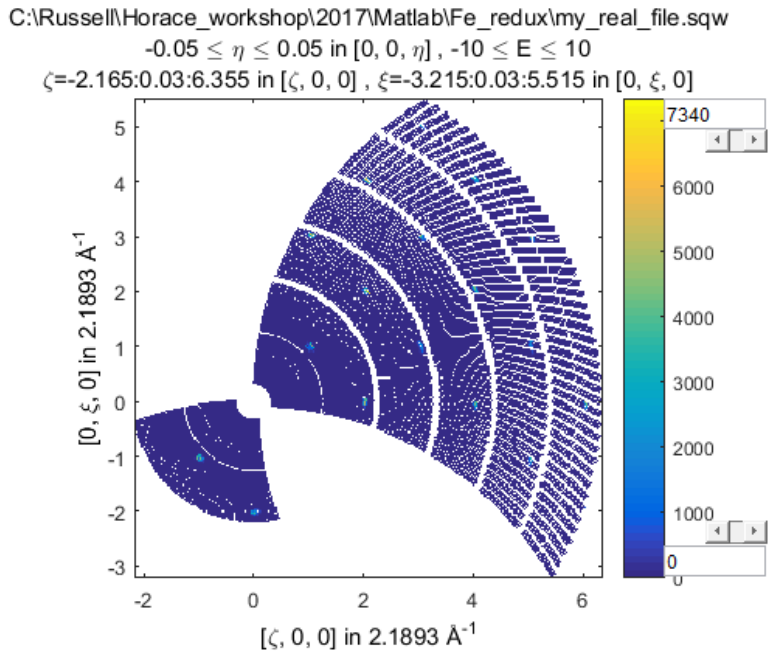
Contents

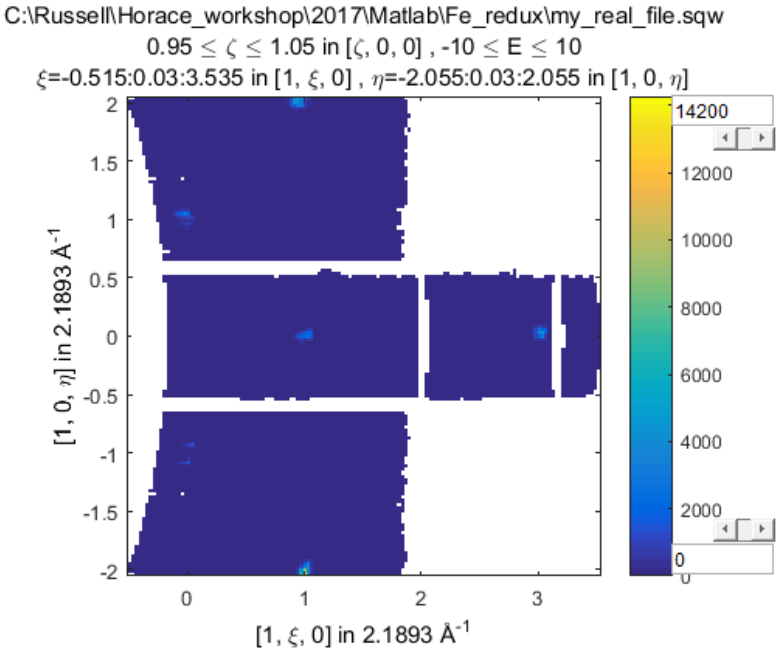
Correcting for sample misalignment

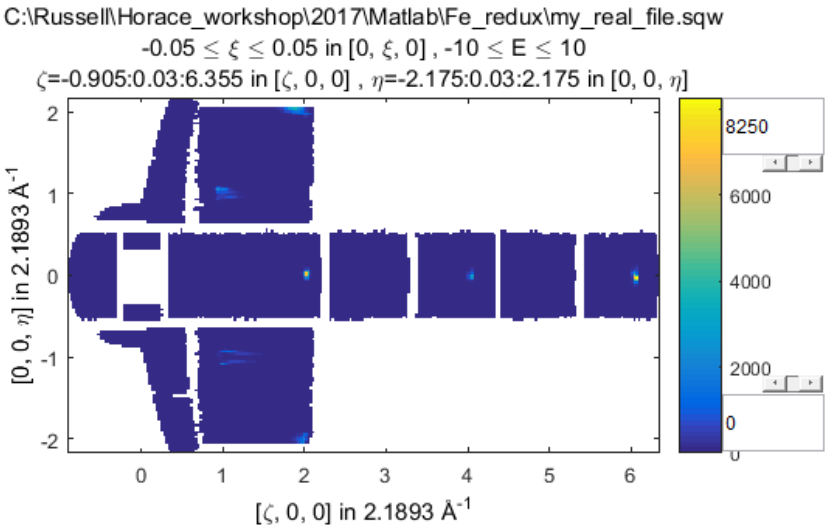
```
%If your sample is misaligned compared to the notional alignment used when
%generating the sqw file, you can correct for this without having to
%regenerate the sqw file (since this can be quite time-consuming)

%Make a series of hk-slices at different l, in order to work out what Bragg
%positions we have. Step sizes and energy integration should be customised for your data
%Step sizes should be as small as possible, and energy integration tight.
alignment_slice1=cut_sqw(sqw_file,proj2,[-5,0.03,8],[-5,0.03,8],[-0.05,0.05],[-10,10],'-nopix');
alignment_slice2=cut_sqw(sqw_file,proj2,[0.95,1.05],[-5,0.03,8],[-3,0.03,3],[-10,10],'-nopix');
alignment_slice3=cut_sqw(sqw_file,proj2,[-5,0.03,8],[-0.05,0.05],[-3,0.03,3],[-10,10],'-nopix');

%Look at the 3 orthogonal slices to figure out what bragg peaks are visible
plot(compact(alignment_slice1)); keep_figure;
plot(compact(alignment_slice2)); keep_figure;
plot(compact(alignment_slice3)); keep_figure;
```


C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-0.05 ≤ η ≤ 0.05 in [0, 0, η] , -10 ≤ E ≤ 10
ζ=-2.165:0.03:6.355 in [ζ, 0, 0] , ξ=-3.215:0.03:5.515 in [0, ξ, 0]
[0, ξ, 0] in 2.1893 Å-1
[ζ, 0, 0] in 2.1893 Å-1
7340
6000
5000
4000
3000
2000
1000
0


C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
0.95 ≤ ζ ≤ 1.05 in [ζ, 0, 0] , -10 ≤ E ≤ 10
ξ=-0.515:0.03:3.535 in [1, ξ, 0] , η=-2.055:0.03:2.055 in [1, 0, η]
[1, 0, η] in 2.1893 Å-1
[1, ξ, 0] in 2.1893 Å-1
14200
12000
10000
8000
6000
4000
2000
0



Define which Bragg peaks we want to use to align - should not be near edge of Q-space coverage

```
%Our notional Bragg peaks
bp=[4,0,0; 2,0,0; 1,1,0; 4,4,0; 1,0,1];%list of accessible Bragg peaks (in data they may be off from these notional positions)


%Get true Bragg peak positions.
%This routine takes radial and transverse cuts around the Bragg peaks listed above. See the help for further information
