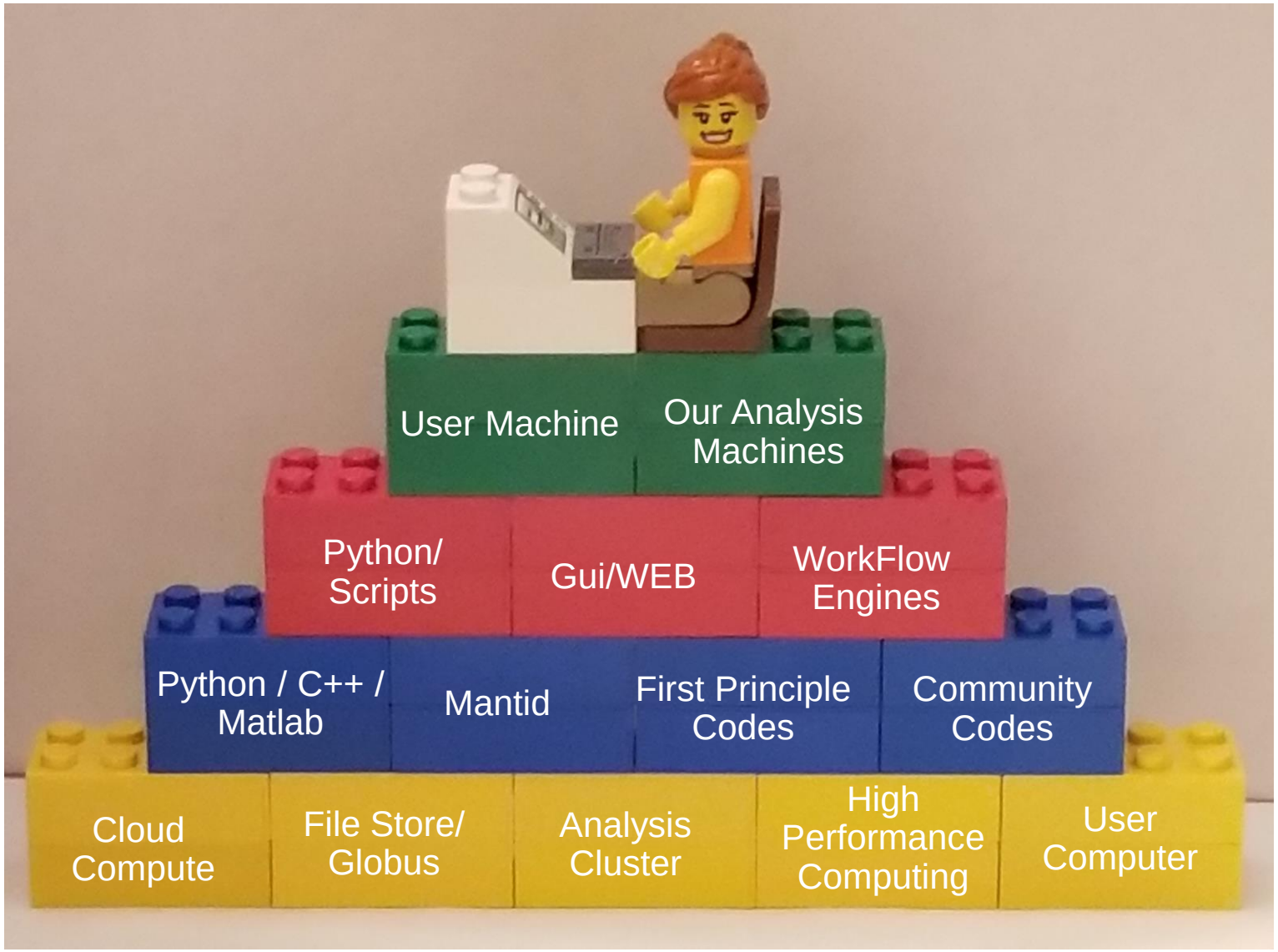


Data

- < 5M events /s /instrument ~ 60 MB/s/instrument of raw data on the stream
- Saved to HDF5 files using NeXus schema (https://www.nexusformat.org/)
- Capturing as much metadata as we can
- Cataloging using MongoDB based solution Oncat. (Oncat.ornl.gov)
- Users usually
  - work with large data on our machines downloading results via sftp client
  - Small data they download via sftp client to their own machine
  - Can use globus to transfer large data (Leveraging ORNL computing)

