Data Reduction and Analysis Overview
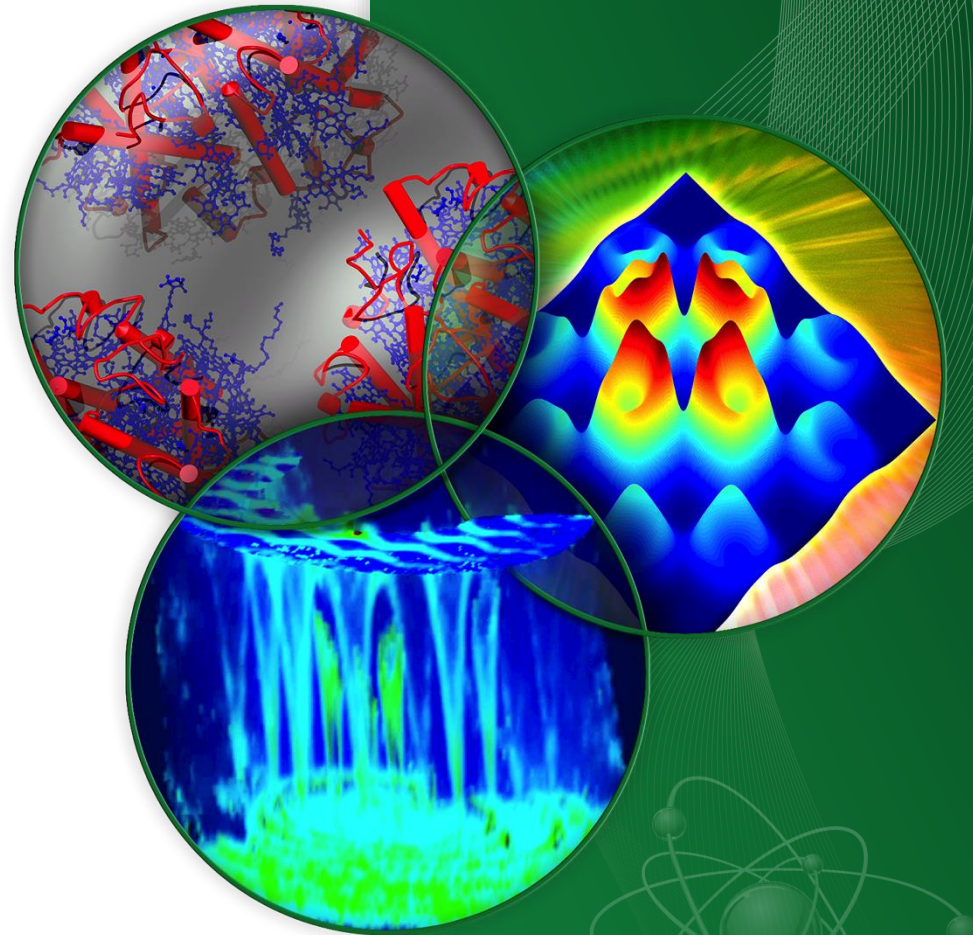
Garrett E. Granroth

Neutron Data Analysis and Visualization Division

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Outline

- Demos in breakout session

- Other highlights
  - Web monitor updates
  - Visualization updates
  - Work on modeling diffuse scattering
  - HPC workflows/MD simulations
  - Virtues and DFT for Molecular spectroscopy

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Overview of Breakout session

- FastGr/Addie an interface for reducing and working with pdfs on NOMAD – Marshall McDonnell

- Reducing from events and viewing data for Single Crystal Diffuse and Direct Geometry Spectroscopy Data – Andrei Savici

- Simulation of samples on Chess and CNCS with McVine using jupyter notebooks– Gabriele Sala

- PyVDrive, an interface for Vulcan with event slicing – Wenduo Zhou

- The imaging software suite including iBeatles and jupyter notebooks – Jean Bilheux

