



# McStas Advanced Samples



**MDANSE 2018**

**Simulation of Inelastic Neutron Scattering using McStas and material dynamics models**

Sept. 24<sup>th</sup> – 28<sup>th</sup> 2018

Puerto de la Cruz – Tenerife

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# 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?

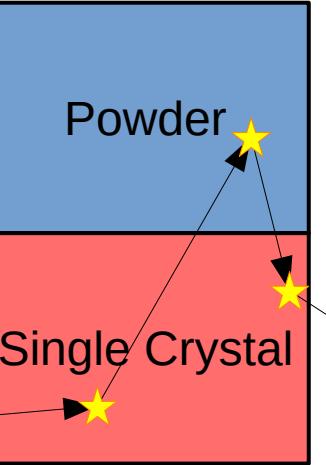
```

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

```

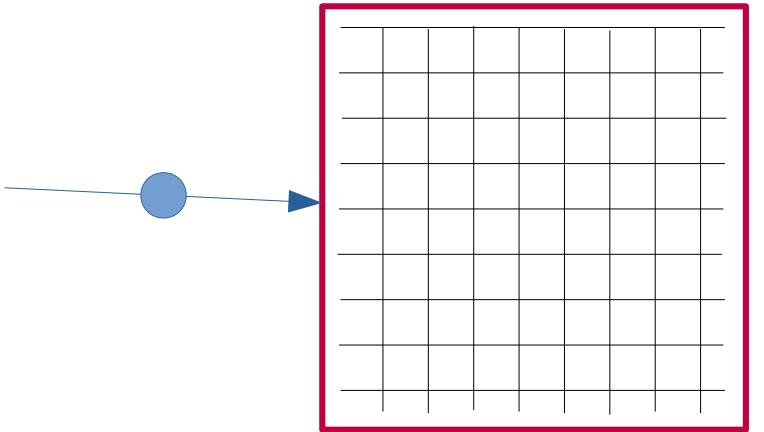




# Extending that idea

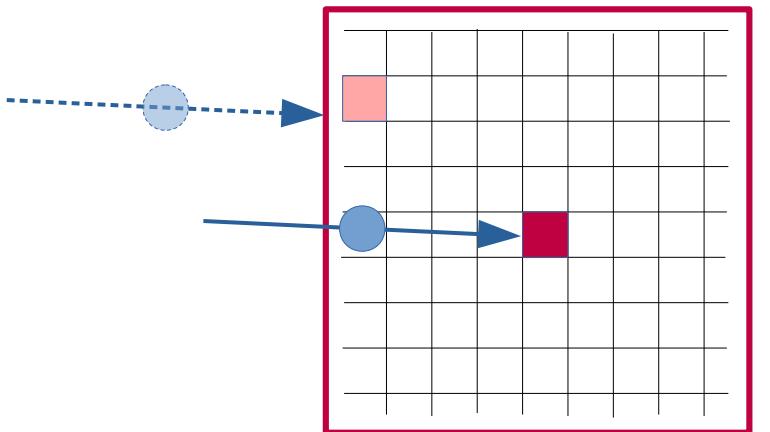
A polycrystal as many Single crystals

The idea: Cheat a single Single\_crystal into  
believing it is many...



