McStas advanced language features

- and other important, not so well known details

NOBUGS McStas Training
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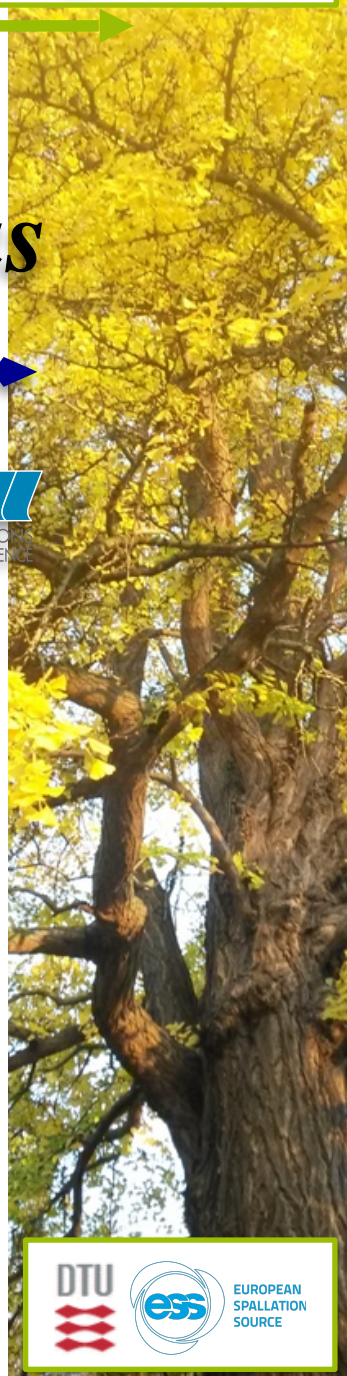
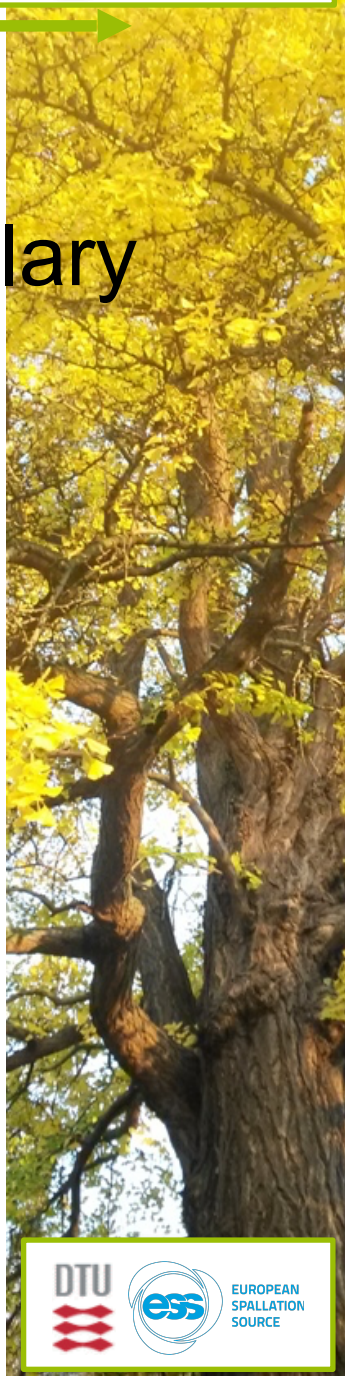
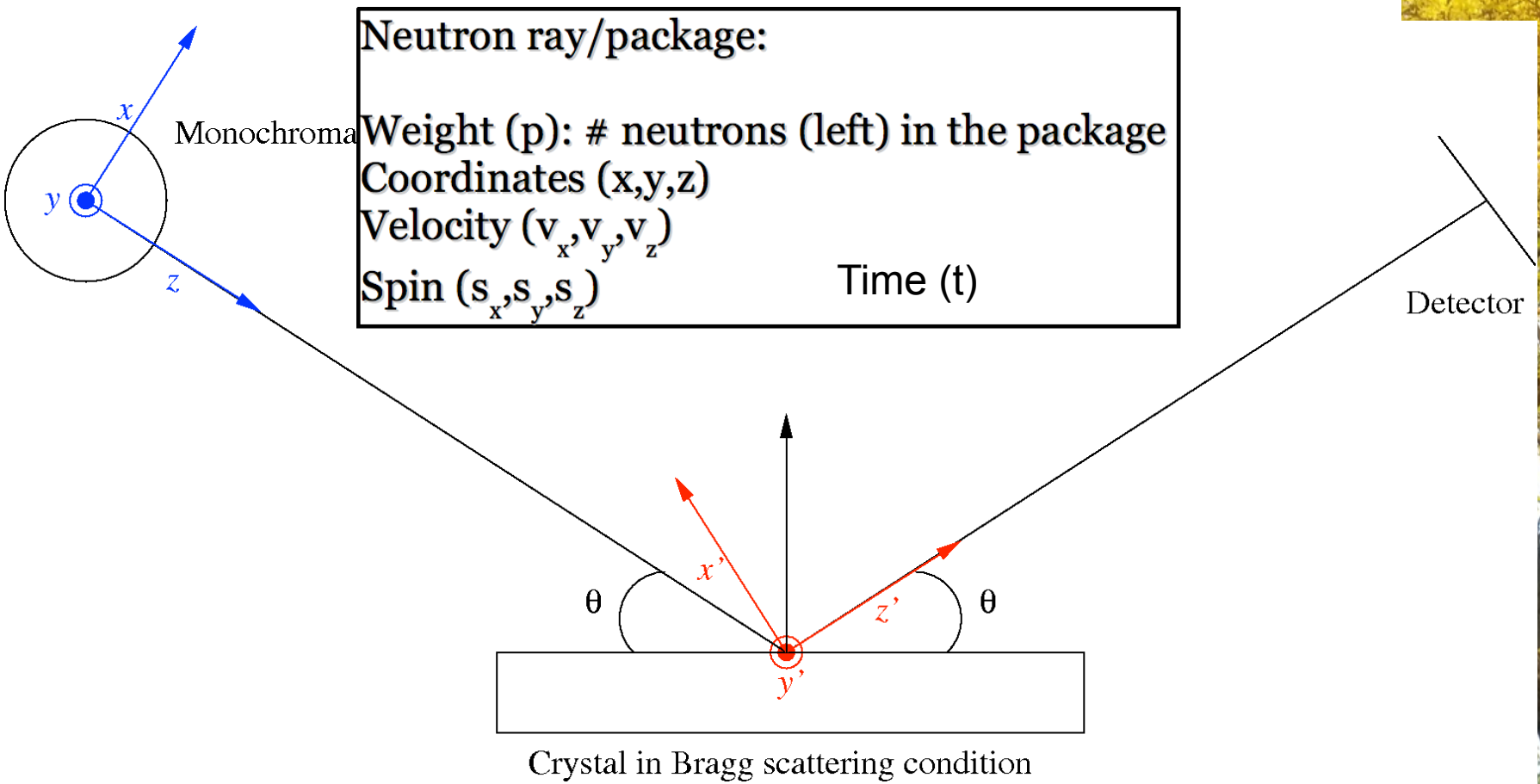


