SEQUOIA Fine-Resolution Fermi Chopper Spectrometer

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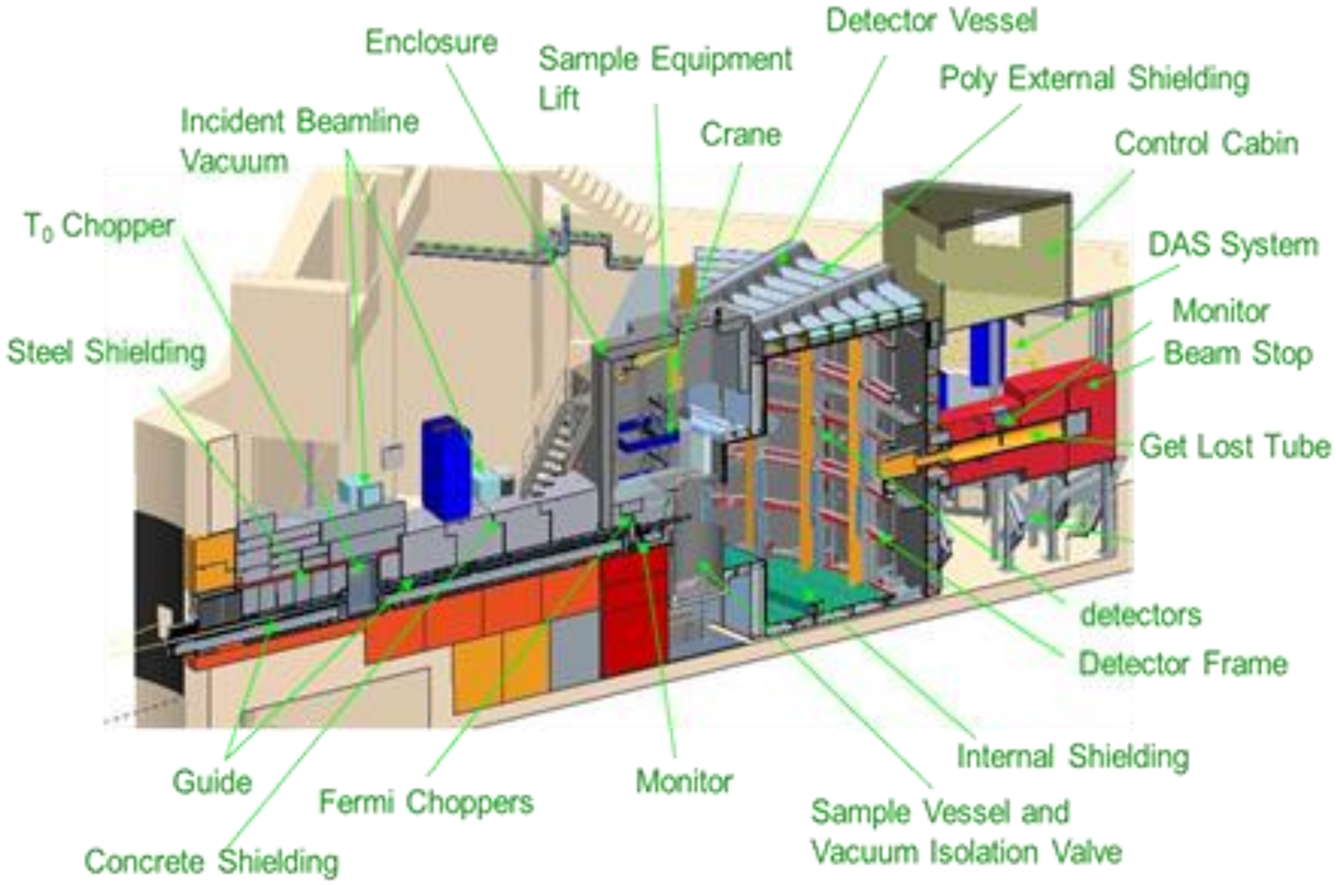
Beamline Review Checklist

1. SEQUOIA overview
2. Scientific Mission and Impact
3. General user program and beam time usage
4. Beamline Productivity
5. Adequacy and reliability of software, sample environment and ancillary equipment
6. Science Highlights
7. Risks
8. Future instrument science and development plan
9. Response to instrument specific recommendations from last review
10. Summary

1. SEQUOIA Overview

- SEQUOIA is a high-resolution, time-of-flight, direct-geometry spectrometer (DGS), optimized for measurement of excitations with good wave-vector and energy resolution at thermal neutron energies.



1. SEQUOIA Overview

Moderator	Decoupled ambient water
Source – Fermi chopper distance	18 m
Chopper – sample distance	2 m
Sample – detector distance	5.5-6.3 m
Incident energy range	8 — 5000 meV
Resolution (elastic scattering)	1 — 5% E_i
Detector coverage horizontal	30°-60°
Detector coverage vertical	-18° — 18°
Minimum detector angle	2.5°
Beam Size	5 cm x 5 cm

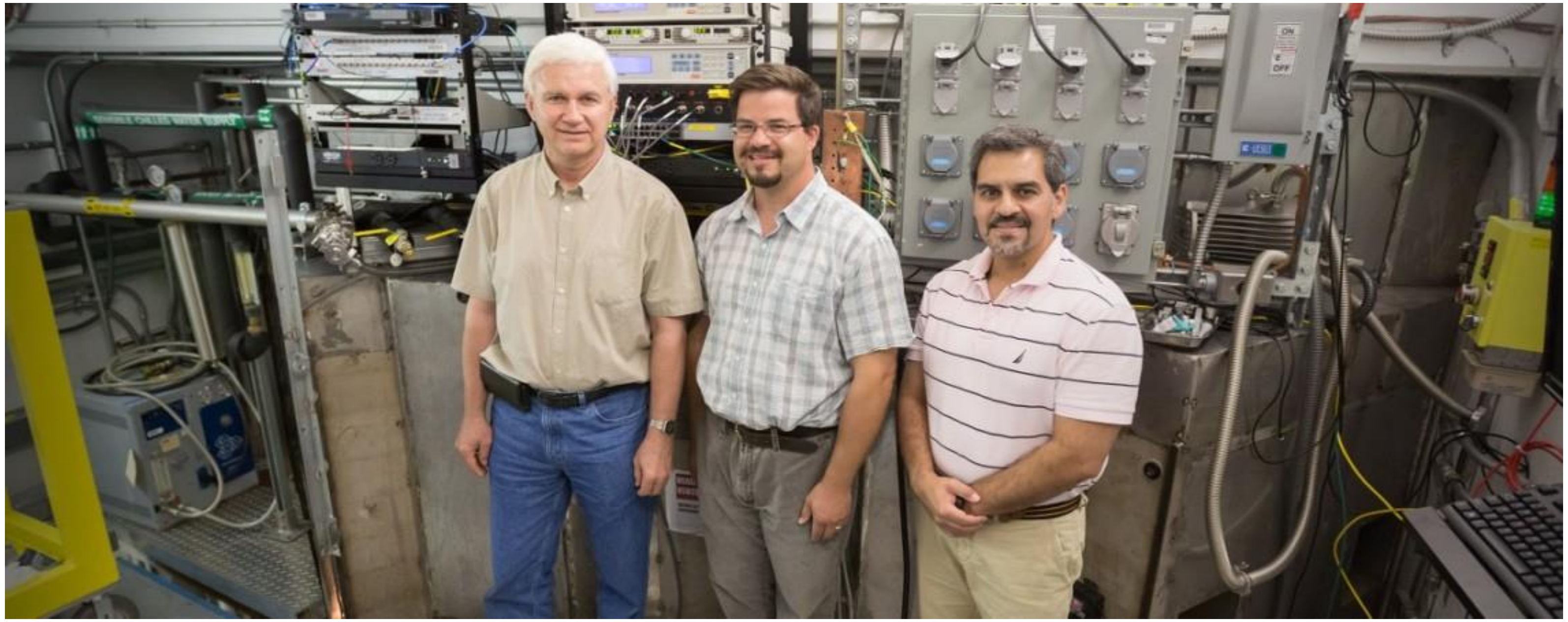
(Green: Supports Polarization Analysis)	Cold Moderator / 2 meV < Ei < 100 meV	Thermal Moderator / 5 meV < Ei < 2000 meV	
1-3% elastic E resolution / less flux	CNCS	**SEQUOIA**	Direct Geometry Spectrometers
3-5% elastic E resolution / high flux	**HYSPEC**	ARCS	
Highest time-averaged flux, localized & finite Q, ω	CTAX	HB1A, **HB1**, HB3	Triple-Axis Spectrometers
High energy resolution with flat dispersion / high throughput	BASIS	VISION	Indirect Geometry Spectrometers

