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# Advanced language features

- Macros and tricks for your instrument...





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# DECLARE / INITIALIZE

- Use the DECLARE section define user variables and functions.
  - `DECLARE %{`
  - `double some_global_var;`
  - `%}`
- Use USERVARS for particle-dependent flags
  - `USERVARS %{`
  - `double myvar;`
  - `%}`
- Use INITIALIZE for initialization of user variables and calculations.
  - `INITIALIZE %{`
  - `myvar = sqrt(PI*input_var)*rand01();`
  - `%}`
- - Both use normal c-syntax.
- BEWARE: (example) What you do in the c-style areas is c-standard, e.g. trigonometric functions from `math.h` use radians! - McStas placement specifiers work in degrees, etc...



K & R. / GNU



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n →

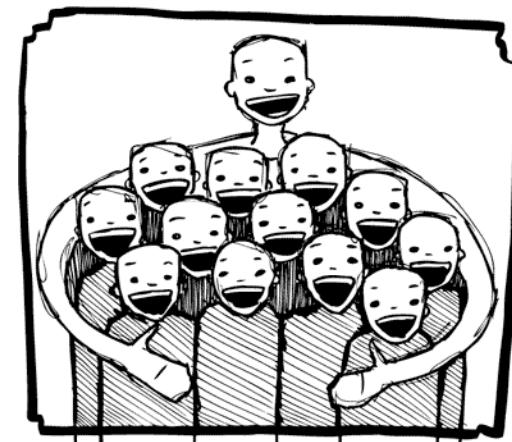


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# %include

- Instrumentfiles can include external c-code or other instrumentfiles... See the examples:
  - ILL\_H15\_IN6.instr:%include "monitor\_nd-lib"
  - ILL\_H16\_IN5.instr:%include "ILL\_H16.instr"
  - ILL\_H25\_IN22.instr:%include "ILL\_H25.instr"
  - ILL\_H25\_IN22.instr:%include "templateTAS.instr"
- Used in the DECLARE section





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# Syntax in one, complex view...

```
{SPLIT} COMPONENT name = comp(parameters) {WHEN condition}  
AT (...) [RELATIVE [reference|PREVIOUS] | ABSOLUTE]  
{ROTATED {RELATIVE [reference|PREVIOUS] | ABSOLUTE} }  
{GROUP group_name}  
{EXTEND C_code}  
{JUMP [reference|PREVIOUS|MYSELF|NEXT] [ITERATE number_of_times | WHEN condition] }
```