- Global fitting of QENS data– Jose Borreguerro

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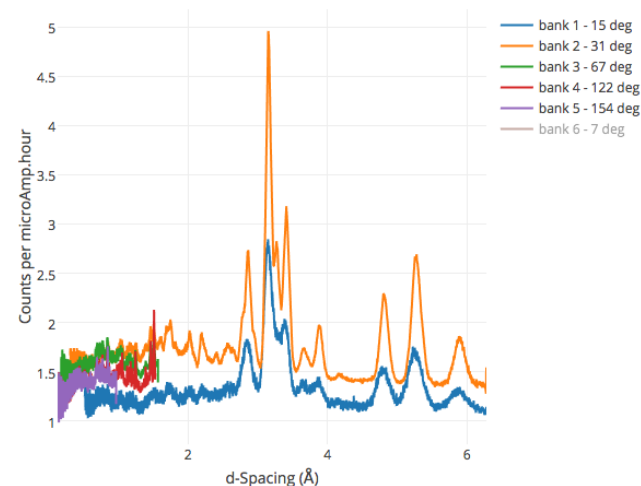National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

Monitor.sns.gov

- ## Plotly plots
  - interactive allow zooming, scale change, etc.

- ## Live Data
  - can be implemented for Adara instruments
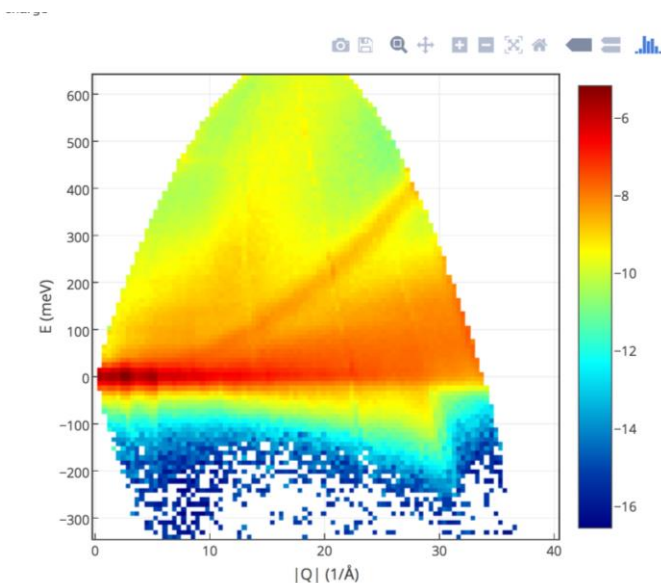
Visualization

- Paraview/vtk is our technology of choice for 3D vis

  – Behind VSI in Mantid

  – Parallel backend for large vis. (Sorting out proper hardware)