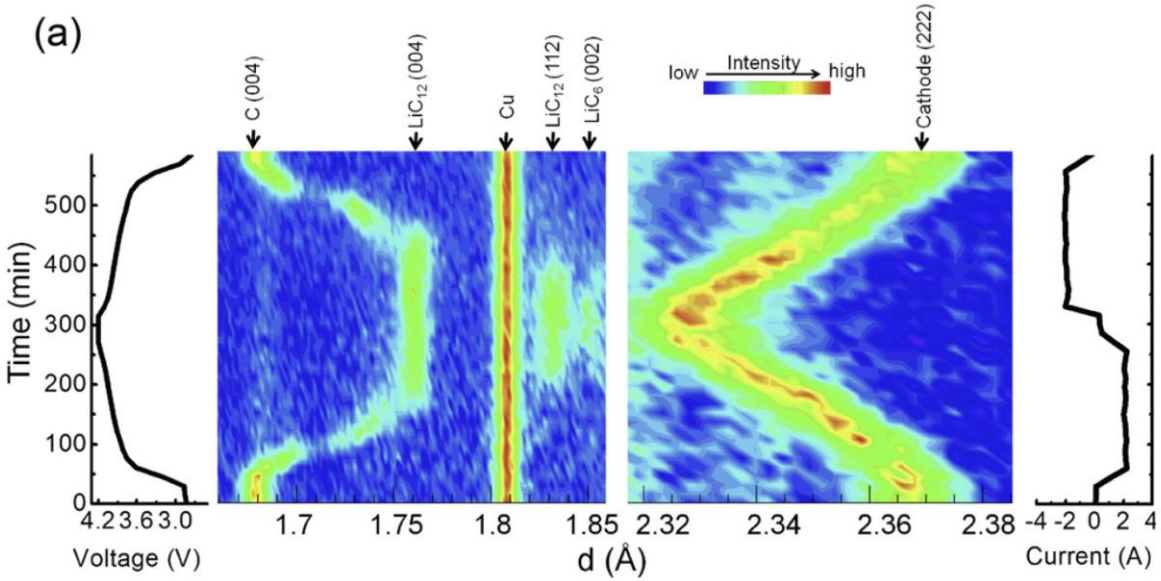
Software Ecosystem

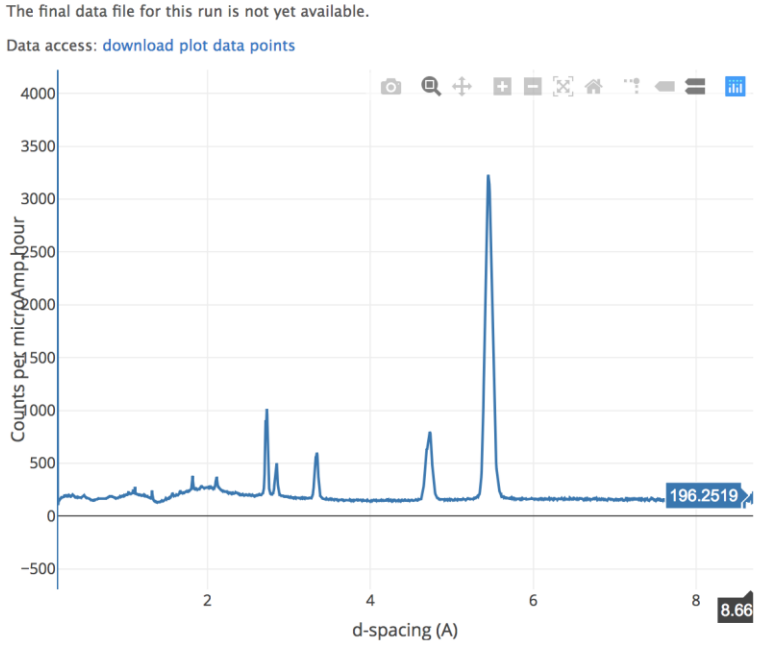
- Modular codes easily glued together
  - Some critical codes not easily glueable
- Workflow engines
  - can leverage HPC, and Cloud
  - User provided compute is harder
  - Easily configure novel workflows