Topics

- A quick recap of the most important vocabulary
- McStas language macros
- Other important details

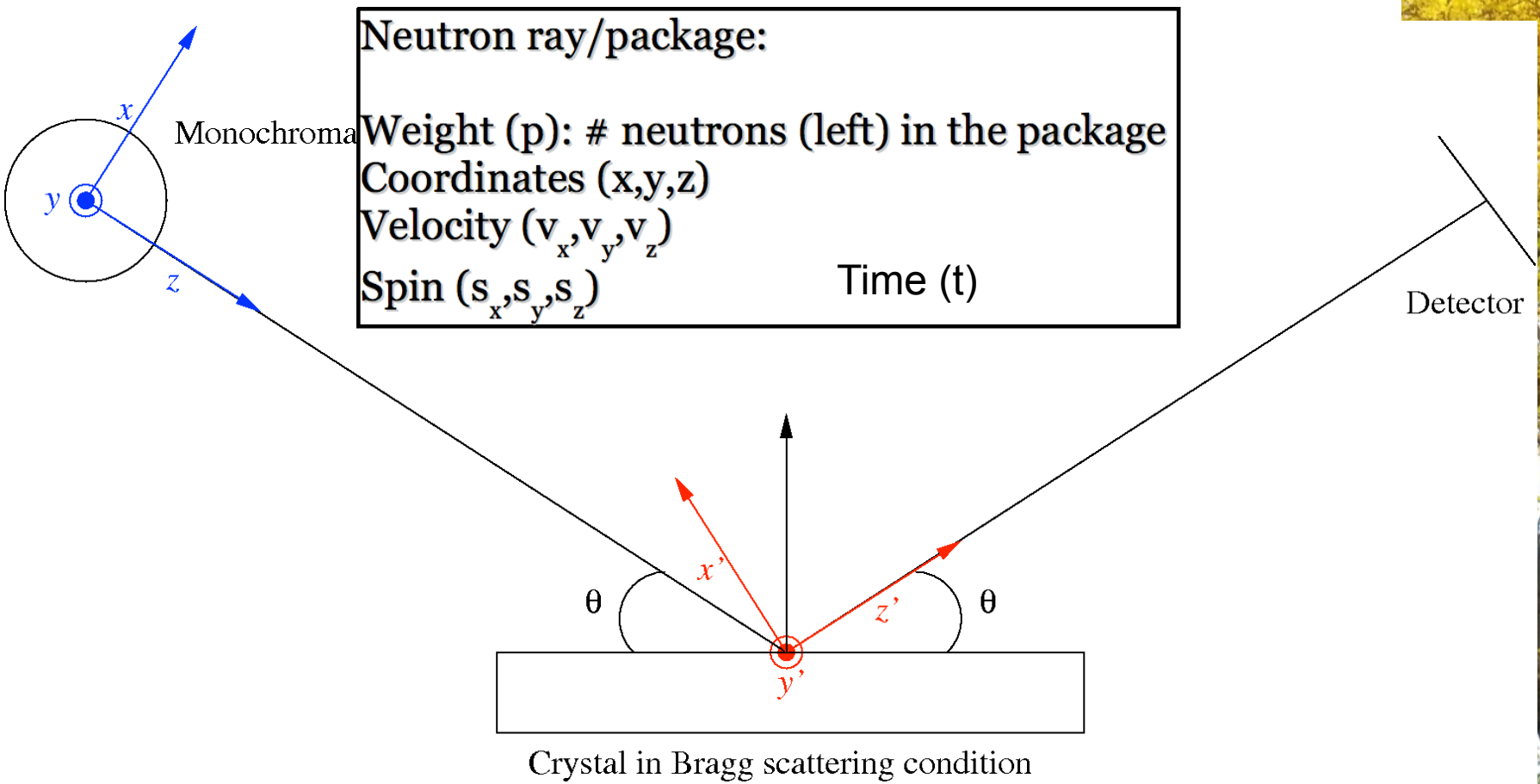


McStas: key concepts

