Data Analysis Software Project

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- Obtain data in useful units (i.e., get $S(\vec{Q}, E)$).
- Focus of my talk – Connect data to models and simulations.
  - *Big idea*: Full experiment smulations
  - *Mid-Size idea*: Invert dynamical models.

$S(\vec{Q},\omega)$ **Approach**

- $S(Q,\omega)$ is a minimum standard for what users need to take home
- Absolute units [barns, meV, Å^{-1}]
- Efficient instrument calibration
- How to handle E, $\vec{Q}$ resolution and background?
- Special considerations for single crystals ($\vec{Q}$, not Q)
  - Real-time information on locations of dispersive excitations (guidance of goniometer?)
  - Data visualization

Magnetic Dynamics (local model)

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E} \propto \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(\vec{Q}\cdot\vec{r}-\omega t)}\, \Gamma_{\alpha\beta}(\vec{r},t)\, \mathrm{d}\vec{r}\,\mathrm{d}t$$

$$\Gamma_{\alpha\beta}(\vec{r},t) = \sum_{l} \sum_{l'} \langle\, \hat{S}_l^\alpha\, \hat{S}_{l'}^\beta(t)\,\rangle \int_{-\infty}^{\infty} \delta(\vec{r}+\vec{R}_l-\vec{r}\,')\, \delta(\vec{r}\,'-\vec{R}_{l'}(t))\, \mathrm{d}\vec{r}\,'\, \mathrm{d}t$$

spin correlations nuclear correlations

- Need simulations of magnetic and lattice dynamics, using both exchange forces and springs.
- To scatter from simulations, transform to wavepackets:

$$\mathrm{e}^{\mathrm{i}(\vec{k}\cdot\vec{r}-\omega t)} \rightarrow G^{\Delta\vec{r}}(\vec{r})\, G^{\Delta t}(t)\, \mathrm{e}^{\mathrm{i}(\vec{k}\cdot\vec{r}-\omega t)}$$

$$\mathrm{e}^{\mathrm{i}(\vec{k}'\cdot\vec{r}-\omega' t)} \rightarrow G^{\Delta\vec{r}\,'}(\vec{r})\, G^{\Delta t'}(t)\, \mathrm{e}^{\mathrm{i}(\vec{k}'\cdot\vec{r}-\omega' t)}$$

In $\{E, \vec{Q}\}$, this is equivalent to convolutions of broadened incident and scattered wavepackets.

Magnetic Dynamics (susceptibility approach)

$$
\begin{aligned}
\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E} &\propto (1+n(\omega)) \sum_{\alpha,\beta} (\delta_{\alpha,\beta} - \hat{Q}_\alpha \hat{Q}_\beta)\, \mathcal{I}m[\overline{\chi}^{\alpha\beta}_{\vec{Q}}(-\omega)] \\
\overline{\chi}^{\alpha\beta}_{\vec{q}}(-\omega) &= \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\omega t} \langle [\hat{T}^{\alpha}_{\vec{Q}}(t), \hat{T}^{\beta}_{\vec{Q}}(0)] \rangle \, \mathrm{d}t \\
\hat{T}^{\alpha}_{\vec{Q}}(t) &= \sum_{l} \mathrm{e}^{-W(\vec{Q})}\, \mathrm{e}^{\mathrm{i}\vec{Q}\cdot\vec{l}}\, G^{\Delta t}(t)\, G^{\vec{\Delta} l}(\vec{l})\, \hat{S}^{\alpha}_{l}
\end{aligned}
$$

- Should we modify $\overline{\chi}$ by the Δt, $\vec{\Delta} l$, or should we modify the $\mathrm{d}^2\sigma/\mathrm{d}\Omega\,\mathrm{d}E$?
- Does the susceptibility approach belong in the $S(\vec{Q}, E)$ approach, or the full experiment simulation approach?
- Can we provide a seamless user interface across both approaches?

