EUROPEAN SPALLATION SOURCE

Data Management and Software Centre

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www.europeanspallationsource.se

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What is DMSC ?

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- Data Management and Software Centre (DMSC)

- A Division of ESS Science Directorate…
  - Just like Instrument Technologies, Neutron Instruments etc.
  - Two campuses: ESS Lund & ESS Copenhagen
    (Universitetsparken, Københavns Universitet)
  - DMSC building to be constructed in Copenhagen

- Responsibility: design, develop & implement for the ESS instruments:
  - Software (user control interfaces, data acquisition, reduction & analysis)
  - Hardware (servers, networks, workstations, clusters, disks, pfs etc.)

Mission

ESS is an experimental facility – users will come here to do neutron scattering experiments:

- *Collect the most (appropriate) data during their beam time*
- *Understand that data as much as possible/practical*

DMSC's mission is to create a computational infrastructure that gives ESS users:

- The ability to acquire (capture) neutron & associated data & control the instrument
- The ability to reduce, and analyze, the data (as it is being acquired)
- Data files created instantly after acquisition (no matter how big)
- The ability to reduce a data set post-acquisition *(could be 1 min, 1 month, 1 year later)* in ~1 minute
- Archival, and cataloguing, of the data
- Access to the resources (software/hardware) for users to do post-acquisition reduction, analysis, visualization, modeling

How do we make it happen?

General Framework + Customization

Generic Data Framework

- Event mode data for later reprocessing/filtering
- Stream the data ➔ on the fly data processing (live view)
  ➔ on the fly file creation
  ➔ to a location where appropriate post-acq. resources are available
- Create standard HDF5 data files (NeXus or other)
- (Where possible) Automate data reduction & analysis
- Catalogue the data & meta-data for fast processing

Don't re-invent the wheel

➔ Existing projects: ICAT, MANTID, ADARA – Join these

Customize for ESS Instruments

- User Control Interface, detector type, IOC's for sample environment etc.

Data Acquisition, Reduction & Control

Generic Framework

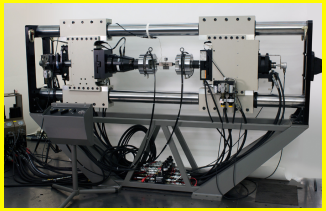
- Instrument Control
- Data Acquisition
- Data Reduction & Visualization

NEUTRON TECHNOLOGIES

Choppers

Motion Control

Sample Environment



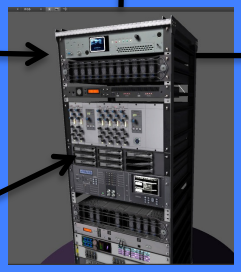
Fast Sample Environment

Detectors & Monitors

INTEGRATED CONTROL SYSTEMS

Timing

EPICS



Control Box

Bulk Data Readout (Detector Group)

DATA MANAGEMENT & SOFTWARE CENTRE

Data Aggregator & Streamer (ADARA)

Instrument Control Room

User Control Interface

Mantid
Live, Local & Remote Data Reduction

Data Analysis Interfaces

Automated Data Reduction
Mantid
Lund Server Room

Automated Data Reduction
Mantid
Copenhagen Server Room

Technologies & Collaborations

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Data Acquisition, Streaming & Reduction

EPICS

Used by ESS accelerator/target, SLS, Diamond, US light sources, to be used by ISIS & SNS

ISIS

ADARA

Publish/subscribe software & protocol for streaming data (neutron + meta)

SNS SPALLATION NEUTRON SOURCE

Mantid

Data reduction framework in Python & C++ developed by ISIS & SNS

Data Management

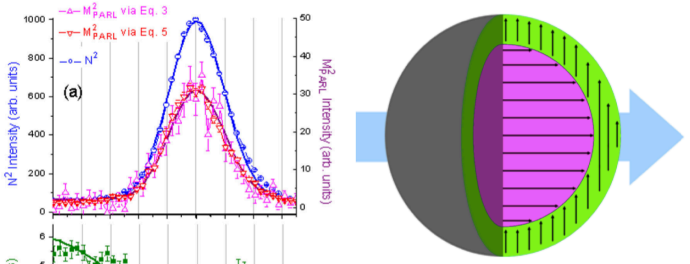
pandata

ICAT data cataloguing software developed under NMI3 by PanData collaboration of 19 European facilities (+ SNS in US)

Data Analysis

- Data on disk is useless!
  - It is published *results* from the data that makes progress
- Need to ensure that ESS users have access to
  - appropriate software packages for data analysis
  - the necessary computational resources to exploit the software to obtain those results
  - analysis software during experiment to influence the data taking strategies
- Roll out in-sync with instruments

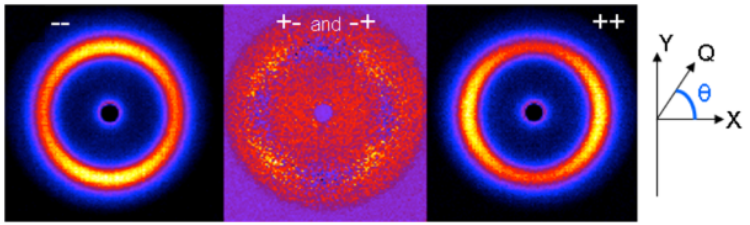
Structure of Nanomaterials



K. L. Krycka et al. **Core Shell Magnetic Morphology of Structurally Uniform Magnetite Nanoparticles** *PRL* **104**, 207203 (2010)

Polarized SANS demonstrated that these nanoparticles have uniform nuclear structure but core-shell magnetic structure.

