Virtual Experiments

LaMnO3 sample: adding all contributions

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Our goal

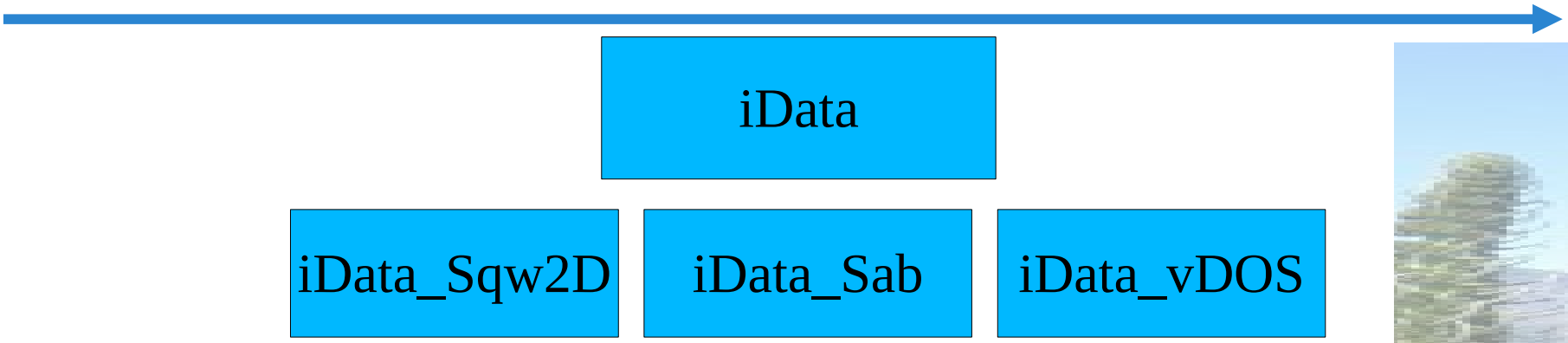
- Model a ToF with a LaMnO3 sample
- This material has contributions:
  - Structure (Bragg peaks)
  - Phonons
  - Spin-waves
  - Incoherent scattering

- We shall prepare all this and actually assemble a full model.
- Dropbox: 28th: VE LaMnO3

Limitations

- We shall use a simple ToF direct spectrometer.
- The sample will be assumed in powder state.
- The intensity of the contributions will have to be scaled with the proper cross sections. Will not be absolute.
- No phonon-spinon coupling as contributions are computed separately.
- Antiferromagnet, with localized coupling (BZ boundary).

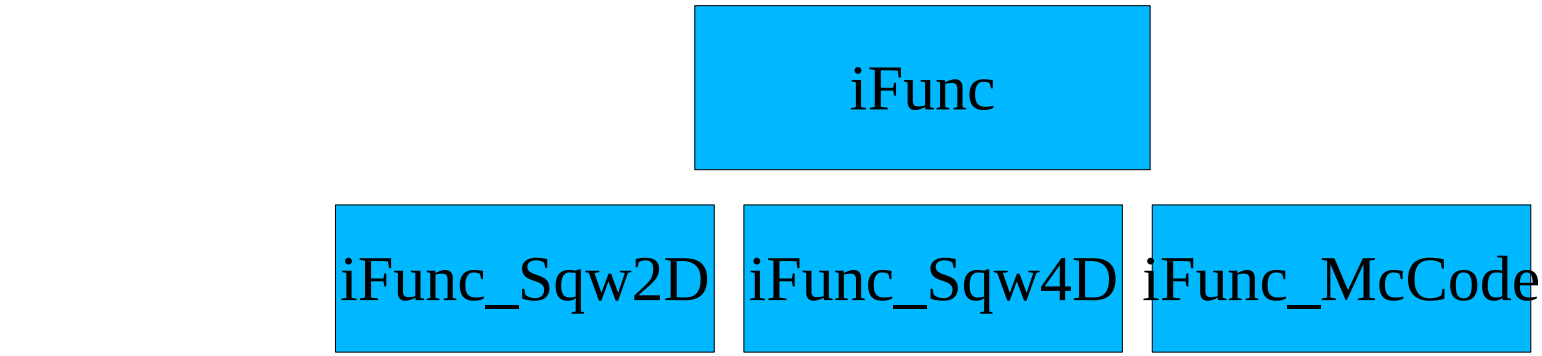
iFit: data sets



- Import a data file:
  - data = iData('filename') *% many formats*
  - data = iData(x,y,z,…, signal)
- Convert to a flavour:
  - data = iData_Sqw2D(data)
- Can apply many operators between data sets
  - +-/* trigo … 193 operators.