%about how the routine works - you will in general have to adjust some of the inputs here, especially the energy window
[rlu0,width,wcut,wpeak]=bragg_positions(sqw_file, bp, 0.8, 0.06, 0.4,...
                                        0.8, 0.06, 0.4, 8, 'gauss','bin_ab');

%Check how well the function did (note the command line prompts to allow you to scan through the cuts made above)

%bragg_positions_view(wcut,wpeak)

%Opens an interactive tool to check the results
```

Calculate corrections, with options of whether the lattice is fixed or not (see more detailed help pages for more info)

```
%Determine corrections to lattice and orientation (in this example we choose to keep the lattice angles fixed,
%but allow the lattice parameters to be refined, keeping a cubic structure by keeping ratios of lattice pars to be same):
[rlu_corr,alatt,angdeg] = refine_crystal(rlu0, alatt, angdeg, bp,'fix_angdeg','fix_alatt_ratio');


%Apply changes to sqw file
change_crystal_horace(sqw_file, rlu_corr);


%Check the outcome: Get Bragg peak positions and look at output: should be much better
[rlu0,width,wcut,wpeak]=bragg_positions(sqw_file, bp, 1.5, 0.06, 0.4,...
                                        1.5, 0.06, 0.4, 20, 'gauss','bin_ab');
bragg_positions_view(wcut,wpeak)
keep_figure

%=========
%Generally you only want to figure out the misorientation once, then apply some correction to subsequent data.
% You can do this by finding the values of the notional goniometers gl, gs, dpsi that are used in gen_sqw:

[alatt, angdeg, dpsi_deg, gl_deg, gs_deg] = crystal_pars_correct (u, v, alatt0, angdeg0, omega0_deg, dpsi0_deg, gl0_deg, gs0_deg, rlu_corr);
%u and v are the notional scattering plane, alatt0, angdeg0, etc are the original values for those parameters you used in gen_sqw
%rlu_corr is the misalignment correction matrix determined above. The routine outputs the corrected lattic parameters (if these were
%refined) and the values of dpsi, gl and gs to use in future regenerations of the sqw file
```

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