Example script to simulate MnF2 powder data using SpinW.

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Assumes that you have already installed Horace and SpinW!

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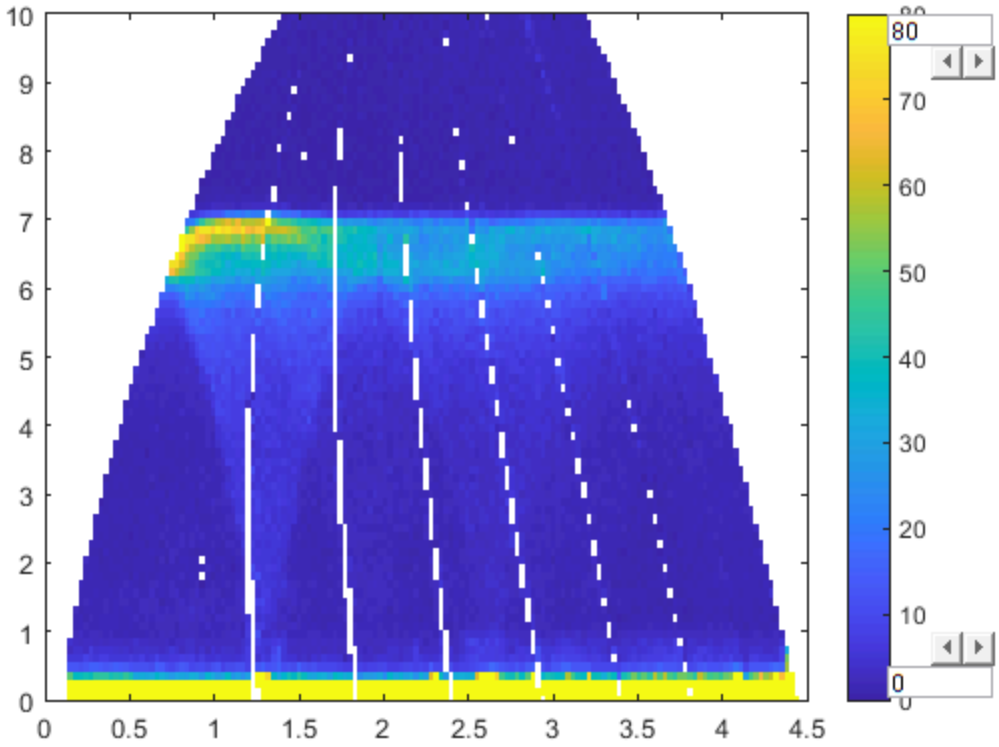
Step 1: convert to a generic data format

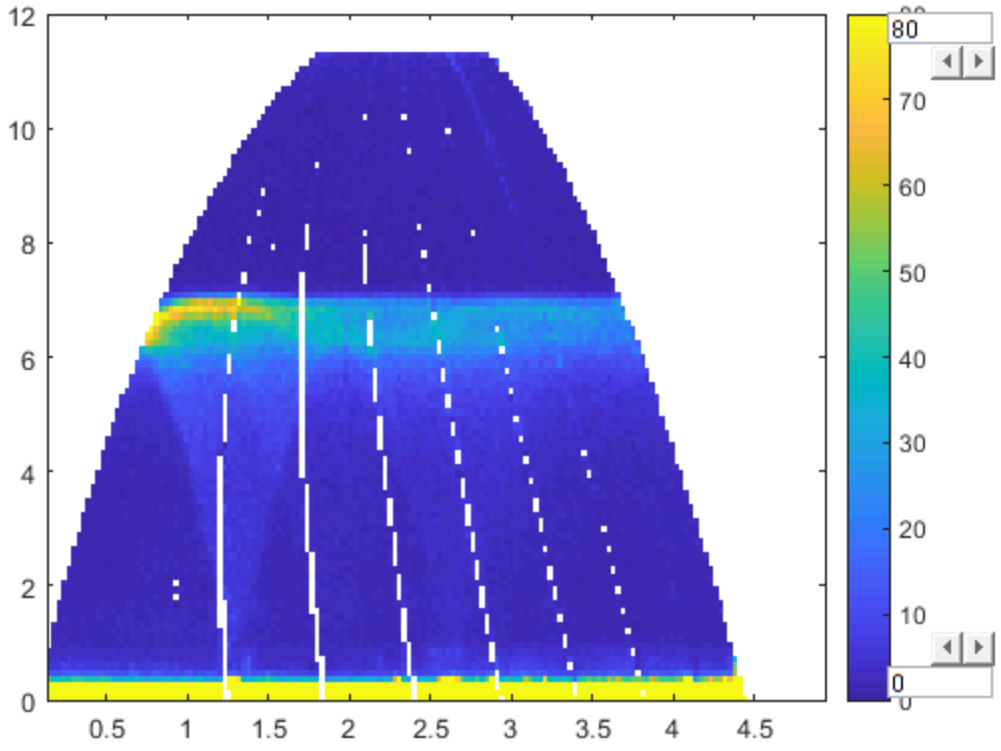
```
%This avoids accidentally using Horace methods that give unexpected
%behaviour later.


%First step is to convert the data (from mnf2_example_plotting.m) into
 yet another format!
mnf2_IX=IX_dataset_2d(mnf2_cut.p{1},mnf2_cut.p{2},mnf2_cut.s,sqrt(mnf2_cut.e));

%Notice that this has zero intensity whereas before there were NaNs to
%specify parts of QE space where there are no detectors. Change this
 back
%so we know where we measured.

mnf2_IX.signal(mnf2_IX.error==0 & mnf2_IX.signal==0)=NaN;
plot(mnf2_IX)
lz 0 80;%colour scale
lx 0 4.5;%x-axis limits
ly 0 10;%y-axis limits
%shold look the same as before
```