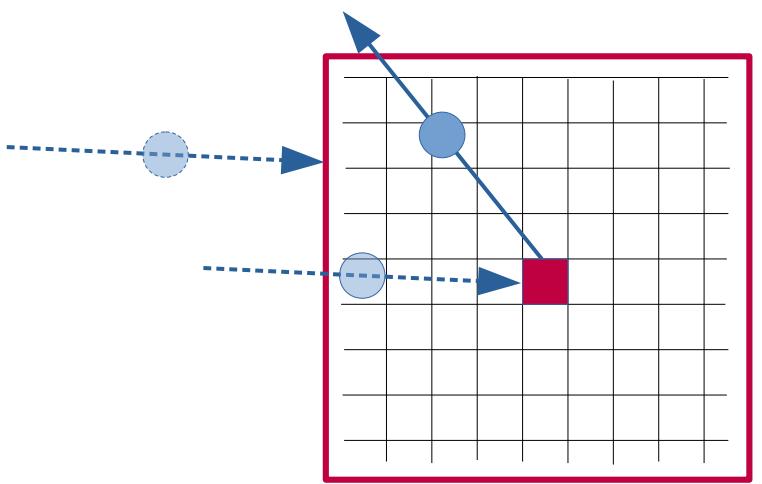


Apply translation

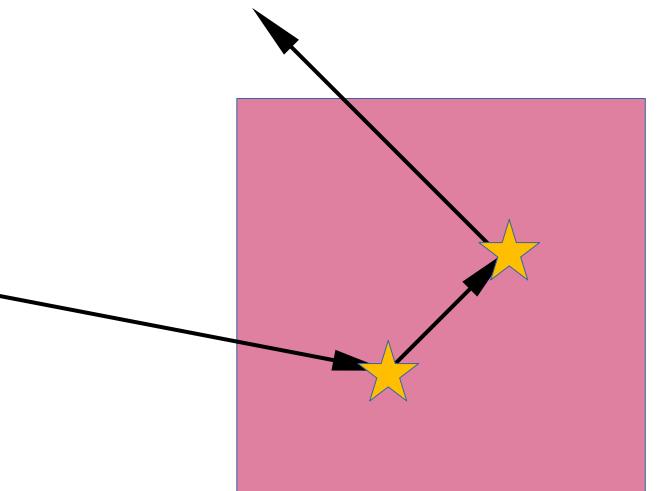




# Single\_crystal as polycrystal



Apply translation

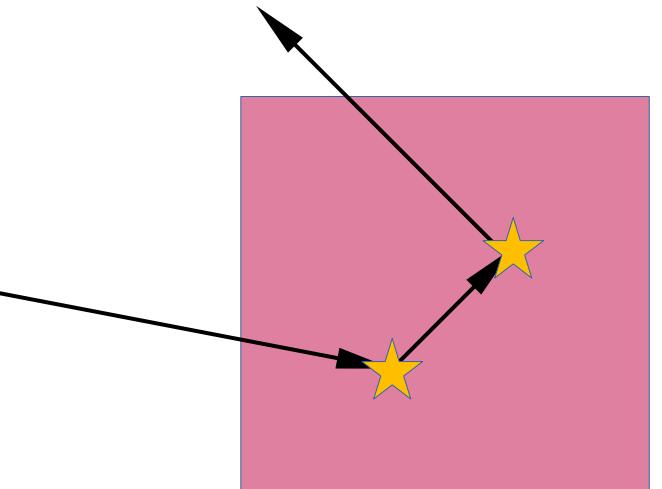
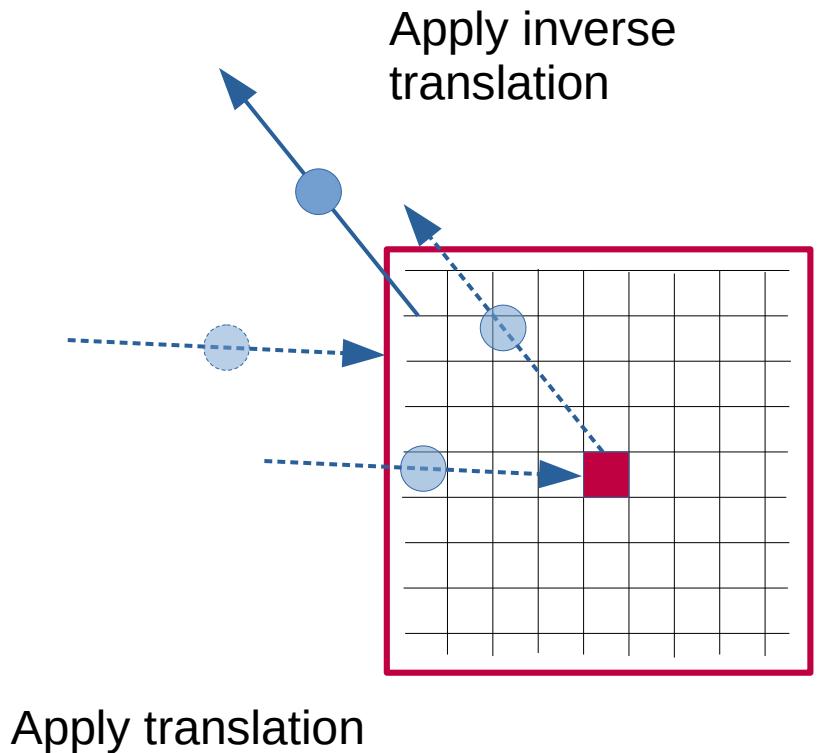


Scattering events happen  
in the crystal  
neutron exits.





# Single\_crystal as polycrystal



Scattering events happen  
in the crystal  
neutron exits.



