

# Reduction and analysis challenges across the STS instrument suite

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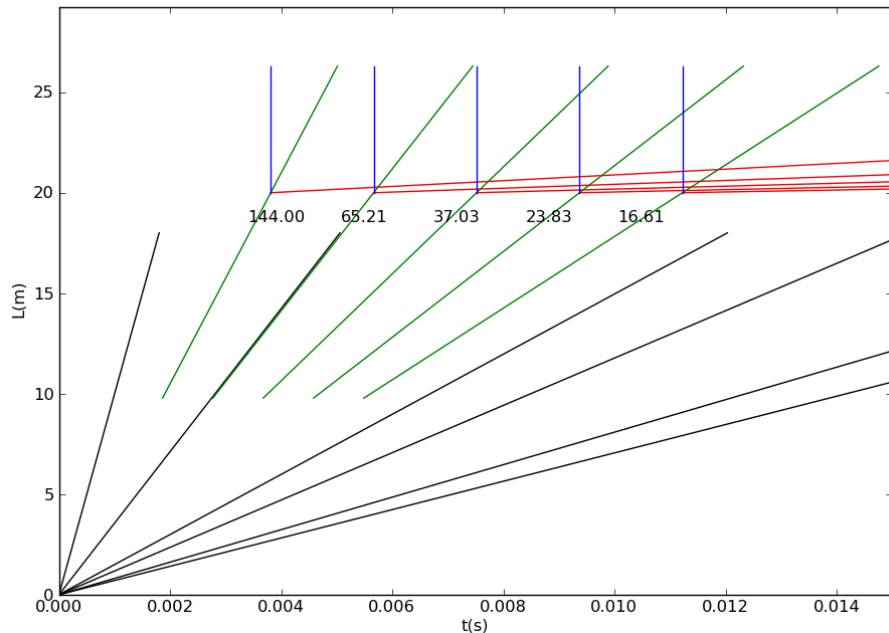
# Outline

- Analysis of Repetition Rate Multiplication
- Analysis of hierarchical structures (the overlap between SANS and diffraction)
- Effective Collection and UX for Cinematic Mode
- Designing instruments to exploit super resolution

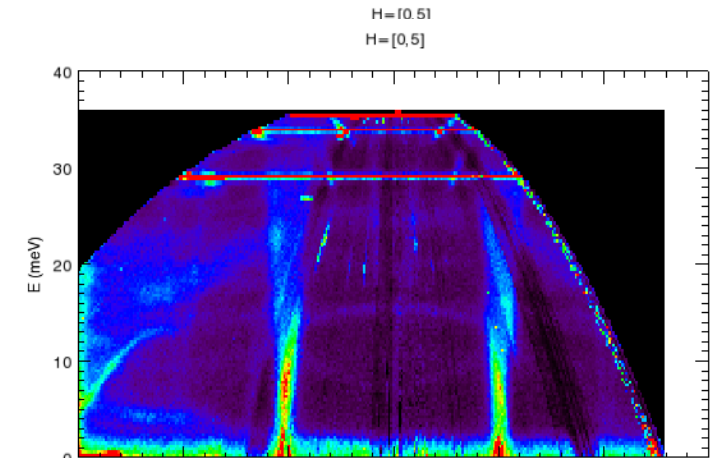
# Repetition Rate Multiplication

- Measuring more than one Incident energy in a given frame.
- Longer frames mean it can be exploited more.
- Currently in use at LET, Amateras, HRC, and in a limited case on SEQUOIA
- Measurements from SEQUOIA show the potential

