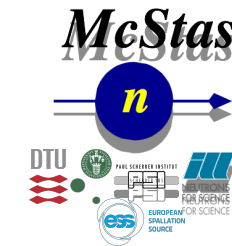




McStas Advanced Samples



MDANSE 2018

Simulation of Inelastic
Neutron Scattering
using McStas and
material dynamics models

Sept. 24th – 28th 2018

Puerto de la Cruz – Tenerife

(c) A. Mart (2012)





Agenda

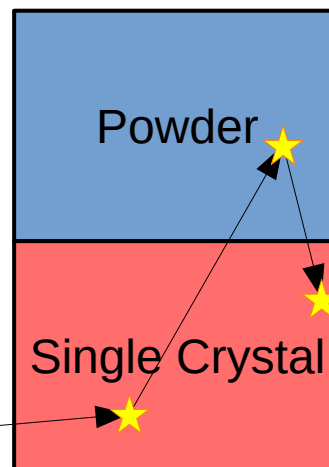


- ★ *Combining a powder sample with a Single Crystal*
- ★ *Polycrystal*
The Union concept
- ★ *External Connections:*
 - *nCrystal, nxs, cif2hkl**In General: MCPL*

Powder SX combination

- Use a **GROUP!**
- ... but also allow reentry – How?

```
COMPONENT a1 = Arm()
AT(0,0,0) RELATIVE sample_pos
EXTEND
%{
    sample_scatter=0;
%}
COMPONENT pow = PowderN( ... )
AT(0,h/2,0) RELATIVE a1
GROUP sample
EXTEND
%{
    if(SCATTERED) sample_scatter=1;
%}
```



```
COMPONENT sx = Single_crystal( ...)
AT(0,-h/2,0) RELATIVE a1
GROUP sample
EXTEND
%{
    if(SCATTERED) sample_scatter=1;
%}
```

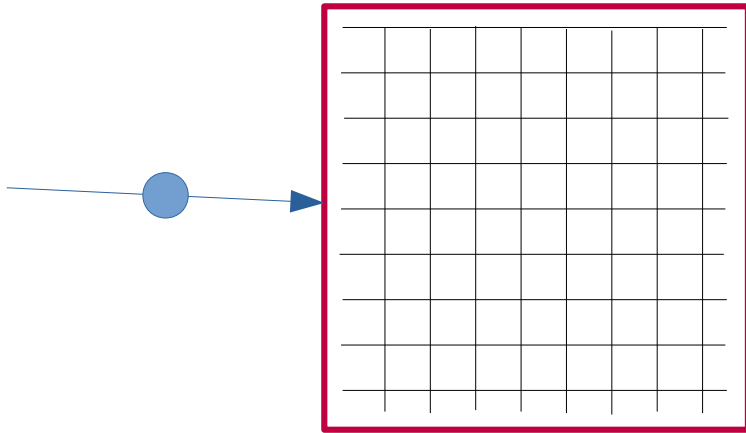
```
COMPONENT a2 = Arm()
AT (0,0,0) RELATIVE a1
WHEN (scatter) JUMP a1
```