1b. SEQUOIA's role in the ORNL spectroscopy suite

- Large detector array with good energy and wave-vector resolution. 100 eight-packs
- Versatile operation with neutron energies between ~8 and ~5000 meV with energy resolution between 1 and 5% of incident energy

- Large science cross-section
- Planned upgrades focus on improving signal:noise, and extending measurement capabilities

1c. SEQUOIA Instrument Team



Instrument team (left to right):

- Sasha Kolesnikov
- Matthew Stone
- Victor Fanelli

2. Scientific Mission and Impact

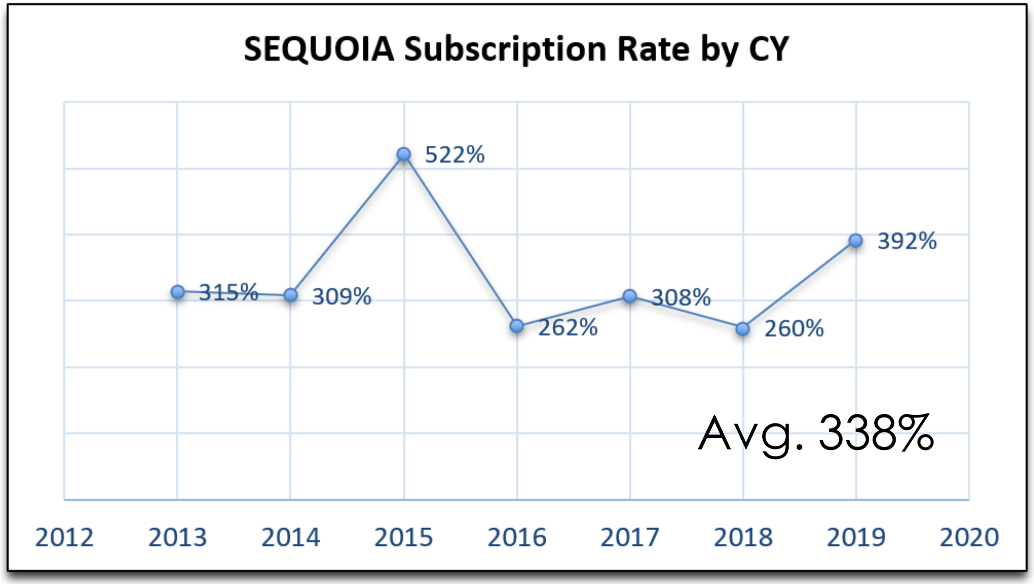
Mission

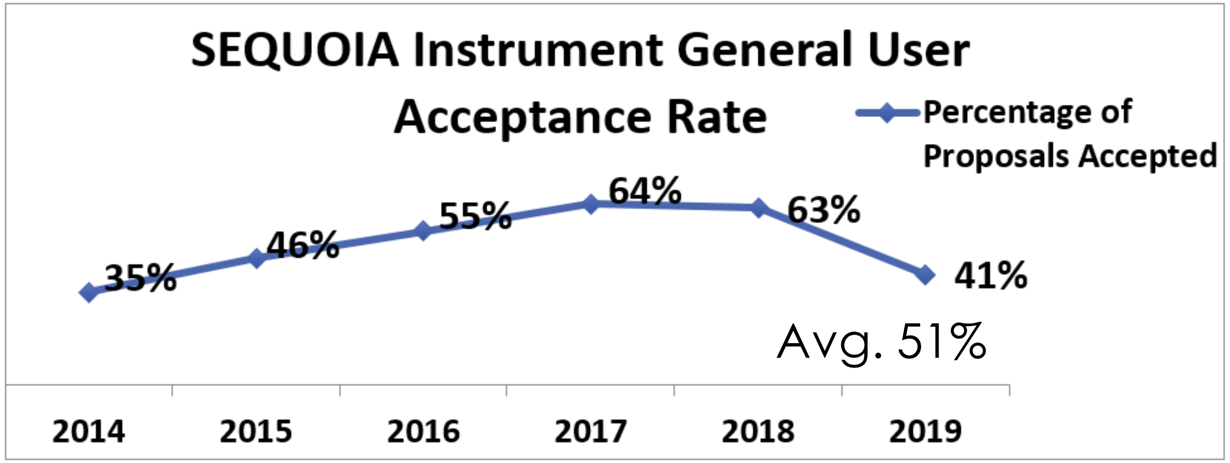
- Unconventional superconductors
- Quantum magnetism
- Itinerant magnets
- Ferroelectrics
- Thermoelectrics
- Multiferroics
- Confined water
- Metal hydrides
- Hydrogen dynamics

