OAK RIDGE National Laboratory

Reduction and analysis challenges across the STS instrument suite

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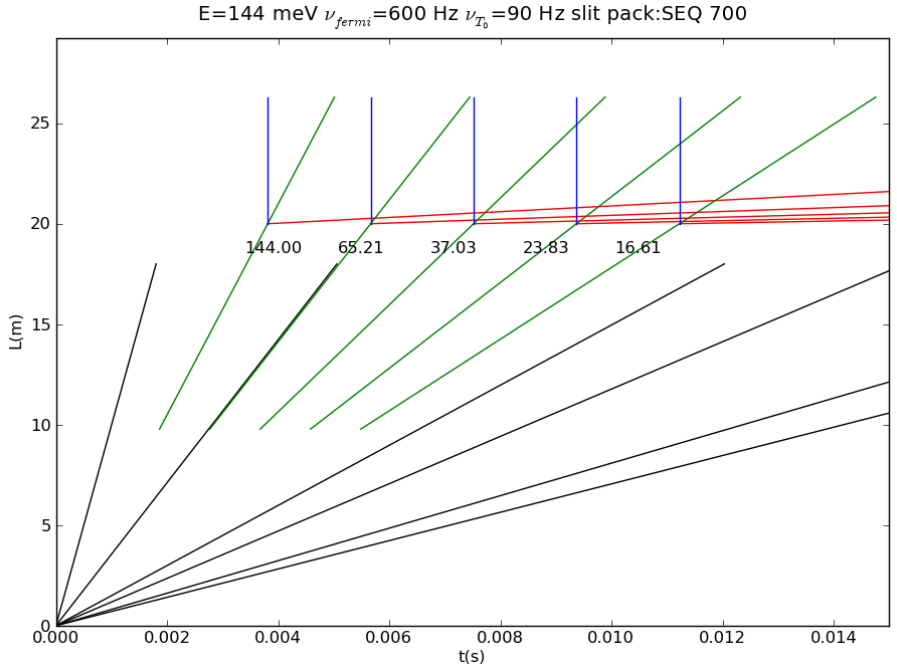
U.S. DEPARTMENT OF ENERGY

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

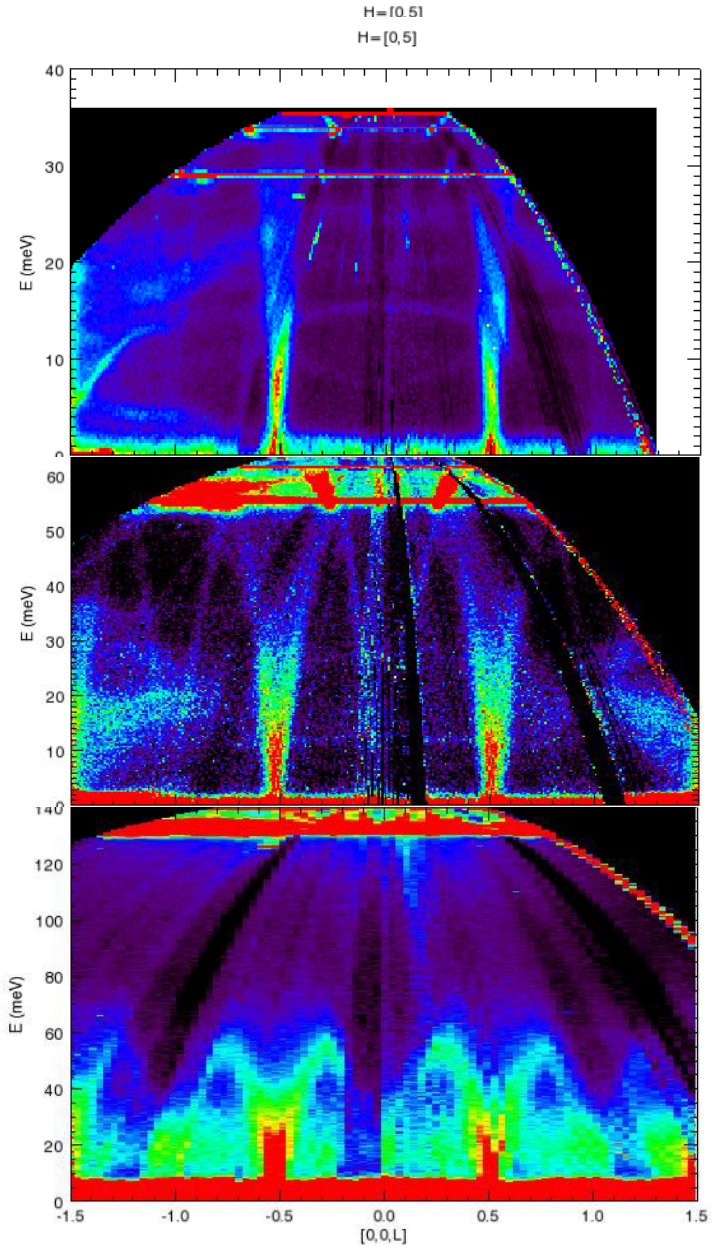
- Measuring more than one Incident energy in a given frame.
- Longer frames mean it can be exploited more.
- Currently in use at LET, Amateras, HRC, and in a limited case on SEQUOIA
- Measurements from SEQUOIA show the potential