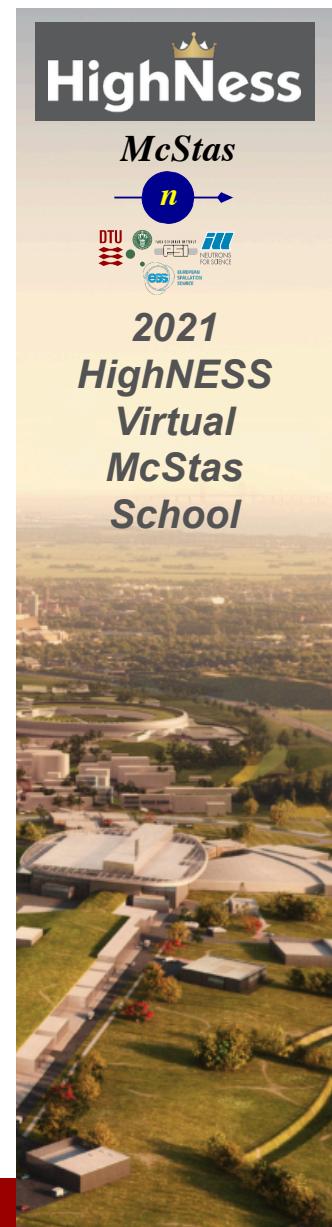




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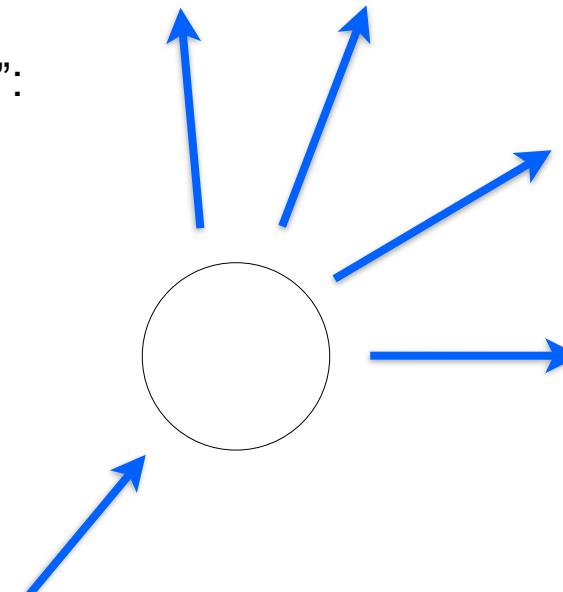


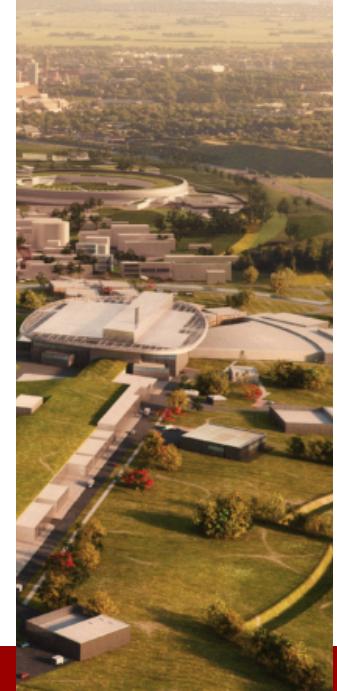
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# SPLIT

- Increase statistics beyond this point in the instrumentfile
- SPLIT n MyArm = Arm()
- AT somewhere
- will “formulate an if-statement”:
- for j=1:n
- comp1
- comp2
- comp3
- ...
- end (of instrument)
- ONLY meaningful in case of Monte Carlo choices after SPLIT point...





# Problem: McStas Single\_crystal.comp “slow” for large unit cell diffraction studies

- Example: Rubredoxin

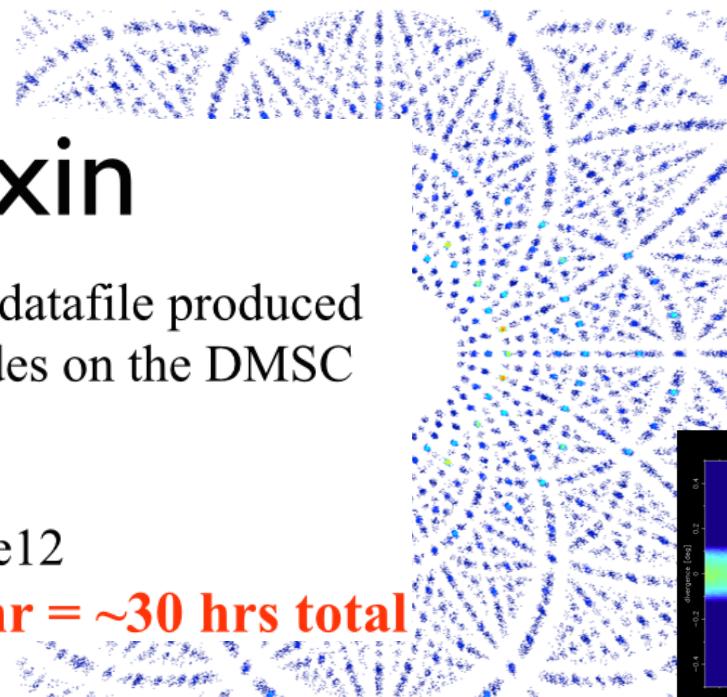
1 timebin, 1000 x,y-bins

## Rubredoxin

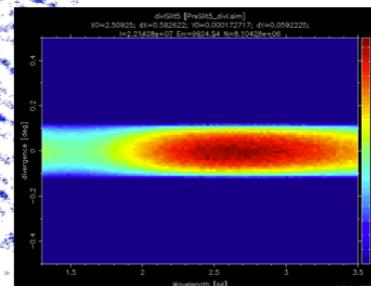
Images created from simulated datafile produced August 20th 2012 using 25 nodes on the DMSC cluster.

