

Running an experiment part 1 - generating an sqw file

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data_path='C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\';

%par_file=[data_path,'4to1_102.par'];
par_file='';
sqw_file=[data_path,'my_real_file.sqw'];
efix=400;
psi=[0:2:90];
runno=[15052:15097];
emode=1;
alatt=[2.87,2.87,2.87];
angdeg=[90,90,90];
u=[1,0,0]; v=[0,1,0];
omega=0; dpsi=0; gl=0; gs=0;

alatt0=[2.87,2.87,2.87];
angdeg0=[90,90,90];
omega0_deg=0; dpsi0_deg=0; gl0_deg=0; gs0_deg=0;

for i=1:numel(psi)
    spefile{i}=[data_path,'map',num2str(runno(i)),'_ei400.nxspe'];
end

gen_sqw (spefile, par_file, sqw_file, efix, emode, latt, angdeg,...
        u, v, psi, omega, dpsi, gl, gs)

%test adding a file that does not exist yet:
% psi=[0:2:100];
% runno=[15052:15102];
% for i=1:numel(psi)
%     spefile{i}=[data_path,'map',num2str(runno(i)),'_ei400.nxspe'];
% end
% accumulate_sqw (spe_file, par_file, sqw_file, efix, emode, latt, angdeg,...
%                 u, v, psi, omega, dpsi, gl, gs)

%A comment on accumulate_sqw
%accumulate_sqw (spe_file, par_file, sqw_file, efix, emode, latt, angdeg,...
%                 u, v, psi, omega, dpsi, gl, gs)

%Or
%accumulate_sqw (spe_file, par_file, sqw_file, efix, emode, latt, angdeg,...
%                 u, v, psi, omega, dpsi, gl, gs,'clean')

%This is a way of appending newly processed spe files to an existing
%dataset. The key point is that the psi and spe_file arrays contain a list
%of PLANNED files and run-numbers - only those that actually exist will be
%included in the file.

%Can run this periodically overnight, say.

%Note that if one has access to a high performance cluster on which sqw files can be generated
%quickly then this routine need only be run once around the time the sqw file is required.

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