Mantid – Community Code for Reducing neutron data

- Convert from events to histograms (reduce data)
  - In some cases data size grows.
  - Format for that users can work with
- Event filtering for time varying stimuli
  (J. Appl. Cryst. **51**, 616 (2018))
- Facility for live reduction
- Stores a history in metadata
- Python API allows,
  - Autoreduction, custom guis, expanded workflows
- C++/Python framework
- Collaboration of STFC, ORNL, ESS, ILL
- PSI, ANSTO, Juelich contribute
- Mantidproject.org





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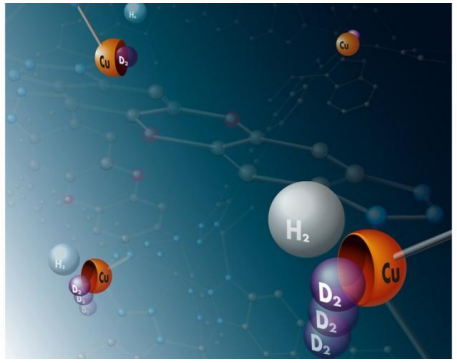
MANTID

Materials Models need More compute

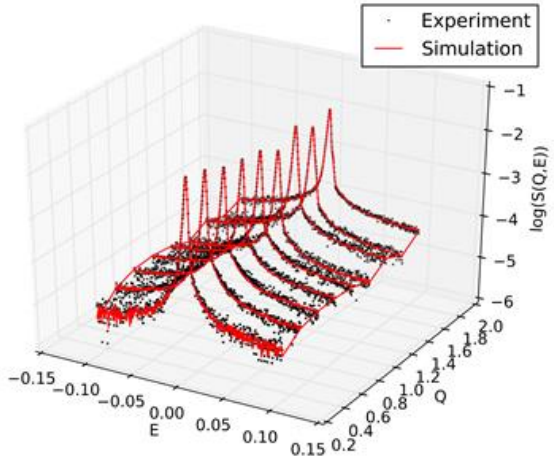
- Density Functional Theory (DFT)

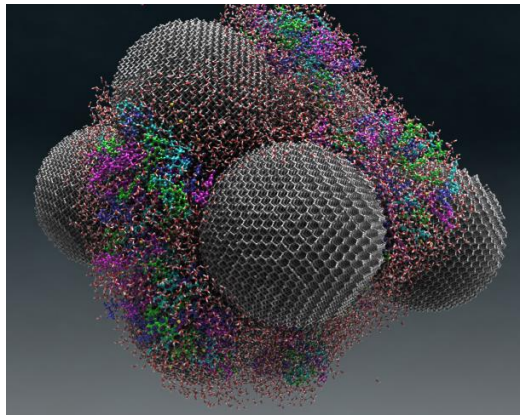


Molecules of the heavy hydrogen isotopes deuterium and tritium preferentially bind to copper atoms in a metal-organic framework compound.