Required development of both data reduction and data analysis methods and tools.



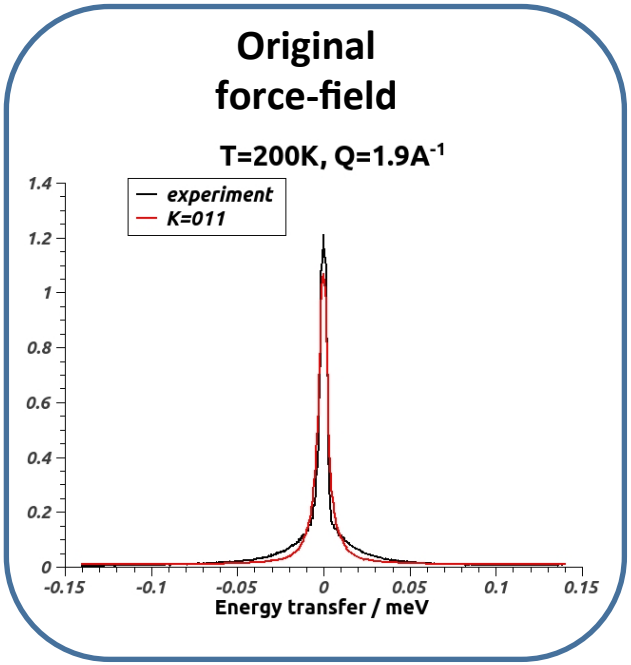
Data Analysis Development

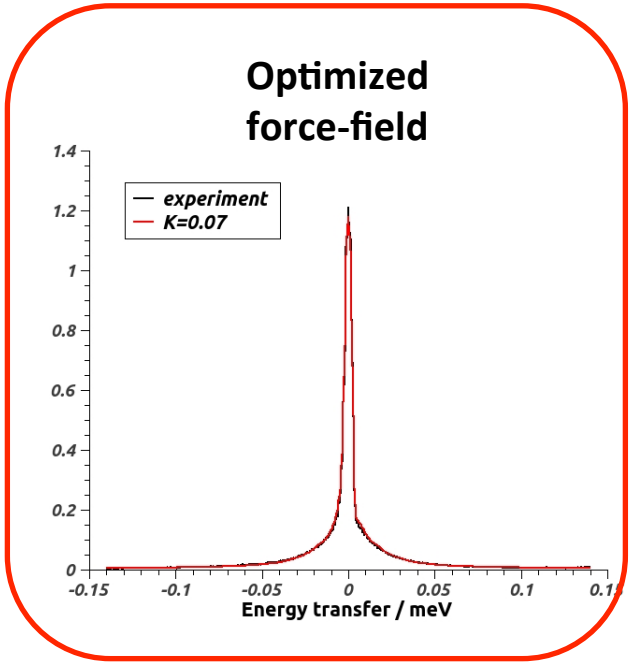
Integration of Analysis with Advanced Modeling Techniques

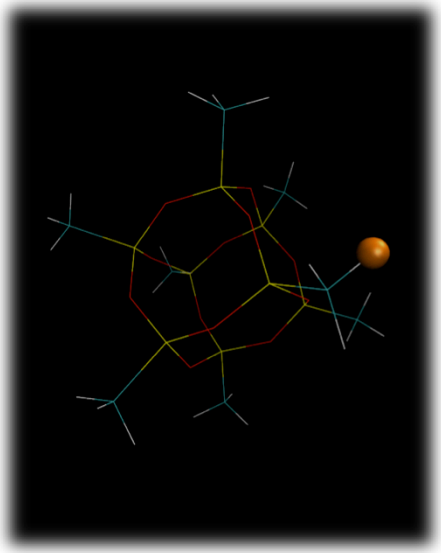
Molecular Dynamics & Density Functional Theory (DFT) Techniques

Jose Borreguero (SNS/NDAV) Mike Crawford (Dupont) & Niina Jalarvo (Julich): BASIS experiment / MD simulation studies of Methyl rotations in methyl-Polyhedral oligomeric silsesquioxanes (POSS)