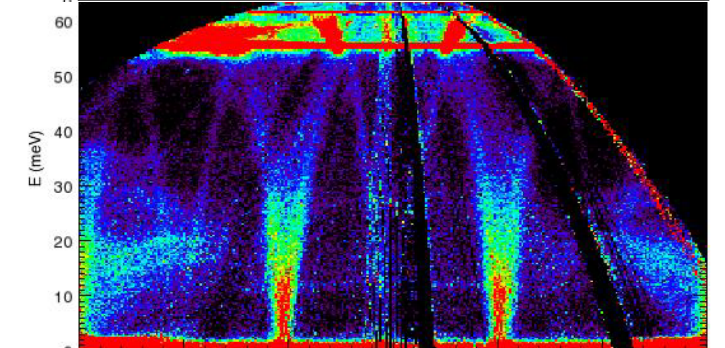
$E=144$  meV  $\nu_{fermi}=600$  Hz  $\nu_{x_0}=90$  Hz slit pack:SEQ 700



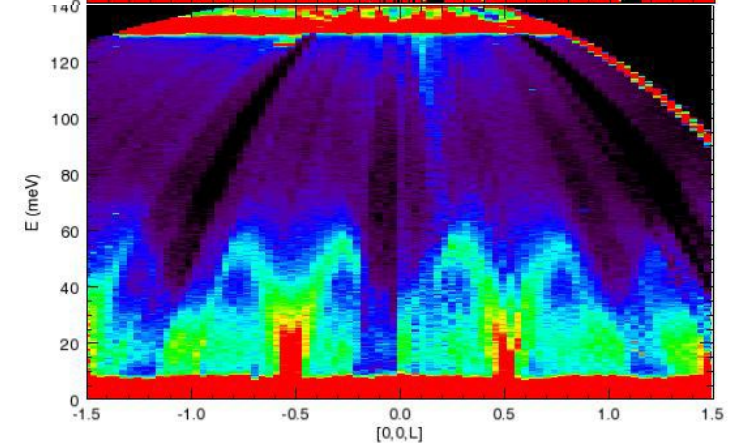
$E_i=37$



$E_i=65$

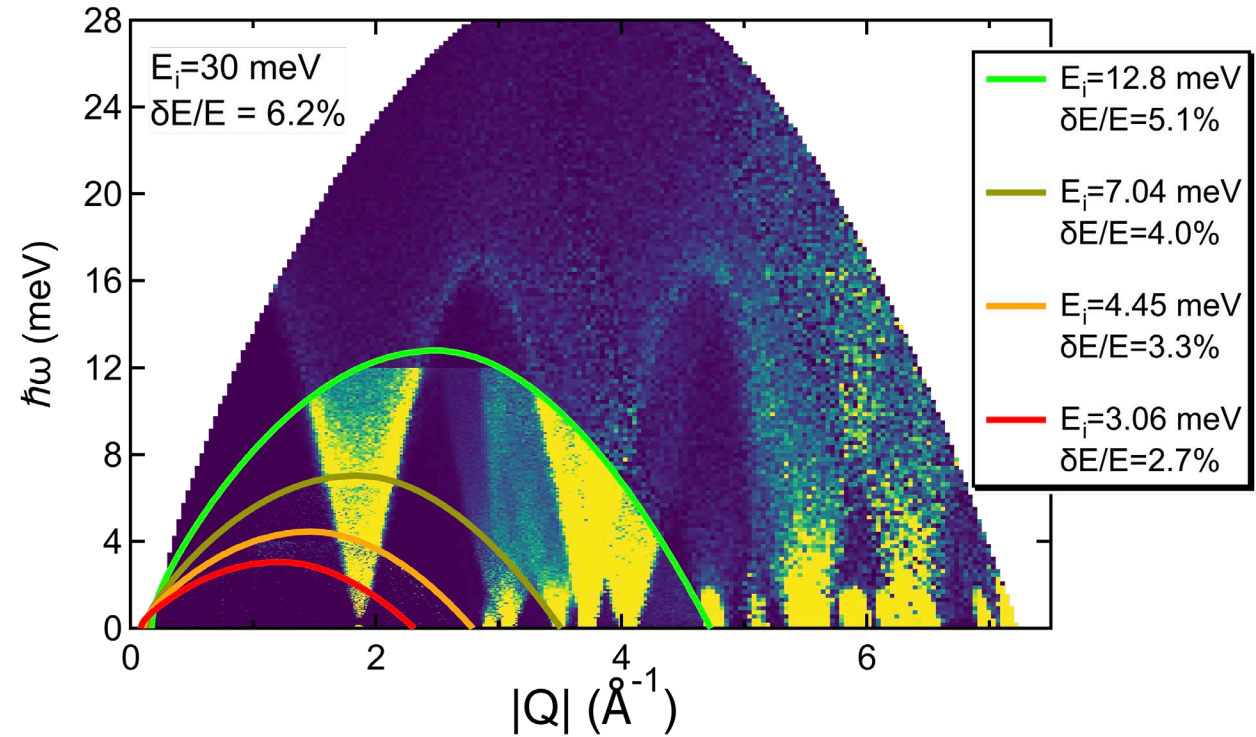


$E_i=144$



# Analysis is a challenge

- Currently each Incident energy is handled independently
  - More than one energy is used only if it provides a large benefit
- Resolution changes greatly over multiple  $E_i$ s
  - (Factor of 2 between 12.8 and 3.06 for Chess)
  - Combining is not Trivial



# What to do

- Auto reduce each energy and store in a combined data structure
- Use methods, pioneered by Jiao, to extract a single combined dispersion
- Tool to easily flip back and forth between combined and individual EIS



neutrons.ornl.gov/content/no-cost-way-improve-neutron-scattering-resolution-500

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ORNL scientists developed a computational technique that improves the resolution of neutron instruments by 500 percent. This solution comes at virtually no cost since it requires no additional hardware and uses open source software. Credit: ORNL/Jill Hemman

55 Shares

'No cost' way to improve neutron scattering resolution by 500 percent

May 5, 2022

Scientists pushing the limits of the world's most advanced neutron scattering instruments know that a small amount of distortion in their measurements is inevitable. For some experiments, this distortion is easily accounted for, but in other types of research it can cause inaccurate findings.

Why does a small amount of distortion matter? It's similar to when a detective lifts a fingerprint from a glass of water. The curvature of the glass distorts the fingerprint slightly, making it difficult to match the print to a suspect's fingerprint on file. In such a case, it would be helpful if there was a way to remove the distortion from the fingerprint found on the glass.