http://ifit.mccode.orgs

iFit: models



- Create a model:
  - model = iFunc('p(1)*x+p(2)')
  - model = gauss
- Convert to a flavour:
  - model = iFunc_Sqw2D(model)
- Can apply many operators between models
  - +-/* trigo … 81 operators.

iFit: predefined models

- Predefined models: 57
  - [o,m] = fits(iFunc) *% optimizers, models*
  - doc(iFunc, 'Models')
- Those we shall use here:
  - **sqw_phonons**: S(q,w) 4D lattice dynamics / DFT
  - **sqw_spinwave**: SPINWAVE model

sqw_phonons

- Uses transparently ASE+PhonoPy to compute lattice dynamics estimate of the Forces in a SX.
- Produces a 4D S(q,w) model [iFunc_Sqw4D]
- Supports all ASE calculators, e.g. QE VASP …
- For complex crystals, computation can be days.
- iFunc Sqw4D flavour methods:
  - vDOS, thermochemistry, plotting, powder average, ...

sqw_phonons (2)

- Will use MPI and all CPU's
- Can input CIF/PDB/… file, as well as common ASE Atom builder (python)
- Can also input a 'cod: formula'
- **Syntax:** sqw_phonons('crystal','calculator', …)
  - sqw_phonons('Al.cif','qe')
  - sqw_phonons('cod: Al','vasp')
  - sqw_phonons('bulk("Al", "fcc", a=4.05)','gpaw')

Exercise 1: sqw_phonons Al

- Generate the ‘default’ Al S(q,w) model:
  - Al = sqw_phonons(‘bulk("Al", "fcc", a=4.05)’,’emt’)
- Plot the dispersion and the BZ cube
  - plot(Al) *% dispersion and DOS*
  - plot3(Al) *% 3D cube*
  - slice(Al) *% play with isosurface and cuts*
- The views have contextual menus on figure, axis and plots.

sqw_spinwave

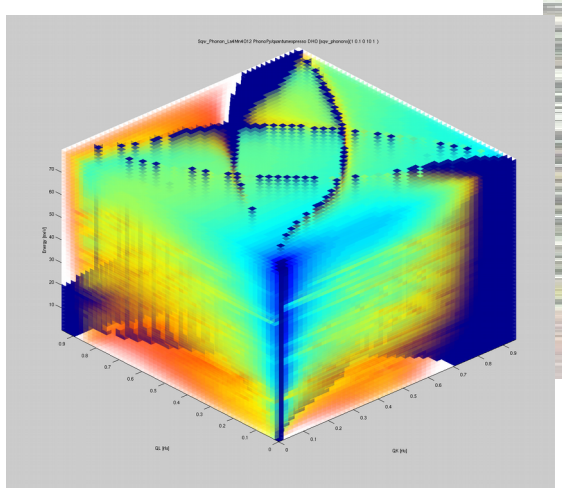
- Uses transparently SPINWAVE.
- Has a special ‘powder’ mode (that we shall use).
- Can define variable model parameters $par
- Produces a 2D/4D S(q,w) model [iFunc_Sqw2/4D].
  - sqw_spinwave(‘file’)
  - sqw_spinwave(‘file’,’powder’)
  - sqw_spinwave(‘file’,’edit’) *% then insert $par, e.g. J1...*

LaMnO3: Structure

- Just need to generate a LAZY/PulverX Laz file
- Matlab/iFit:
  - cif2hkl('cod: La Mn O3','LaMnO3.laz')
- Then use it with e.g. **PowderN**

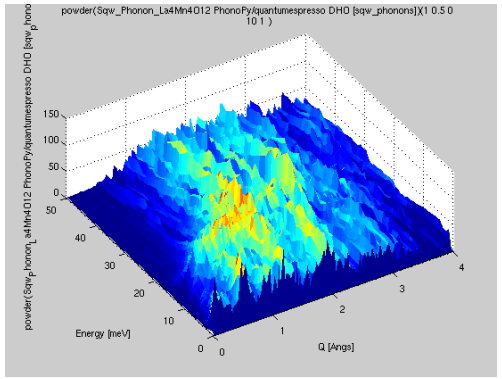
LaMnO3: Phonons

- Calculation done with QE:
  - s=sqw_phonons('cod: La Mn O3','qe') *% 15 h, 24 cpus*
- Start Matlab/iFit:
  - load LaMnO3
  - disp(s) *% a 4D model*
  - figure; plot3(s) *% use contextual menu 'invert transparency'*
  - slice(s)