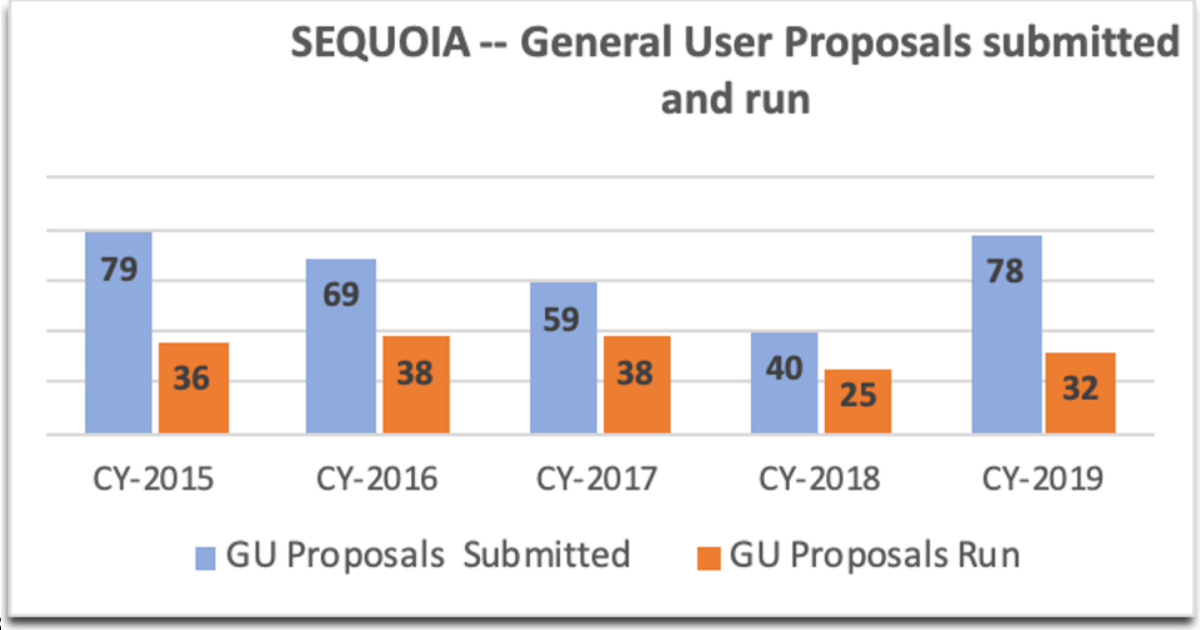
Impact

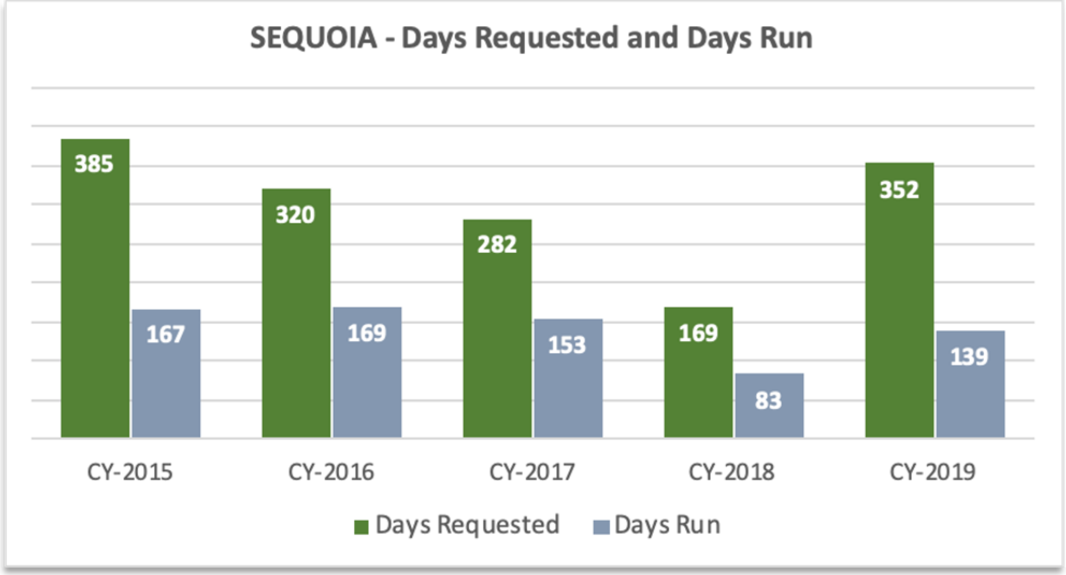
- Started operation in 2009
- Instrument h-index = 26
- 213 publications
- 13 publications with >50 citations
- 33 publications with >7 impact factor
- 31 Ph.D. Dissertations
- Covid-19 experiments

3a. General user program and beam time usage

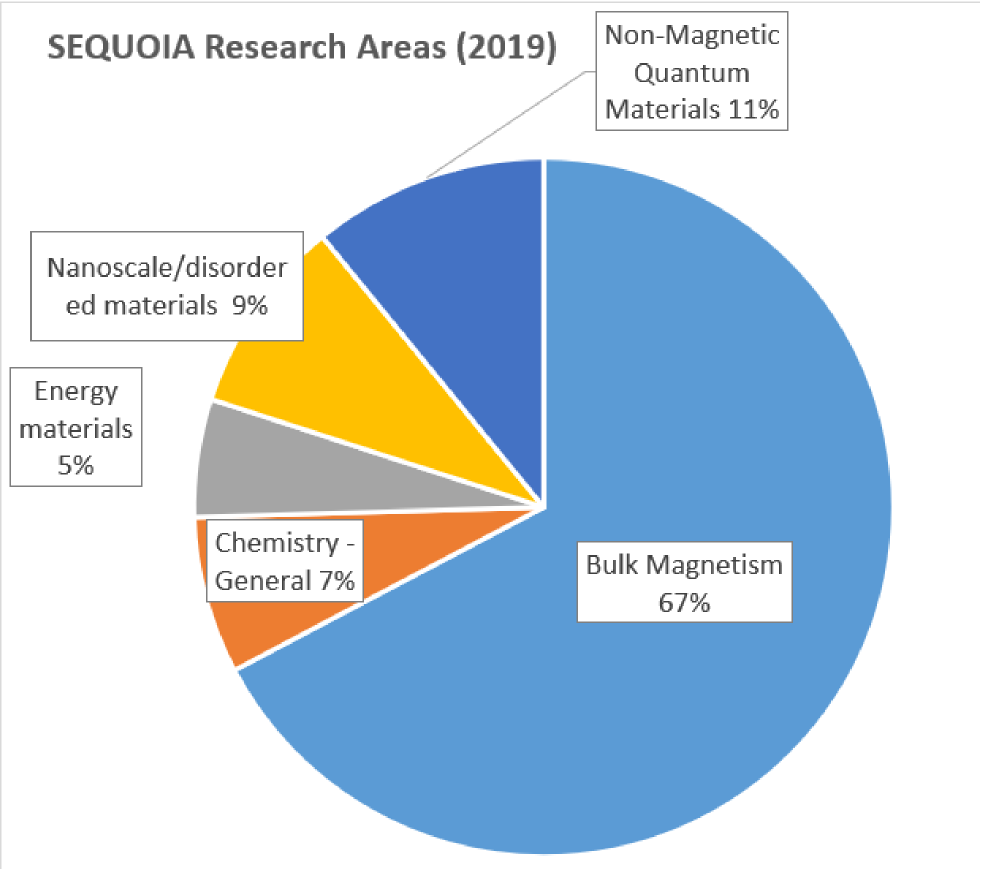








3a. General user program and beam time usage



Compare to 2018:

