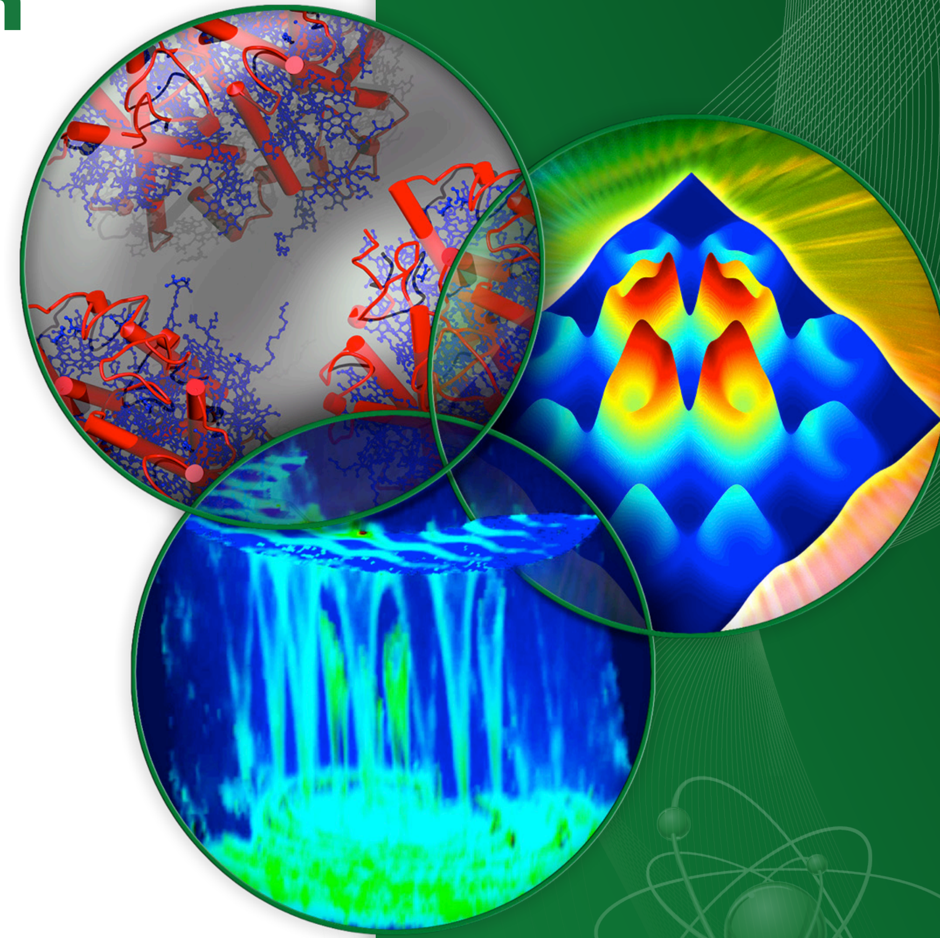
Reduction and Analysis of Neutron Data



G. E. Granroth

Scientific Data Analysis Group Lead

Neutron Data Analysis and Visualization Division

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

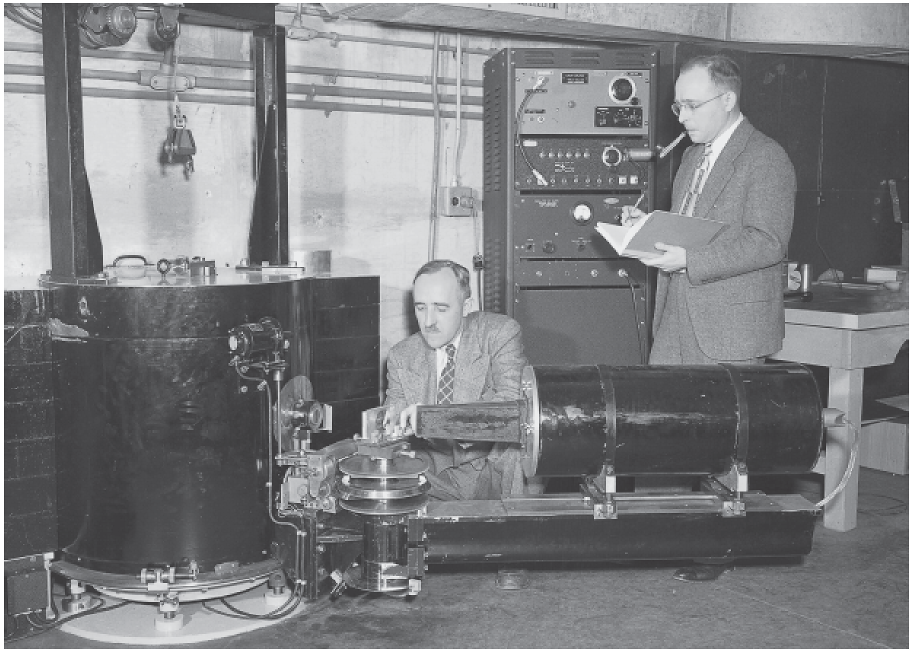
OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

Examples of Analysis and Reduction

- Overview
- Early Days at ORNL
- An example of magnetic excitations in Gd
  - Studying this magnet as
    - Instruments change, data sizes increase, and analysis methods change
- Novel Processing – Event based Reduction
  - Continuous T scans
  - Pulsed Magnet
- Complex analysis
  - Moving from simple fitting to more complex models to computing intensive codes
    - Ab-initio

Wollan teams with Shull

- In the early days counts were fastidiously recorded in a notebook.
- Shull and Wollan at the Graphite reactor
- 1994 Nobel Prize



First neutron powder diffraction

- Pioneered by Wollan and Shull in the late 1940's.
- Monochromatic

$$\lambda = 2d \sin \theta$$

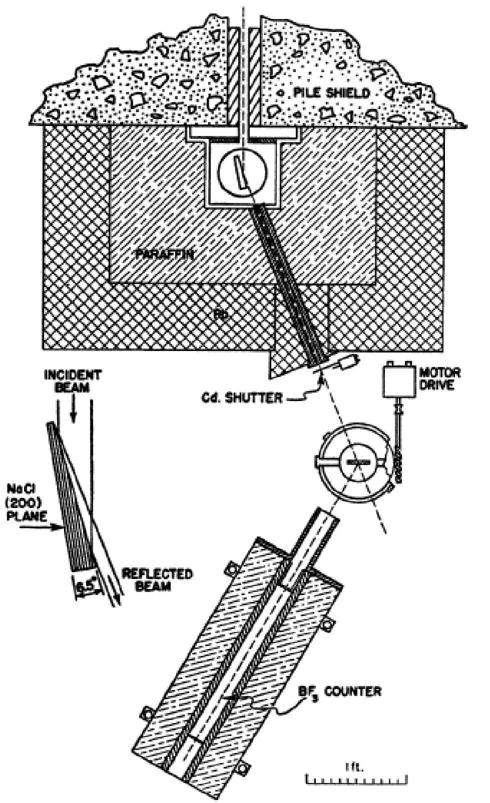
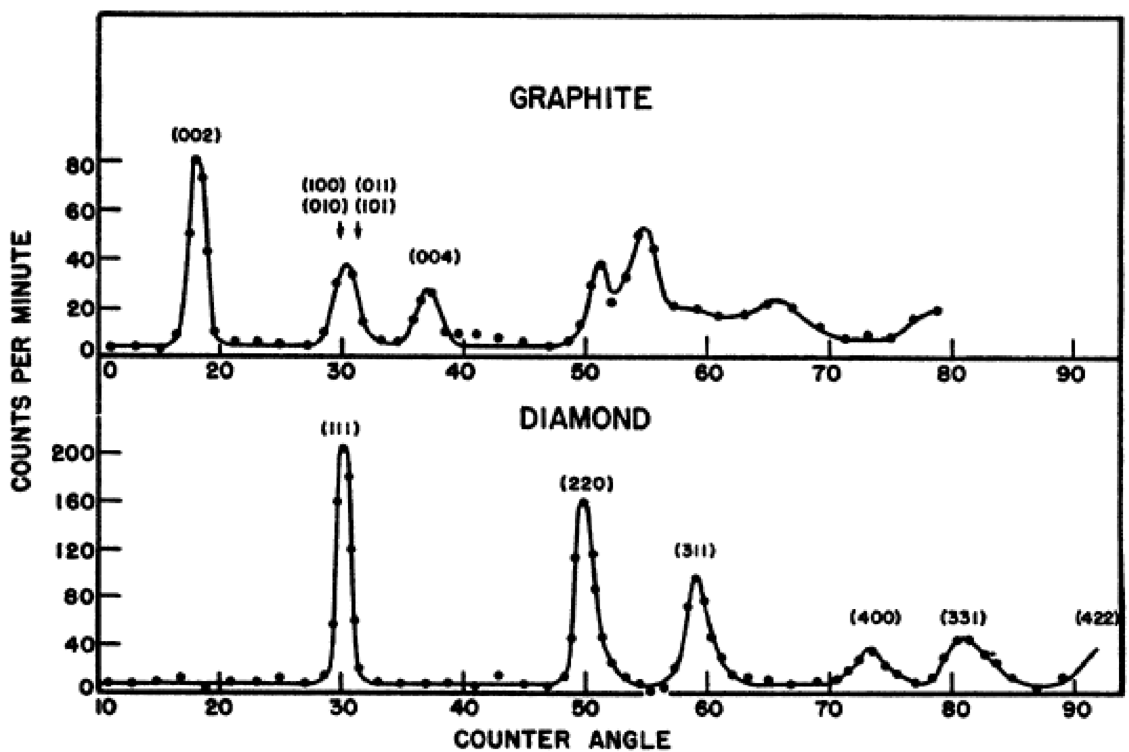


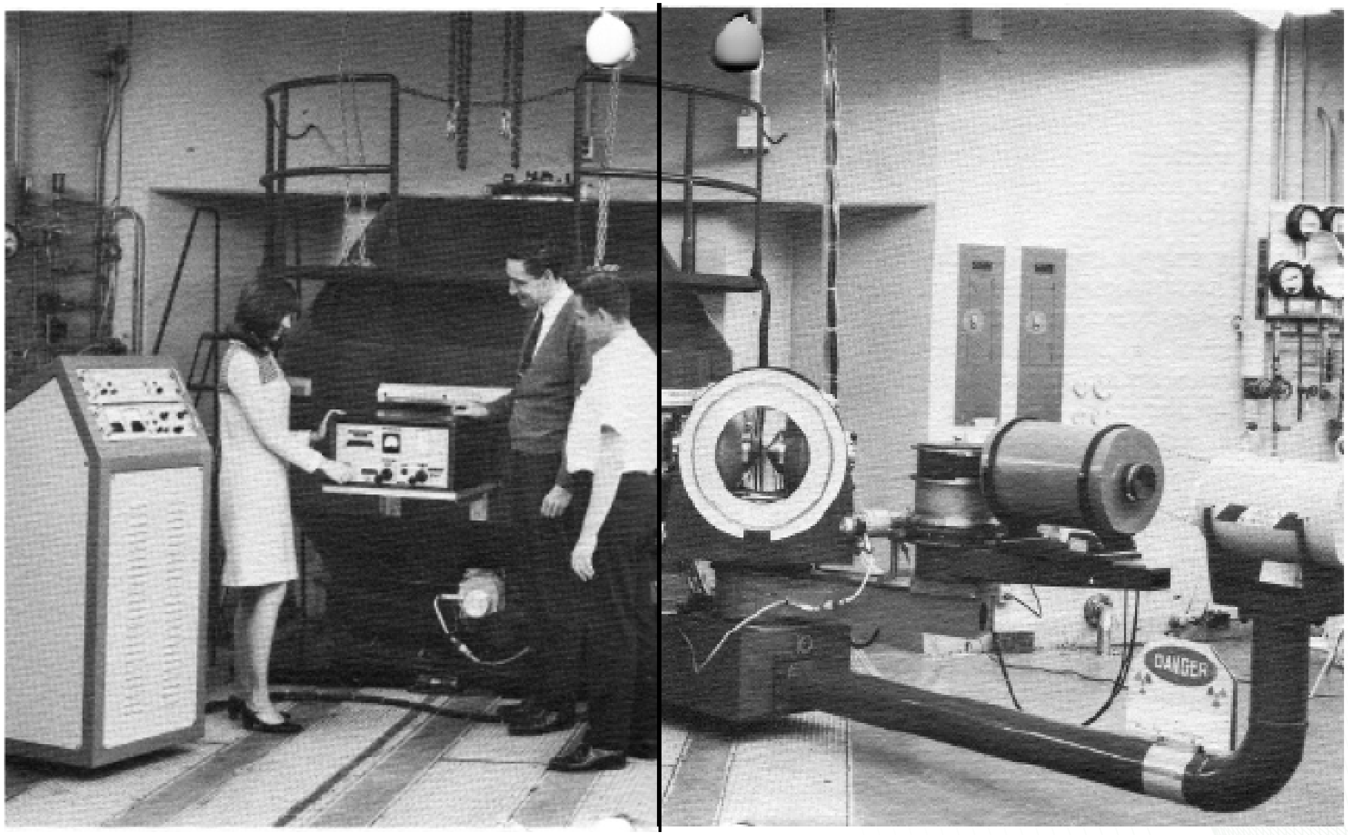
FIG. 1. Arrangement of apparatus, showing the monochromating crystal (detailed in left center) collimating slits, shielding, second spectrometer with location of powder specimen and counter.



