OAK RIDGE National Laboratory

STS Experiment Automation Needs

preliminary analysis from an instrument scientist's perspective: why and what do we need?

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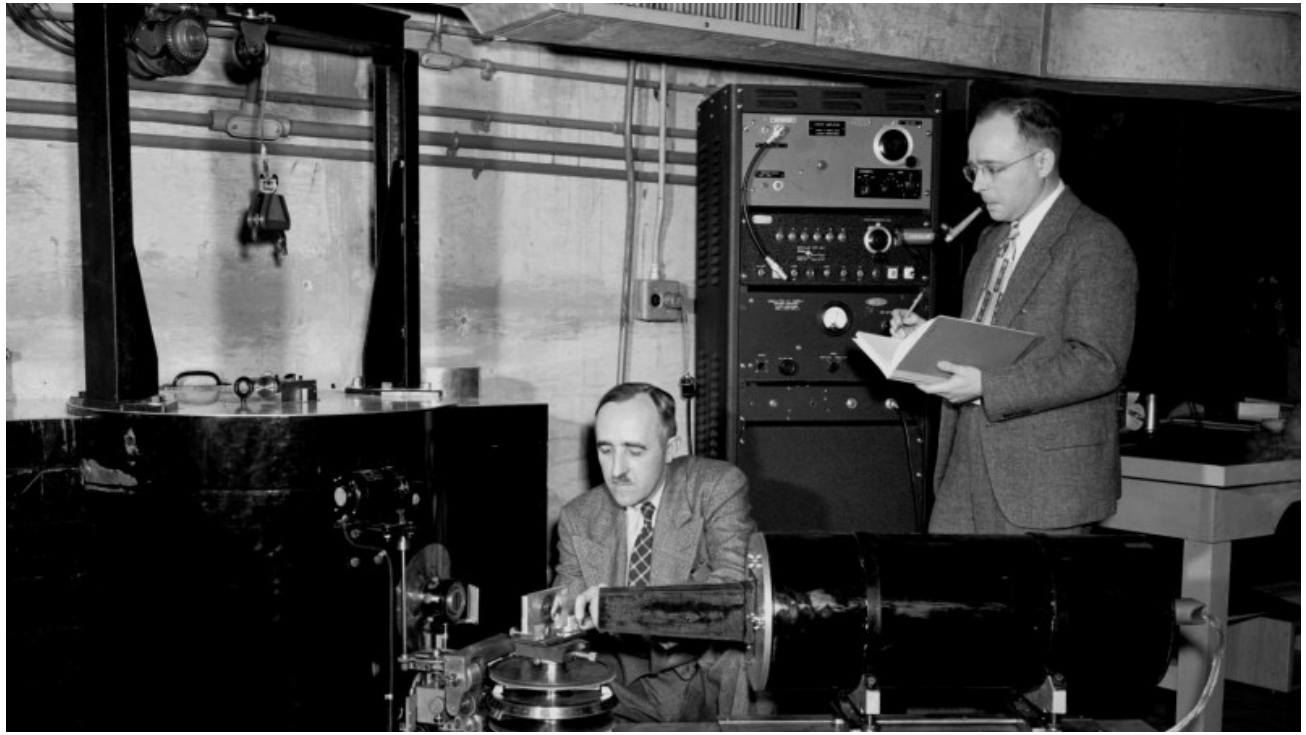
Second Target Station/Computer Science & Math Workshop

June 23, 2022

U.S. DEPARTMENT OF ENERGY

ORNL has a glorious history of implementing experiment automation capabilities for neutron scattering instruments.