Something like this occurred when scientists from Oak Ridge National Laboratory (ORNL) used the world-class SEQUOIA neutron scattering spectrometer at ORNL's Spallation Neutron Source (SNS). The researchers were measuring spin wave dispersions from a magnetic crystalline material. They discovered that the data (the fingerprint) obtained from SEQUOIA (the glass) was slightly distorted by the resolution limits of the instrument, despite its state-of-the-art design.

To resolve the issue, the researchers developed a new computational technique that improved SEQUOIA's effective resolution by 500 percent in order to match the data to known spin wave dispersion values. Plus, this solution comes at virtually no cost since it requires no additional hardware and uses open source software.

The results of their efforts, titled, [A super-resolution technique to analyze single-crystal inelastic neutron scattering measurements using direct-geometry chopper spectrometers](#), were published in the AIP journal Review of Scientific Instruments.

"We predicted that if we could measure the amount of distortion inherent in SEQUOIA's data collection, we could then apply a

KEY CONTRIBUTORS



Matthew Stone



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Gabriele Sala

# Hierarchical Structures

- Information between the traditional SANS and the traditional diffraction regime
- One person's background is another person's signal
  - Typical for SANS it is treated as a correction factor at High Q
  - Typical for Diffraction it is cutoff or treated in a spherical SANS approach to provide a low Q background (Farrow and Billinge Acta Cryst. A **65** 232-239)