E_i=37

E_i=65

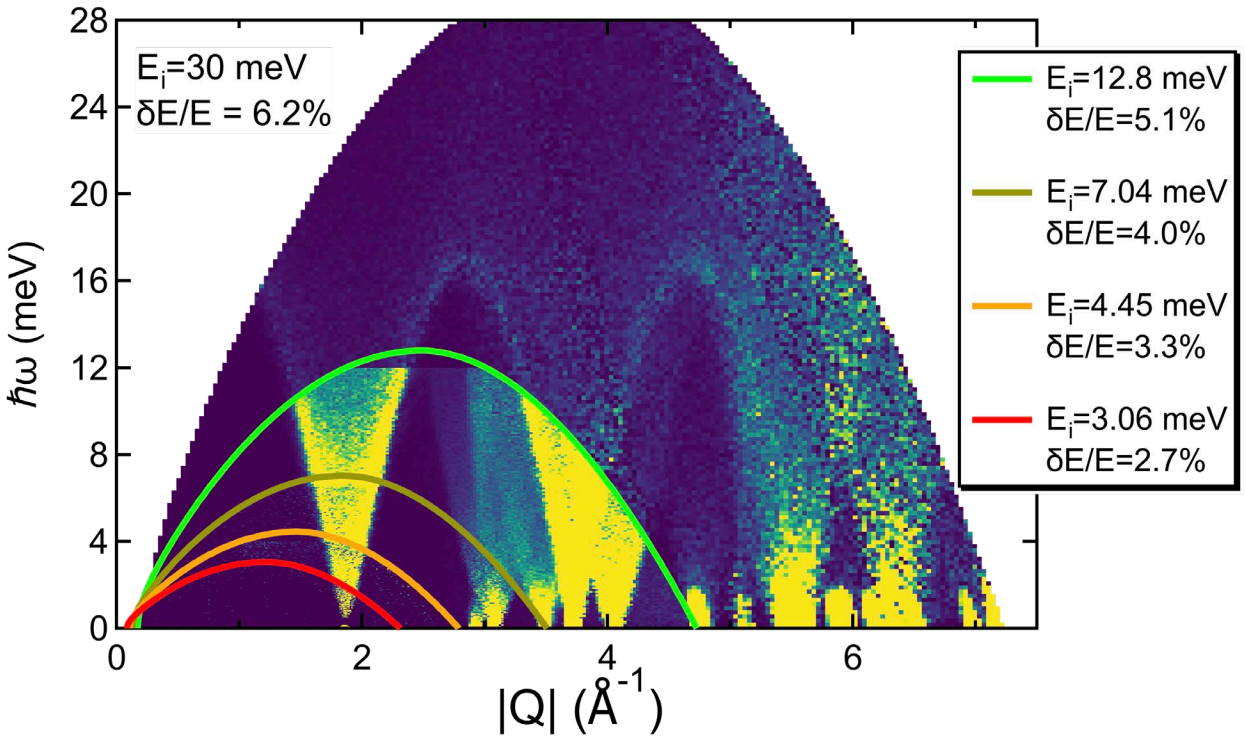
E_i=144



G. E. Granroth, J. Phys. Soc. Jpn. **80B**, SB016 (2011)

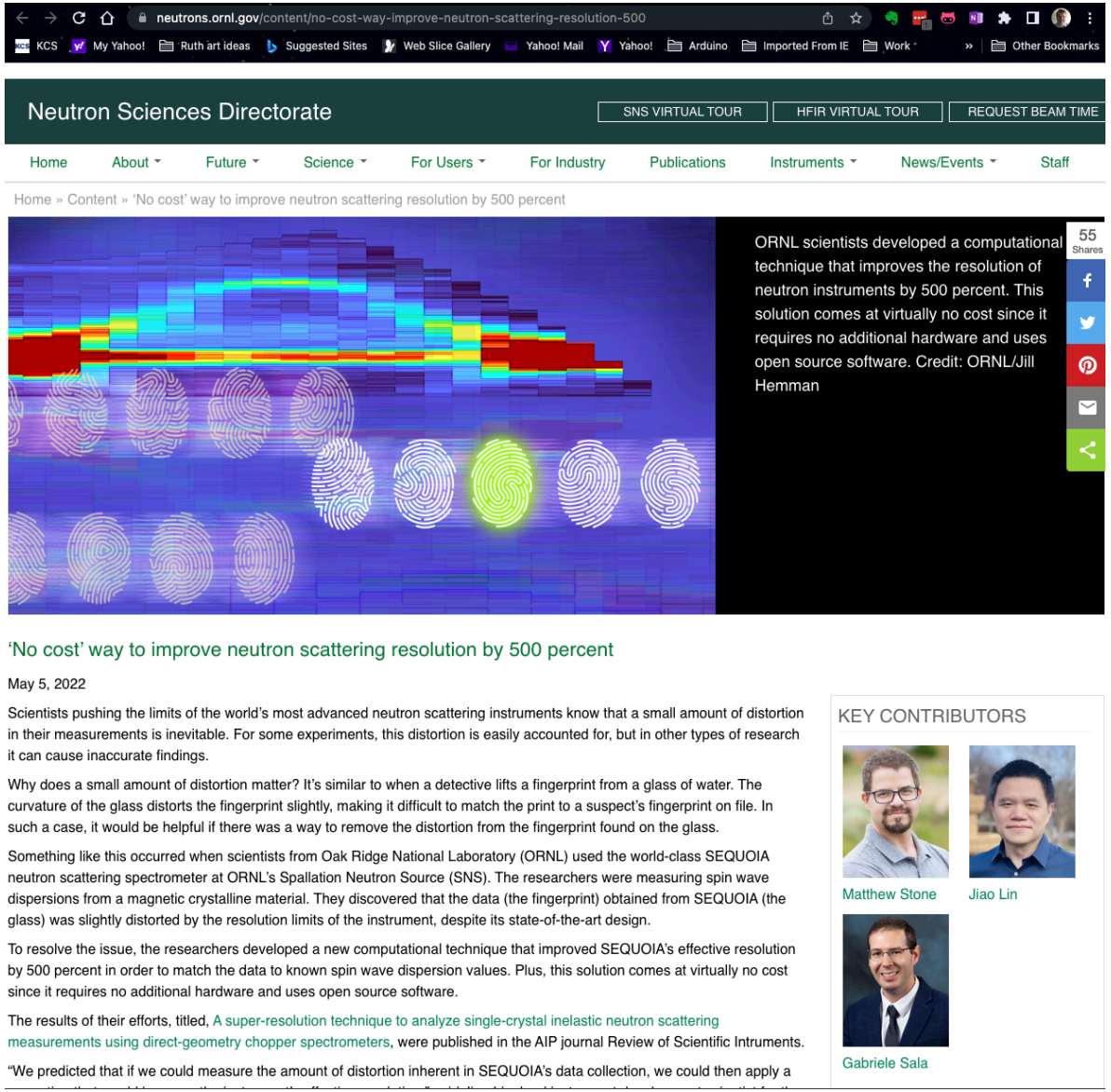
Analysis is a challenge

- 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 Eis
  - (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