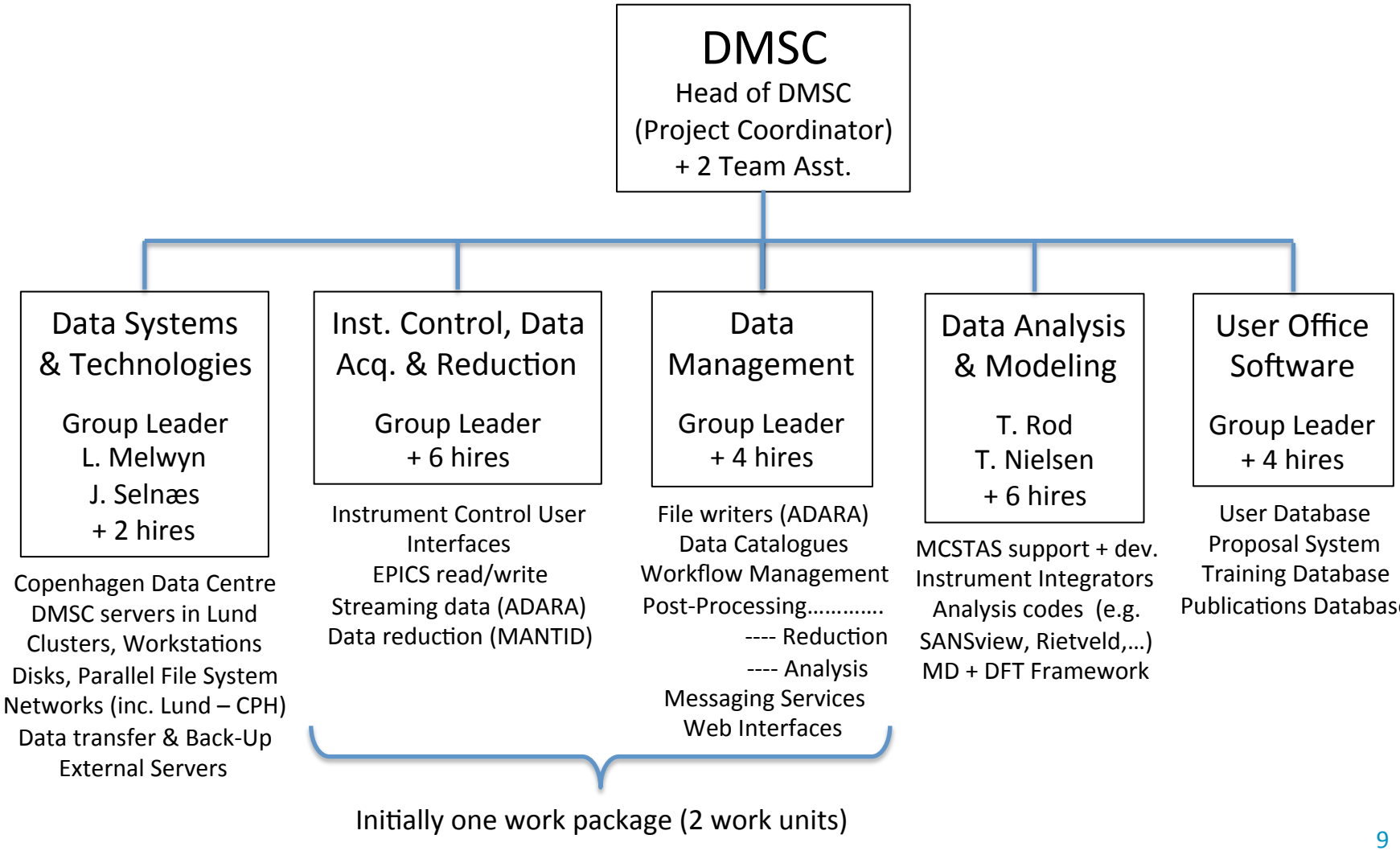
Optimization of dihedral potential governing the rotational jumps in methyl hydrogens. Preliminary simulations indicate that the dihedral potential barrier must be decreased ~37% in order to match experimental data







Organization



During the construction years

- Primary goal: To be ready for hot commissioning of first ESS instruments in 2020.
- Includes significant amount of NRE (Non-Recurrent Engineering) for subsequent ESS instruments.
- Establish the basic facilities at both campuses.
- Front loaded with instrument-centric work + scope to grow analysis in an integrated way

Conclusion

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- DMSC's mission is the computational (software/hardware) infrastructure for the ESS *data chain* - instrument control, data acquisition, reduction & analysis
- Generic framework customized for each of the instruments – utilizes data streaming to account for large data files/live processing
- Don't re-invent the wheel – work with collaborators ISIS, SNS, PanData (+ others?) to develop/customize existing software – EPICS, ADARA, MANTID, ICAT…
- Customize for each of the ESS instruments in-sync as they roll out
- In-sync with instrument roll out work with instrument teams to ensure analysis software is available (doesn't necessarily mean develop)
- Longer term goal to develop new data analysis methods for ESS instruments

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QUESTIONS