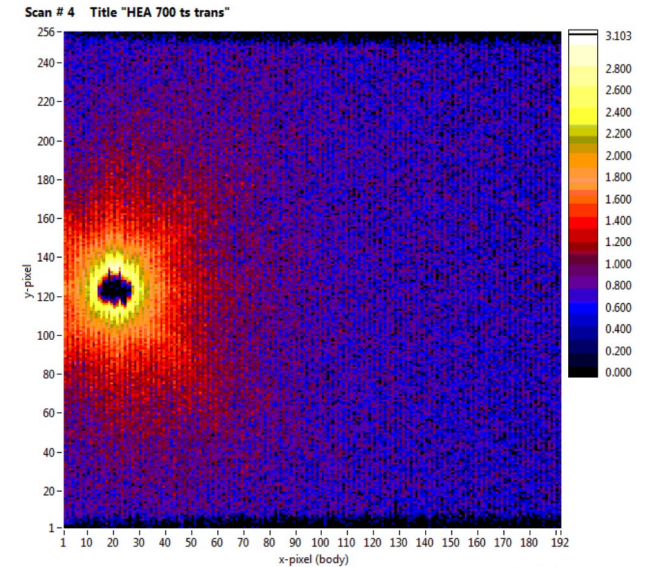
# Compelling science case in Additive manufacturing

- Challenges

- SANS non dilute limit
- SANS not spherically averaged.
- Diffraction is preferred orientation appropriate?
- Understanding the interface between non spherically averaged SANS and preferred orientation

- Path Forward

- SANS Fourier Transform from shape and grains
- Understanding where in Q grain orientation changes to preferred orientation limit
- Nano Particle work provides a framework for starting. Farrow and Billinge Acta Cryst. A **65** 232-239)



# Other things to consider

- Technological materials may have interesting magnetic structures on the same length scale (skyrmions)
- This functionality might be the interesting science when STS comes on line