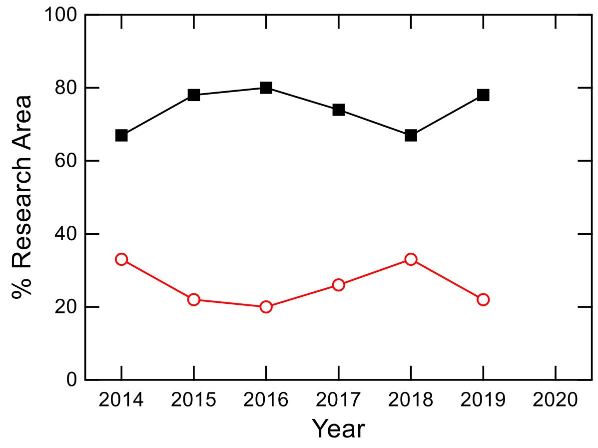
Bulk Magnetism up 25%

Nanoscale Materials up 4%

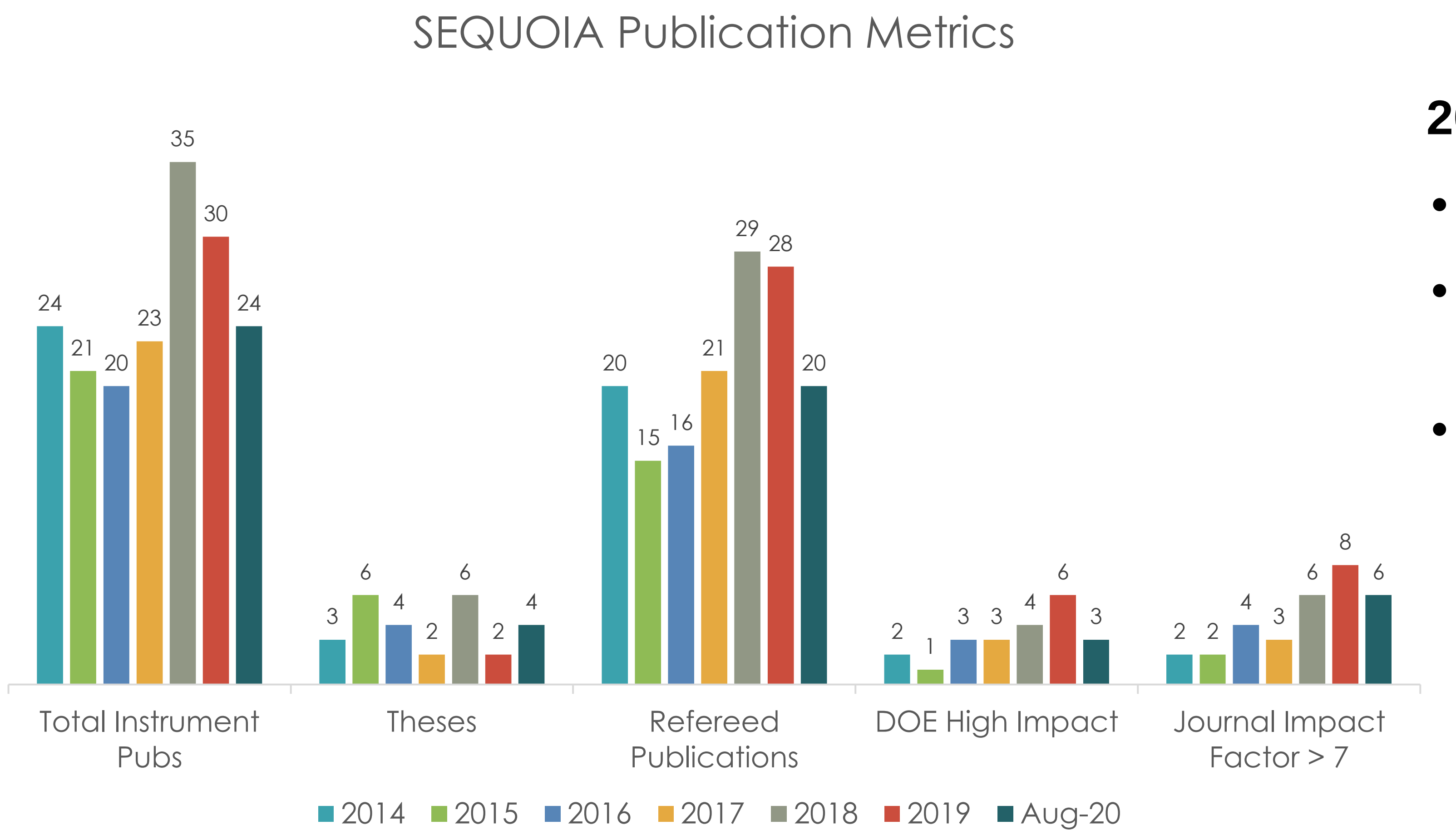
Non-Magnetic Quantum down 13%

Energy Materials down 13%

3b. Condensed view of categories



4. Beamline Productivity



2017-2019:

- 95 GU experiments
- 88 Publications (17 with IF >7)
- 3.2 Oversubscription rate on average

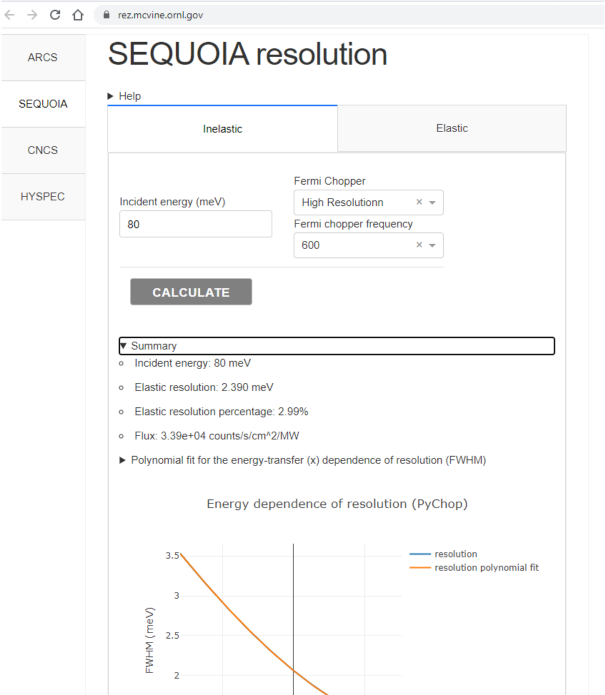
5a. **software**, sample environment and ancillary equipment

Data Acquisition

- **EPICS / CSS / ADARA /OnCat**
  Live event data broadcasting
- **Remote monitoring**

Experiment Planning

- **DGS Planner**
  In MantidWorkbench
- **Online Flux / Res. calculator**



Data Reduction

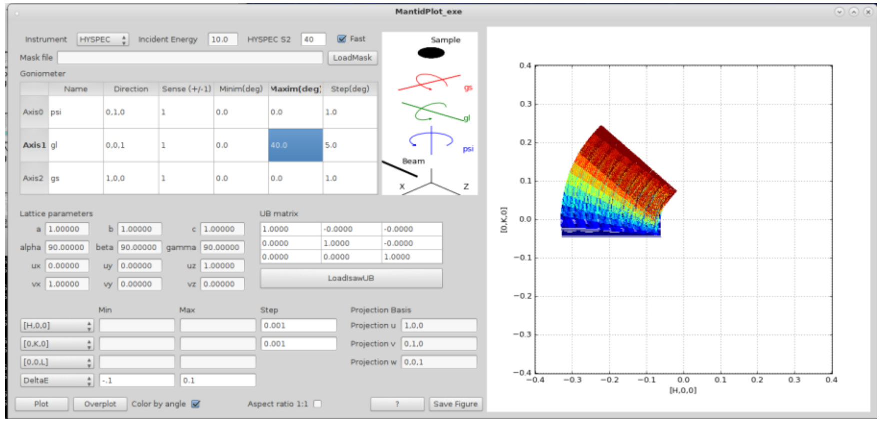
- **Autoreduction** (Mantid)
  - **Powders, single crystals, and rep-rate multiplication.**

Visualization and Analysis

- **Dave-Mslice - Horace**
- **Mantidplot**

Modeling

- **McVine**



5a. **software**, sample environment and ancillary equipment

- Normalize DAS & planning tools of other DGS's
  - Implementing latest CSS upgrades
  - Standardize the TOF spectrometer DAS interface
- Ongoing
  - Automated reduction of a multidimensional workspace (i.e. data are combined as rotation scans are performed)
- Future
  - DGS-common (resolution function, modeling, etc.)
- Analysis Primer for new(ish) users

5a. software, **sample environment** and ancillary equipment

- SEQUOIA's dedicated workhorse ~80% of experiments
  - Bottom loading CCR-22 (5-325 K)
  - Expanded temperature range with auxiliary heaters (10-800 K)
  - 3-sample changer for powder samples (very popular)
- Top loading CCR
  - Gen 1 has 100 mm bore shared with ARCS
    - 5-325 K and 10-550 K
    - Slow and high background
  - Gen 2 will be 70 mm bore shared with ARCS
    - Purchasing
    - Will be faster cooldown and improved background.