LaMnO3 → Sqw phonons coherent

- Matlab/iFit:
  - p=powder(s) *% powder average model*
  - q=0.01:0.025:4; w=0:0.05:50;
  - coh=iData(p,[ ], q , w);
  - coh=iData_Sqw2D(coh);
  - figure; plot(coh)
  - saveas(coh, 'LaMnO3_pow_coh.sqw','mcstas')



LaMnO3 → Sqw incoherent

- Matlab/iFit: with same (q,ω) range as coherent.
  - g=dos(s, w); *% vDOS with coh 'ω' values*
  - plot(g)
  - inc = g.incoherent('q', q, 'm', 242, 'T', 10);
  - figure; subplot(inc)
  - sinc = deBosify(plus(inc));
  - ylim(sinc,[-0.15 50]); sinc{1}=w; sinc{2}=q;
  - saveas(sinc, 'LaMnO3_pow_inc.sqw','mcstas')

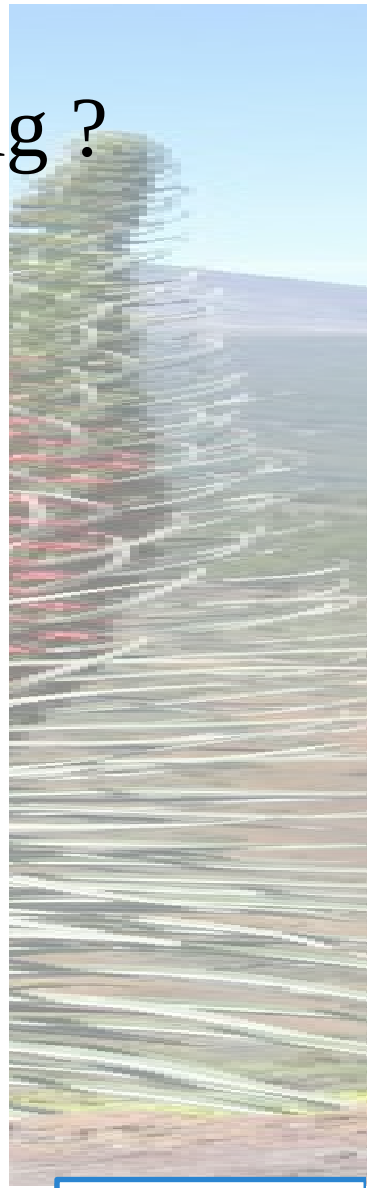
LaMnO3: SpinWaves → Sqw

- Create the spin-wave model:
  - SW=sqw_spinwave('LaMnO3.txt','powder')
- Evaluate on our axes:
  - dSW=iData(SW, [], q, w); *% **SLOW** (20 min)*
  - dSW=iData_Sqw2D(dSW);
  - dSW.saveas('LaMnO3_pow_sw.sqw','mcstas')

Now is the time to … mix

Check data files

- Edit the LaMnO3.laz file. Something wrong ?
  - Molar mass: 242 g/mol for LaMnO3
  - σ_{coh} = 23.0 barns / LaMnO3
  - σ_{abs}=22.3
  - σ_{inc}=1.53
  - Density = 6.56 g/cm3
- Check other files



Use LaMnO3 data files

- We start from the templateTOF.
- We remove the container, then add
  - Isotropic_Sqw(Sqw_coh=”coh”, Sqw_inc=”inc”, norm=1)
  - Isotropic_Sqw(Sqw_coh=”sw”, norm=1)
  - PowderN(reflections=”laz”)
- **Sqw: T=-1** (no detailed balance), and **norm=1** (data files as is).

S classical – S quantum

- $S^*(q,w) = S(q,w)\ e^{-hw/2kT}$
- If T=10 K ~ 1 meV, and w ~ 30 meV
  - $e^{-hw/2kT} \sim e^{30} = 10^{13}$ oups…
- This is solved in iFit, but not in Isotropic_Sqw
  - T=-1

RUN !

- templateTOF_LaMnO3.instr
- ncount=1e8. Takes 10 minutes.