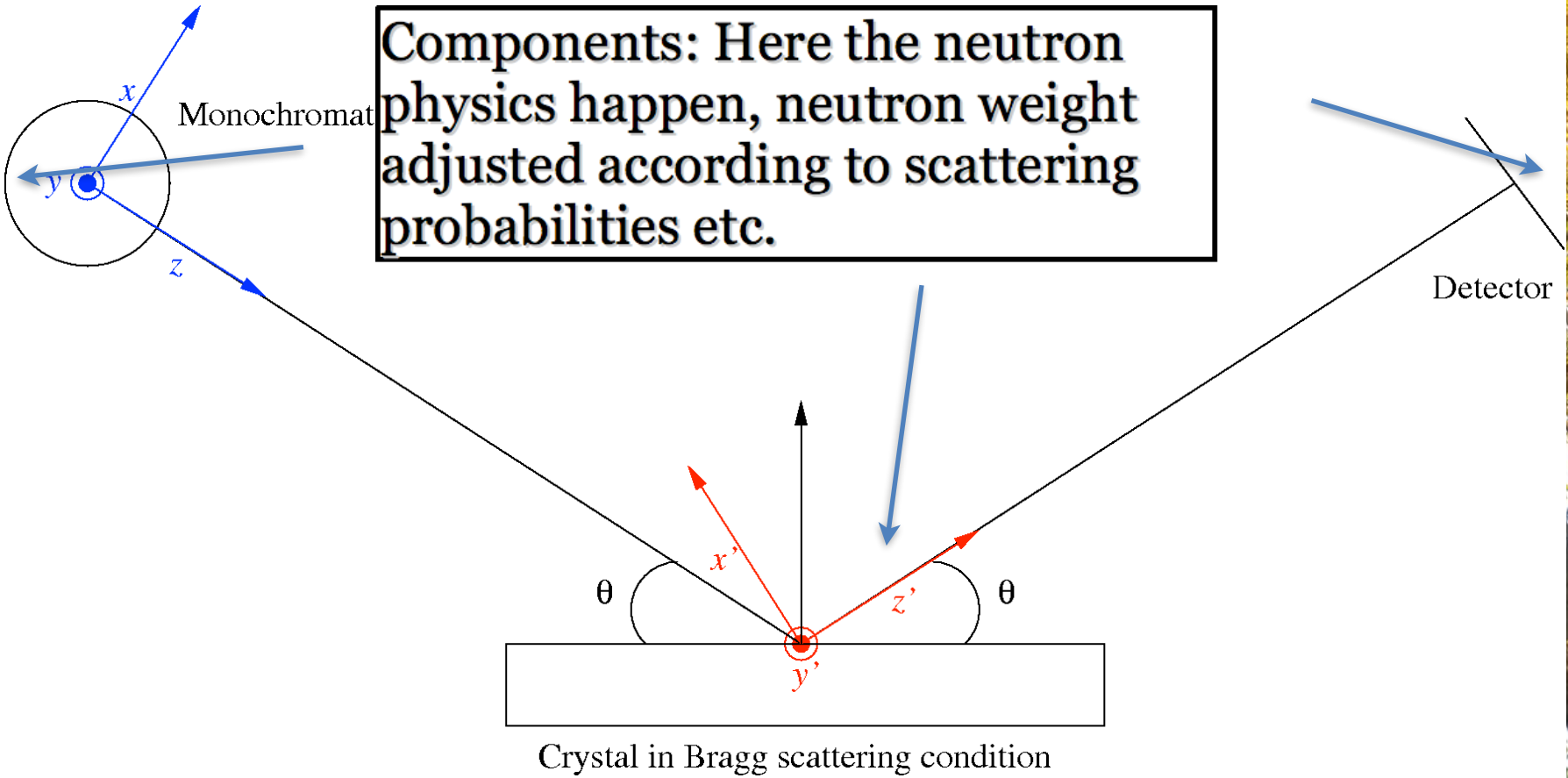


McStas: key concepts

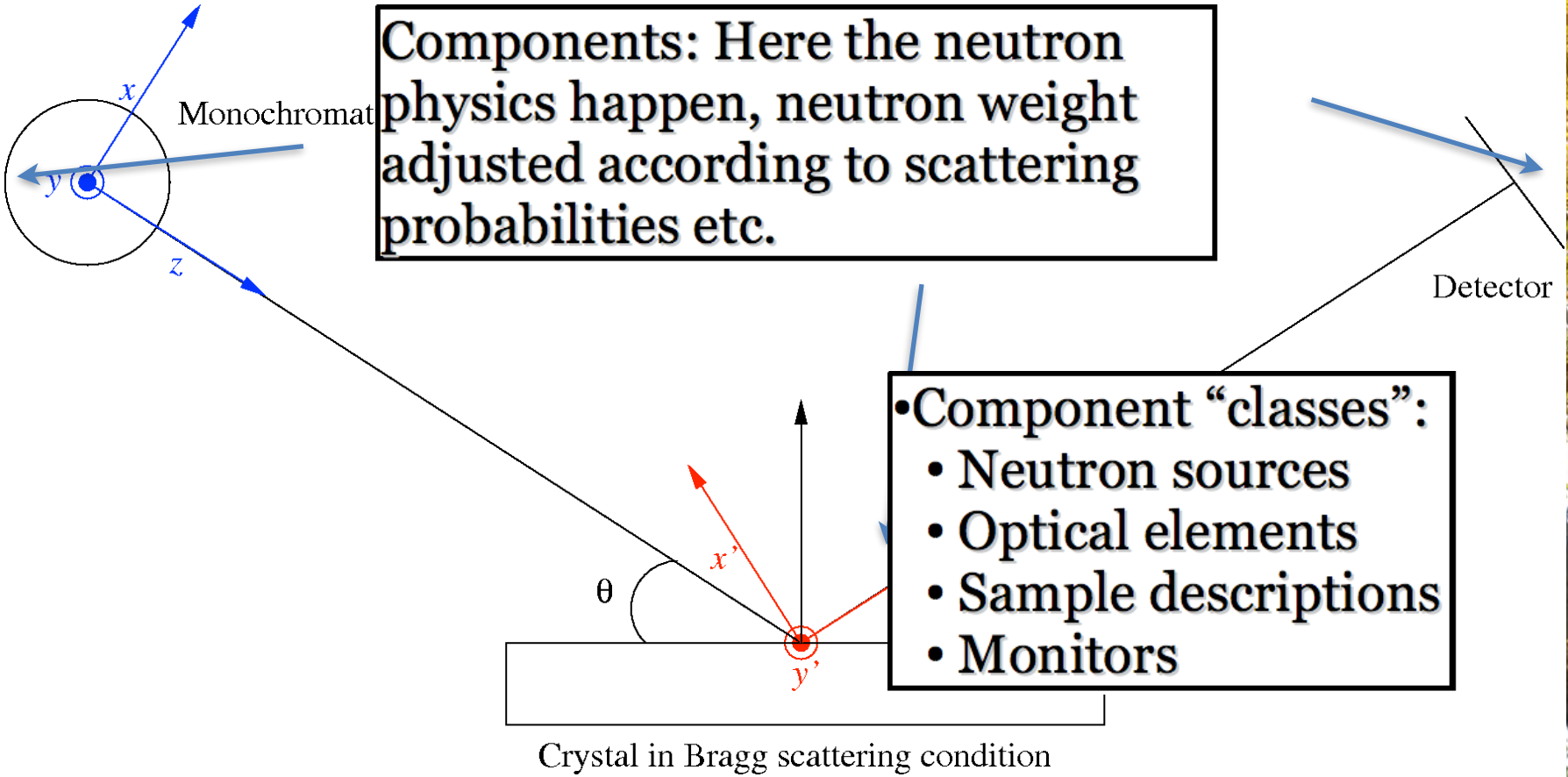
Neutron state parameters are global variables!