- Other sample equipment from pool available
  - Orange cryostats, Furnaces, ^{3}He, Dilution refrigerators, Pressure cells, pulsed magnet, Vertical field magnets

5a. software, **sample environment** and ancillary equipment

14 T magnet


SPALLATION NEUTRON SOURCE

TECHNICAL SPECIFICATION

14-Tesla Magnet System

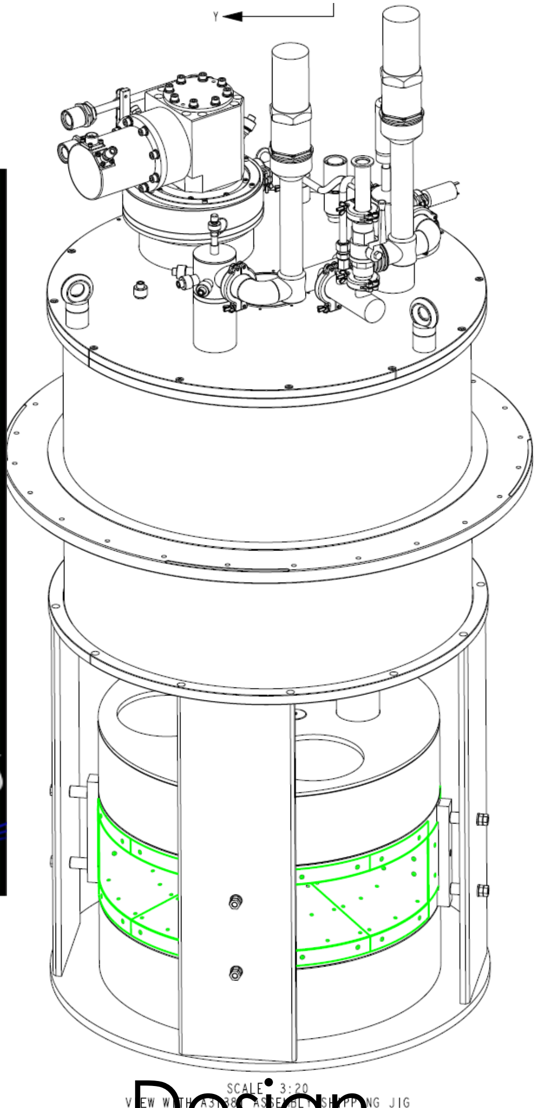
January 2016

NEUTRON SCIENCES

SNS

HFIR

Specification

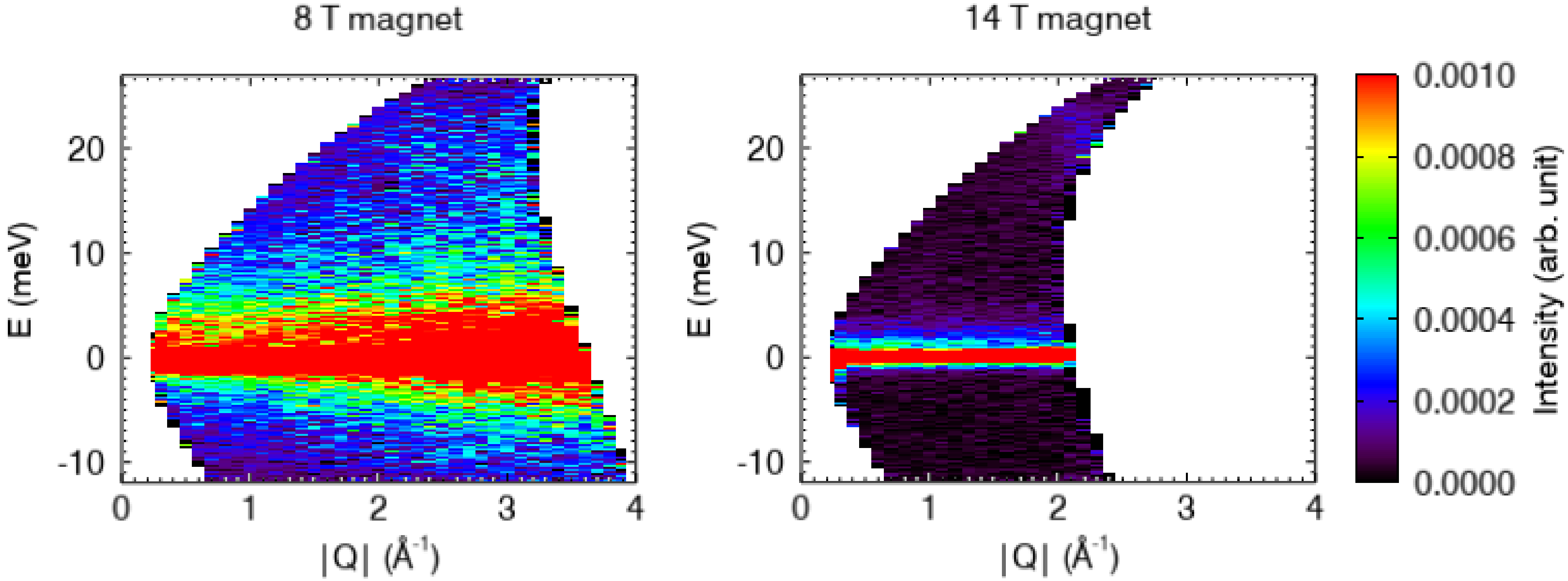


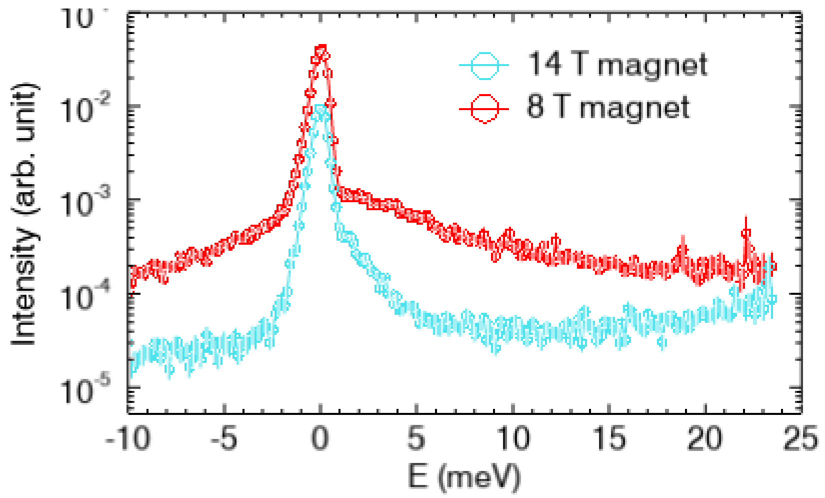
Design

Build

Commission

Background from empty magnets





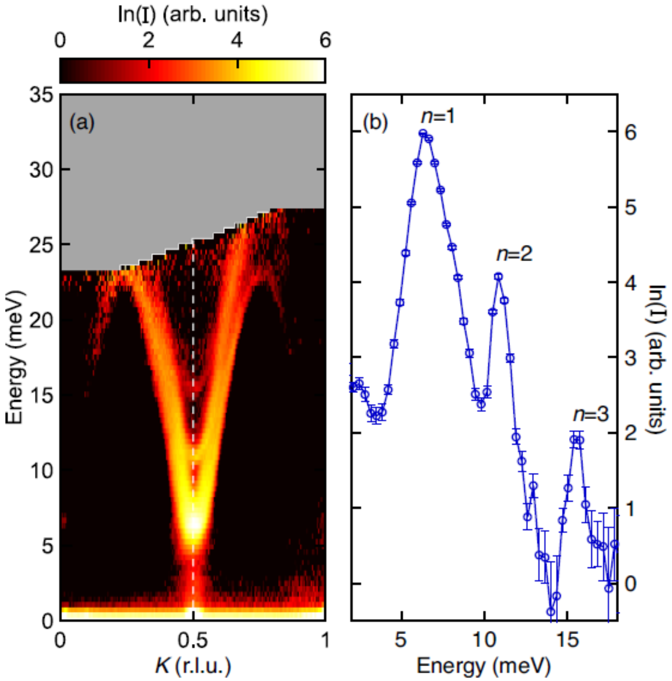
Empty 14 T magnet has ~5 times less background than the 8 T magnet

5a. software, sample environment and **ancillary equipment**

Vacuum System Upgrade

- In 2015, weaknesses in the vacuum system at SEQUOIA were identified
- Turbo-pumps installed on both detector and sample chambers for redundancy and leak checking
- Standardization of roughing pumps, gauges and transducers, and facility interface.
- Remove high voltage hazard from controls cabinet
- Was completed in Spring 2018 during IRP outage

6. Three-Magnon Bound State in the Quasi-1d Antiferromagnet α-$NaMnO_2$



(a) Measured excitation spectrum of a-$NaMnO_2$ and (b) cuts through the antiferromagnetic zone center (white dashed line in (a)) demonstrating the observation n=1, n=2, and n=3 magnon modes.

Worked performed on the SEQUOIA instrument at ORNL's SNS, a DOE Office of Science User Facility.

Rebecca L. Dally, Alvin J. R. Heng, Anna Keselman, Mitchell M. Bordelon, Matthew B. Stone, Leon Balents, and Stephen D. Wilson, *Physical Review Letters*, **124**, *197203* (2020).

Scientific Achievement