Nature Comm. **8,** 14496 (2017)

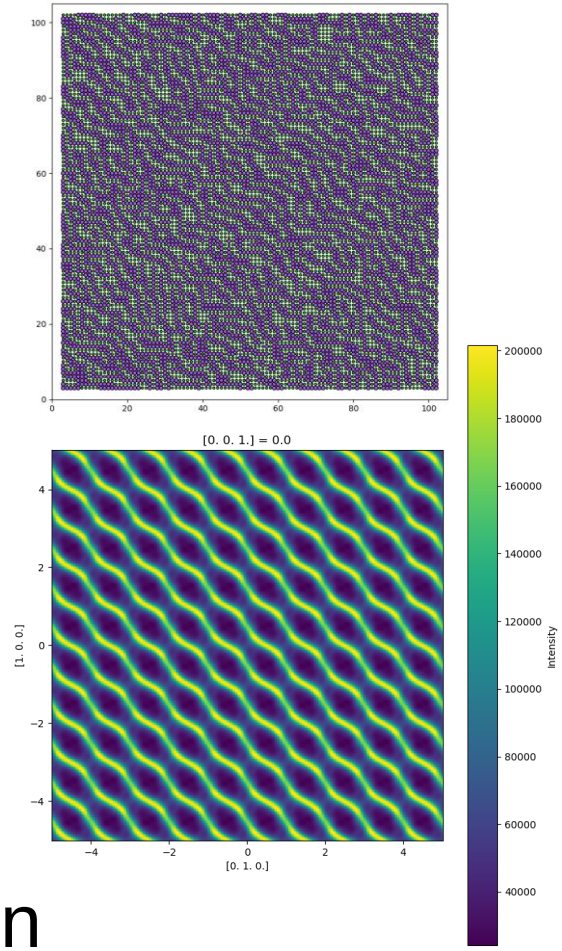
- Molecular Dynamics (MD)





