Advanced language features 2:

SPLIT, EXTEND, WHEN & GROUP

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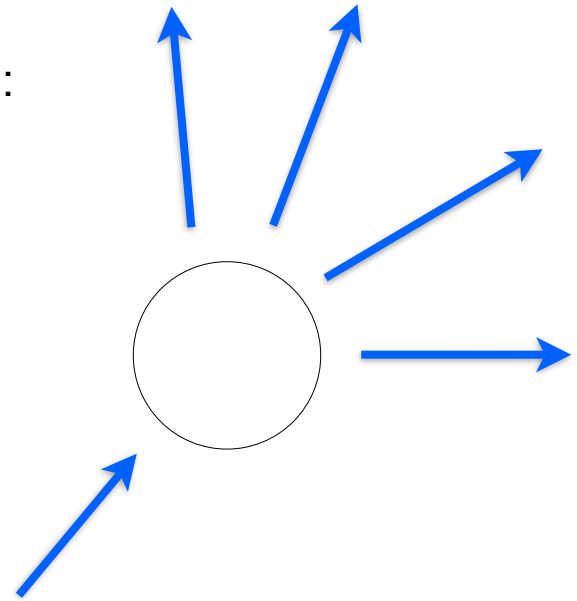
SPLIT

- 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...

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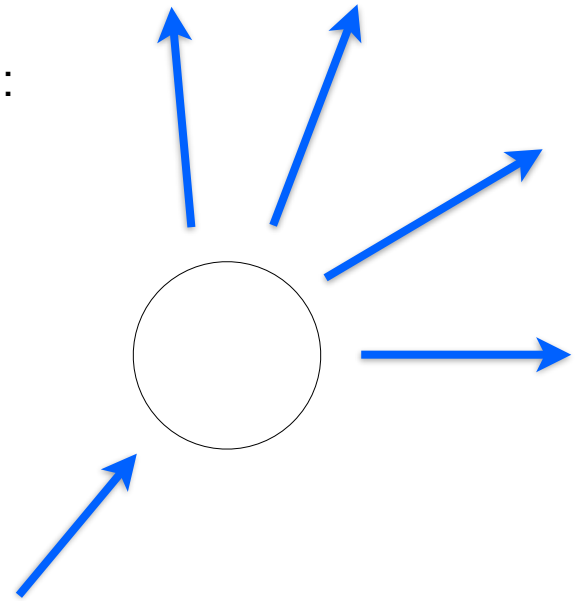


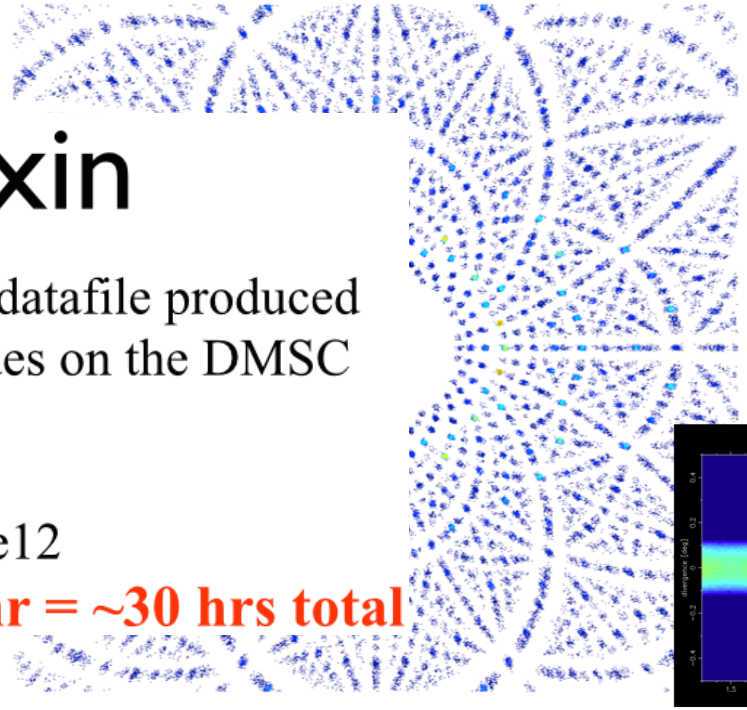
- ONLY meaningful in case of Monte Carlo choices after SPLIT point...

slight sidetrack….

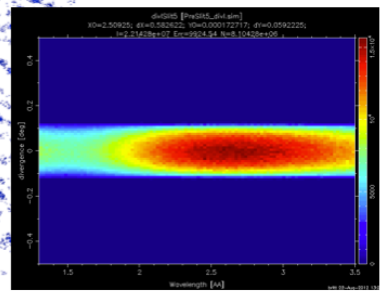
Problem: McStas Single_crystal.comp “slow” for large unit cell diffraction studies

- Example: Rubredoxin

1 timebin, 1000 x,y-bins



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
λmin = 1.3 Å
λmax = 3.5 Å
Timespan: 51.39 to 143.4 ms
Divergence = 0.2 degs



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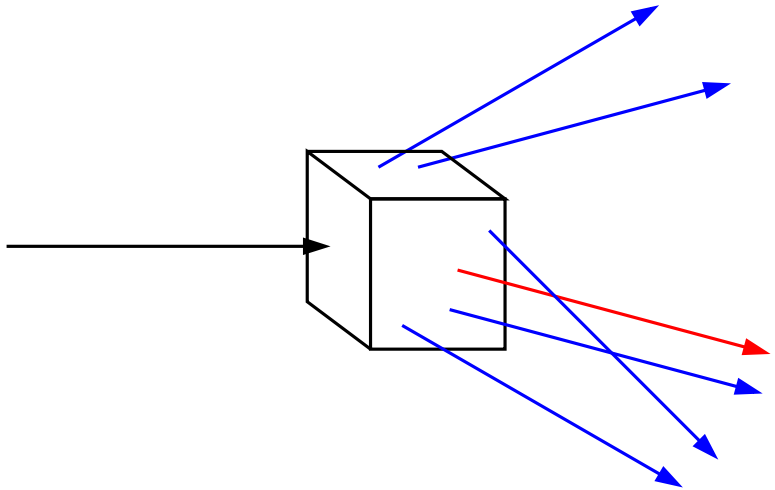
slight sidetrack….

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**!



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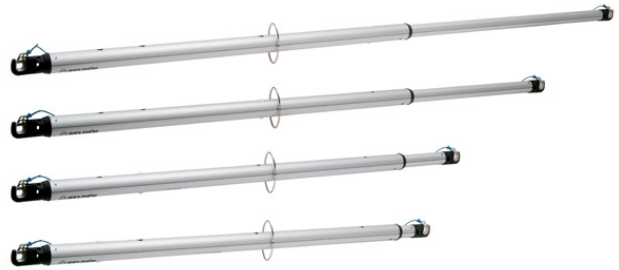
GROUP - components working in parallel

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



- 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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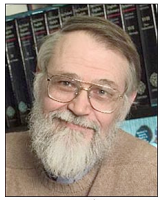

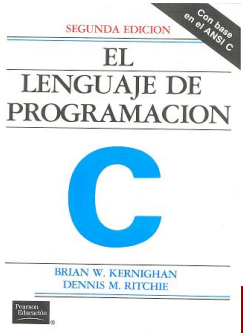

WHEN

- 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.

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

COMPONENT Mon = PSD_monitor(...)
WHEN (myvar==1) AT (0,0,0) RELATIVE Sample

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