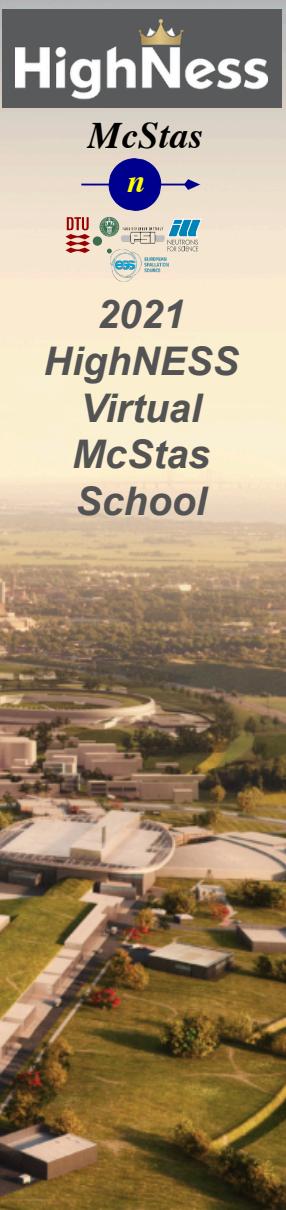
Neutron count: 1e12

**Simulation time: ~10 + ~20 hr = ~30 hrs total**



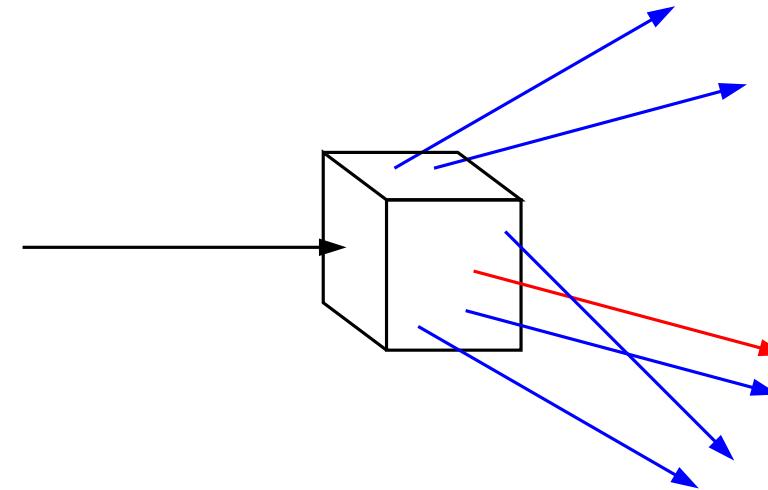
Neutroncount: 1e12  
 No gravitation  
 Xtal size: 0.5 mm  
 Xtal mosaicity: 12'  
 Detector: 50 x 50 cm flat  
 Detector-to-sample distance: 20 cm  
 Guide length: 131 m  
 Guide dimensions: 9.5 cm  
 $\lambda_{\min} = 1.3 \text{ \AA}$   
 $\lambda_{\max} = 3.5 \text{ \AA}$   
 Timespan: 51.39 to 143.4 ms  
 Divergence = 0.2 degs





# Algorithm improvement: Use incoming neutrons more efficiently - scatter each one on all possible reflections

- **Red:** Original algorithm, one incoming neutron used only once
- **Blue:** Improved algorithm, each incoming neutron scattered (via SPLIT keyword) all possible times
- Component makes **estimate on average number of “active” diffraction spots** - in the case Rubredoxin this is around **50!**



!!! For now, does not work in our GPU implementation !!!



# GROUP - components working in parallel



*AT (0,0,-LMM) RELATIVE Cradle ROTATED (0,A1/2,0) RELATIVE Cradle  
GROUP IN6Monoks*

*AT (0,0,0) RELATIVE Cradle ROTATED (0,A2/2,0) RELATIVE Cradle  
GROUP IN6Monoks*

- One comp after the other is “tried” in sequential order until the neutron was SCATTERED.