E. O. Wollan and C. G. Shull, *The diffraction of neutrons by crystalline powders*, Phys. Rev. **73**, 830-841 (1948).

Computer controlled acquisition

- Increased Flux (New high flux reactor)
- More efficient detectors



Sharron King (left), adjusting the *rf* spin reversal circuit with Ralph Moon (middle), and Jim Sellers.

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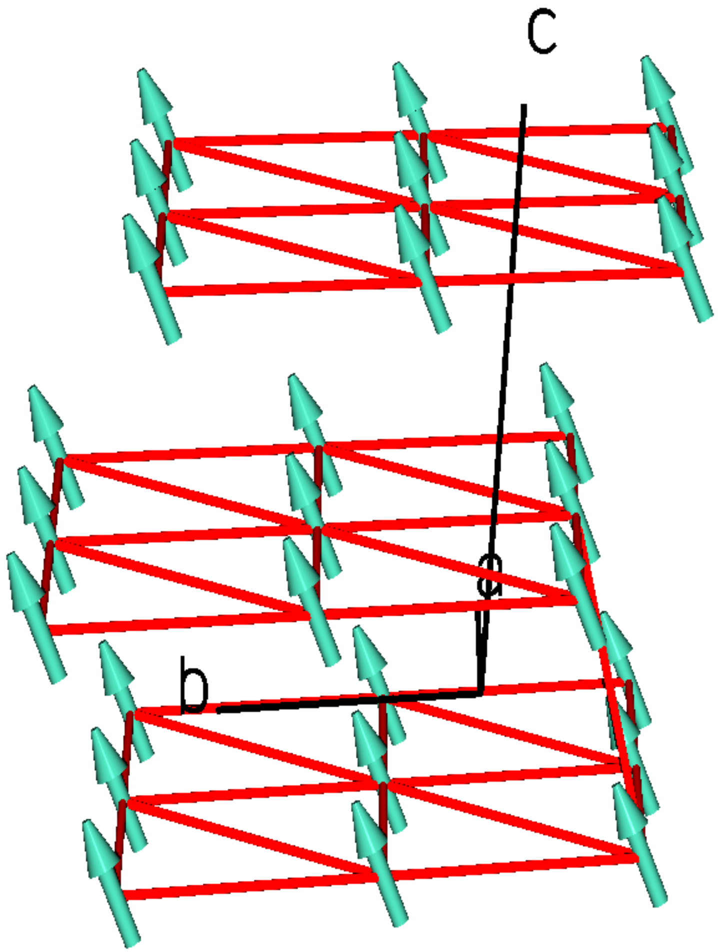
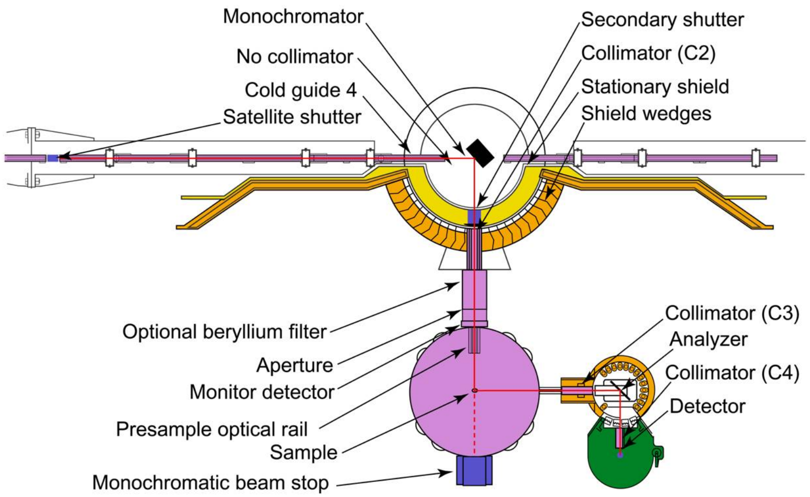
Gd

- Study Spin waves to understand interactions
  - Conduction electrons mediate exchange
- Sample
  - "Textbook" HCP localized Ferromagnet?
  - $7.6\mu_B$ moment
  - Hexagonal lattice a=b=3.643, c=5.781
  - μ canted ~ 30° from c
    - PR 165, 733 (1968); PRB 5, 997 (1972)



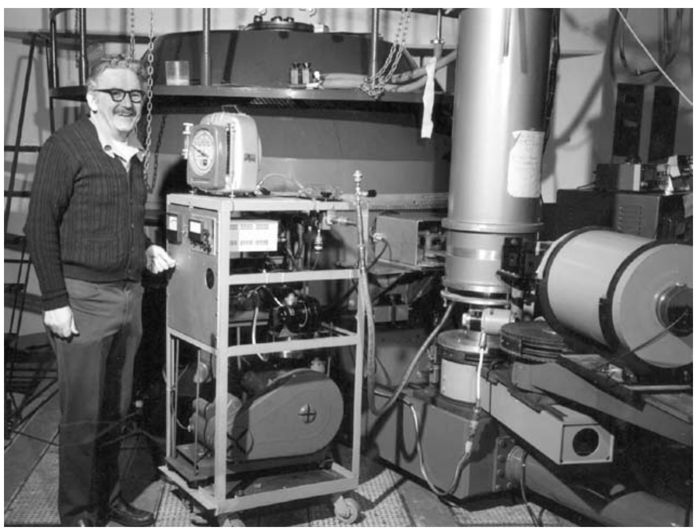
Triple axis is useful for measuring spin waves

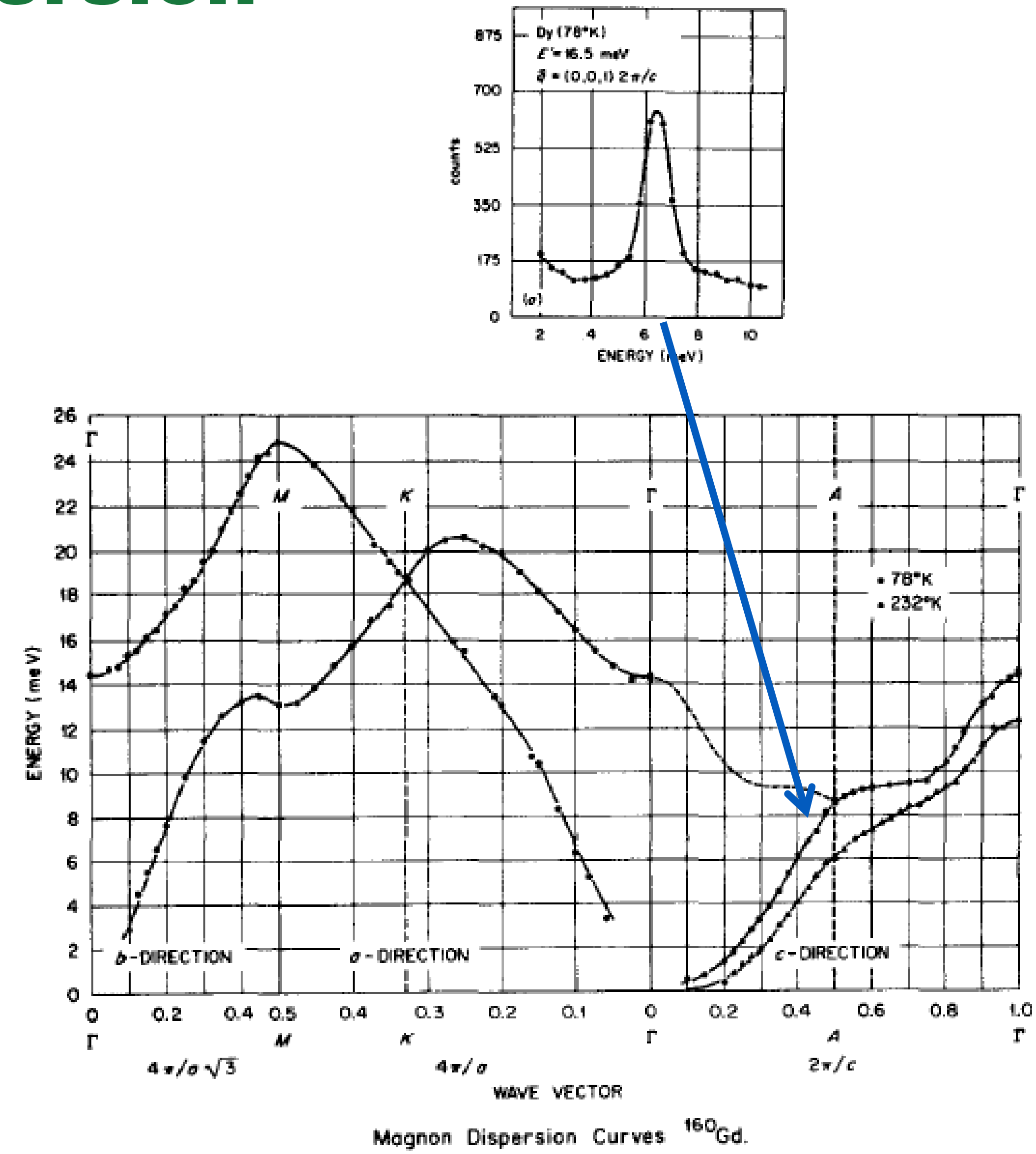
- Monochromator crystal (axis 1) selects a narrow incident energy wavelength distribution
- Analyzer crystal (axis 3) selects a narrow final energy distribution
- Axis 2 selects orientation of sample
- Straight forward to perform scans in E at constant Q or vice versa



Mapping the Dispersion

- Take a series of constant Q scans
  - Along high symmetry directions
- Fit the peak of each scan
- Plot the peak position vs. Q

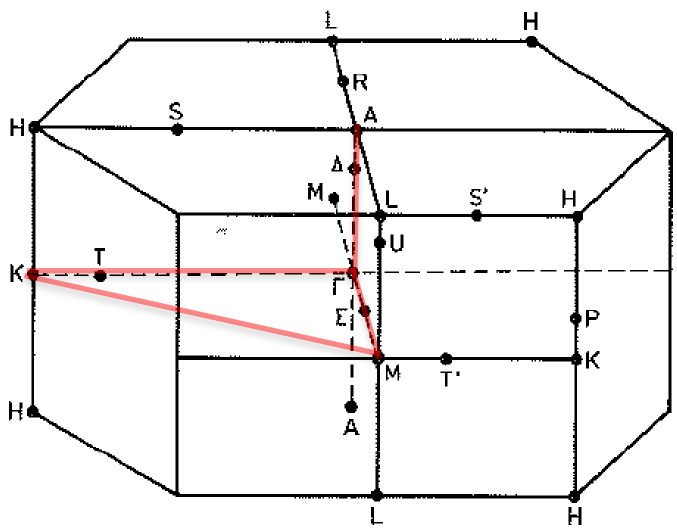


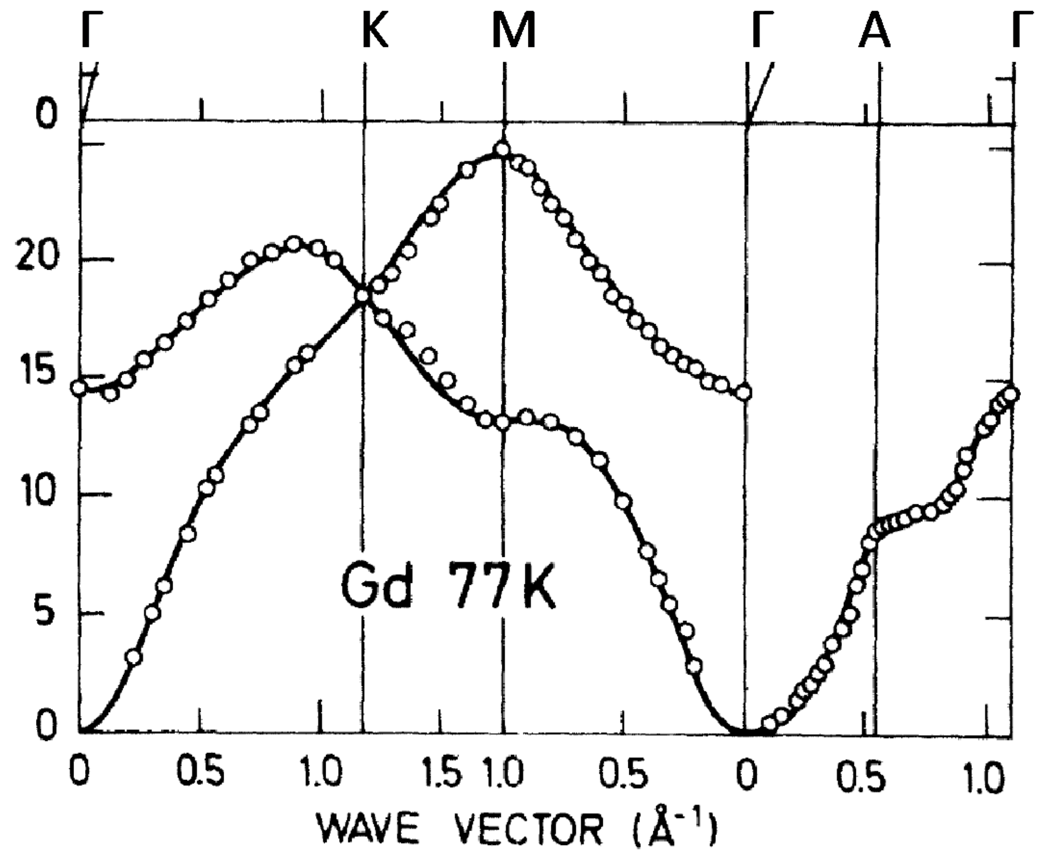


Koehler *et al.* PRL **24**, 16 (1970).