Simulations

- Monte Carlo Simulations of Dynamics
  (true simulation – iterate parameters of simulation)
  - Molecular dynamics packages exist.
    (Should we pick one for phonon scattering?)
  - What about realistic magnetic dynamics packages?
    (Can we find a suitable classical dynamics model with, for example, magnetovibrational coupling? Is there interest from theorists in a quantum dynamics simulation?)

Models

- Inversions of Analytical Models
  (not a true "simulation" – iterate parameters of model)
  - Lattice dynamics – Well underway, example below.
  - Magnetic dynamics – Your ideas and opinions are solicited!

Born–von Kármán Inversions of Phonon DOS

- No problem from "neutron weighting" by σ/m (use dynamics to calculate actual data, including neutron weights)
- Extreme case – inelastic nuclear resonant x-ray scattering from ^{57}Fe – for Pt$_3{}^{57}$Fe, $\sigma_{\mathrm{Pd}}/m_{\mathrm{Pd}} = 0$

Invert the ^{57}Fe Phonon Partial DOS of $Pt_3{}^{57}Fe$

- Definition of phonon DOS

$$g(\varepsilon) \equiv \sum_{j}^{modes} \delta(\varepsilon - \varepsilon_j)$$

- Definition of Fe phonon partial DOS

$$g^{\mathrm{Fe}}(\varepsilon) \equiv \sum_{j}^{modes} |\vec{\sigma}_{\vec{q}}^{\mathrm{Fe}}|^2 \, \delta(\varepsilon - \varepsilon_j)$$

- Using normalization of $1|\vec{\sigma}_{\vec{q}}^{\mathrm{Fe}}|^2 + 3|\vec{\sigma}_{\vec{q}}^{\mathrm{Pd}}|^2 = 1$ for four-atom unit cell of Pt_3Fe

$$g(\varepsilon) = 1 g^{\mathrm{Fe}}(\varepsilon) + 3 g^{\mathrm{Pd}}(\varepsilon)$$

- We measure only $g^{\mathrm{Fe}}(\varepsilon)$. To calculate $g^{\mathrm{Fe}}(\varepsilon)$, we must have the full lattice dynamics. We therefore get $g^{\mathrm{Pd}}(\varepsilon)$ as a byproduct. Is this $g^{\mathrm{Pd}}(\varepsilon)$ reliable?

Neutron Simulation Codes

- NISP
  - FORTRAN
  - LANL
- MSLICE
  - Matlab
  - ISIS
  - closer to $S(\vec{q}, \omega)$ approach
- Vitess
  - tcl
  - HMI
- McStas
  - C
  - Riso
- ISAW
  - java
  - ANL

Caltech Activity – Hardware

- Beowulf Cluster (partly tested)
  - 16 node, each with one 1.4 GHz Athlon processor, 512 MB RAM, 40 GB HD, box
  - switched ethernet interconnection
  - 240 GB Raid drive
  - Red Hat Linux

Caltech Activity – Software

- DOS inversions $g_{Fe}(\varepsilon) \rightarrow \{\phi_{\alpha\beta}({}^{jj'}_{ll'})\}$
  - On Beowulf cluster, each node runs same code but different parameter set
  - Each inversion iteration (32 parameters) requires about 8 h on 0.4 GHz node
  - Two days for robust analysis

Summary of Directions for Software Project

- Develop a software framework for data analysis.
  - Establish the scope of capabilities.
  - Can we provide a common front-end to integrate simulations, models, direct analysis of data?
  - Assess existing neutron simulation packages. Repackage to fit in the framework.
- Magnetic Scattering
  - Assess classes of theoretical models.
  - Workgroup volunteers needed.
- Phonon Scattering
  - Born–von Kármán inversions: Weight in phonon dispersion data. Test the role of noise. $S(\vec{Q}, \omega)$ with mixed coherent/incoherent scattering.
  - Select molecular dynamics package. Timing tests for wavepacket scattering.
- Science
  - Money for science must be used wisely.
  - Must be done to leverage an integrated software development effort.