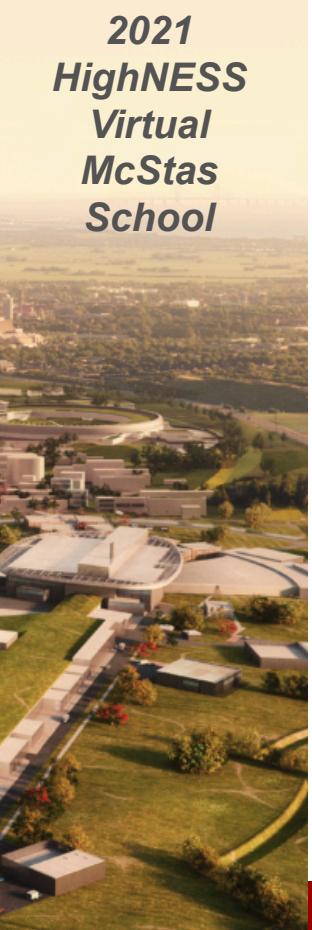
# EXTEND

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- Enrich component behaviour using EXTEND:

```
COMPONENT Mono1 = Monochromator_curved(...)
AT (0,0, -LMM) RELATIVE Cradle ROTATED (0,A1/2,0) RELATIVE Cradle
GROUP IN6Monoks
```

```
EXTEND
```

```
%{
    if (SCATTERED) { myvar = 1; }
%}
```

```
...
```

```
COMPONENT Mono2 = Monochromator_curved(...)
AT (0,0, 0) RELATIVE Cradle ROTATED (0,A2/2,0) RELATIVE Cradle
GROUP IN6Monoks
```

```
%{
    if (SCATTERED) { myvar = 2 ;}
%}
```

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en el ANSI C

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# WHEN

- Syntax:

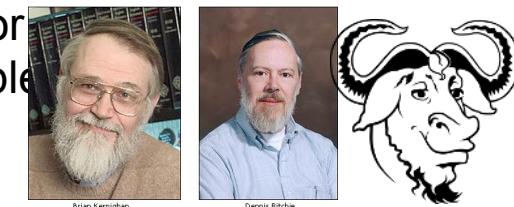
COMPONENT Mine = Yours(blah, blah)

WHEN (c-expression) AT (....)

- Is very powerful when combined with EXTEND and user variables, or as a method to let input parameters select if certain components are active.

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- Example: Use EXTEND to flag if neutron was scattered on one monochromator or another. Then later use WHEN to only show contribution from blade N at sample



COMPONENT Mon = PSD\_monitor(...)

WHEN (myvar==1) AT (0,0,0) RELATIVE Sample



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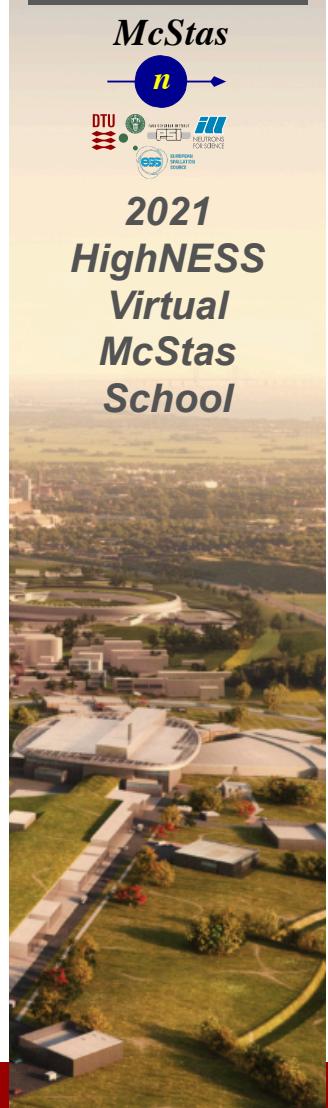