Data Analyzed

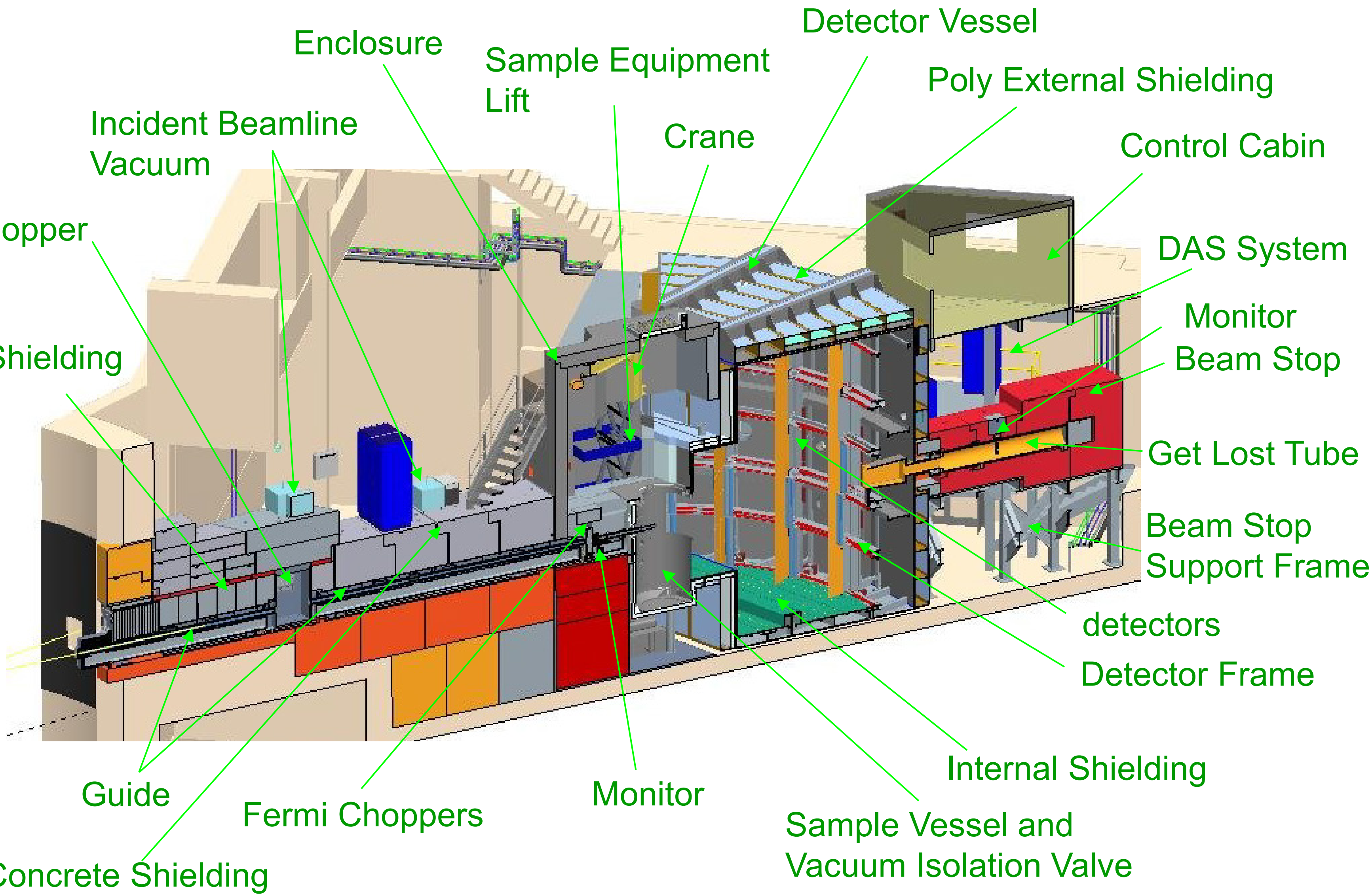
- Used Multiple exchange parameters to characterize RKKY interaction
- Γ 0,0,0 ; K ⅓,⅓,0; M ½,0,0; A 0,0,½





P. Lindgård PRB **17**, 2348(1978)

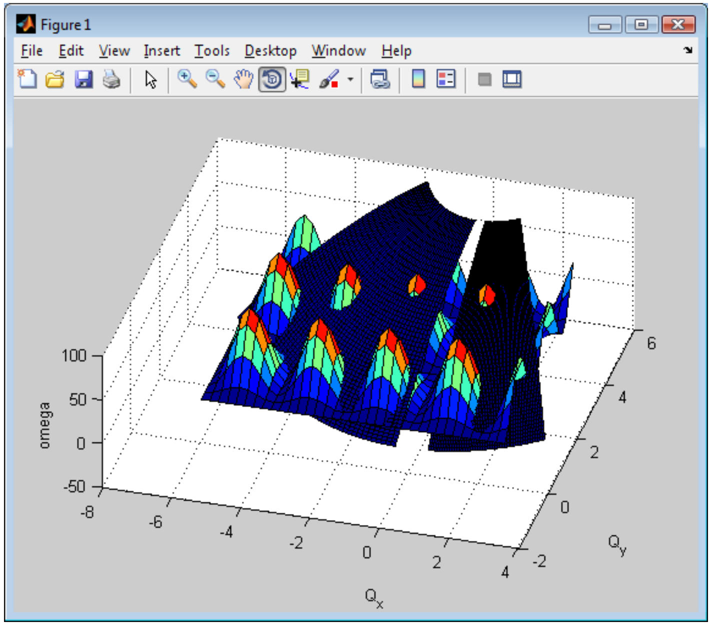
SEQUOIA – highly pixelated array

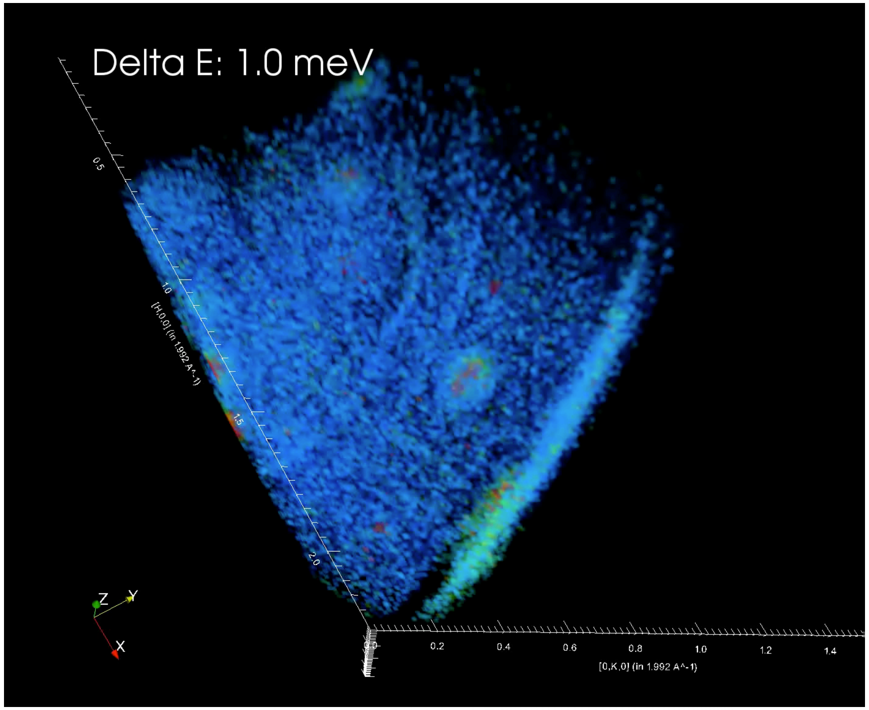


G. E. Granroth *et al.* Physica B 385-386, 1104 (2006). J. Phys.: Conf. Ser. 251, 012058 (2010).

Volumes of Data collected overnight

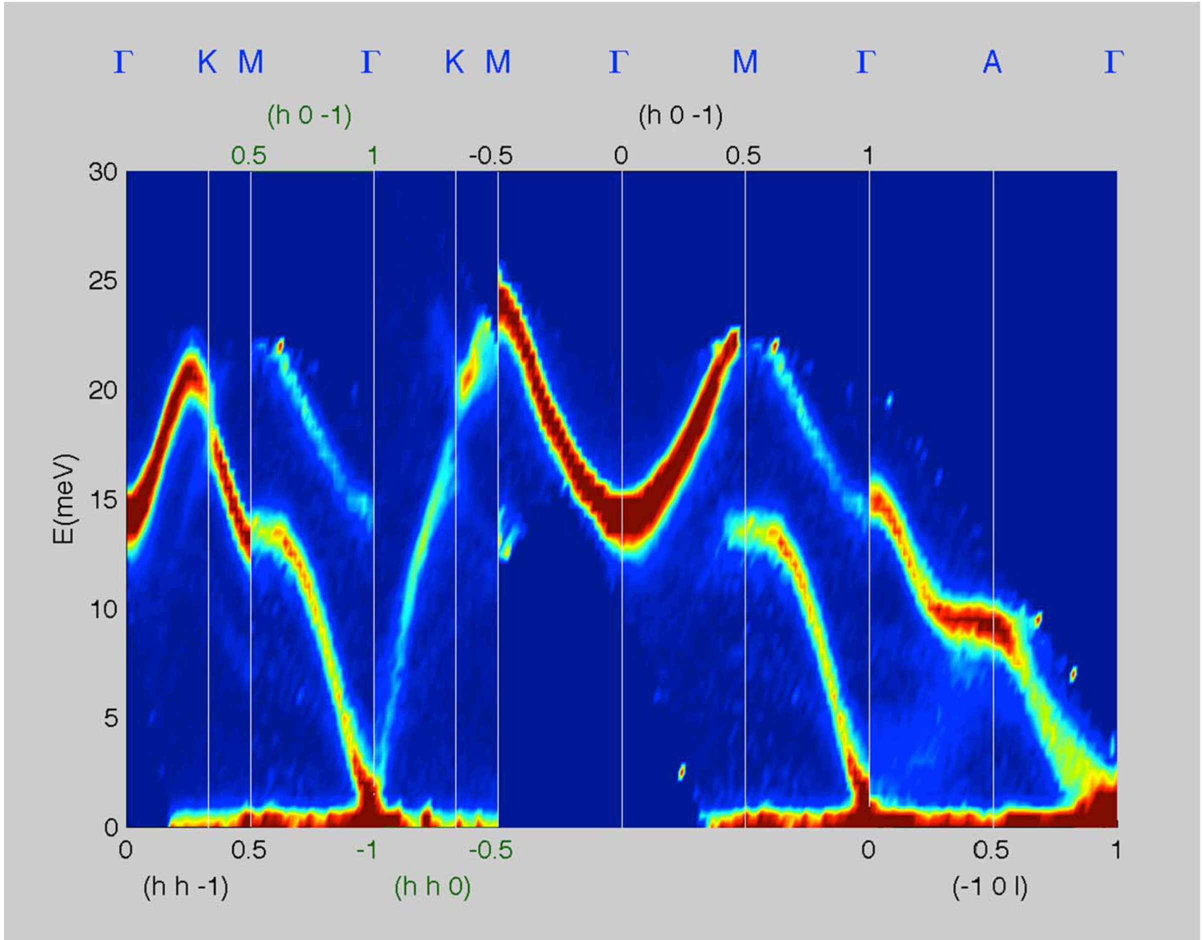
- Take a series of constant E slices
- Each orientation adds a new one.