McStas: key concepts

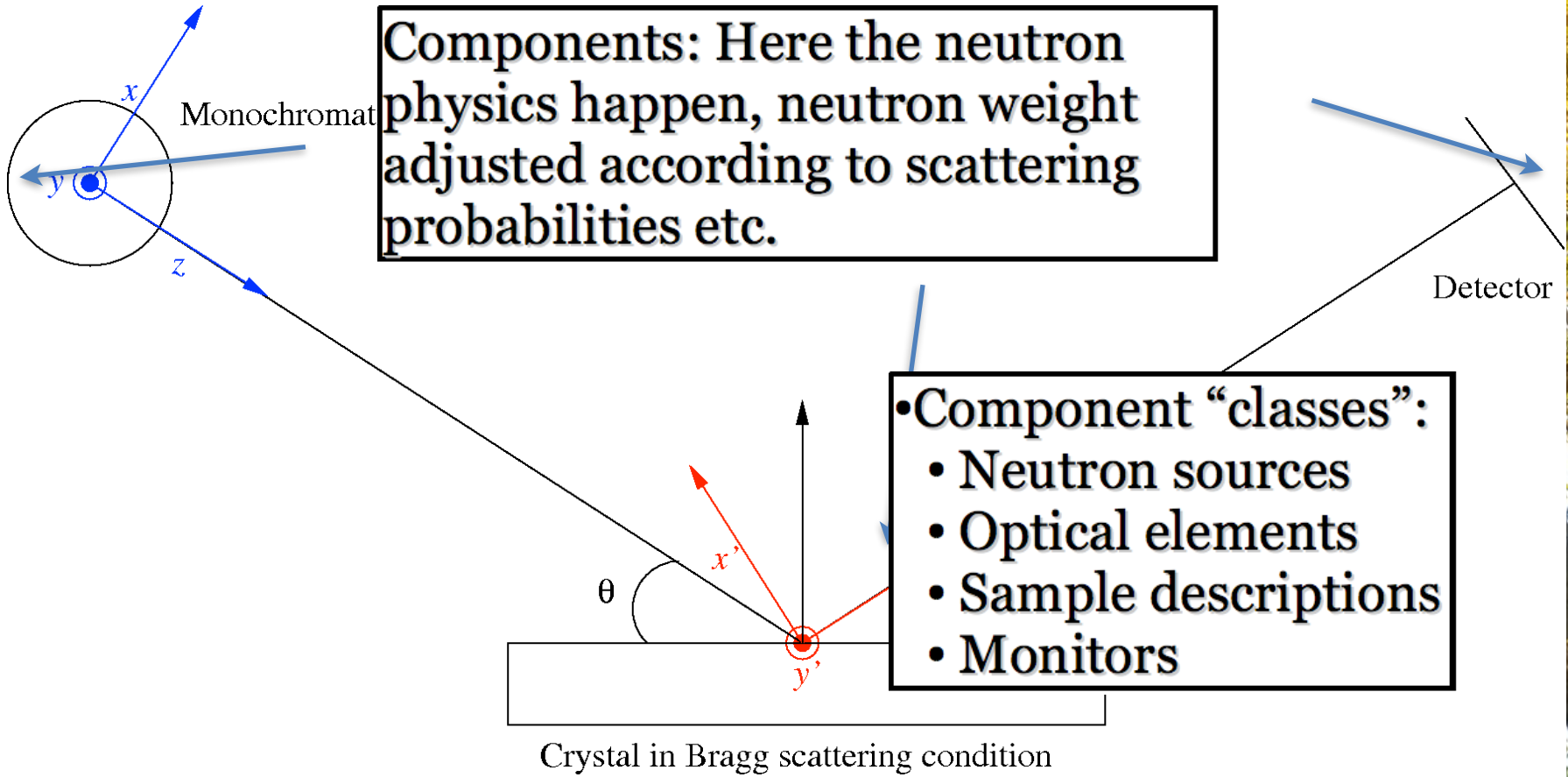


McStas: key concepts

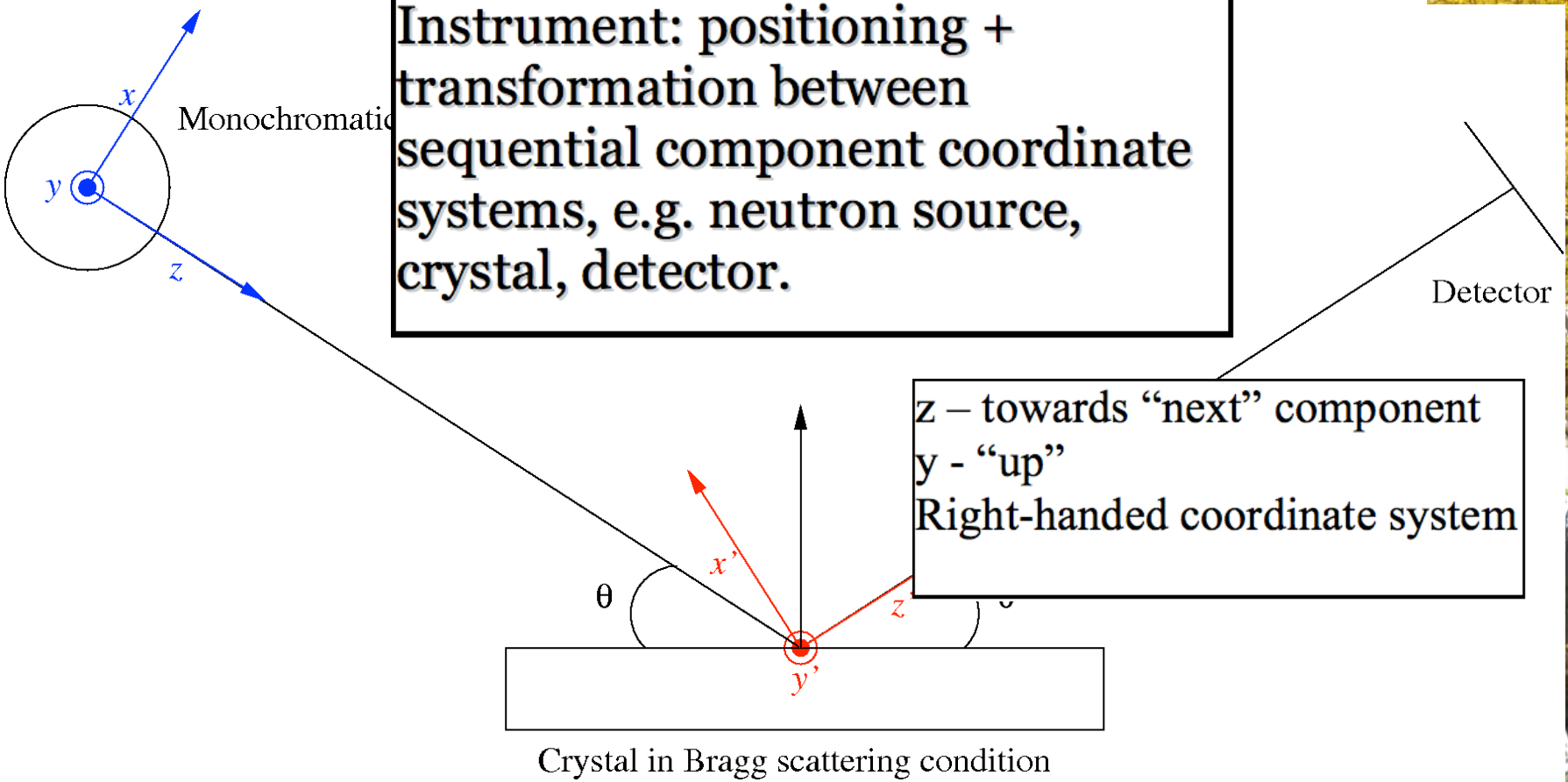


McStas: key concepts

Local, internal coordinate system!