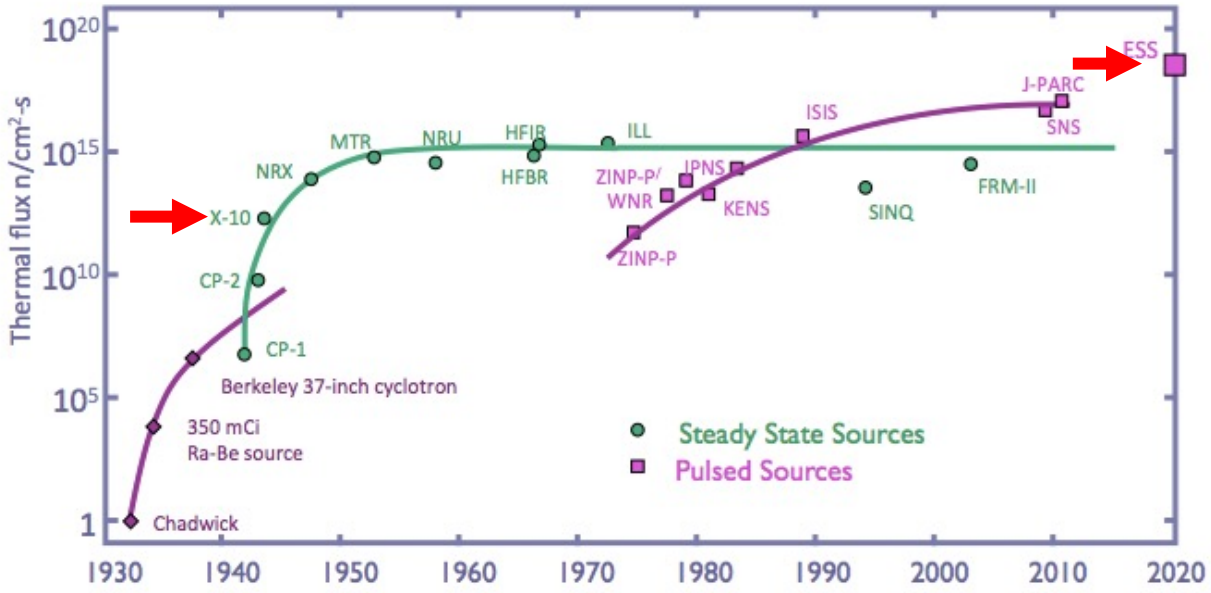
The first instrument exclusively for neutron scattering had been capable of automated data recording, which took the place of pen and paper and allowed researchers to collect data overnight.



Neutron scattering pioneers, Ernest Wollan (left) and Clifford Shull* work with the first instrument exclusively for neutron scattering, a double-crystal neutron spectrometer, ***at the ORNL X-10 Graphite Reactor in 1949***.
*(*C.G. Shull was a co-winner of the 1994 Nobel Prize for the development of the neutron scattering technique.)*

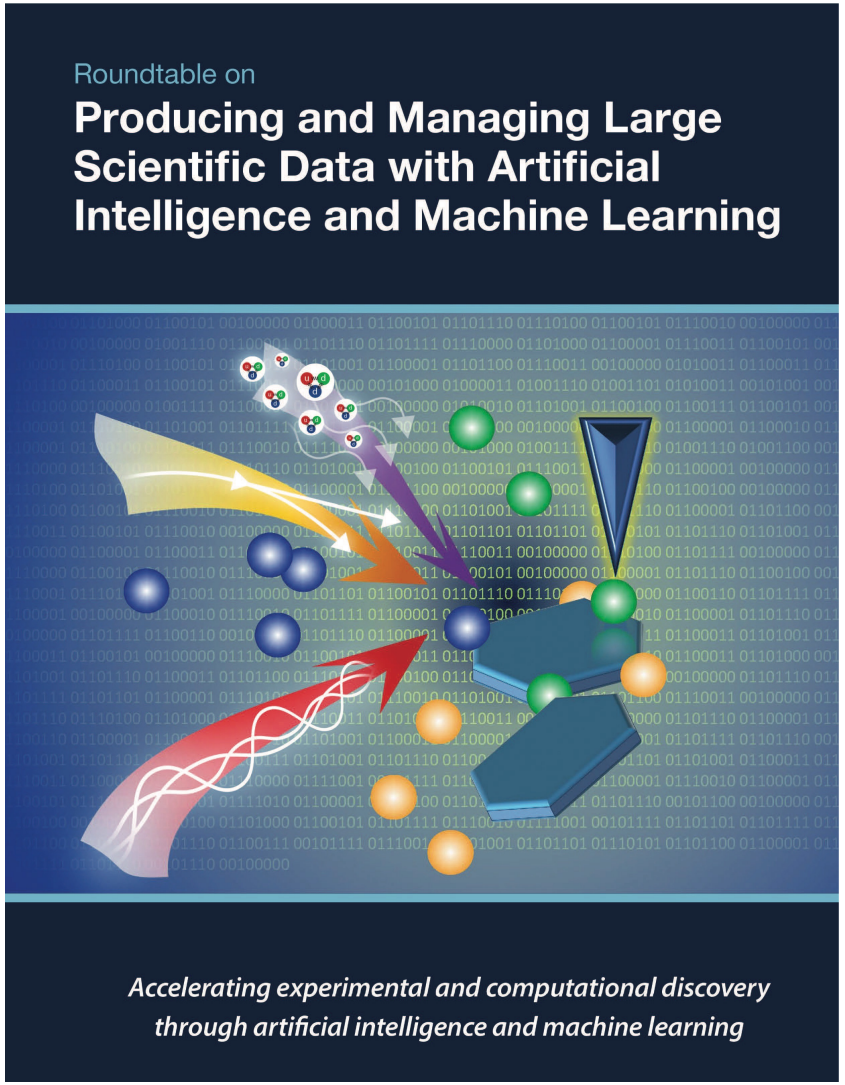
https://neutrons.ornl.gov/content/history-neutron-scattering-ornl