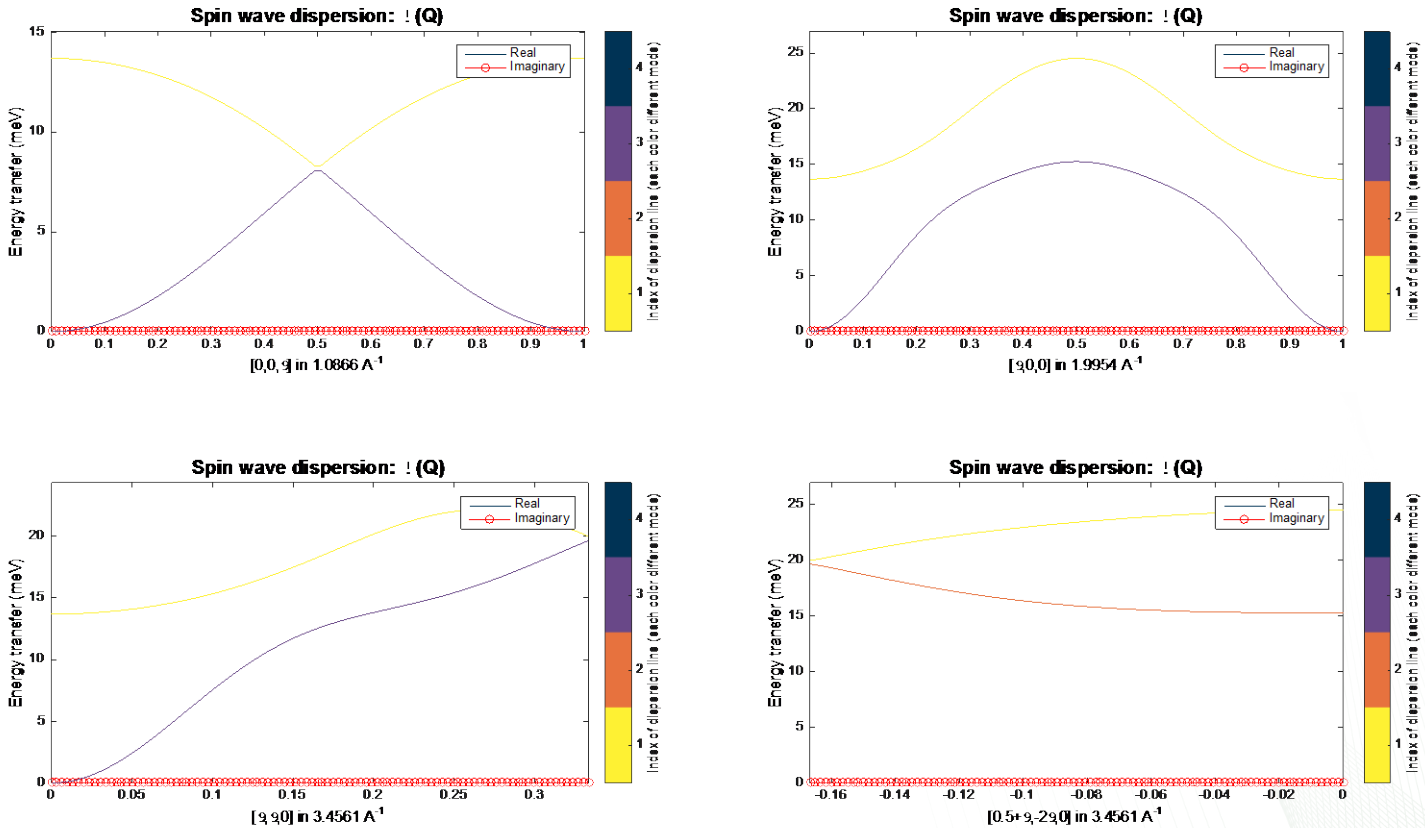
Data reduced in similar way

- Cutting volume data
- Also lots of intensity information
- Provides details of itinerant compontent



More Modern Analysis

- Modeled with Spin W



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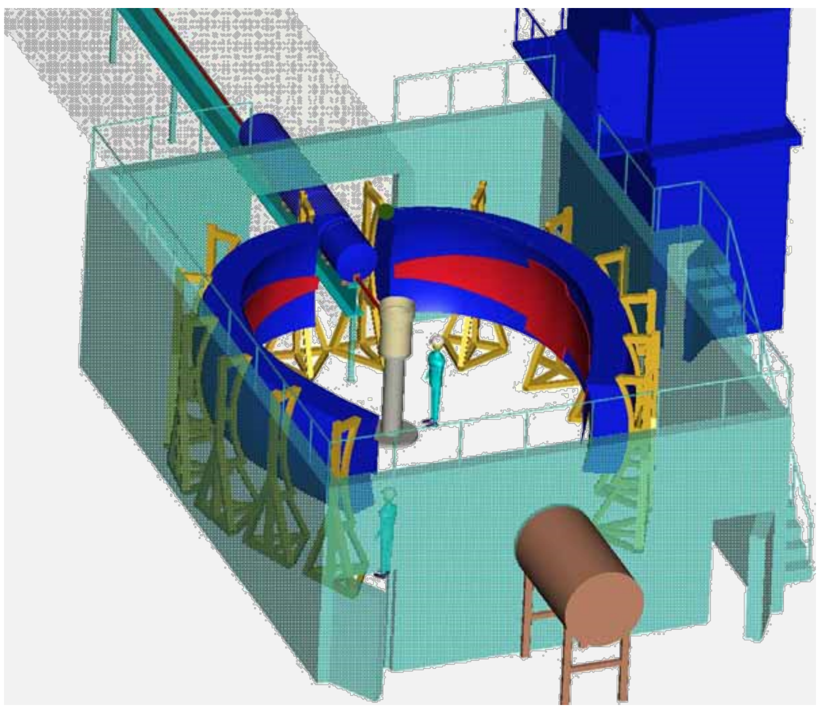
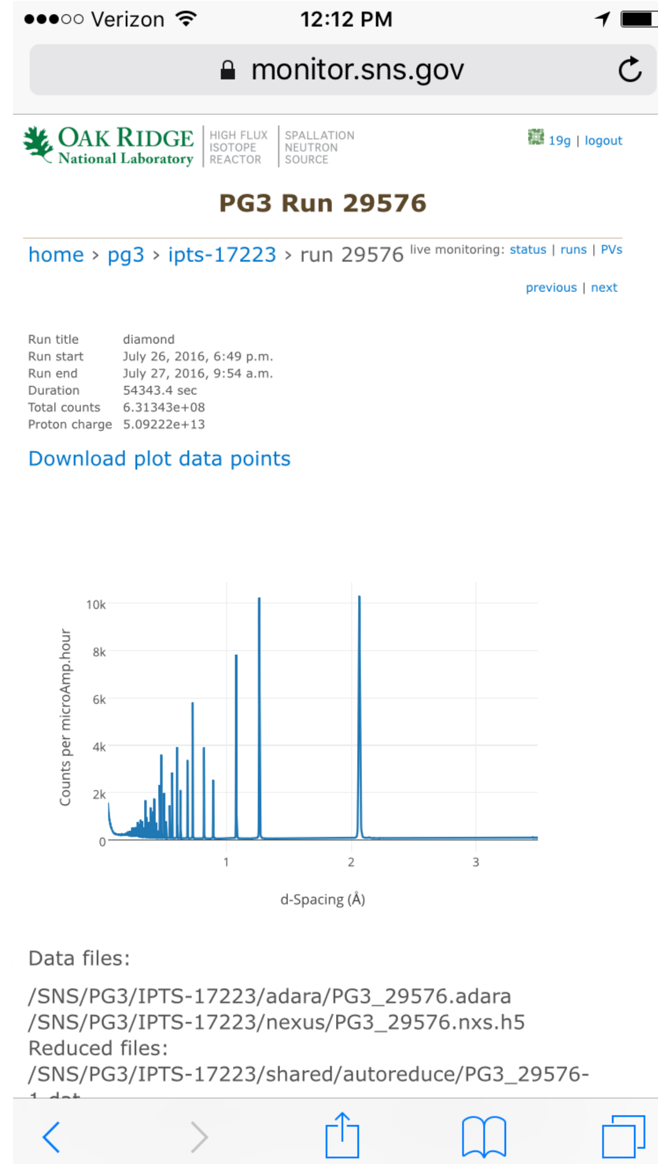
Event Data Processing

- Neutrons are recorded on an event by event basis
  - A list of pixel positions and time of detection
  - Can do
    - Continuously changing parameters such as
      - Temperature
      - Sample rotation
      - Battery charge
      - Gas loading
      - AC electric field
    - Time synchronized collection like pulsed magnet
  - For details of the algorithms for event data see
    - P. F. Peterson *et al.* NIMA **803,** 24 (2015)

POWGen

- Powder diffractometer
- Fixed detector array $\lambda = 2d \sin\theta$
- Tof encoded wavelength
- Data typically displayed in d





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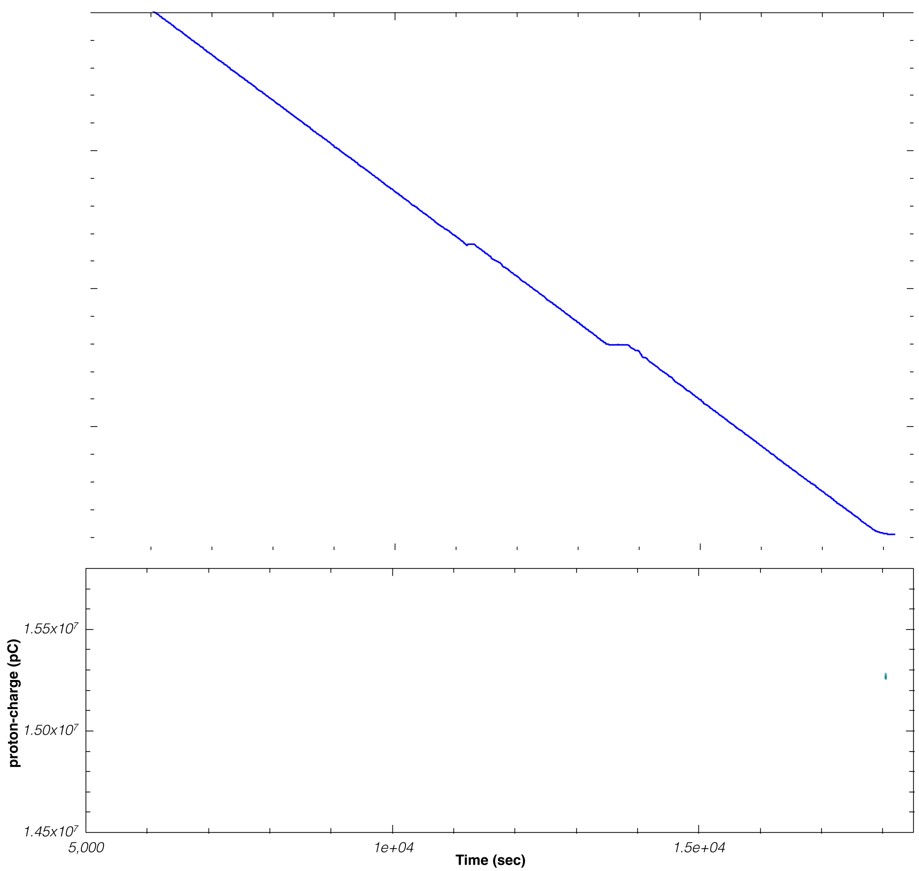
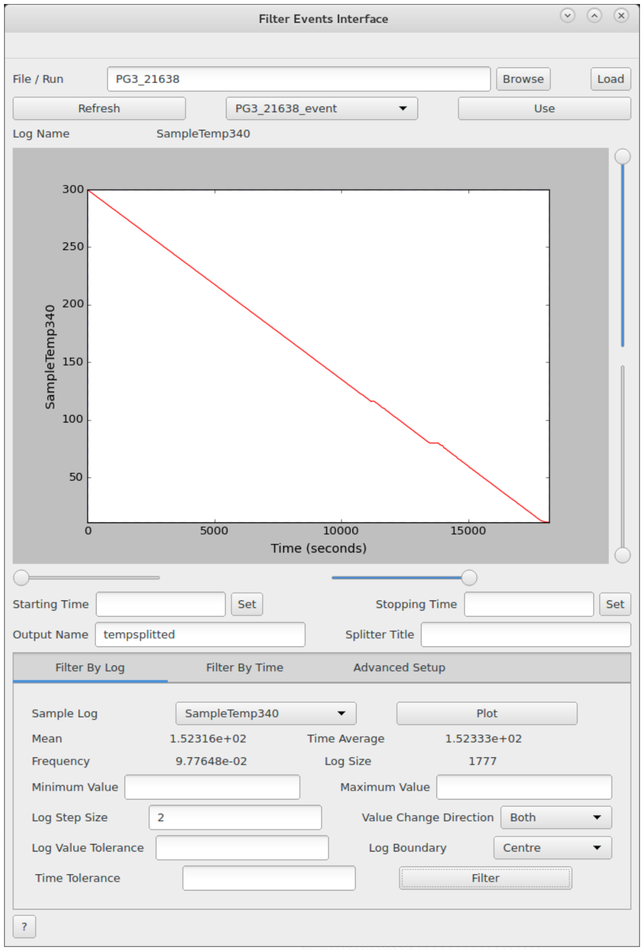
Powder Diffraction – Event Filtering