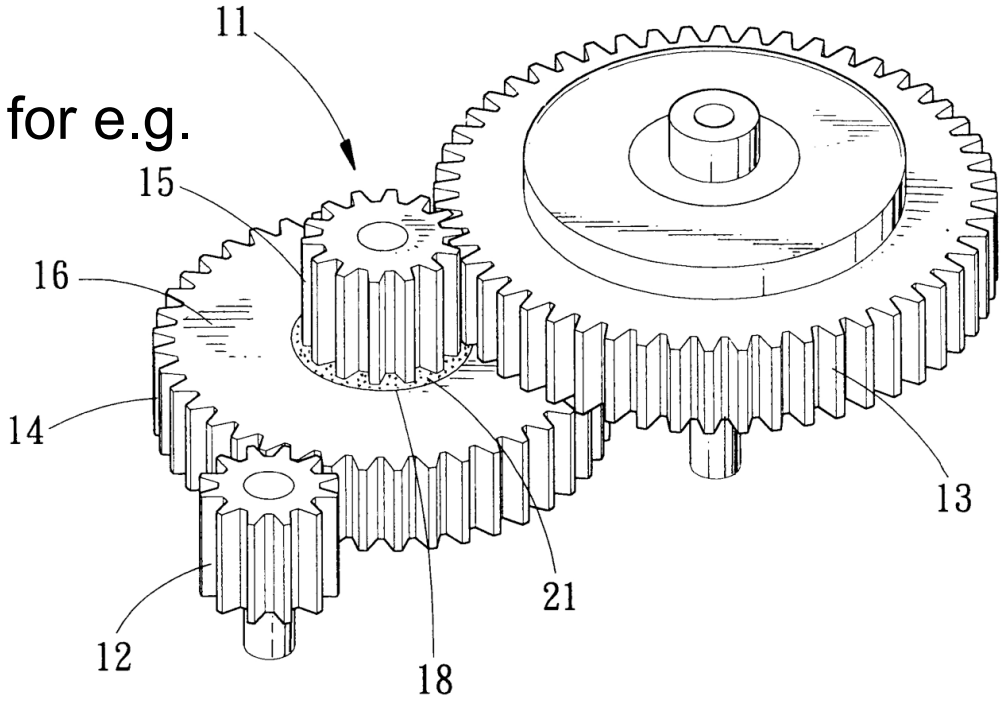


McStas: key concepts



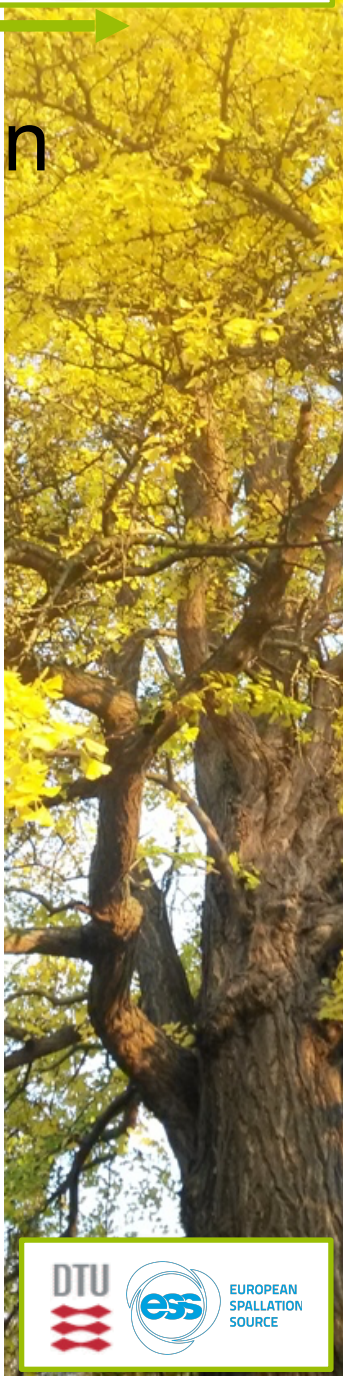
Under-the-hood / inner workings

- Domain-specific-language (DSL) based on compiler technology (LeX+Yacc)
  - Simple Instrument language —Code generation→ ISO C
- Component codes realizing beamline parts (including user contribs)
- Library of common functions for e.g.
  - I/O
  - Random numbers
  - Physical constants
  - Propagation
  - Precession in fields
  - ...

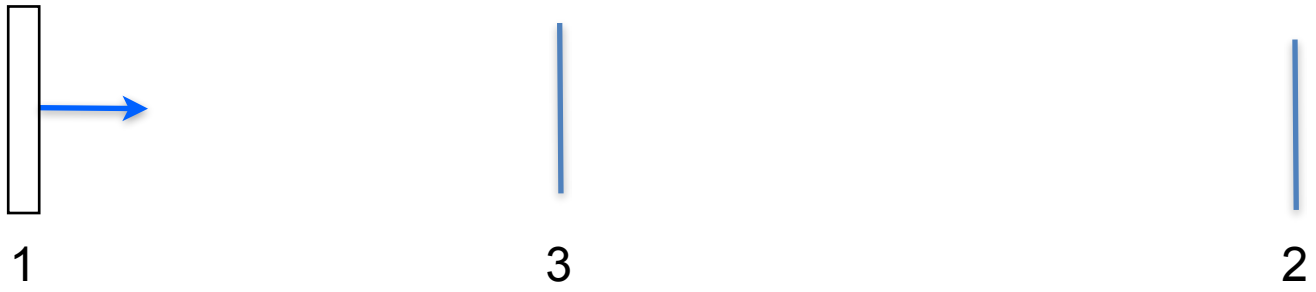


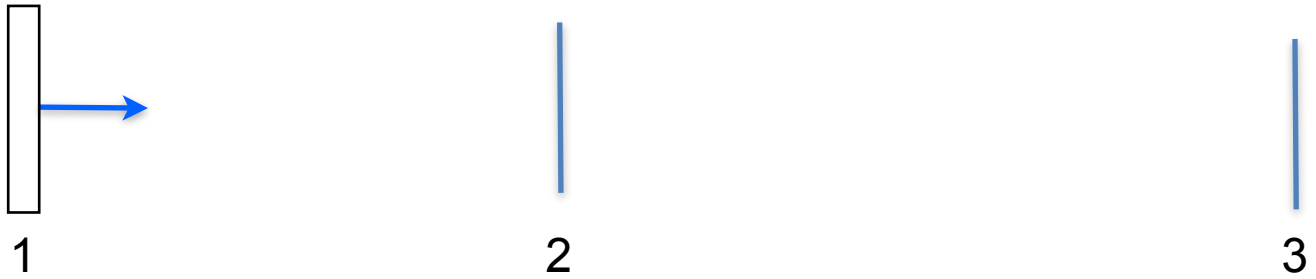
From the “list of frequent questions”

- Why do you need to have the components in this order?