There is a global and continuous trend for increasing experiment automation at neutron, x-ray and nanoscale scientific user facilities due to the improvement of source, instrumentation and computing.

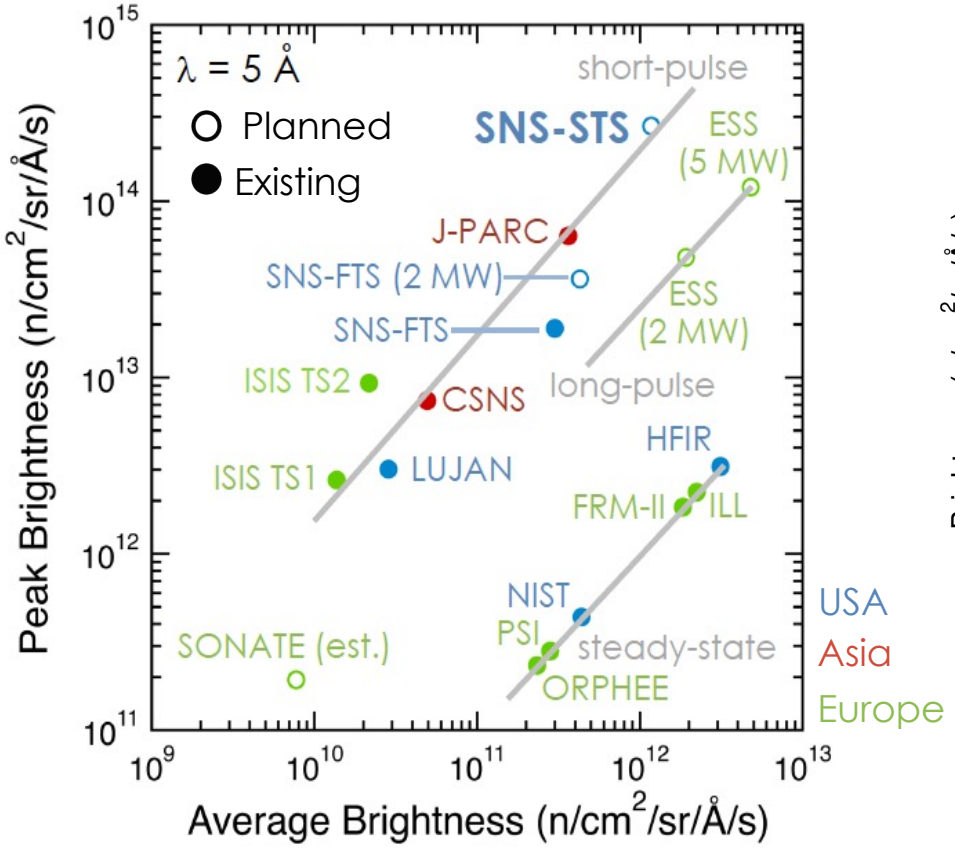


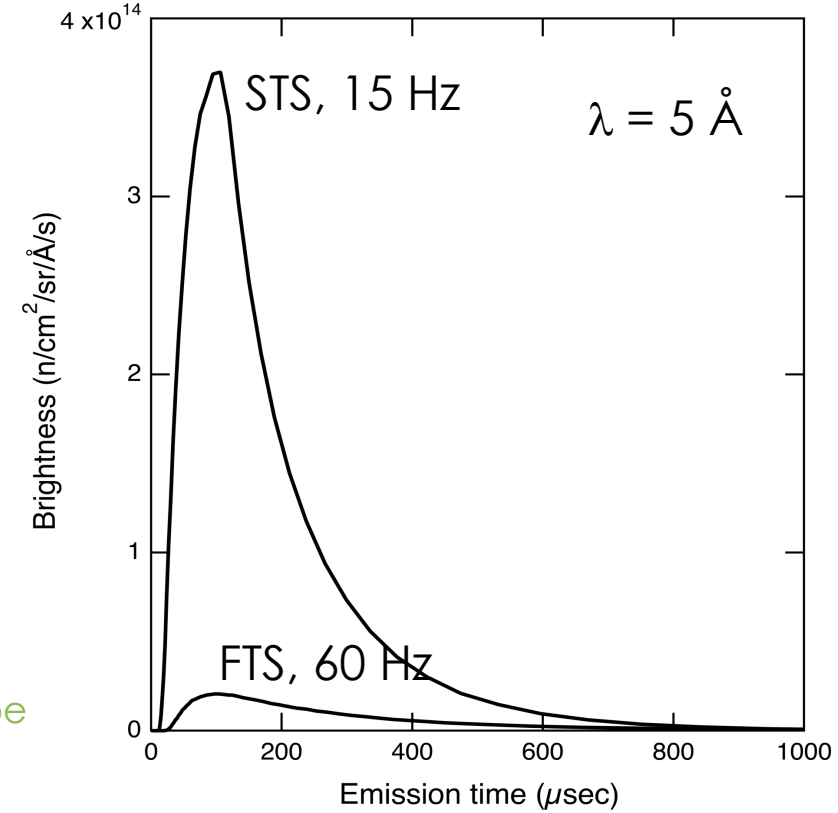
Andersen, K. H., and C. J. Carlile. "A proposal for a next generation European neutron source." In *Journal of Physics: Conference Series*, **746**, 1, 012030 (2016)

[2019 BES roundtable report (right)] In the next 10 years, AI/ML are expected to ***go beyond traditional data analysis*** to aid the design and control of complex facilities, enable real-time capabilities to acquire and analyze large data volumes, ***automatically steer data collection for in-the-loop experiments***, and support experimentalists' use of exascale computing.



STS needs high-level experiment automation to leverage the high-performance neutron source for high-impact science.