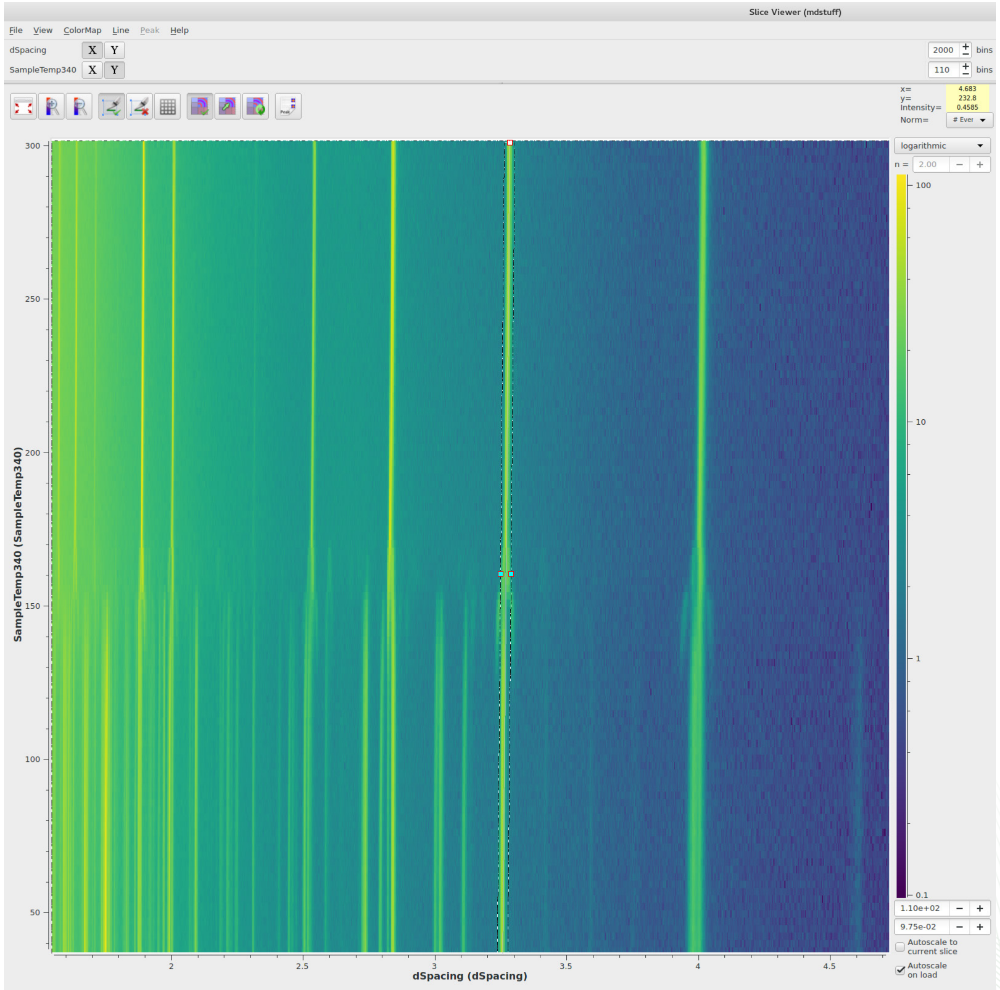
- Routine for continuous T scans
  - Scan pauses when beam down
- Interface for facilitating filtering





Working with Event filtered data

- Split into as many T bins as one wants in this case every 5 degrees
- Plot as another dimension



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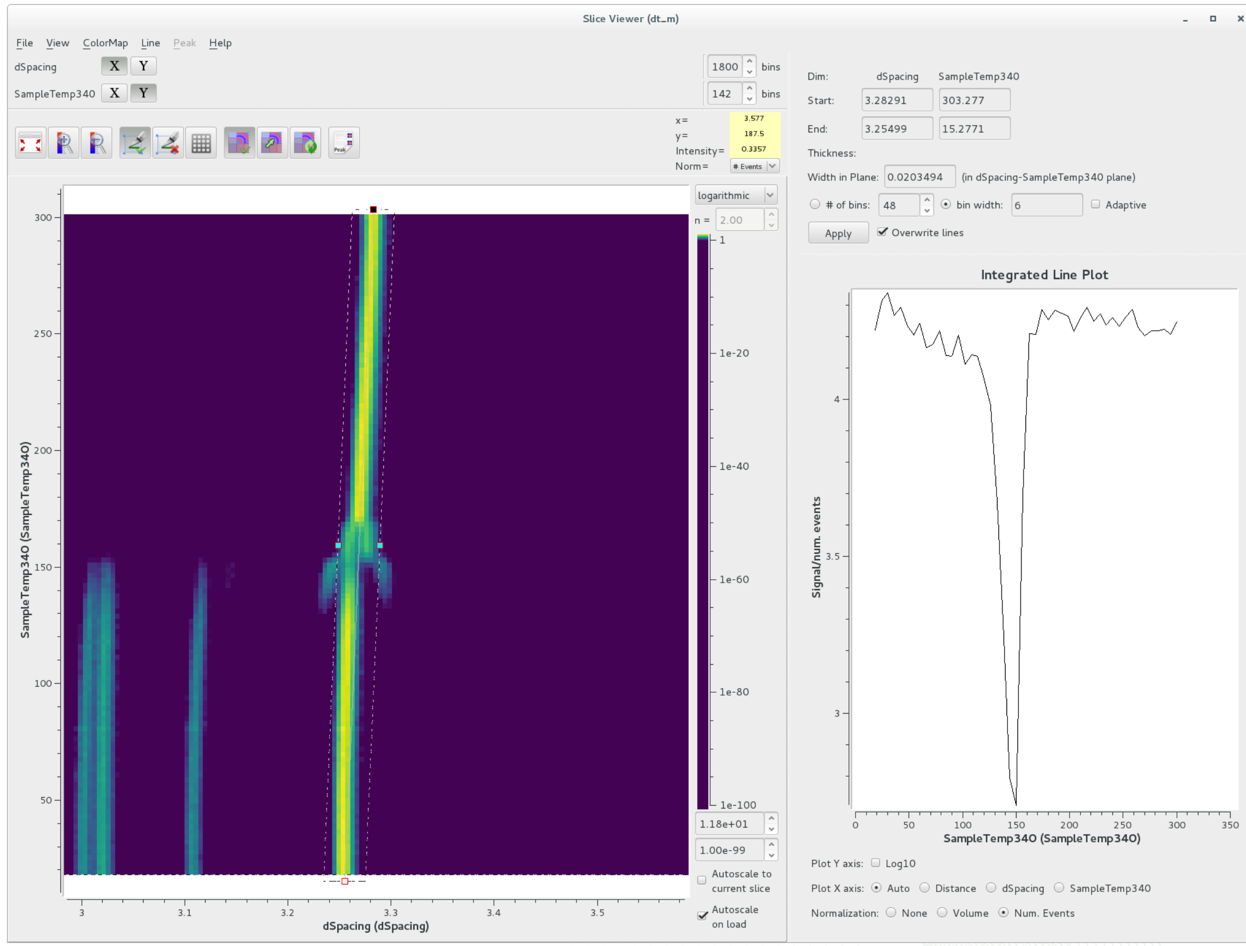
Slice viewer for MultiDimensional data sets

- Allows one to produce cut that takes into account lattice dimension change
- Helps with identifying phase transitions



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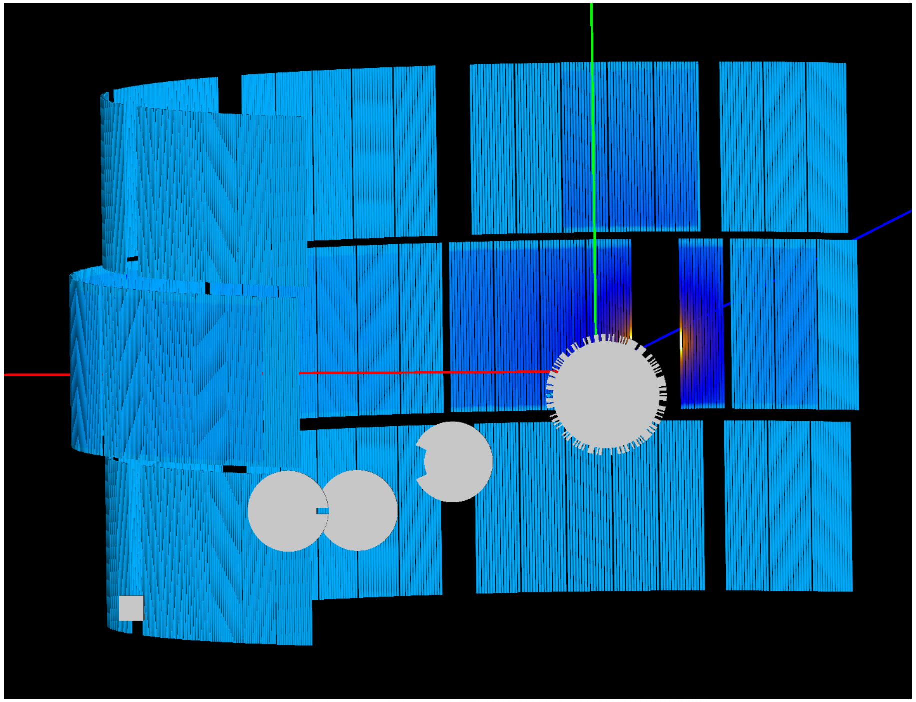
Corelli

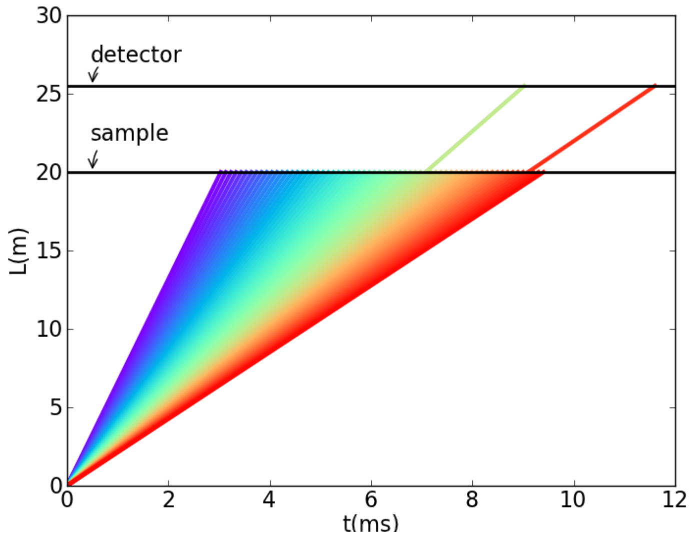
- Single Crystal diffractometer
- Designed for diffuse scattering
- Can discriminate elastic and inelastic scattering truly elastic scattering
- Also has low angle bank, ideal for magnetic scattering
- Fixed detector array