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# JUMP

- A goto. Be careful. Can be used in two situations:
- JUMP to myself
- JUMP to an Arm
- No coordinate transformations are applied... (Meaning that if the Arms you JUMP between do not coincide you will “move” / “reorient” the neutrons...)
- Syntaxes:
- COMPONENT a=b(...)
- WHEN (expr) AT (...) JUMP somewhere
- COMPONENT a=b(...)
- WHEN (expr) AT (...) JUMP myself





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***BEWARE - This IS a***

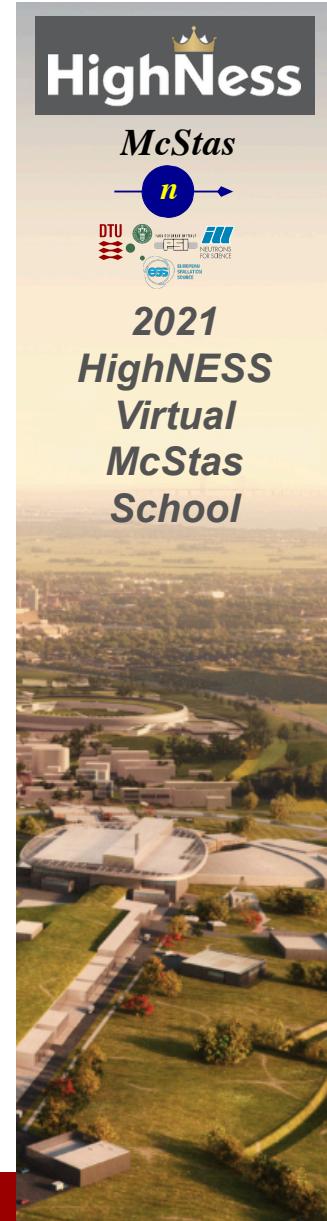


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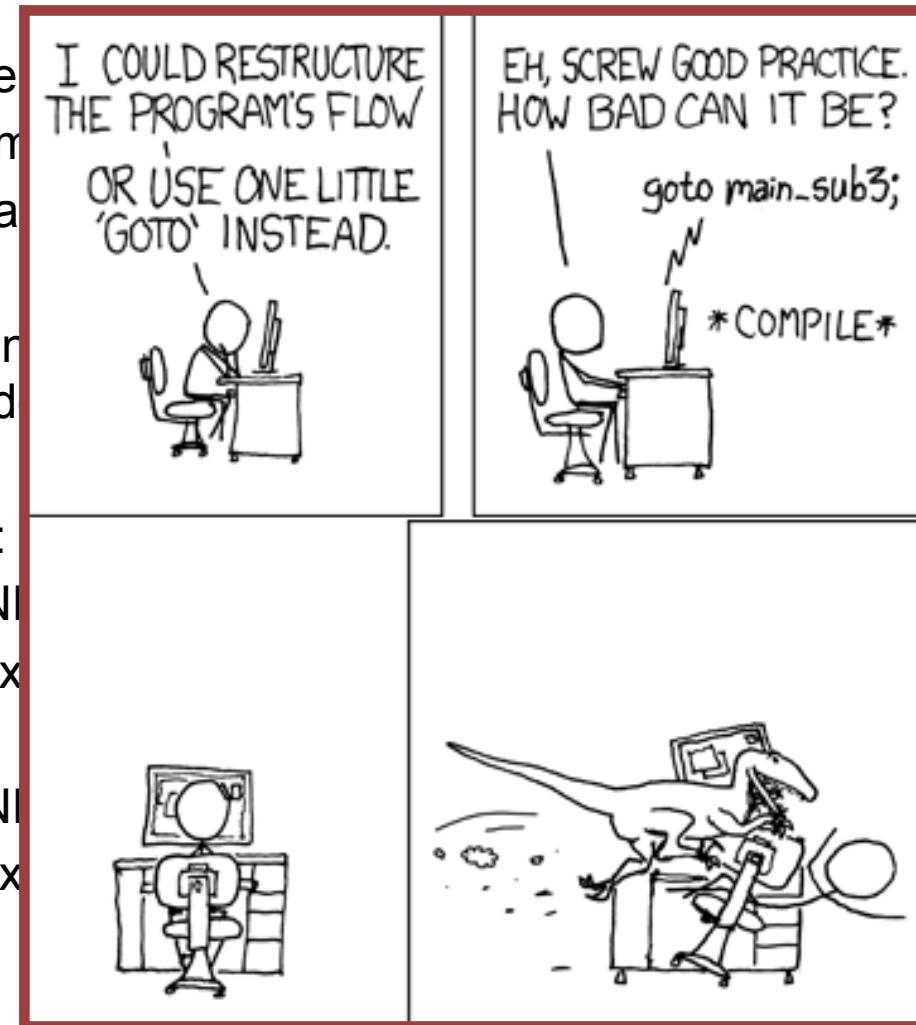