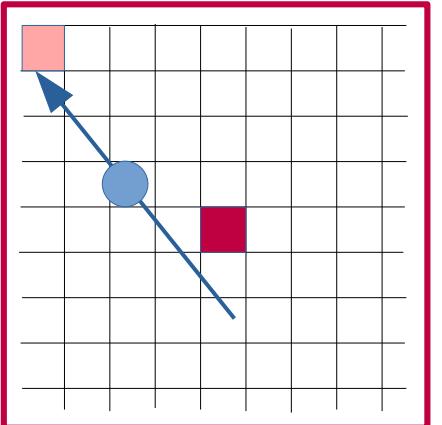


# Single\_crystal as polycrystal

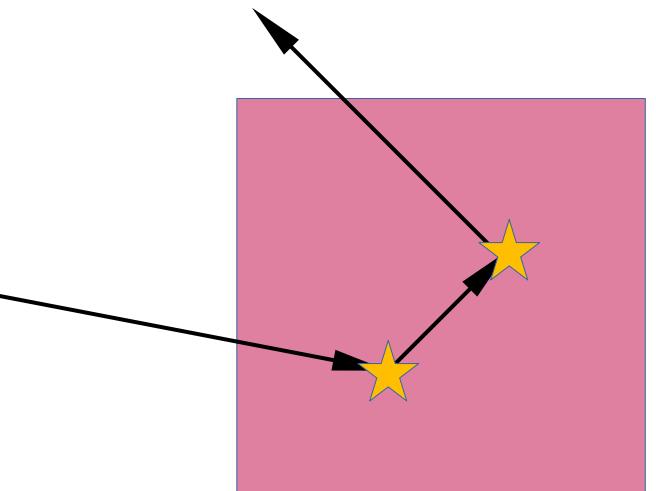


Apply inverse  
translation

Neutron may  
enter a new  
subcrystal...



Apply translation



Scattering events happen  
in the crystal  
neutron exits.

# Union



Jump to another slideshow





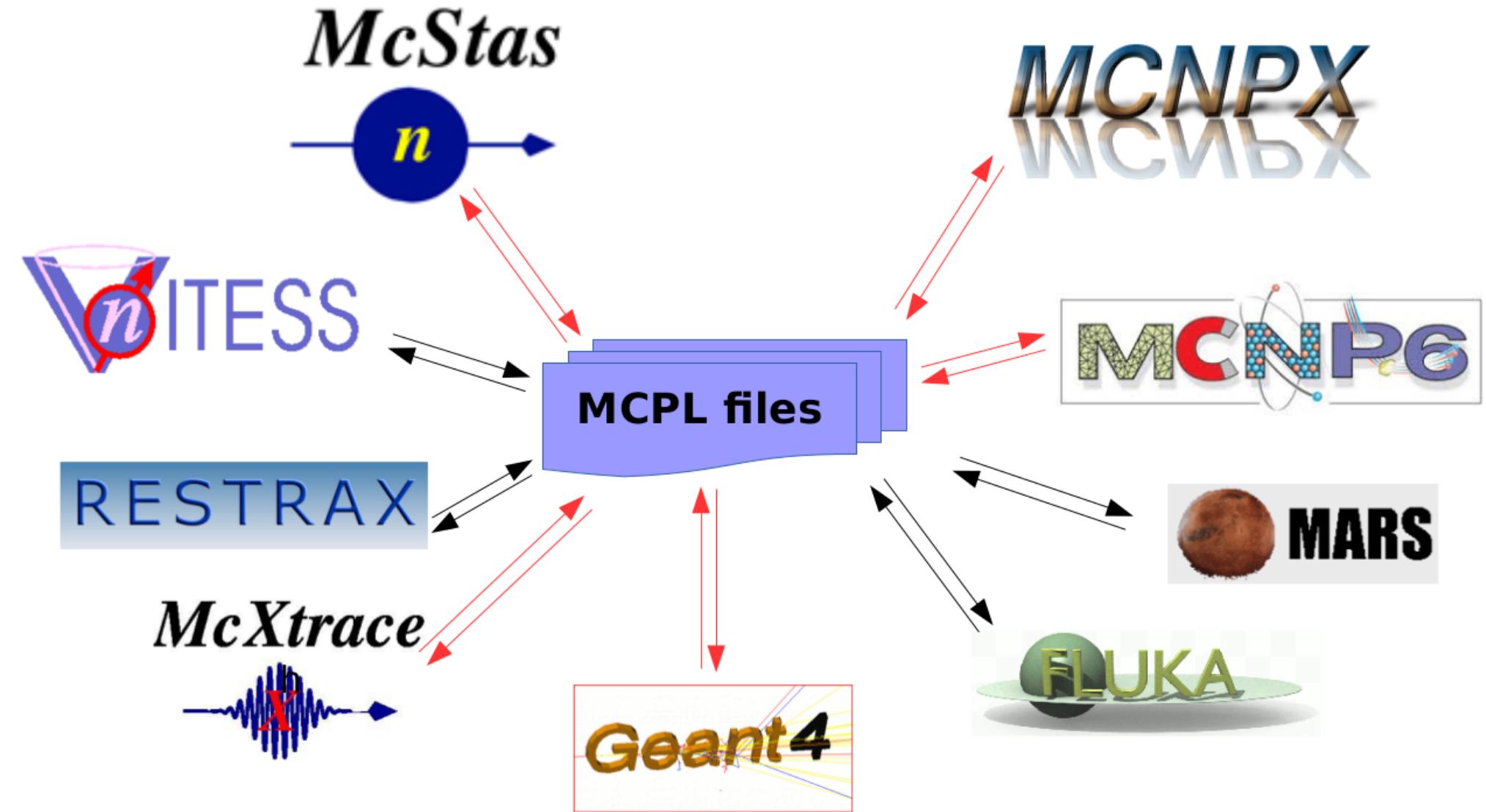
# External Connections

- *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