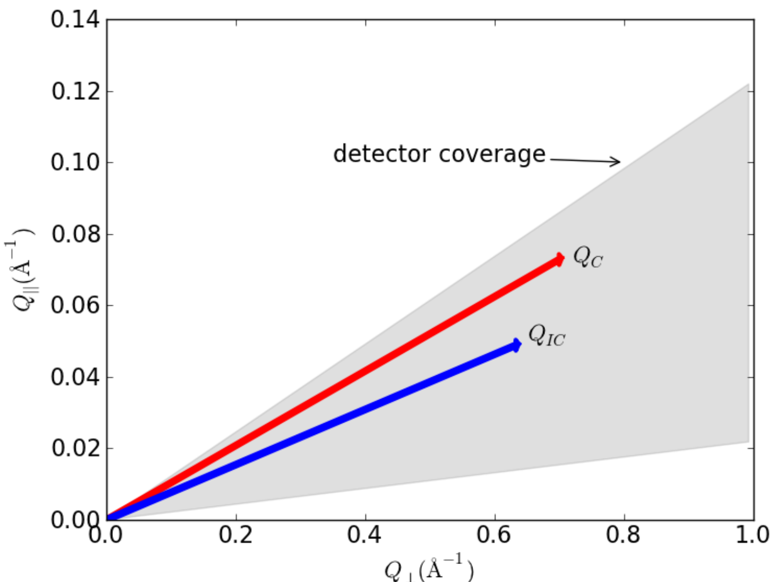
$\lambda = 2d \sin\theta$



TOF Neutron Diffraction

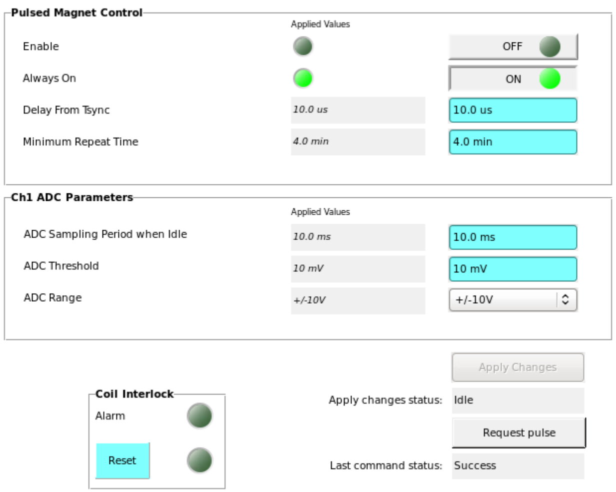
- wavelength is encoded in TOF $\lambda = 2d \sin\theta$
- Fixed detector array
- Laue pattern; but TOF allows identification of individual peaks
- Means multiple Bragg reflections for a single orientation

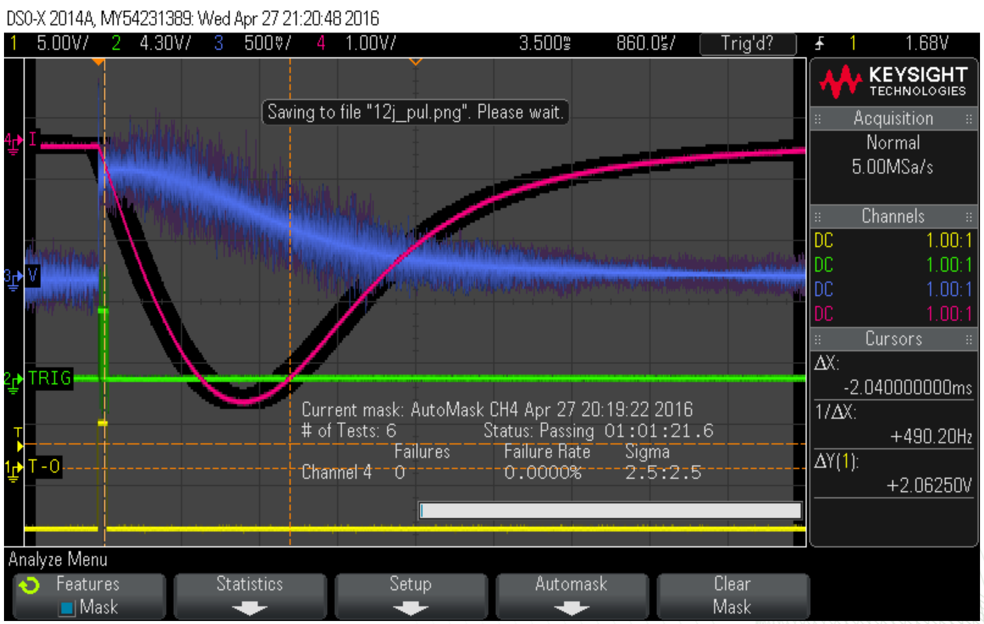




Interface to pulsed magnet

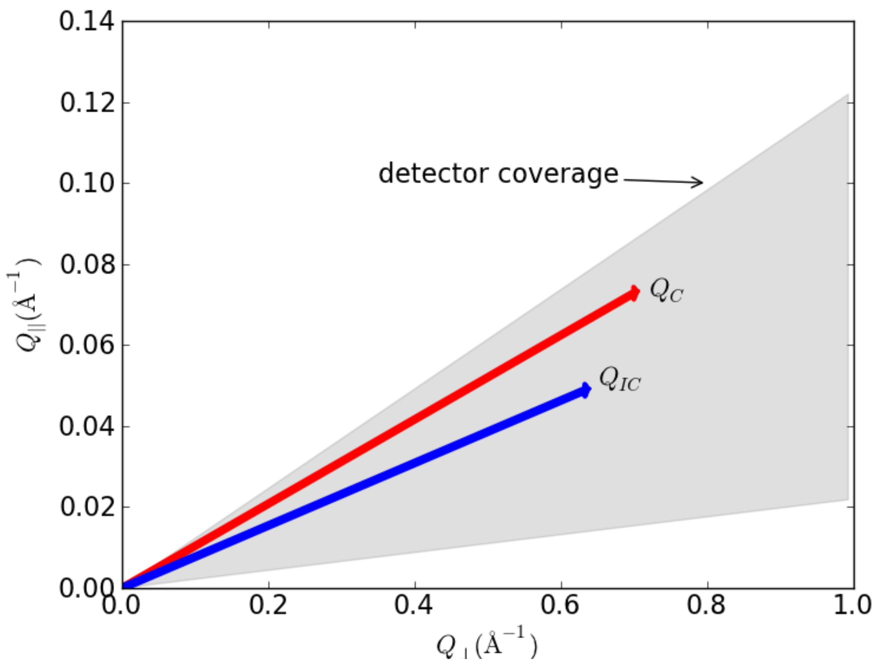
- Send trigger based on when proton hits the target.
- Use offset to set field at a given wavelength

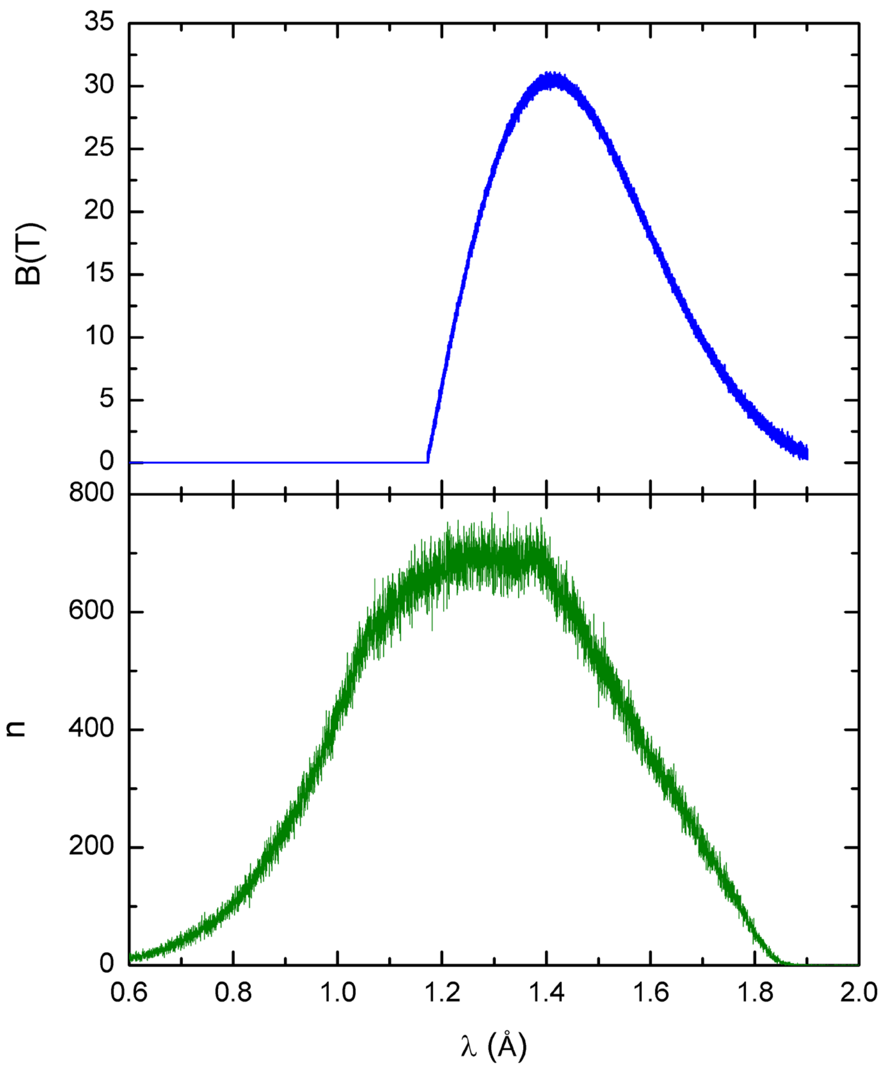




TOF neutrons + pulsed magnet

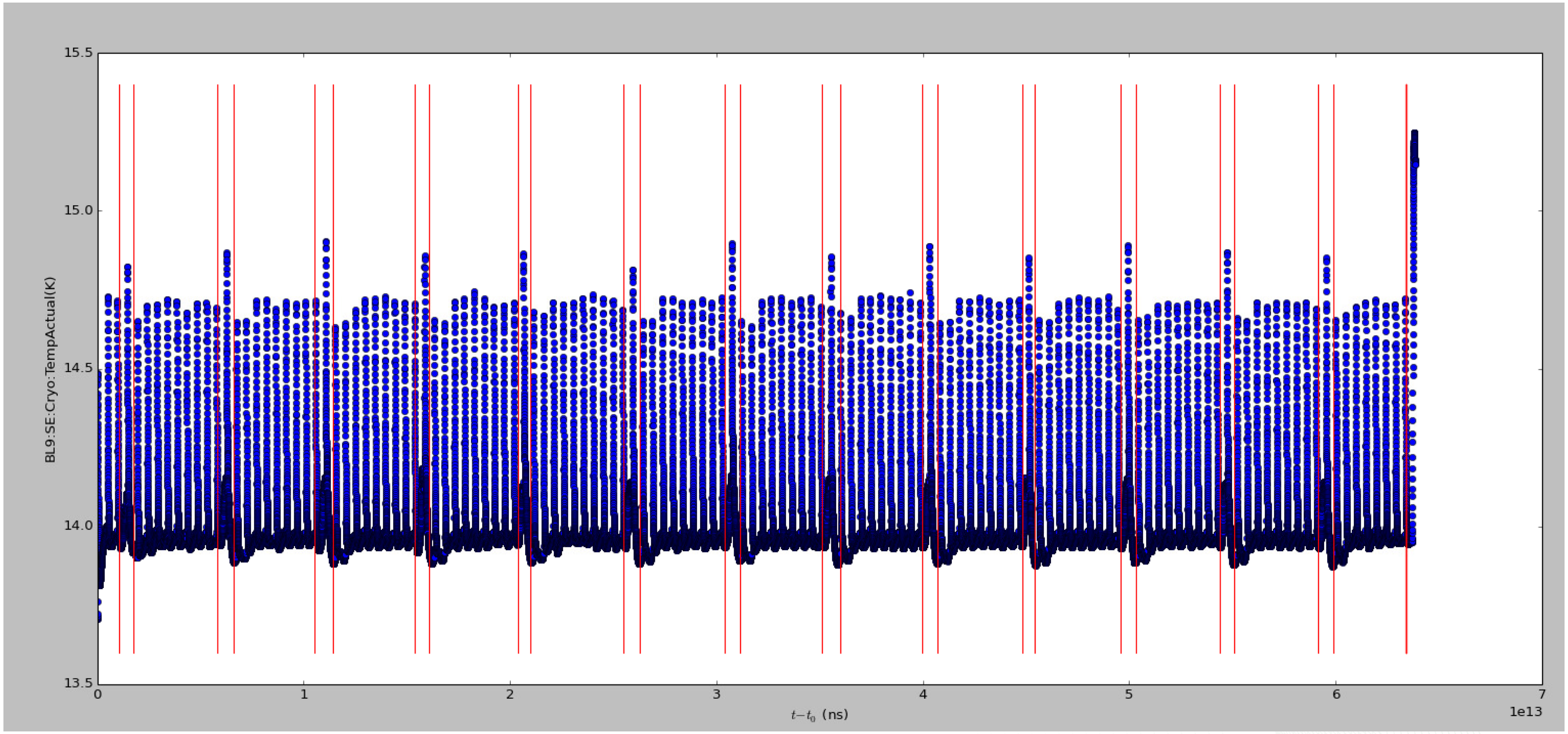
- Independently vary field and wavelength band as a function of time