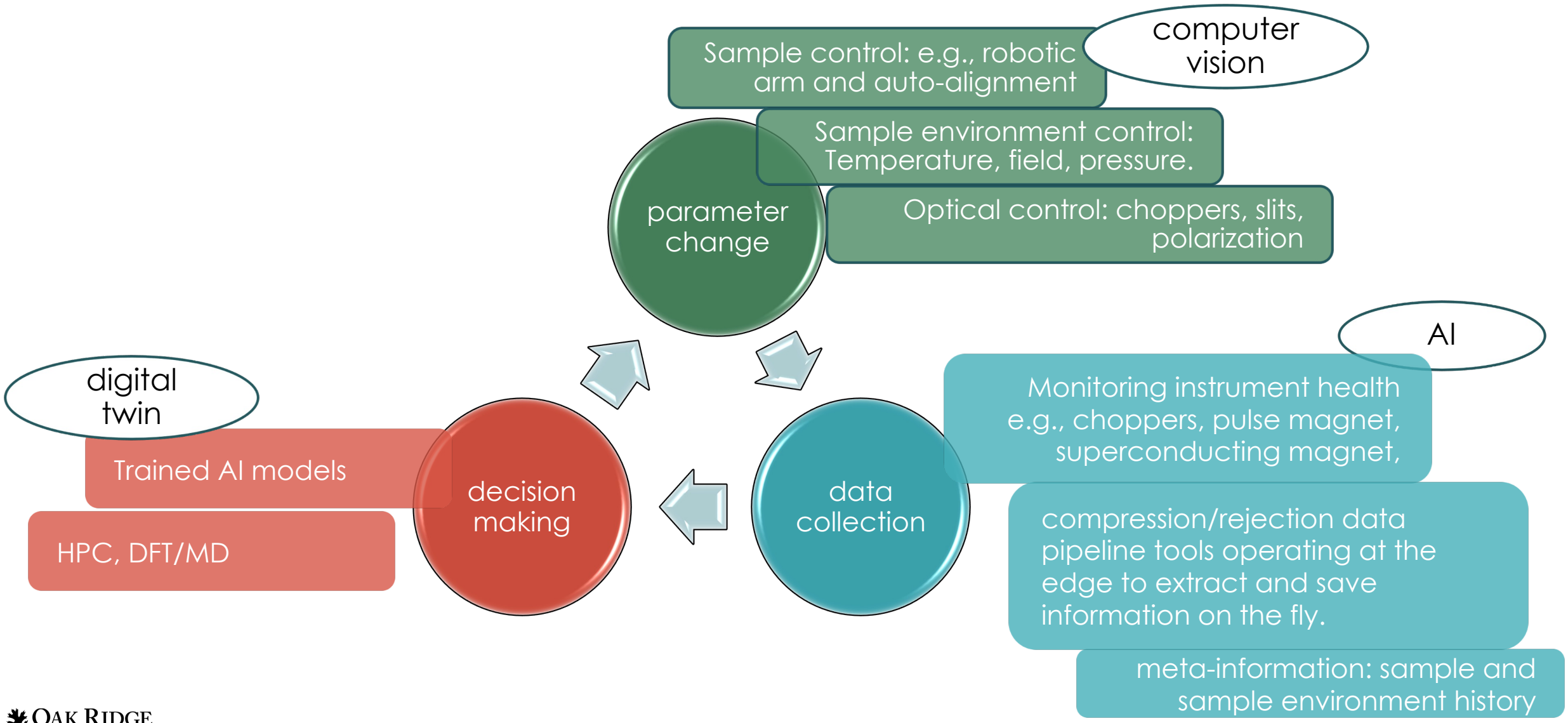




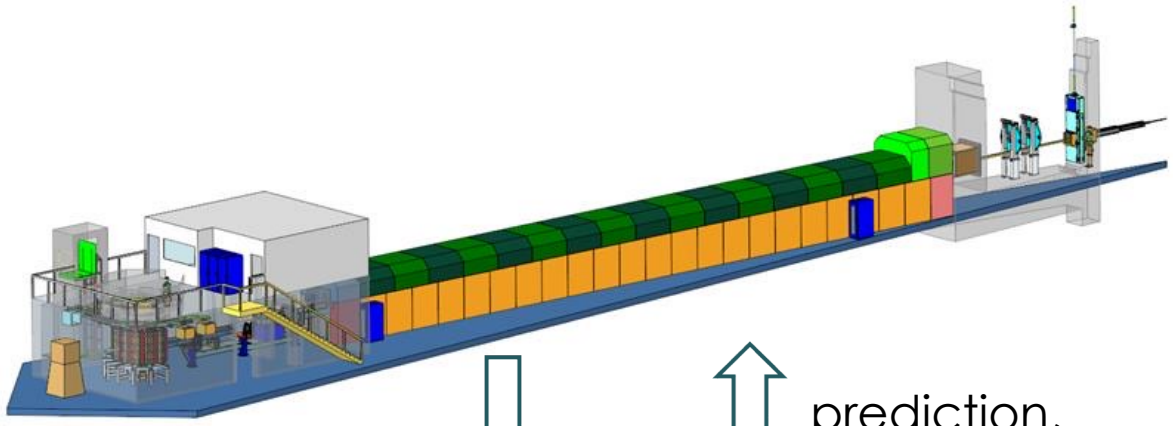
- STS provides the brightest cold neutron source.
- STS instruments will have 10–1000 x flux on samples and 4 x wavelength band, compared to similar ones at FTS.