A three-magnon bound state is observed in the quasi-1d antiferromagnet a-$NaMnO_2$ and can be described by a semiclassical theory that maps the excitations onto a few-body droplet model of interacting bosons.

Significance and Impact

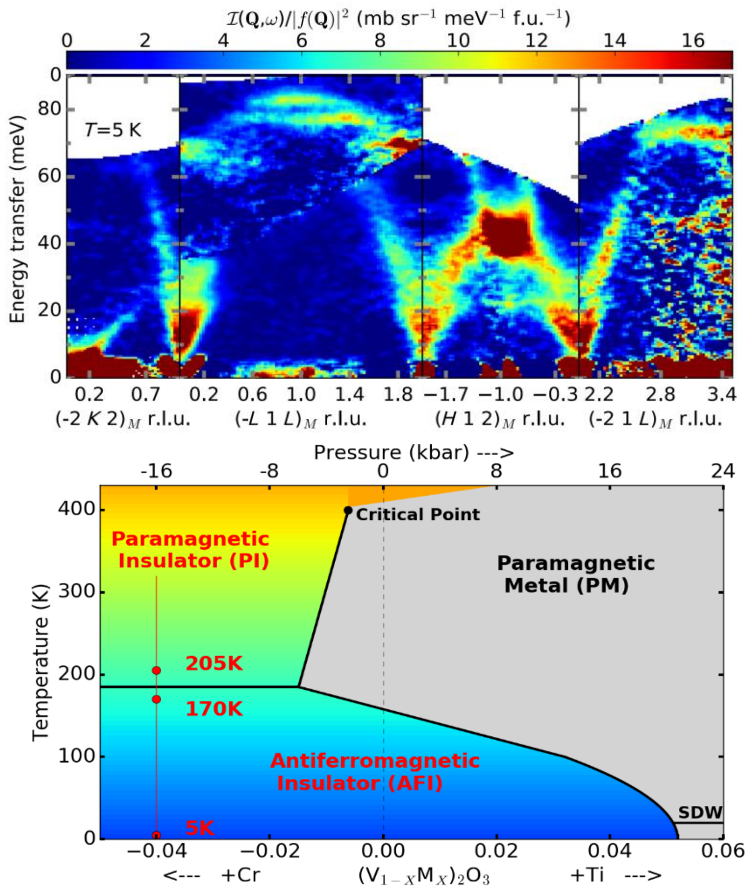
This work establishes a strong analogy between the physics of interacting magnons in antiferromagnets with uniaxial anisotropy and interacting bosons typically studied via ultracold atoms experiments.

Research Details

- The magnetic excitation spectrum was measured with inelastic neutron scattering, with the observation of single magnons as well as two and three-magnon bound states.
- The results were well-described by a semi-classical theory with spectral functions calculated using density matrix renormalization group and time evolution calculations.

NIST UC SANTA BARBARA NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

6. Magnetic Frustration as Origin of the Mott Insulating State of $(V_{1-x}Cr_x)_2O_3$



(Top) Neutron scattering from spin waves across four high symmetry directions. (Bottom) Phase diagram of V_2O_3 indicating the paramagnetic-insulating phase originating from frustrated magnetic interactions.

Scientific Achievement

The paramagnetic Mott insulating phase in $(V_{1-x}Cr_x)_2O_3$ owes its existence to frustrated magnetic interactions in quasi-2D honeycomb layers.

Significance and Impact

This work resolves the long-standing question of what drives this metal-insulator transition (MIT), which is unusual in that it doesn't involve magnetic or structural symmetry breaking.

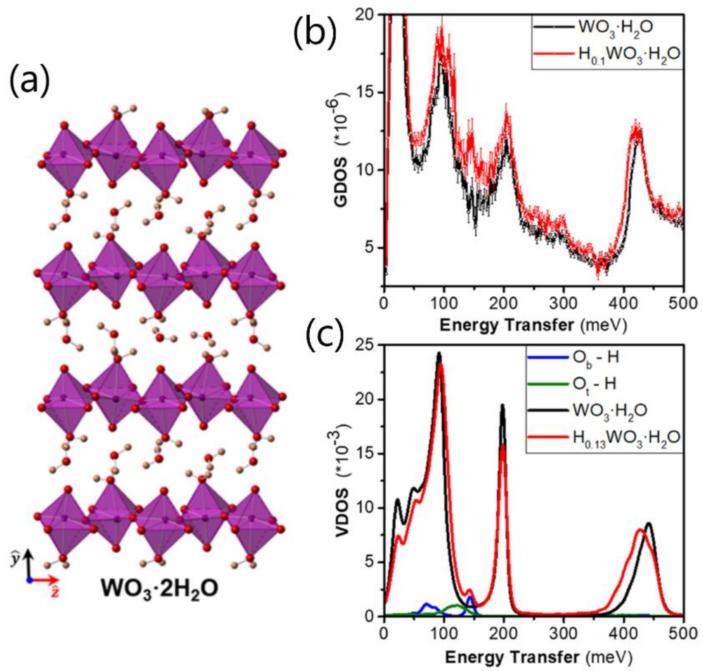
Research Details

– Inelastic neutron scattering on $(V_{0.96}Cr_{0.04})_2O_3$ was combined with density functional theory (DFT) to derive an accurate set of exchange interactions.