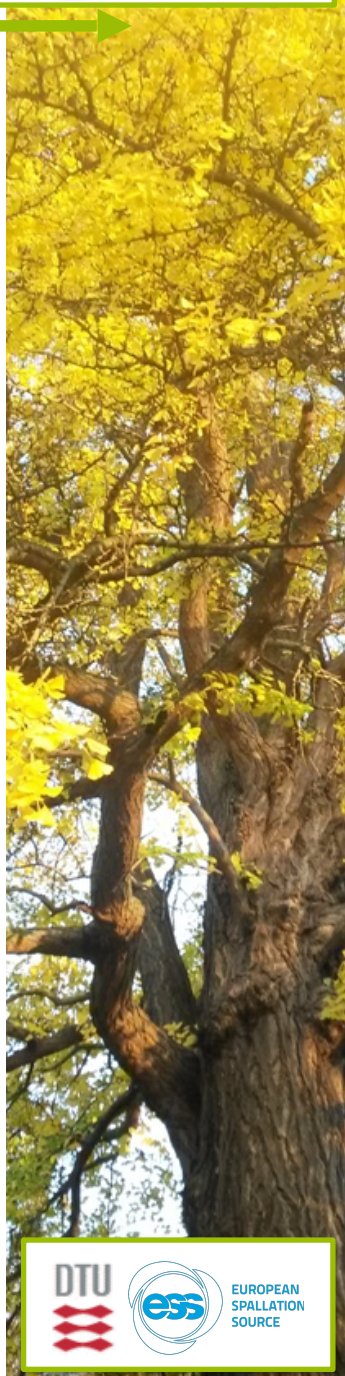


Order of components is important





Starting at the source



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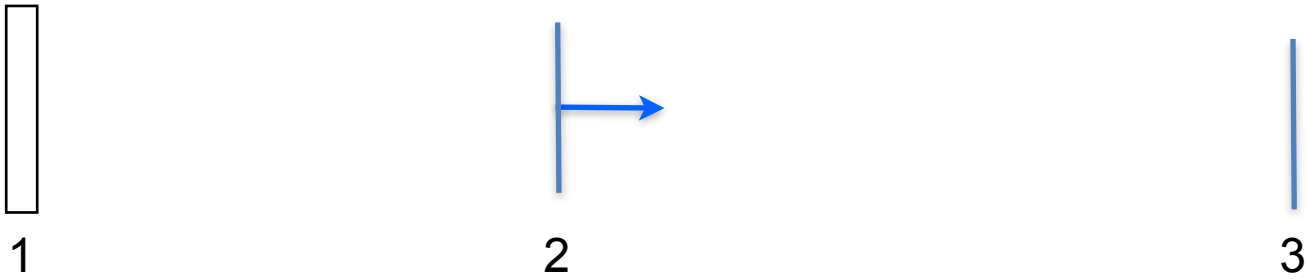
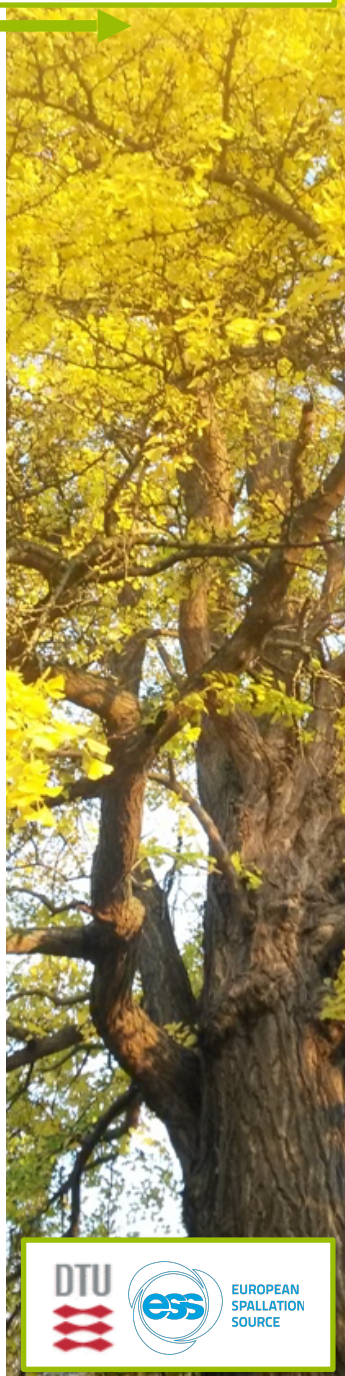


Moving to first comp in the list



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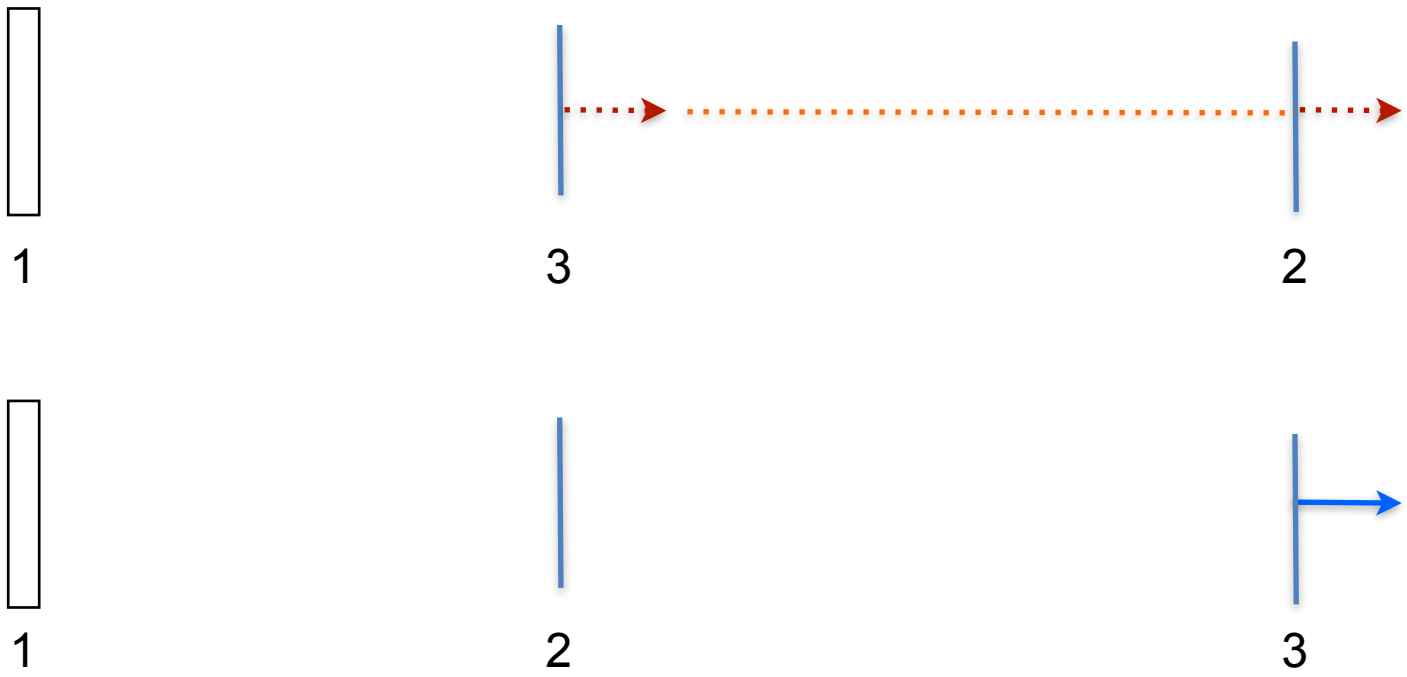
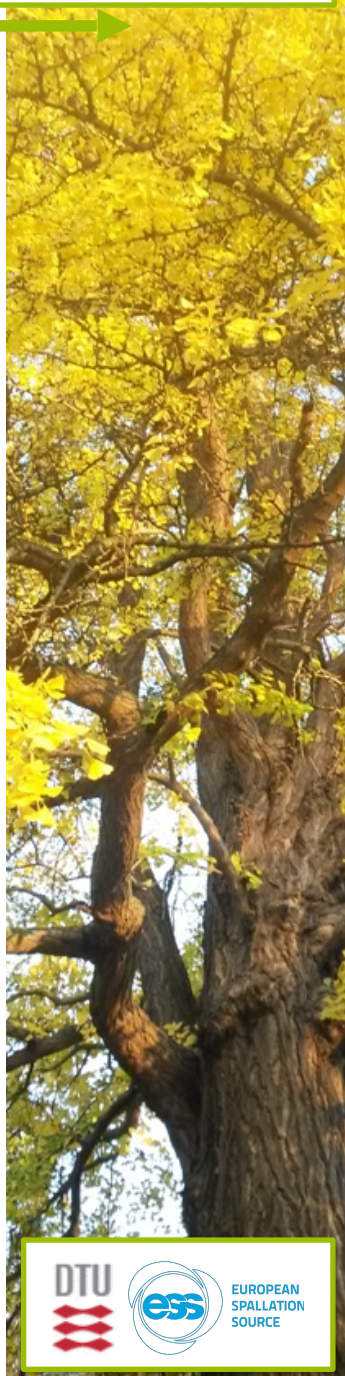