Step 2: perform simulation using Horace and SpinW together

```
%Use the Horace multifit tool to simulate and/or fit a spinwave mode.
 See
%spinw_mnf2.m for details of doing a regular simulation,
 spinw_mnf2_fit.m
%for use with these routines

%First just evaluate the cross section using the known correct values
 for
%J:
scalefac=1;%intensity scale factor
J=[-0.0575,0.3161];%exchange (correct values used here)
D=0;%single ion anisotropy
bg=10;%background

%Tell the function which bits of QE space are OK (i.e. are not NaN):
ok=~isnan(mnf2_IX.signal);
Ei=12;
dE=0.36;%Check with your instrument scientist! This can also be the
 name of
%a  file that gives the resolution as a function of energy transfer
dQ=0.04;
```

```
s=rng(1);%random number seed, so that you get the same result each
 time
%(the SpinW powder averaging routine takes the average of many Q
 points
%with the same value of |Q|, randomly chosen, for the powder average -
 by
%seeding the random number generator we ensure that these Q points are
 the
%same every time we run the simulation, which aids fitting)


% <REALLY IMPORTANT POINT>:
% In the ExcitationsPowder routines that you downloaded, you must copy
 the file "powspec_ran.m"
% to the folder in your SpinW installation .../swfiles/@spinw (this is
 where the regular powspec.m
% file lives - check by typing in Matlab "which powspec"). The routine
 ensures that the same random
% number seed is used every time - see above comment for details


[wfit,fitdata]=multifit(mnf2_IX,@spinw_mnf2_fit,
{[scalefac,J,D,bg],ok,Ei,dE,dQ,s},...
    [1,1,1,0,1],'evaluate');
%
% We use the 'evaluate' keyword so that a fit is not done, simply the
% function is evaluated using our initial guess. If we omitted this
 keyword
% a fit would be done, with the first 3 parameters (scale factor and
 Js)
% being fitted, but D fixed and background fitted: [1,1,1,0,1] - 1 for
 free, 0 for fixed.

%compare data and simulation:
plot(mnf2_IX); ly 0 12; lz 0 80; keep_figure;
plot(wfit); ly 0 12; lz 10 10.6; keep_figure

%We can see that we can get an excellent agreement if we use the right
%parameters!

Creating the bond list (maxDistance = 5 Å, nCell = 2x2x2)...
...14 bonds are retained out of 300 generated!
Calculating powder spectra...
The magnetic form factor is included in the calculated structure
 factor.
No g-tensor is included in the calculated structure factor.
Calculation is finished in 00:00:11 (hh:mm:ss).
Calculation finished.
Finite instrumental energy resolution is applied.
Finite instrumental momentum resolution of 0.040 A-1 is applied.
Energy transfer is limited to instrument, using ki=2.406 A-1.
```


12
10
8
6
4
2
0
0.5
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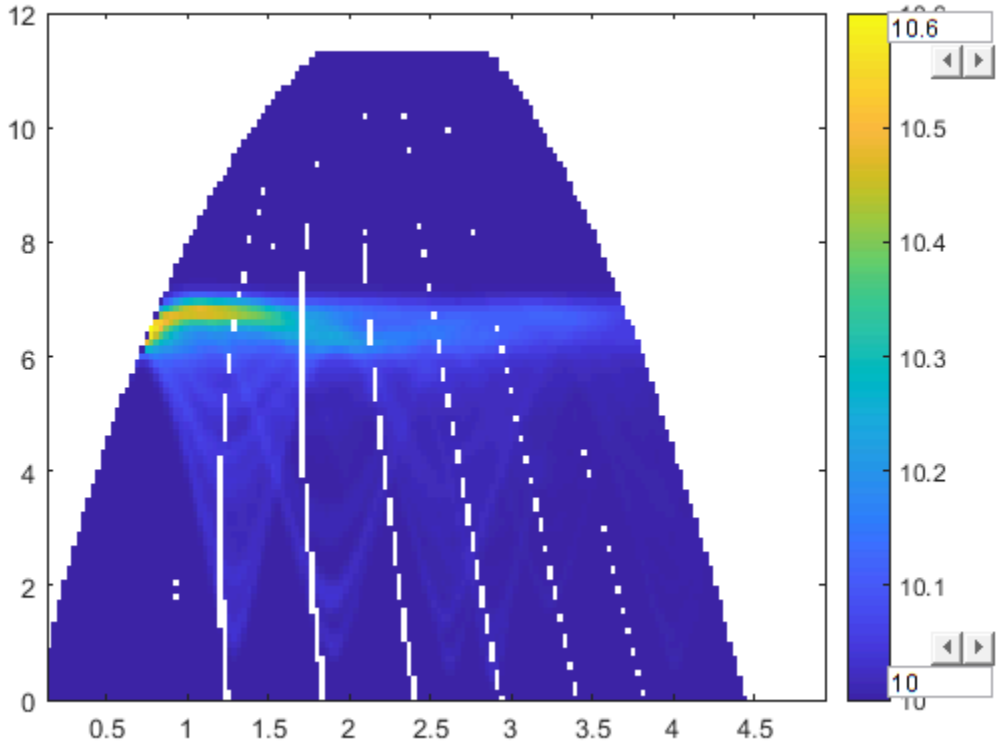
2
2.5
3
3.5
4
4.5
80
70
60
50
40
30
20
10
0


12
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3
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10.6
10.5
10.4
10.3
10.2
10.1
10

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