– This leads to the conclusion that frustrated magnetic interactions prevent magnetic order above 185 K, enabling a non-symmetry breaking MIT above this temperature (see phase diagram on bottom left).

J. C. Leiner, H. O. Jeschke, R. Valentí, S. Zhang, A. T. Savici, J. Y. Y. Lin, M. B. Stone, M. D. Lumsden, Jiawang Hong, O. Delaire, Wei Bao, and C. L. Broholm, *Phys. Rev. X* **9**, 011035 (2019)

6. Confined Interlayer Water Explains Fast Proton Intercalation



(a) Crystal structure of monoclinic $WO_3 \cdot 2H_2O$ showing the interlayer water. (b) Generalized vibrational density of states (GDOS) from INS and (c) ab initio molecular dynamics simulations of the vibrational density of states (VDOS) establish the locations of protons in the material.

J.B. Mitchell, N.R. Geise, A.R. Paterson, et al., *ACS Energy Letters*, **4**, 2805 (2019).

Scientific Achievement

Confined interlayer water in tungsten oxide hydrates ($WO_3 \cdot nH_2O$) stabilizes the layered structure, which explains the fast electrochemical proton intercalation found in these materials.

Significance and Impact

The work shows that the introduction of confined fluids into redox-active layered materials provides a new strategy for energy storage with both high power and high energy density.

Research Details

– Quasielastic neutron scattering showed the confined nature of water in $WO_3 \cdot nH_2O$.
– Inelastic neutron scattering (INS) and density functional theory (DFT) calculations showed that protons occupy bridging oxygen sites.
– X-ray diffraction measurements characterized the *operando* electrochemically induced structural transformations.

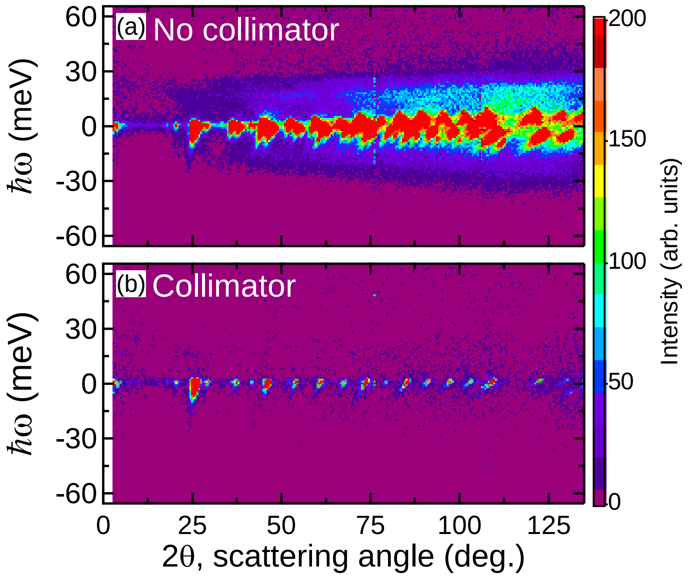
NC STATE SLAC UCR VT

7. Risks

- Detector array in high vacuum
- High oversubscription may frustrate potential users
- Remote operations
- Typecasting of SEQUOIA’s science
- Complacency with detector coverage and current level of background

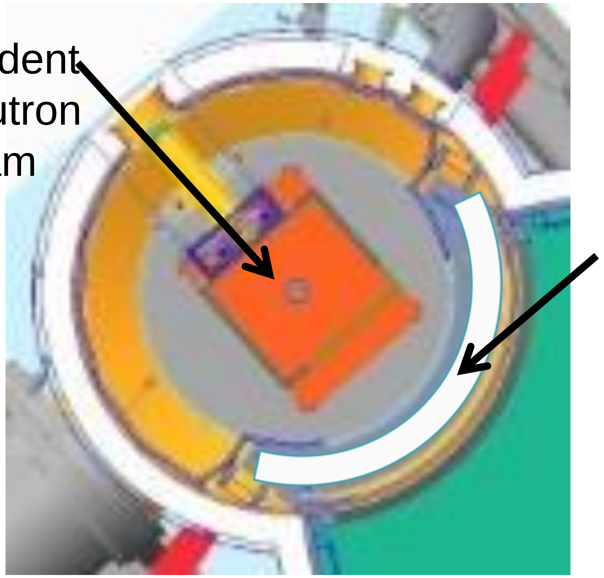
8. Future instrument science and development plan

- A radial collimator at SEQUOIA will significantly reduce background scattering due to sample environments and spurious scattering within the instrument vacuum chambers.
- Collimator will reside within the sample vacuum tank to allow full range of sample environments



ARCS collimator improves background

Incident Neutron beam



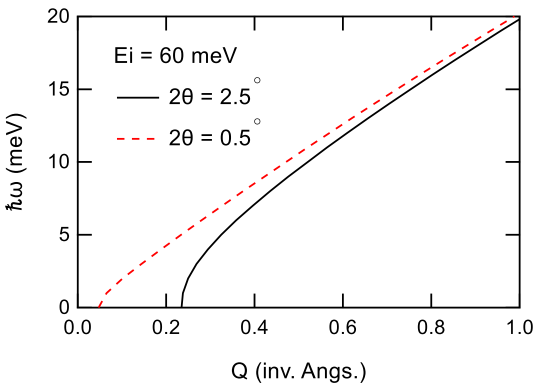
Collimator

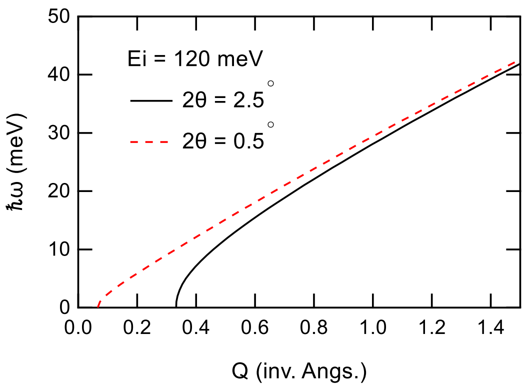
- Collimator will be designed so that 32" sample environments can use a radial collimator

8. SEQUOIA Brillouin scattering upgrade

- Extending detector coverage down to 0.5 degrees scattering angle will allow for greater coverage within the first Brillouin zone of crystals or amorphous materials
- This option would be useful for examining spectra of
  - Ferromagnets
  - 4d and 5d magnetic materials
  - Molecular excitations in hydrogenous materials
  - Amorphous materials and liquids
- This technique is not available currently at the ORNL facilities
- This upgrade has been successful at the HRC spectrometer at J-Parc