STS will enable more high-throughput and more complex experiments, e.g., time-resolved studies, extreme sample environments, and multi-mode characterization, to gain an accurate understanding of high-dimension parameter spaces.

There is a close loop for scattering experiment automation needs and the live reduction/analysis is a key requirement.

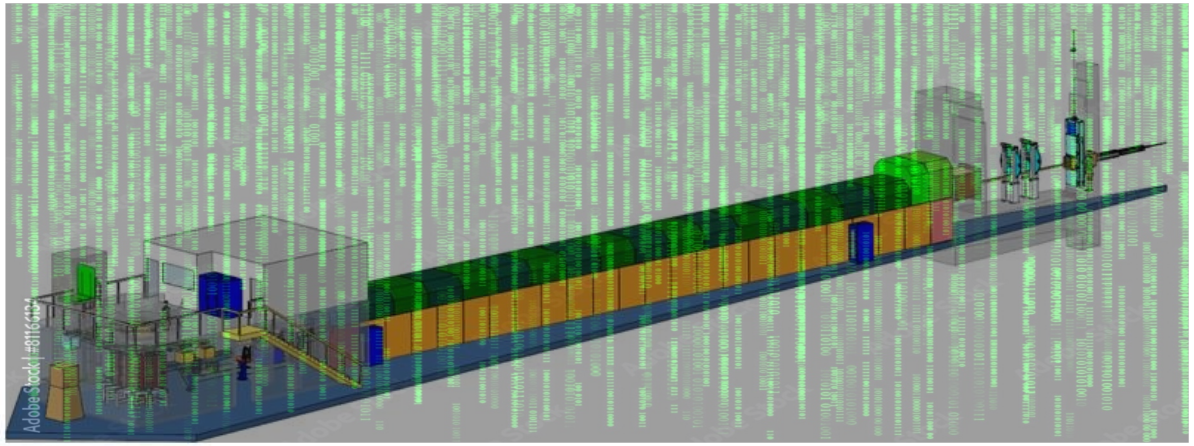


Digital instrument twins are valuable for experiment automation.