  – S. Hahn has made serval 2x speed improvements to Paraview

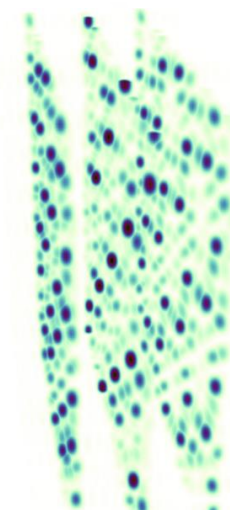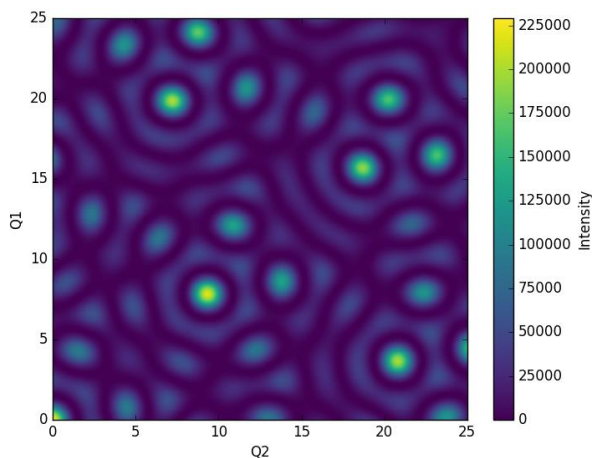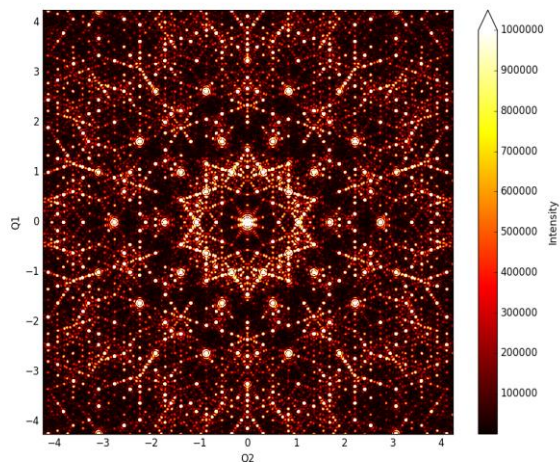- Non orthogonal coordinates now available in Slice viewer
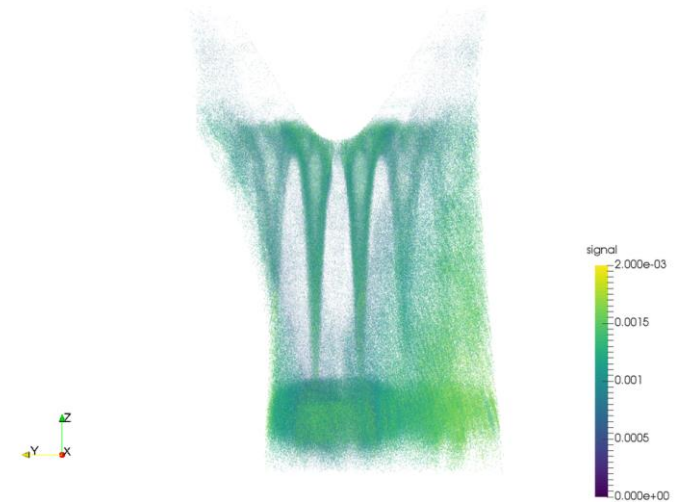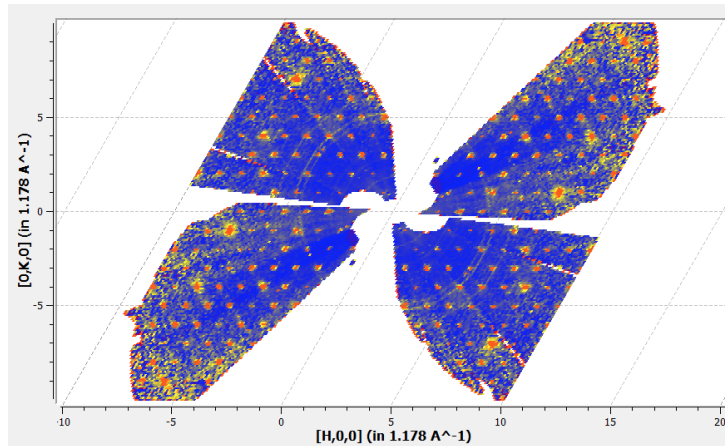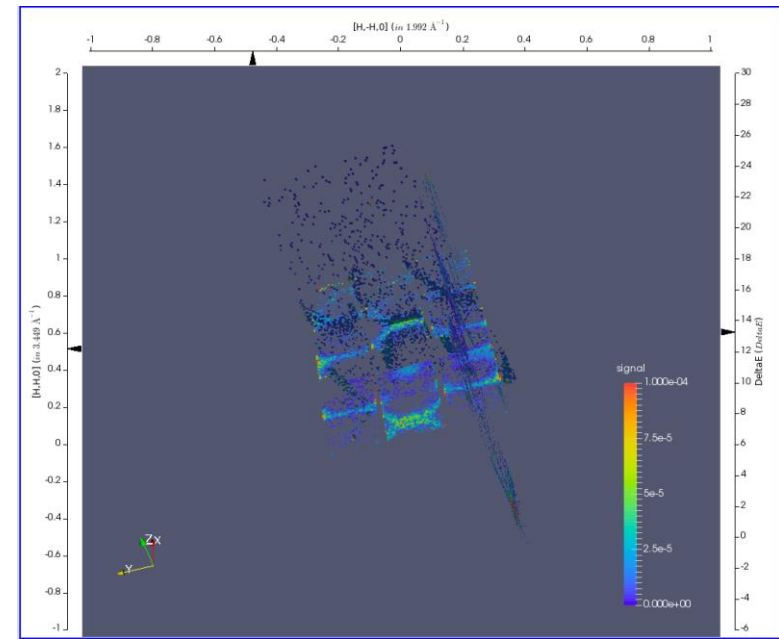
Discus -> Javelin