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that if the Arms you JUMP  
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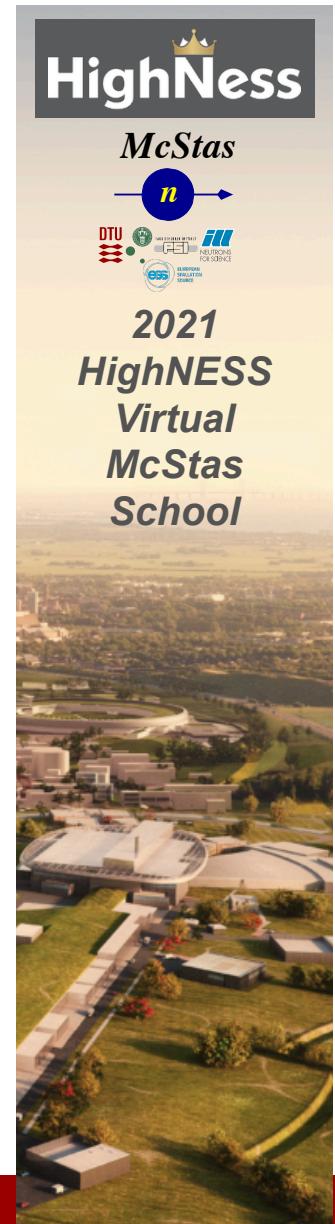


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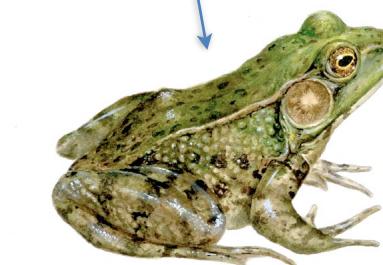
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# COPY- inside instruments

- In instruments: (see ILL\_H25.instr)
  - COMPONENT H25\_1 = Guide\_gravity(
    - w1=0.03, h1=0.2, w2=0.03, h2=0.2, l=L\_H25\_1,
    - R0=gR0, Qc=gQc, alpha=gAlpha, m=m, W=gW)
    - AT (0,0,AI\_Thickness+gGap) RELATIVE PREVIOUS
    - ROTATED (0,Rh\_H25\_1,0) RELATIVE PREVIOUS
  - COMPONENT COPY(H25\_1) = COPY(H25\_1)
    - AT (0,0,L\_H25\_1+gGap) RELATIVE PREVIOUS
    - ROTATED (0,Rh\_H25\_1,0) RELATIVE PREVIOUS
  - COMPONENT COPY(H25\_1) = COPY(H25\_1)(W=2\*gW)
    - AT (0,0,L\_H25\_1+gGap) RELATIVE PREVIOUS
    - ROTATED (0,Rh\_H25\_1,0) RELATIVE PREVIOUS





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# Example: Decompose multiple scattering from Single\_crystal

```
USERVARS %{
    double multiple_scatt;
}

COMPONENT Crystal = Single_crystal(... order=0 ...)
AT (0,0,0) RELATIVE somewhere

EXTEND %{
    multiple_scatt=SCATTERED;
}

COMPONENT PSD_single=PSD_monitor(...)
WHEN (multiple_scatt==1) AT (0,0,0) RELATIVE somewhere_else

COMPONENT PSD_multiple=PSD_monitor(...)
WHEN (multiple_scatt > 1) AT (0,0,0) RELATIVE somewhere_else
```