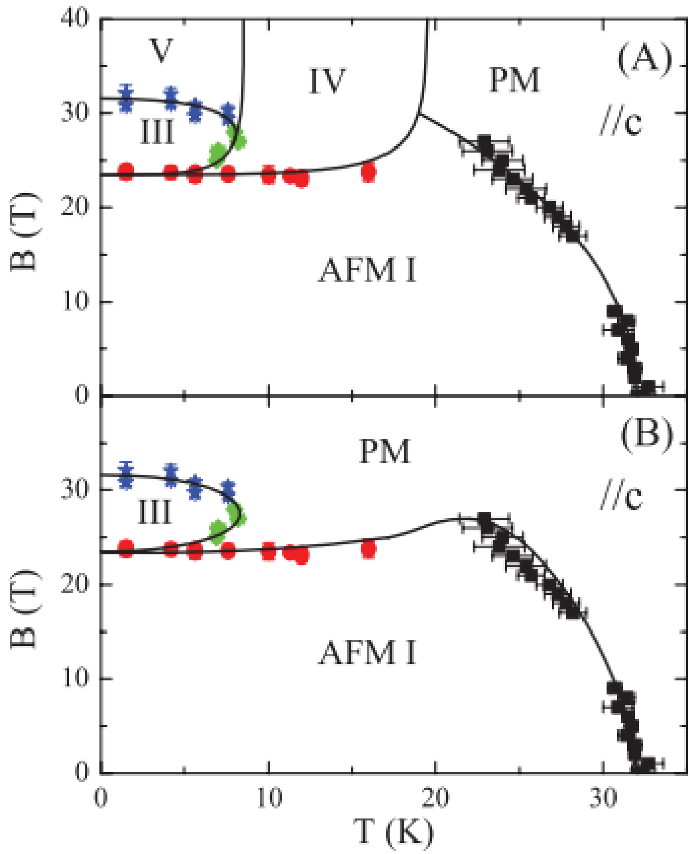


Adding additional filters

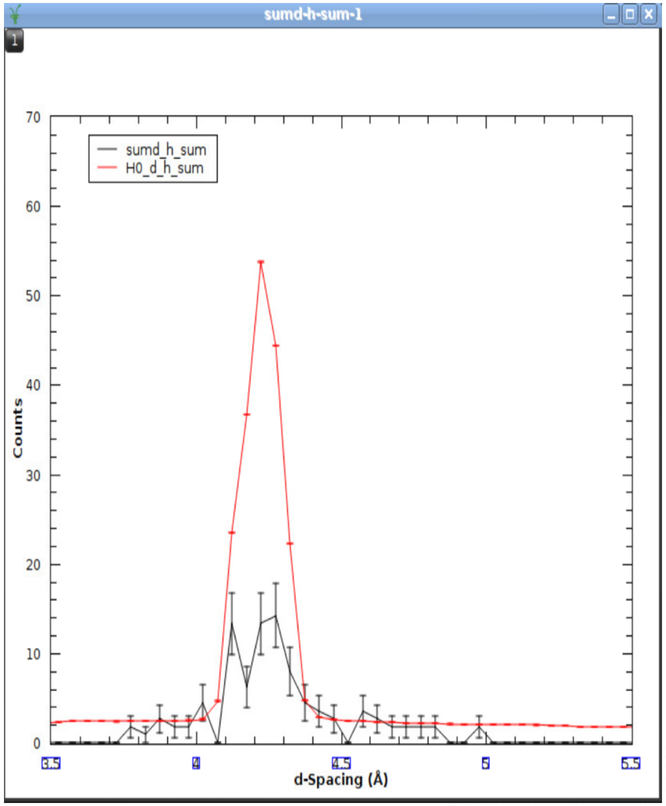
- Filter out temperature excursions too, multiple filters can be applied



UPt_2Si_2



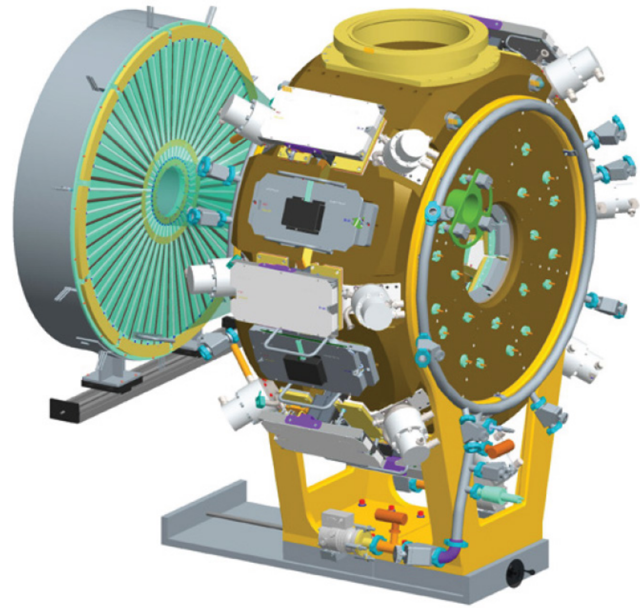
D. Schulze Grachtrup *et al.* PRB 85, 054410 (2012)

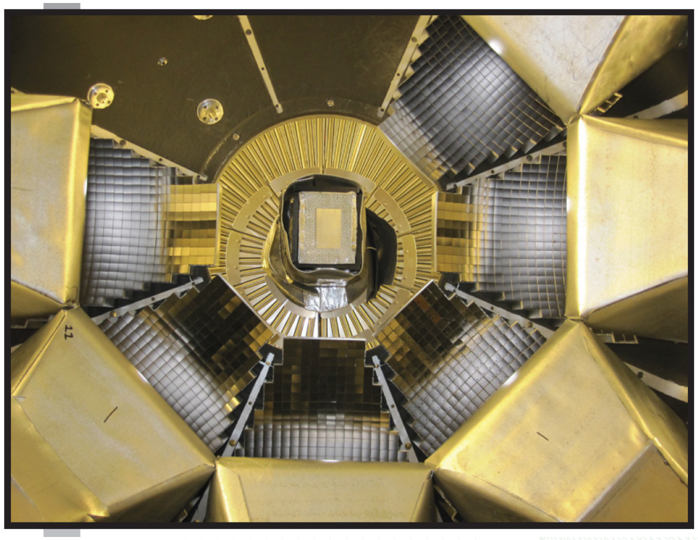


- Field dependence of 1 0 0 peek consistent with the PM phase
- T=14K

Vision

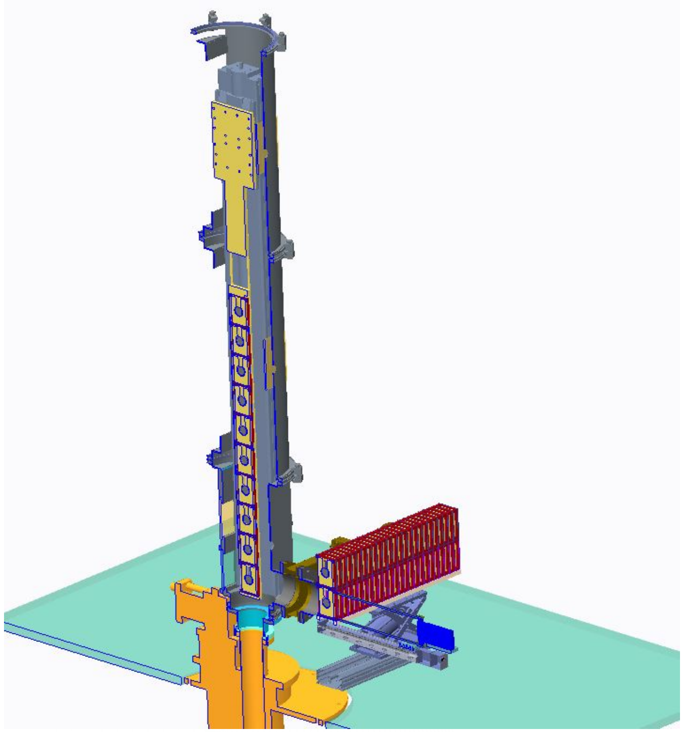
- Inverse Geometry
  - Crystal analyzers select a specific final energy
  - Initial energy is determined by TOF
  - Focuses large scattering volume onto a few detectors

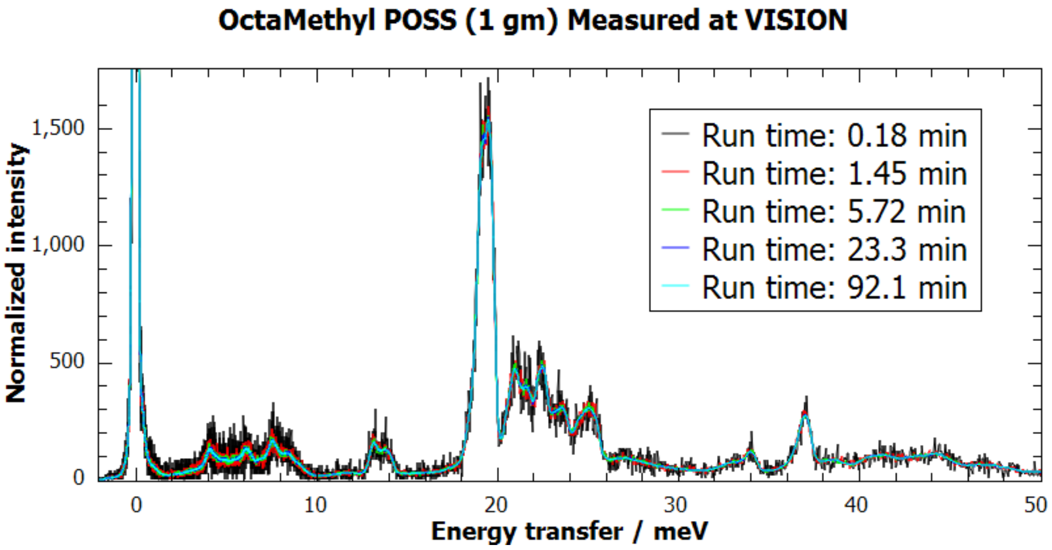




VISION: world's first high-throughput inelastic neutron scattering instrument

- 4000 x TOSCA at ISIS, 1 TB of data/day
- INS measurement in a few minutes to a few hours
- Sample changer is being designed and will be ready by 2016
- Expecting tens of samples a day to be analyzed
- DFT modeling of INS spectra is essential in data analysis and interpretation

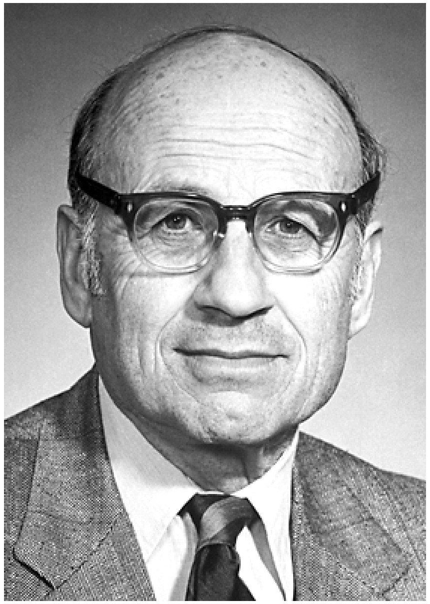




- Major challenges in computation
- Dedicated computer cluster required

Density Functional Theory

- Assumes only valence electrons are relevant
- uses effective wave functions to describe bonding
- Works on each atom in a unit cell
- Thus determines (without fitting)
  - Structure
  - Electronic structure
  - Lattice vibrations
  - Well suited to molecular vibrations
- Many packages
- Require a lot of computing resources



Walter Kohn
Nobel Prize Chemistry 1998

VirtuES Cluster – Hardware Specs

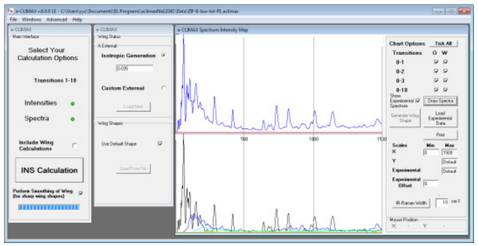
CADES

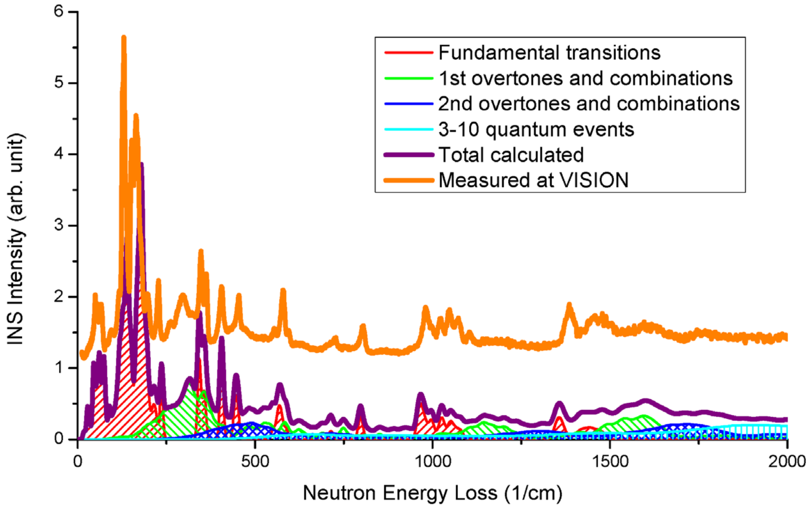
- Dual 16 core Intel Haswell E5-2698v3 2.3 GHz Processors per node
- 50 compute nodes
- 1,600 (non-hyperthreaded) cores
- 128 GB memory/node
- 6.4 TB Total memory
- Each node has 10Gbe and Infiniband networking for connectivity.