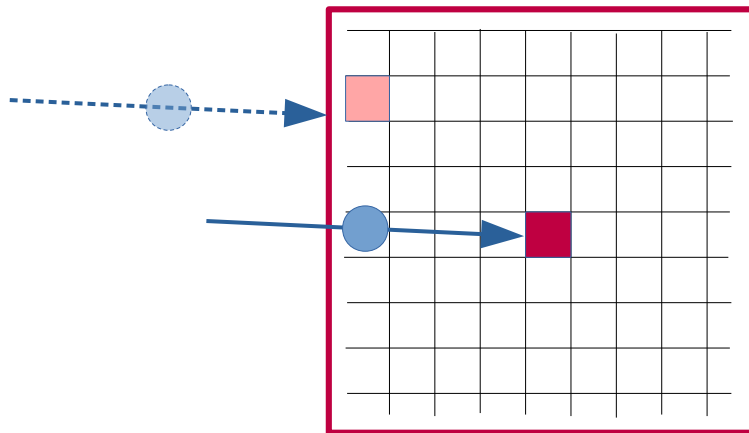
Extending that idea

A polycrystal as many Single crystals

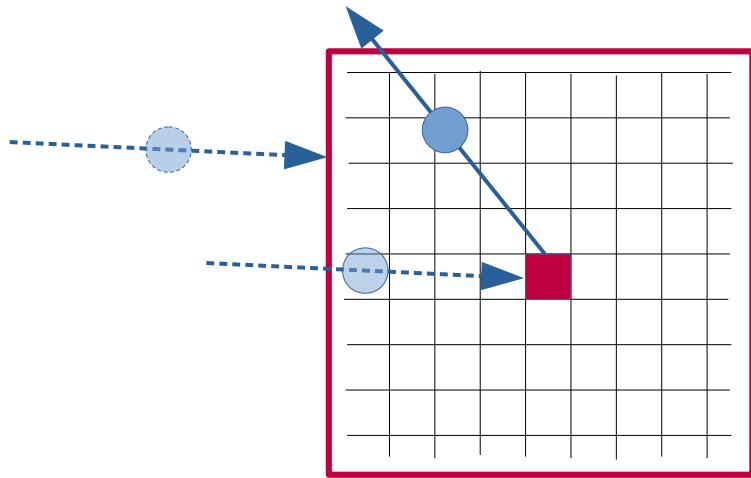
The idea: Cheat a single Single_crystal into believing it is many...