Moving to 3rd comp in list requires “moving back in time”.
Default behavior is to ABSORB this type of neutron.
For monitors use restore_neutron=1 in this case.
For homegrown comps use ALLOW_BACKPROP macro.



Advanced language features

- Macros and tricks for your instrument...

DECLARE / INITIALIZE

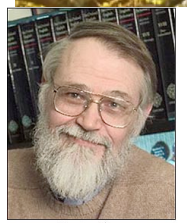
- Use the DECLARE section define user variables and functions.
  - DECLARE %{
  - double myvar;
  - %}

- 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



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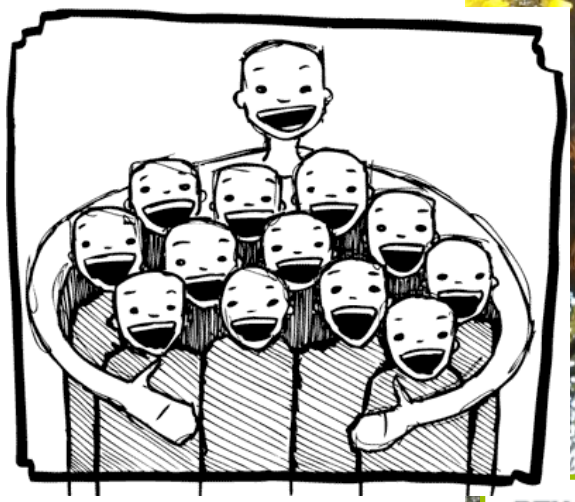
Dennis Ritchie

%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

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] }

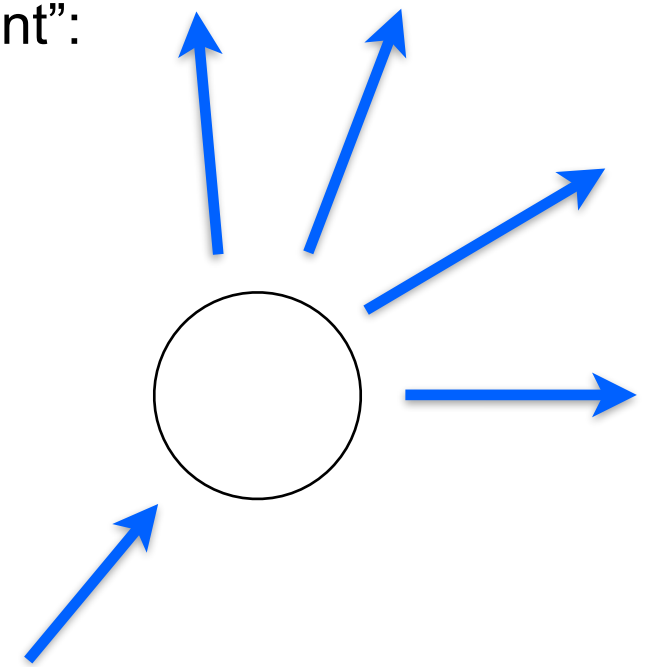
SPLIT

- 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...

WHEN

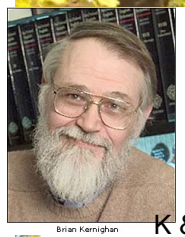
- Syntax:

- COMPONENT Mine = Yours(blah, blah)
- WHEN (c-expression) AT (....)

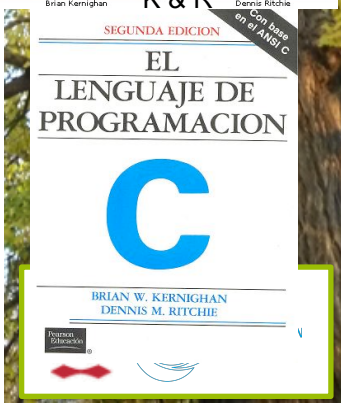
- Is very powerful when combined with EXTEND and user variables, or as a method to let input parameters select if certain components are active.

- 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



K & R

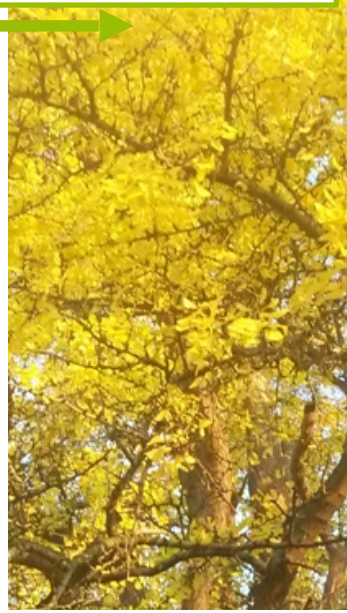


GROUP - components working in parallel


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

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

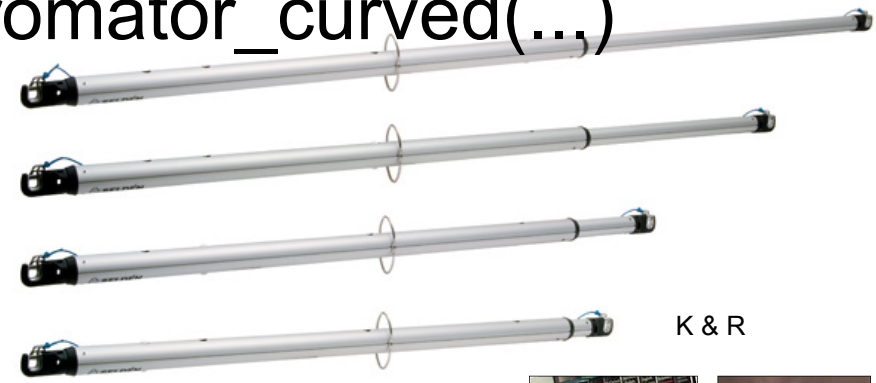
- One comp after the other is “tried” in sequential order until the neutron was SCATTERED.