- Load and Plot experimental data Load Mantid MDHisto workspace (HDF5)

- Calculate diffuse scattering from structures
  - ASE (Nano Tubes)
 - Old Discus files (Quasi Crystal)
- Talk to Ross for more info
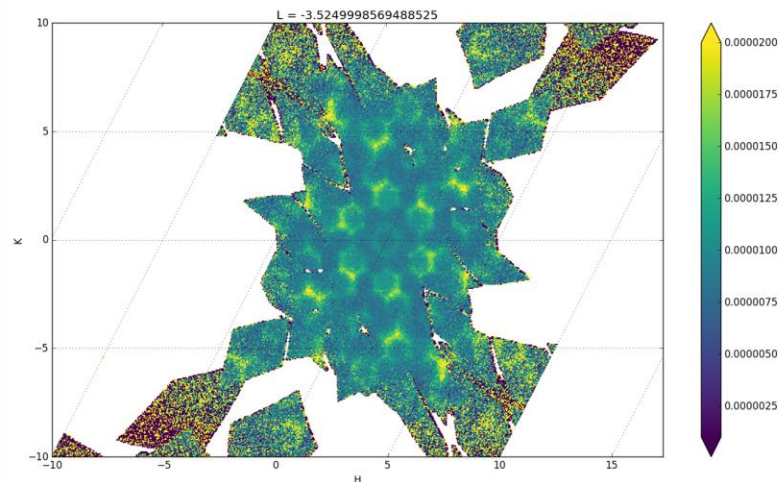
Michaels-Clark, T. M. *et al.* (2016). J. Appl. Cryst. 49, 497-506.

VirtuES Cluster helps Vision users make decisions on-the-fly

- Simulation and data collection start at the same time and finish on a similar time scale. Allowing computation to help direct experimental choices

- Part of the Cades cluster, over 1000 cores

- Result of an LDRD

- Talk to Timmy for more info.
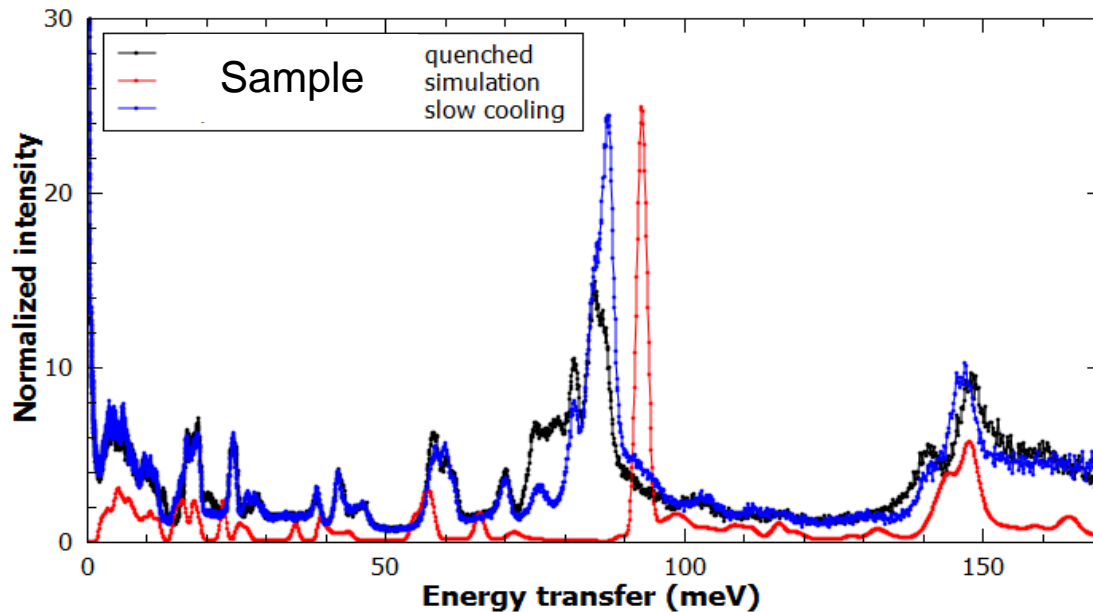
MD and workflows