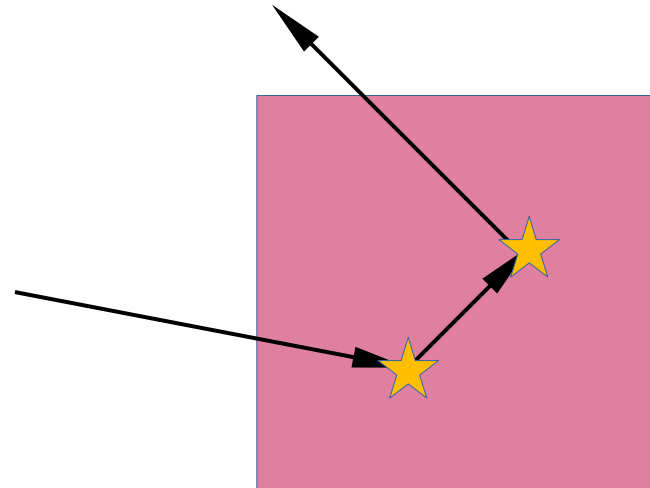
Apply translation



Single_crystal as polycrystal



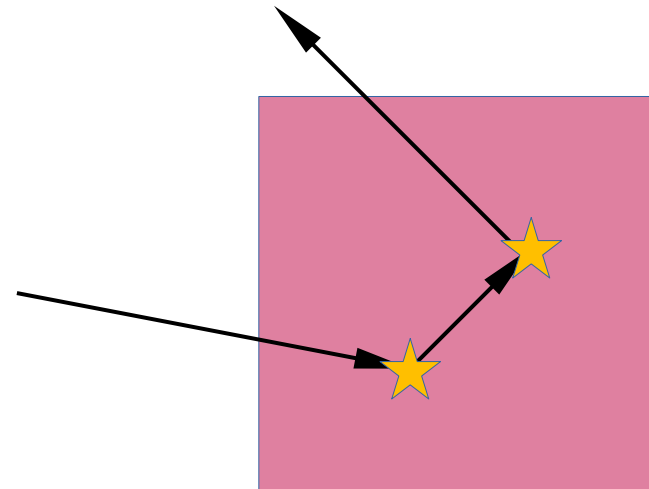
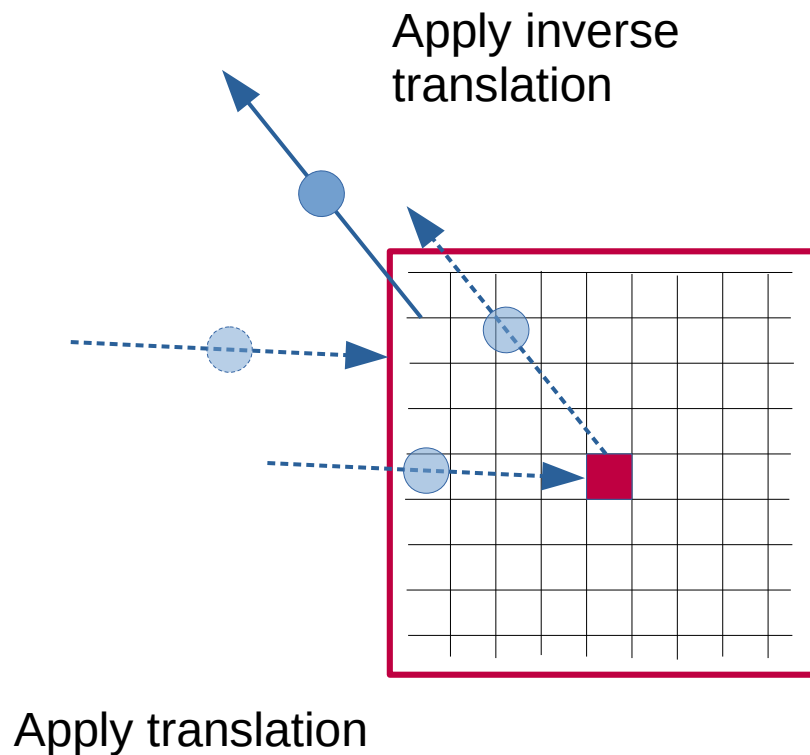
Apply translation



Scattering events happen
in the crystal
neutron exits.



Single_crystal as polycrystal

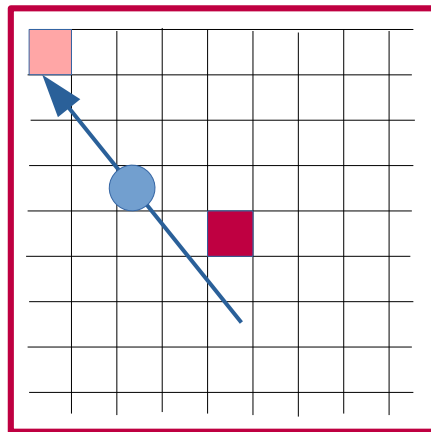


Scattering events happen in the crystal
neutron exits.

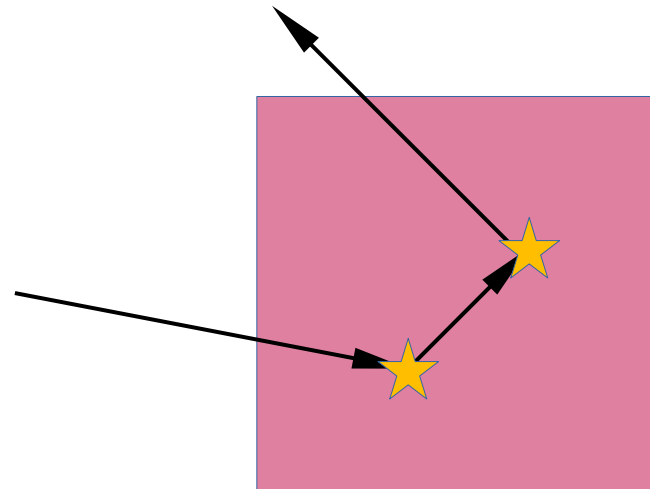


Single_crystal as polycrystal

Neutron may enter a new subcrystal...



Apply inverse translation



Scattering events happen in the crystal neutron exits.