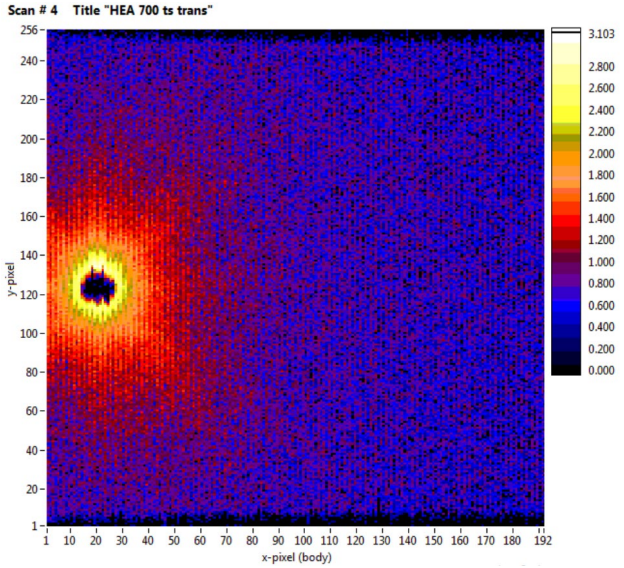


Hierarchical Structures

- 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 orienataion



- 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

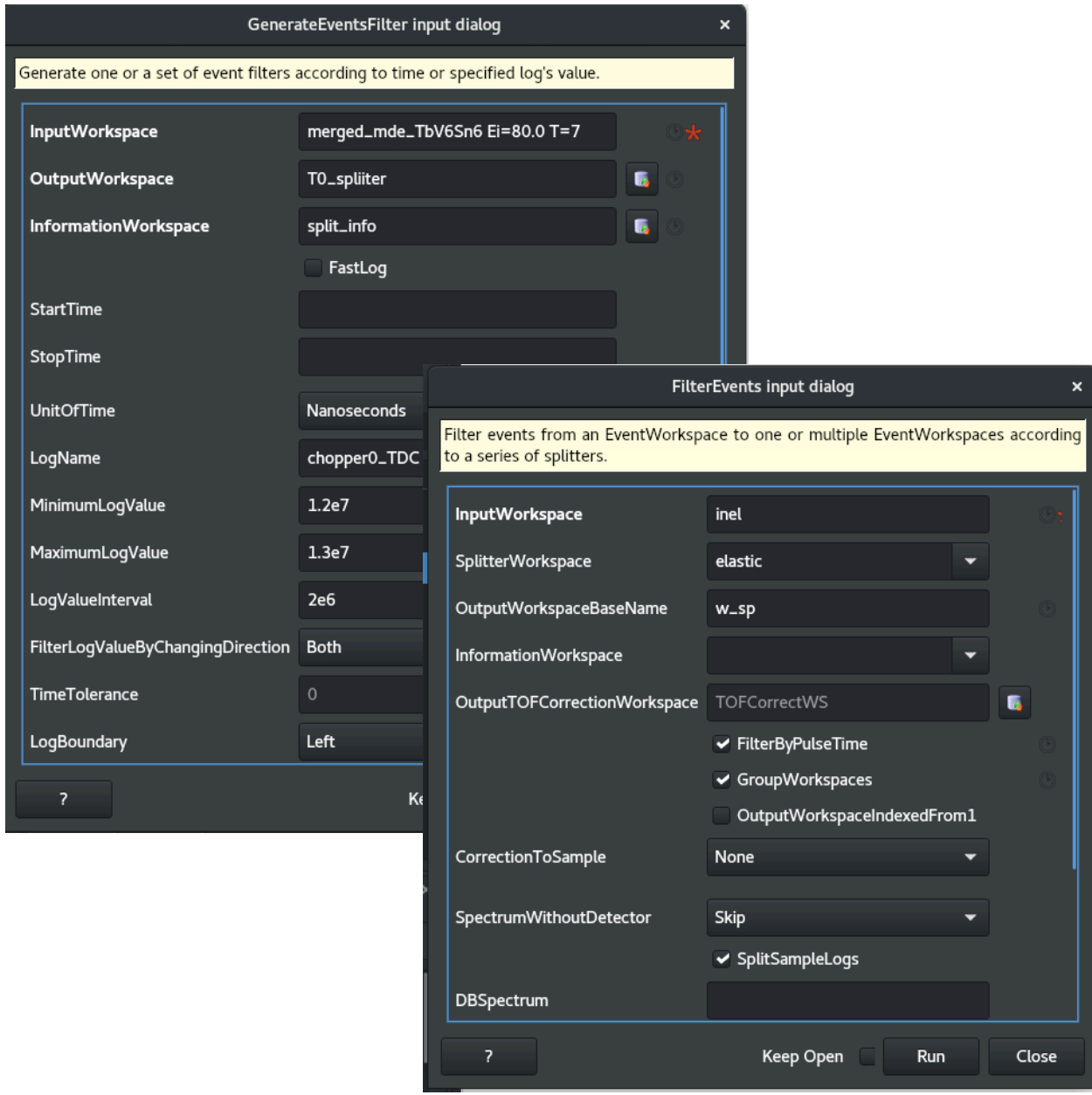
- Technological materials may have interesting magnetic structures on the Same length scale (skyrmions)
- This functionality might be the interesting science when STS comes on line

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 Hirearchical 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
Submitted: 22 June 2019 • Accepted: 1 October 2019 •
Published Online: 18 October 2019

View Online Export Citation CrossMark

Fahima Islam,[1,a] Jiao Y. Y. Lin,[1,a),b)] Richard Archibald,[2] Douglas L. Abernathy,[1] Iyad Al-Qasir,[3] Anne A. Campbell,[4] Matthew B. Stone,[1] and Garrett E. Granroth[1,c)]

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
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Jiao Y. Y. Lin,[1,a] Gabriele Sala,[1] and Matthew B. Stone[2]

MRS Communications (2020), 10, 11–17

doi:10.1557/mrc.2019.166

MRS Communications — Research Letter

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.