J. Phys. Chem. B **120**, 10059 (2016)

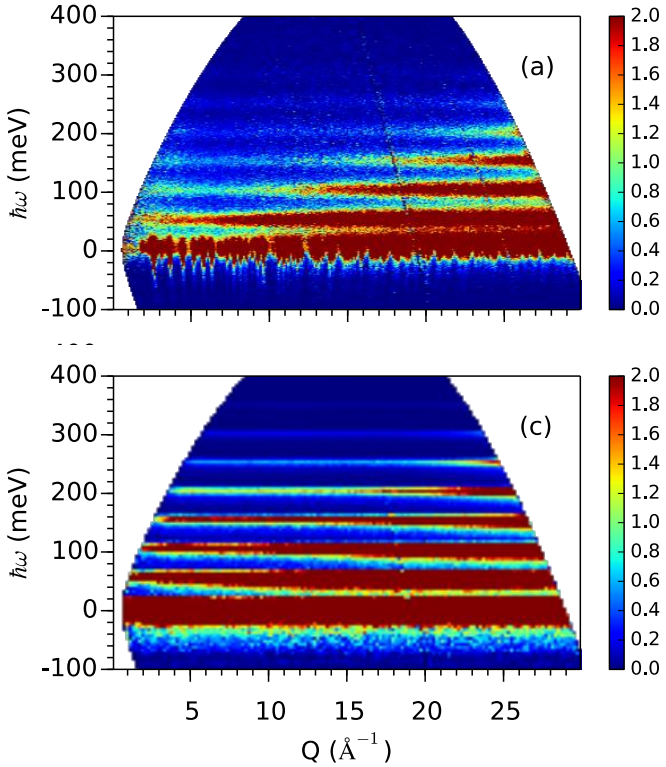
- Big Box Structure calculations



- Javelin
  - https://github.com/rosswhitfield/javelin

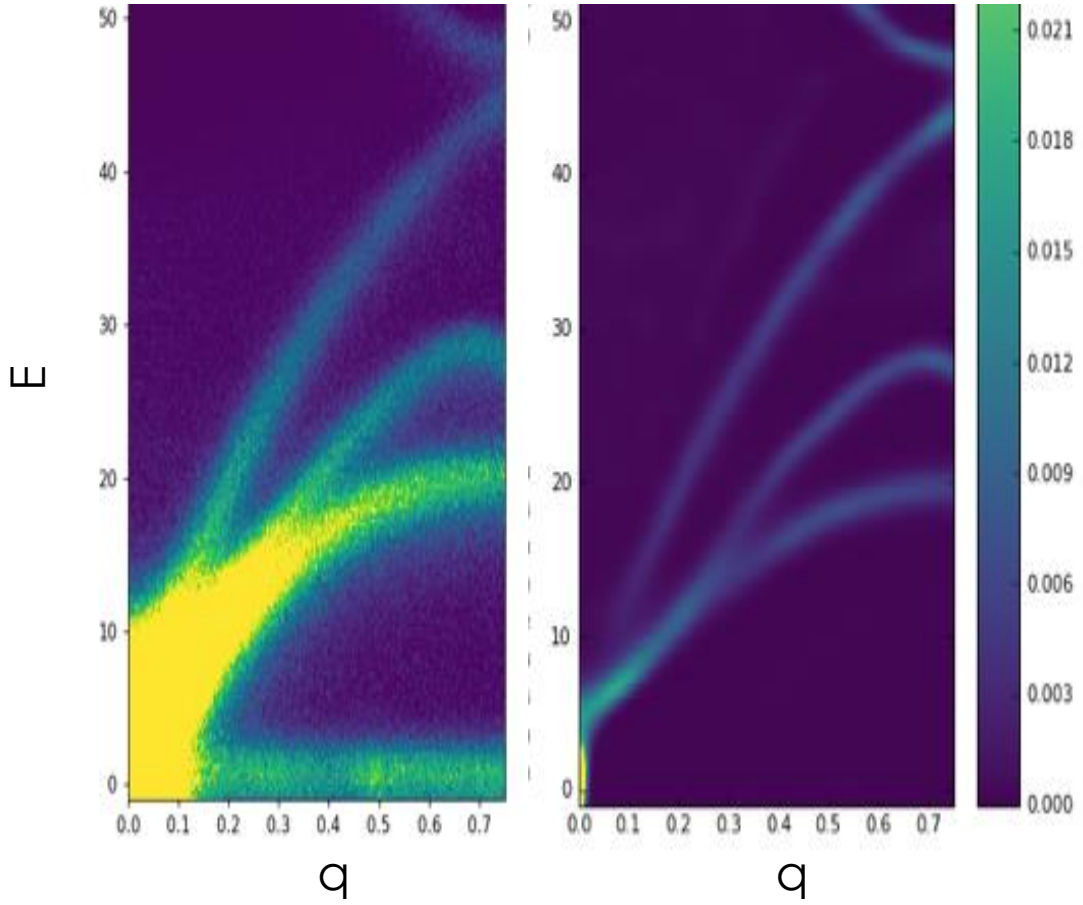
Instrument Models need more compute

- Complex multiple scattering understood by Monte Carlo ray tracing



Physical Review B **89,** 144302 (2014).

- Super resolution techniques are being investigated to remove instrumental effects



Workflow engines can help

- Pegasus (Panorama project) https://panorama360.github.io/
  - MD and quasi elastic scattering
  - Big box models and diffuse scattering
  - Monte Carlo ray tracing of direct deometry spectrometers