Installed as part of the ORNL Compute and Data Environment for Science (CADES)

Integrated modeling for Vision

Computer modeling is crucial to understand and interpret INS data.





CASTEP
VASP
Quantum Espresso
Gaussian
→ Vibrational modes and frequencies → INS simulation (aClimax) → Simulated INS spectra

Sample → VISION → Data reduction and analysis (Mantid) → Measured INS spectra
→ Measured diffraction

Peak assignment
- Structure-dynamics correlation → Understanding mechanisms and properties at atomic level
- (An)harmonicity → Mapping out the local potential energy profile using finite displacement, frozen phonon, molecular dynamics
- Phase transition → Revealing the kinetics and the transition pathway

Summary

- Gd
  - Can now map volumes of excitations (~30GB of data)
  - Volumes reveal information about symmetry
  - Tools like Spin W or Spinwave Genie make spin wave calculations common place
  - Similar changes have been seen for other techniques, e.g. diffuse scattering
- Event based data enables new types of experiments
- Integration of ab initio codes and HPC is enabling more science

Acknowledgements

- NDAV members
  - Jean Bilheux
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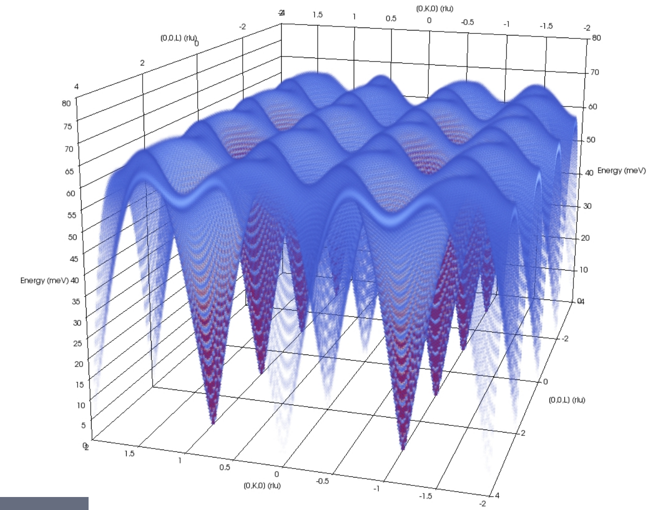
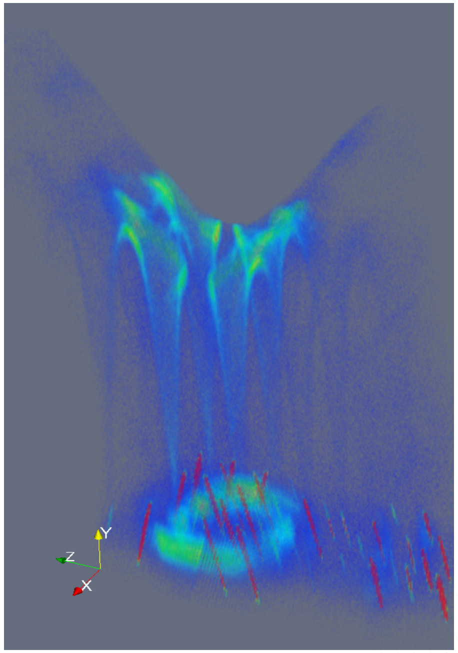
  - Jaime Fernandez-Baca
  - Masa Matsuda
  - Steve Nagler
  - Feng Ye
  - Jooseop Lee
- ORNL – ISD
  - Matt Rucker
  - John Wenzel
  - Andrei Parizzi
  - Harley Skorpenske

$YFeO_3$ a more complex system

- Many exchange terms
- Viewed with Mantid/Paraview
- Modeled with Spin Wave Genie

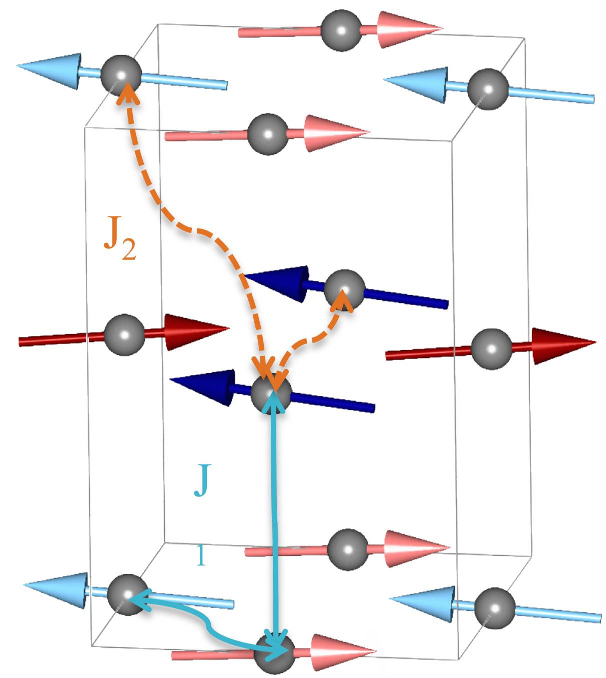




S. E. Hahn *et al.* PRB **89**, 014420 (2014)

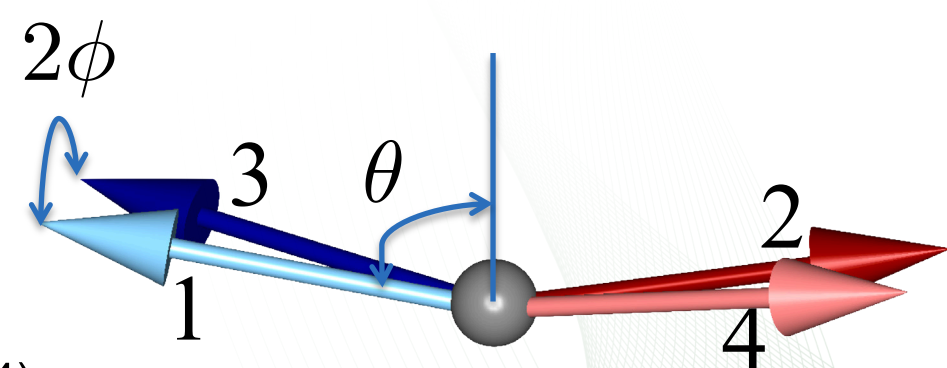
$YFeO_3$ A more Complex System

$$
\begin{aligned}
H = & -J_1 \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - J_2 \sum_{\langle i,j \rangle'} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \\
& - D_1 \sum_{\boldsymbol{R}_j = \boldsymbol{R}_i + a(\hat{x} \pm \hat{y})} \hat{y} \cdot \boldsymbol{S}_i \times \boldsymbol{S}_j \\
& - D_2 \sum_{\boldsymbol{R}_j = \boldsymbol{R}_i + a(\hat{x} \pm \hat{y})} \hat{z} \cdot \boldsymbol{S}_i \times \boldsymbol{S}_j \\
& - K_a \sum_i (\boldsymbol{S}_i^x)^2 - K_c \sum_i (\boldsymbol{S}_i^z)^2
\end{aligned}
$$

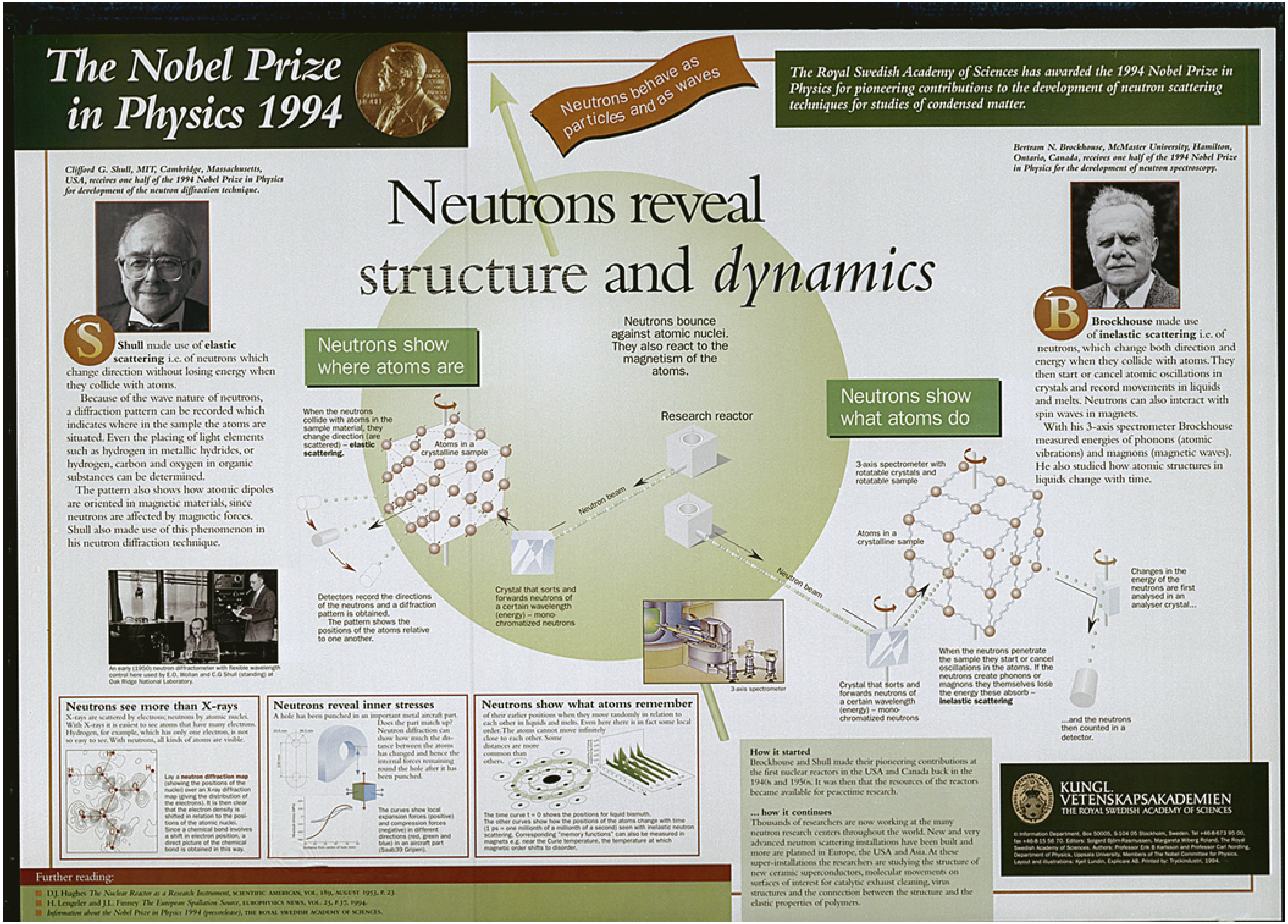


$$\theta = \frac{\pi}{2} + \frac{2D_1}{2J_1 + K_c - K_a}$$

$$\phi = -\frac{2D_2}{4J_1 - 8J_2 - K_a}$$



S. E. Hahn *et al.* PRB **89**, 014420 (2014)



Wollan died in 1984. His surviving family members were Shull's guests at the Nobel ceremonies.