- Using Workflow engines to connect together MD and the neutron data
  - Generating input for HPC simulation, running it on the HPC resource, comparing simulation/ measurement results
  - Using the right resource for the task
  - Beam, Pegasus
  - Talk to Vickie or Jose
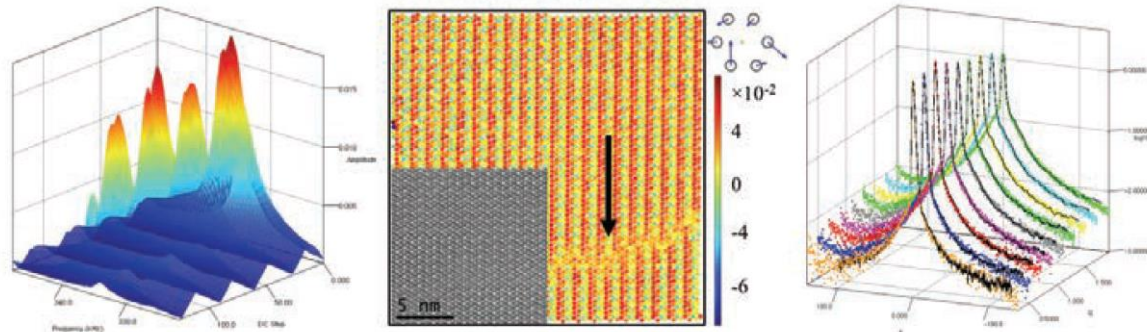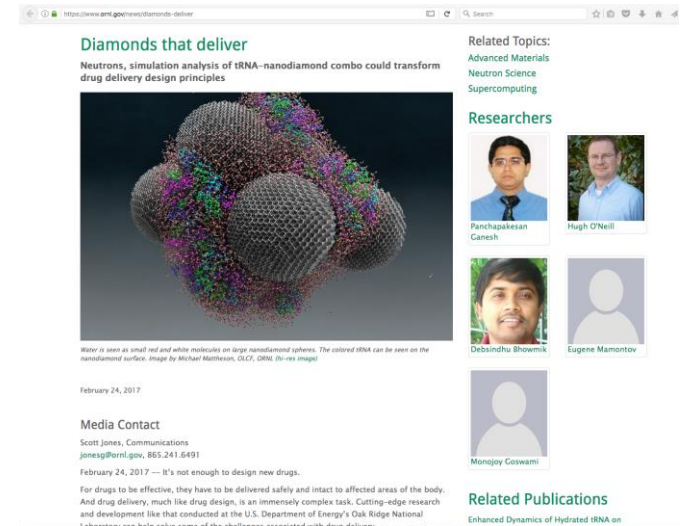
Current Embeeing List

NDAV Staff	Instrument(s)			
Jean Bilheux	Imaging			
Jose Borreguero	Basis			
Mathieu Doucet	EQSANS	USANS	REFL	REFM
Garrett Granroth	HB-1A	HB-1	HB-3	CTAX
Steve Hahn	Vision			
Ricardo Leal	BIOSANS	GPSANS		
Jiao Lin	ARCS	SEQUOIA		
Vickie Lynch	TOPAZ	MANDI	Imagine	
Peter Peterson	NOMAD	Powgen	SNAP	
Andrei Savici	HYSPEC	CNCS		
Ross Whitfield	Corelli	WAND		
Wenduo Zhou	Vulcan	HB-2B	HB-2A	HB-3A