2017 Joint Nanoscience and Neutron User Scattering Meeting

Upcoming New Tools for Structure and Dynamics

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Organizers:
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Closing the loop between materials modeling and neutron scattering data has been the mission of the Center for Accelerating Materials Modeling (CAMM). As part of their effort, CAMM has led the development of advanced workflows and software tools that are now being made available to the wider user community. This workshop will give an overview and demonstrations of new software related to advanced diffraction and dynamics.

Tentative Program

- Overview of CAMM and recent developments – Th. Proffen
- Efficient calculation of volumes of diffuse scattering intensities from disorder materials – R. Whitfield
- Local dynamics and calculation of the dynamic pair distribution function from inelastic scattering data – J. Borreguero
- Calculating S(Q,w) from DFT models – TBD