Union



Jump to another slideshow



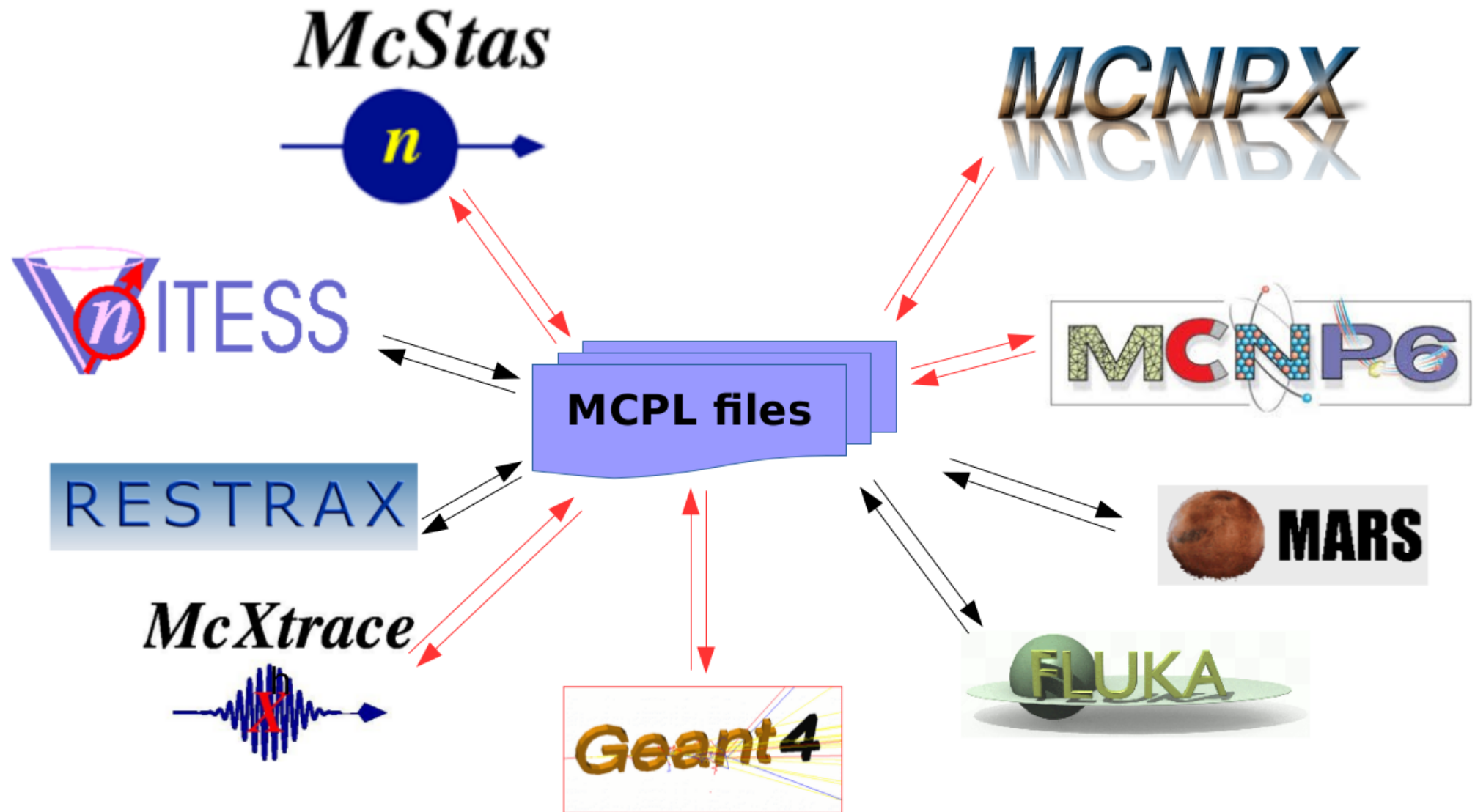
External Connections

- *McStas can be connected to many things, and in many ways:*
 - *Datafiles:*
 - *VASP/MD > Isotropic_Sqw*
 - *cif2hkl (CrysFML) > Single_crystal & PowderN*
 - *MCNP6, VitESS, GEANT-4 > MCPL*
 - *Code-sharing:*
 - *SasView_models*
 - *Direct compilation linkage*
 - *nCrystal*





MCPL





MCPL

McStas



MCNPX



<https://mctools.github.io/mcpl/>



MCPL files

RESTRAX



McXtrace



Geant4