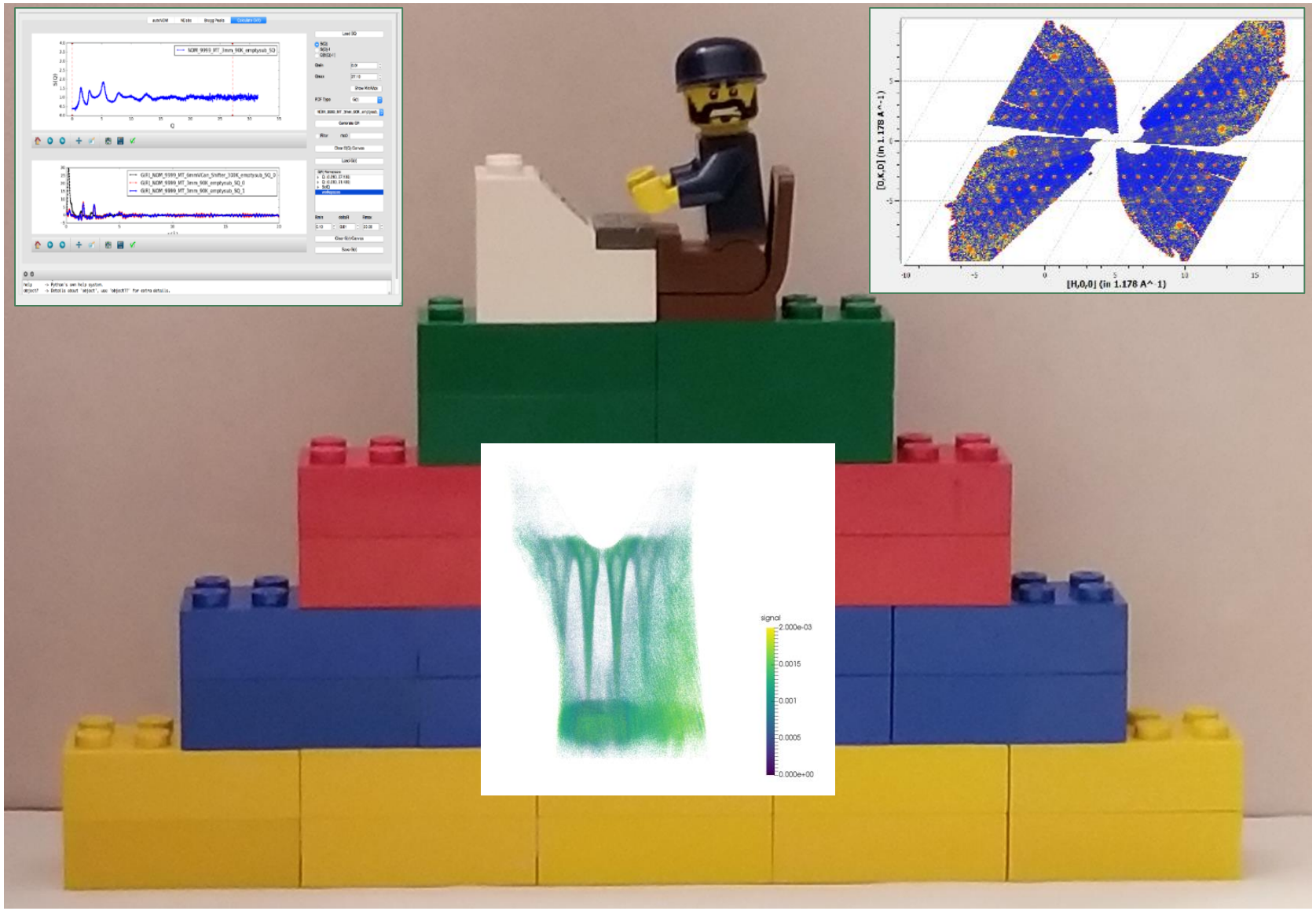
- ICE (Iceman project) https://wiki.eclipse.org/ICE
  - DFT and molecular spectroscopy

- Beam https://doi.org/10.1016/j.procs.2016.05.410
  - MD and quasi elastic scattering
  - Polymer modeling for reflectivity data

Conclusions

- A modular software infrastructure is critical
- We us python to glue codes together.
- Mantid is a key framework for our community
- Workflow engines are helpful, but the ideal is not there yet.

Questions?


[0,K,0] (in 1.178 A^-1)
[H,0,0] (in 1.178 A^-1)
signal
2.000e-03
0.0015
0.001
0.0005
0.000e+00