8. SEQUOIA Brillouin scattering upgrade



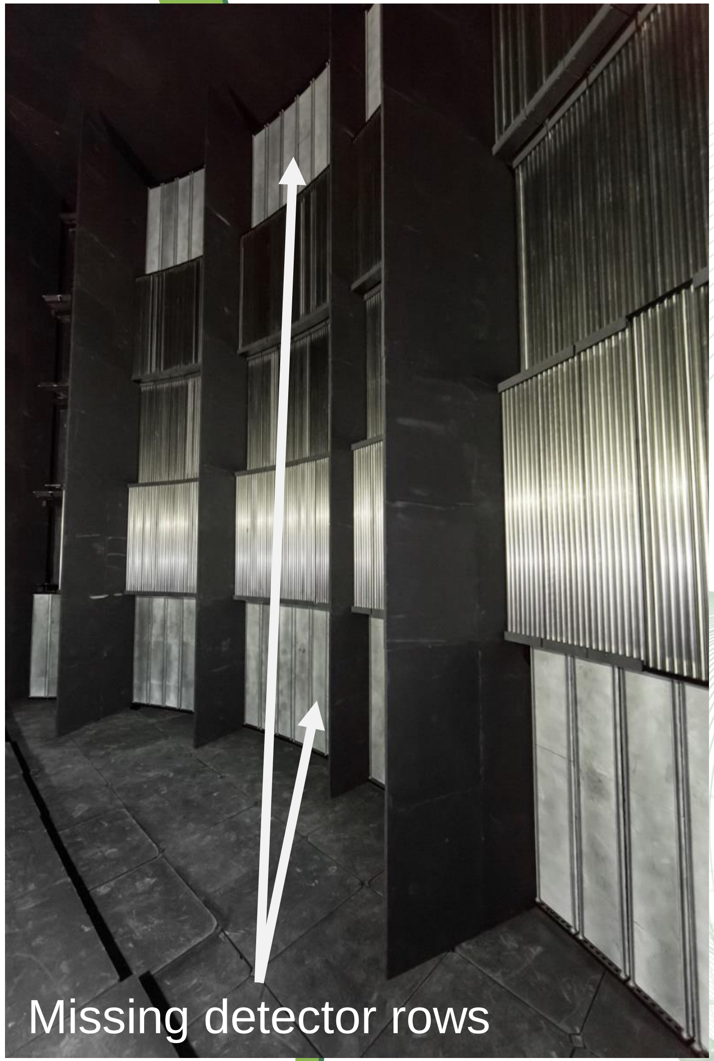


9. Response to instrument specific recommendations from last review

- 3 developments recommended to improve impact
  - Acquisition of radial collimator
    - Project was approved in October 2017. Funding was not awarded due to critical directorate needs
  - Filling out SEQUOIA's detector array
    - Instrument team has purchased 6 detector 8-packs since 2017. Four are installed. Instrument team has applied for funding in 2019 and 2020 for a group of detectors.
  - Brillouin scattering detectors
    - Project was approved October 2017. Funding was not awarded due to critical directorate needs.

10. Summary

- SEQUOIA is in great demand for good reasons
- Scientific output is progressing well
- Room for improvement in software and documentation
- Upgrade projects are in the queue with the neutron directorate
  - Vacuum upgrade project (completed)
  - Brillouin scattering upgrade
  - Radial collimator upgrade
- Long-term plan to complete detector array ($1.2M)



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National Laboratory

Thank you

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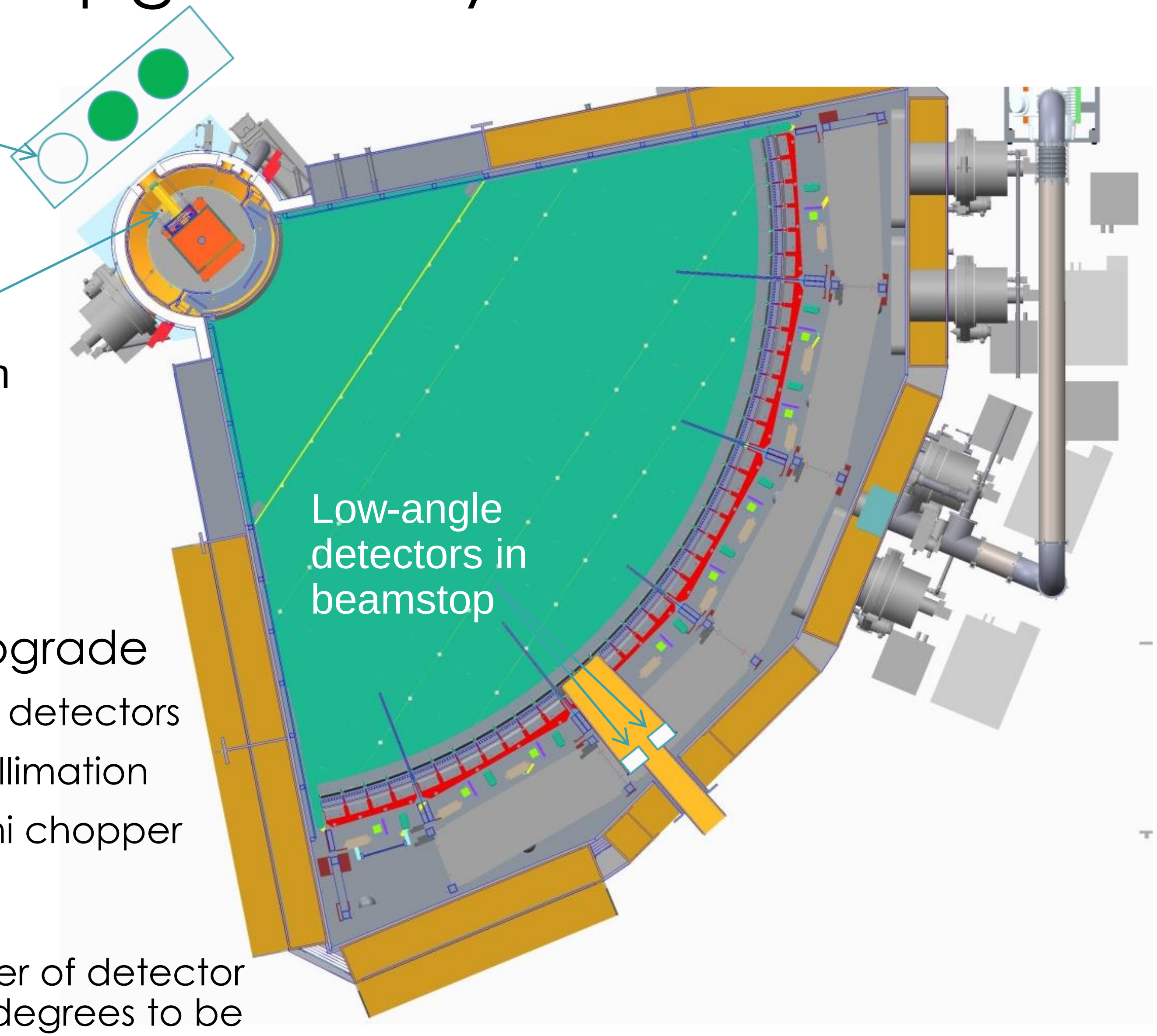
8. SEQUOIA Brillouin Upgrade Layout



- Three parts of upgrade
  - Add small angle detectors
  - Add incident collimation
  - Add a third Fermi chopper
- OPTION
  - Change diameter of detector tubes below 10 degrees to be ½ inch