data from sensors, cameras, monitors, and detectors

prediction, optimization, and diagnosis from simulations

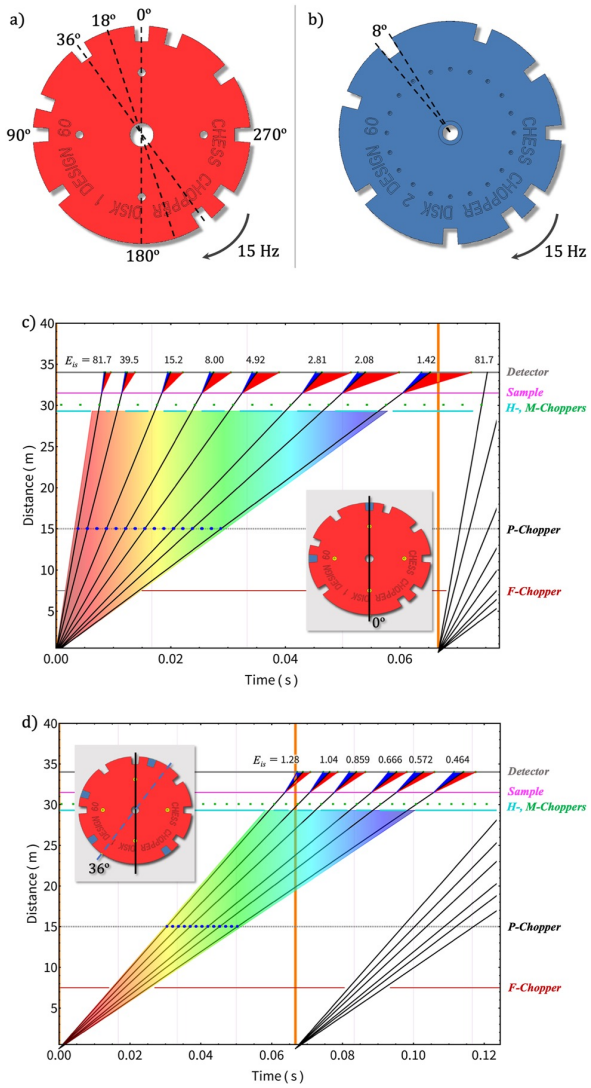


- Pre-train decision-making algorithms using synthetic data from virtual experiments
  - A sharable data infrastructure that provides benchmark datasets for decision-making algorithms training is also needed.
- Virtual diagnostics that provide real-time feedback during experiments.