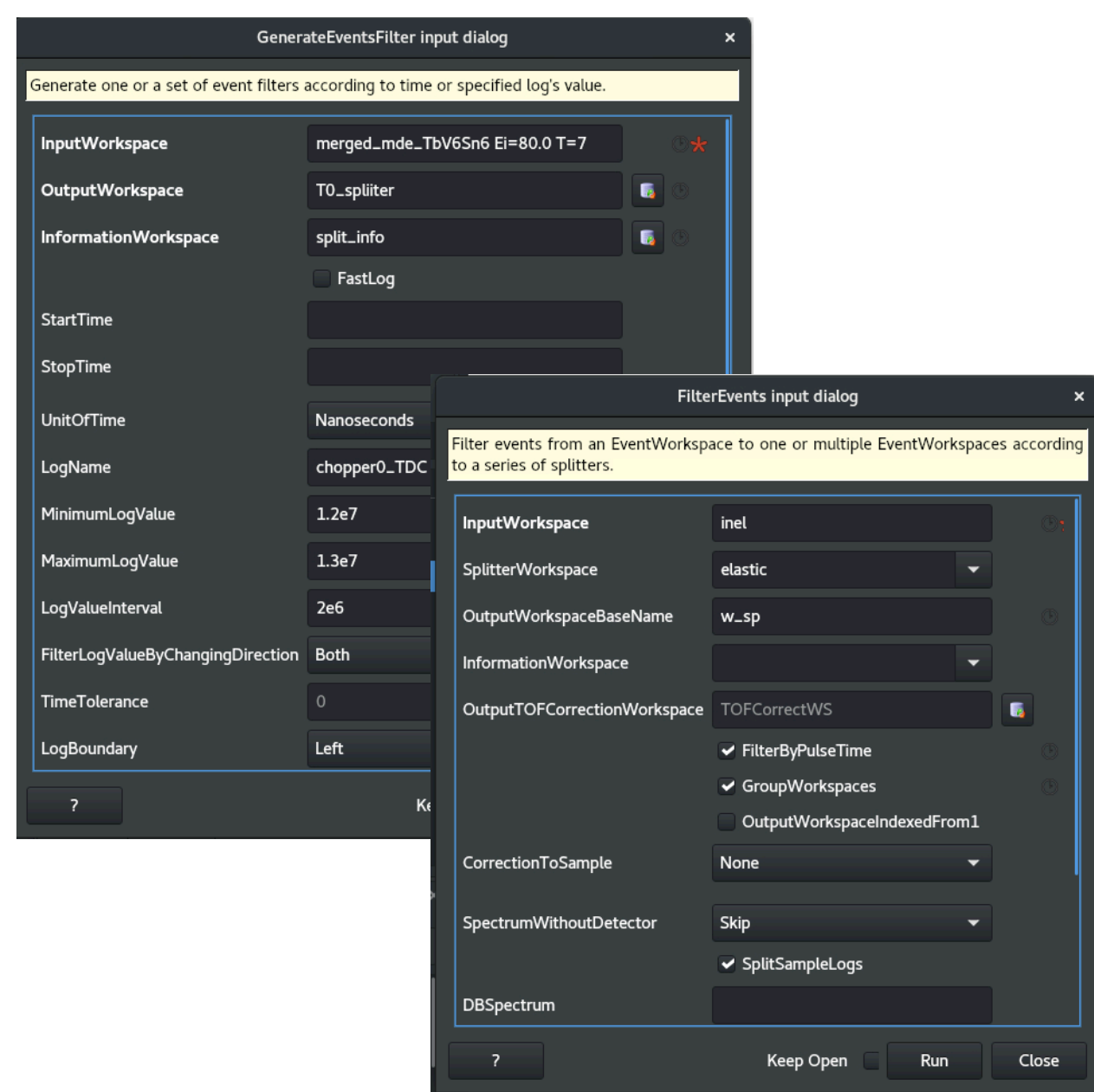


# ORNL has the expertise to give direction

- People that immediately come to mind from a hard materials perspective
  - Andrew Payzant
  - Ken Littrell
  - Lisa Debeer-Schmitt
  - Chris Fancher
  - Matt Tucker
- A separate workshop on Hierarchy structures and wide angle scattering might be needed.

# Cinematic Mode

- One of the big successes of FTS is event based reduction
- It is ubiquitous on Vulcan and POWGEN
- It is used on NOMAD, LR, EQSANS, Vulcan, Corelli, POWGEN, Hyspec, SEQUOIA, ARCS
- Underlying Two step process
  1. Create a list of Parameter vs. times
  2. Filter Events



G. E. Granroth *et al.* J. Appl. Cryst. **51**, 616 (2018)

# User access to filtering

- Too many boxes at the Mantid Level
  - Vulcan and Powgen benefit from custom user interfaces
- For STS need to think through the interfaces for the new communities

# Super Resolution Flurry of Recent papers

## Super-resolution energy spectra from neutron direct-geometry spectrometers

Cite as: *Rev. Sci. Instrum.* **90**, 105109 (2019); doi: [10.1063/1.5116147](https://doi.org/10.1063/1.5116147)

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Research Letter

## A super-resolution technique to analyze single-crystal inelastic neutron scattering measurements using direct-geometry chopper spectrometers

Cite as: *Rev. Sci. Instrum.* **93**, 025101 (2022); doi: [10.1063/5.0079031](https://doi.org/10.1063/5.0079031)

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## Deep learning-based super-resolution for small-angle neutron scattering data: attempt to accelerate experimental workflow

**Ming-Ching Chang** and **Yi Wei**, University at Albany, State University of New York, New York, NY, USA

**Wei-Ren Chen** and **Changwoo Do** , Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

# Uses

- DGS powder uses varying resolution at same  $|Q|$
- SANS uses to reduce measurement time
- Questions
  - Are we designing out these techniques (Spherical Detector Tanks)
  - Can these be exploited for Diffraction?
  - What design changes do we make to exploit them?
    - Sharpness of moderator rising edge more important than time width

# Summary

- For STS to reach its full potential Effort is required in
  - Efficient Analysis of RRM data
  - Understanding Hierarchical structure analysis approaches
  - Improving access to cinematic/event data.
- Super resolution is fantastic. How can we incorporate it to build better instrumentation.