[2019] BES Roundtable on Producing and Managing Large Scientific Data with Artificial Intelligence and Machine Learning

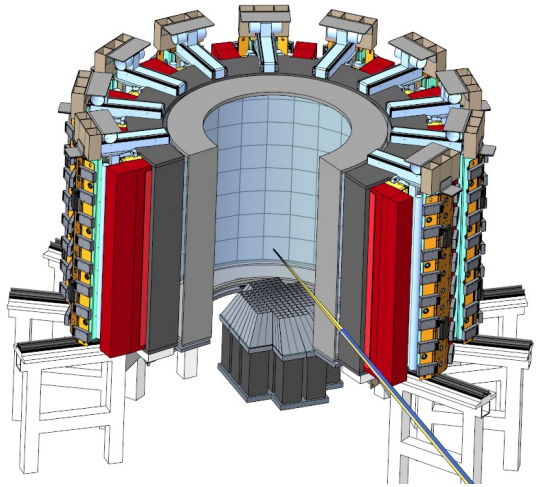
CHESS needs an expert system to guide the chopper settings in real-time.

CHESS, a direct geometry neutron spectrometer.

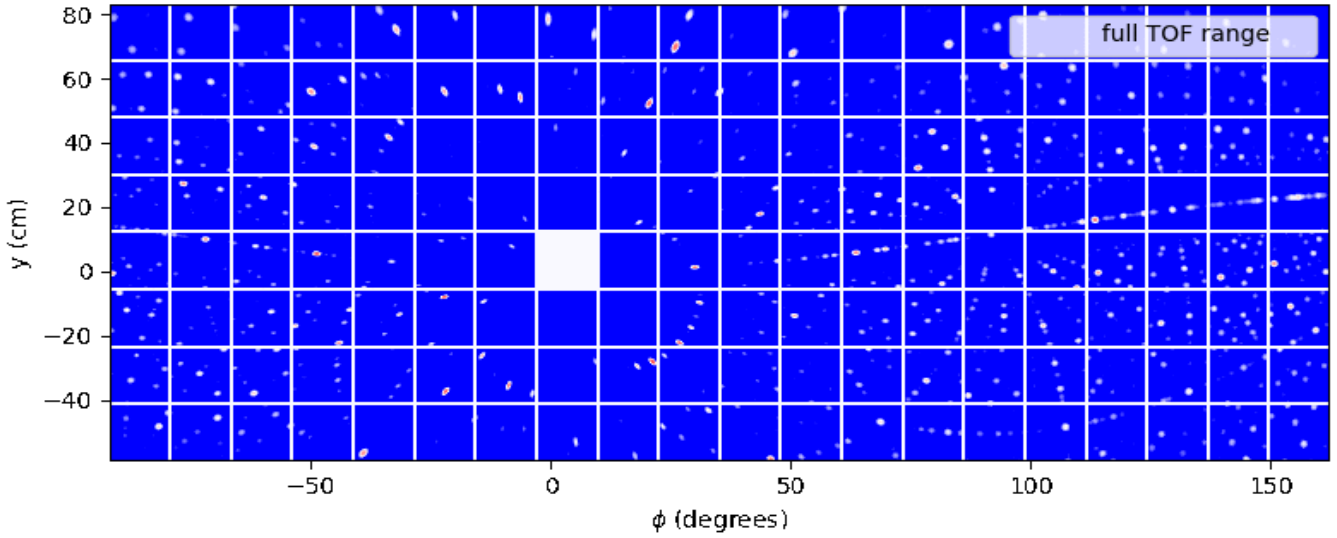


- There is a trade-off between the intensity and the resolution from different chopper settings.
- Which setting is best to address the scientific questions?

PIONEER needs a rapid experimental plan tool to optimize crystal orientations and counting times.

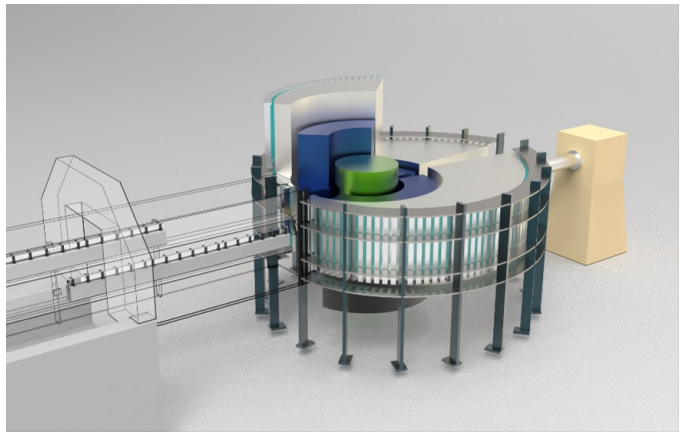


PIONEER, a high Q-resolution polarized single-crystal neutron diffractometer.

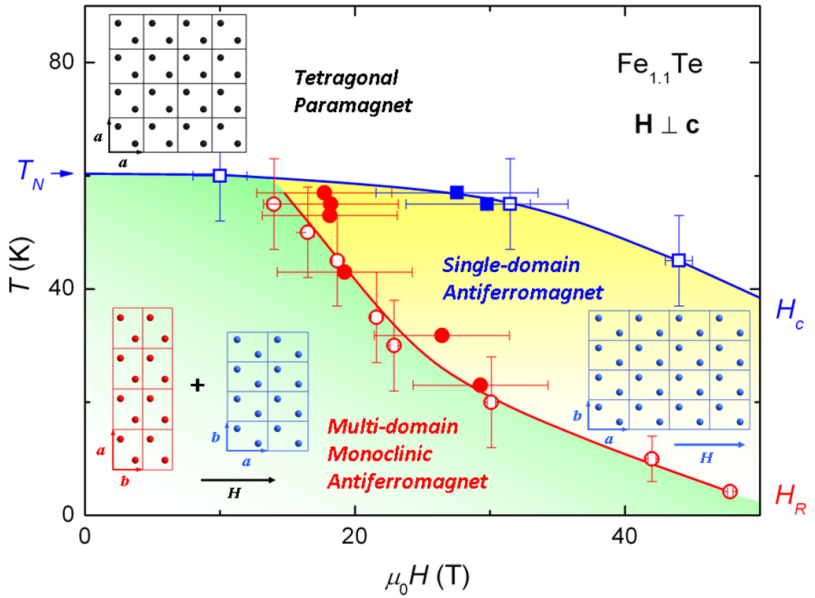


- The planning system shall not only consider the coverage but also consider the signal and background strength and redundancy.
- Many combinations work. Which one is more efficient?

VERDI needs to efficiently map the phase diagram of quantum materials.



VERDI: VERsatile DIffractometer with wide-angle polarization analysis for magnetic structure studies in powders and single crystals



Field-induce structural transition in the antiferromagnet Fe1.1Te, *X. Fabrèges, et al., PRB* ***95****, 174434*

- A typical grid scan is slow in high-dimensional phase space.
- AI-assisted experimental plan tool can be more efficient to identify the region of interest, i.e., the phase boundary.

There is an increasing momentum at ORNL for experiment automation.