EXTEND

- Enrich component behaviour using EXTEND:

- COMPONENT Mono1 = Monochromator_curved(...)

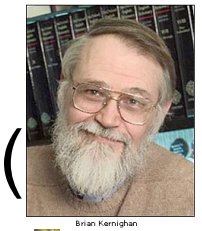


K & R

- AT (0,0, -LMM) RELATIVE Cradle ROTATED (0,A1/2,0) RELATIVE Cradle
- GROUP IN6Monoks
- EXTEND
- %{
- if (SCATTERED) { myvar = ;1 }
- %}

- ...

- COMPONENT Mono2 = Monochromator_curved(



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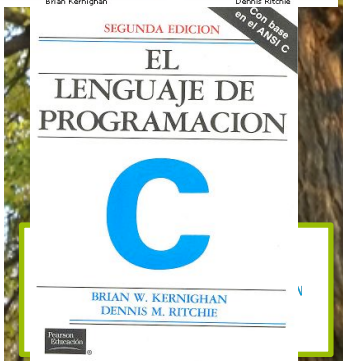
- AT (0,0, 0) RELATIVE Cradle ROTATED (0,A2/2,0) RELATIVE Cradle
- GROUP IN6Monoks
- %{
- if (SCATTERED) { myvar = 2 }
- %}



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

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BEWARE - This IS a GOTO!

- COMPONENT a=b(...)
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JUMP

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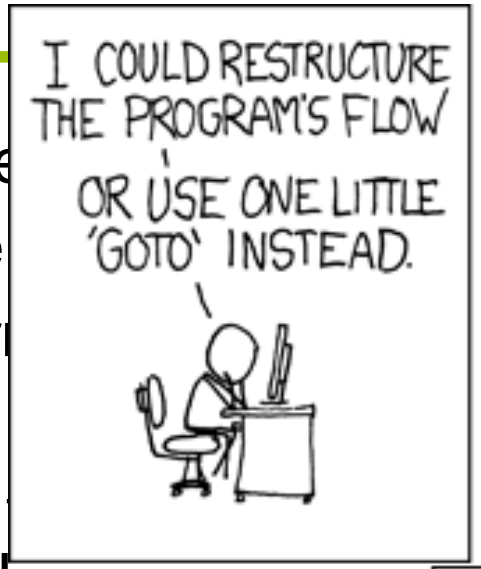
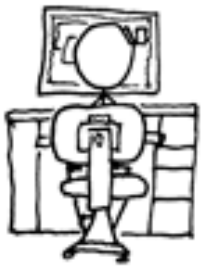
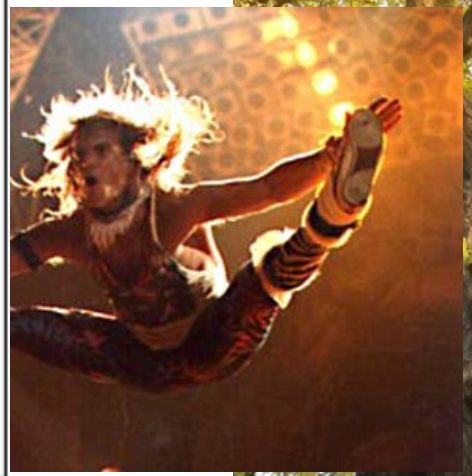


- No coordinate ing that if the Arms you J vill "move" / "reorient" the n

BEWARE

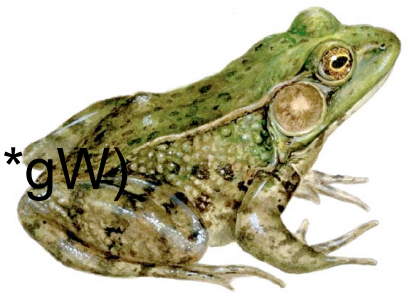
- COMPONENT
- WHEN (expr) A





- COMPONENT a=b(...)
- WHEN (expr) AT (...) JUMP somewhere

COPY- inside instrument



- In instruments: (see ILL_H25.instr)

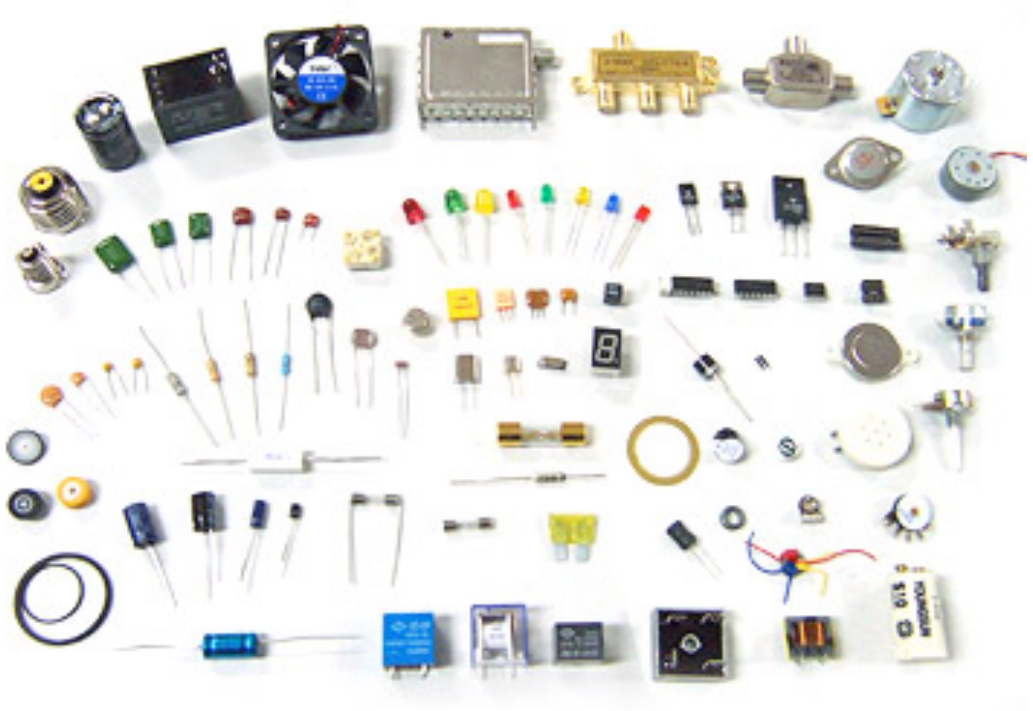
- COMPONENT H25_1 = Guide_gravity(
- w1=0.03, h1=0.2, w2=0.03, h2=0.2, l=L_H25_1,
- R0=gR0, Qc=gQc, alpha=gAlpha, m=m, W=gW)
- AT (0,0,Al_Thickness+gGap) RELATIVE PREVIOUS
- ROTATED (0,Rh_H25_1,0) RELATIVE PREVIO

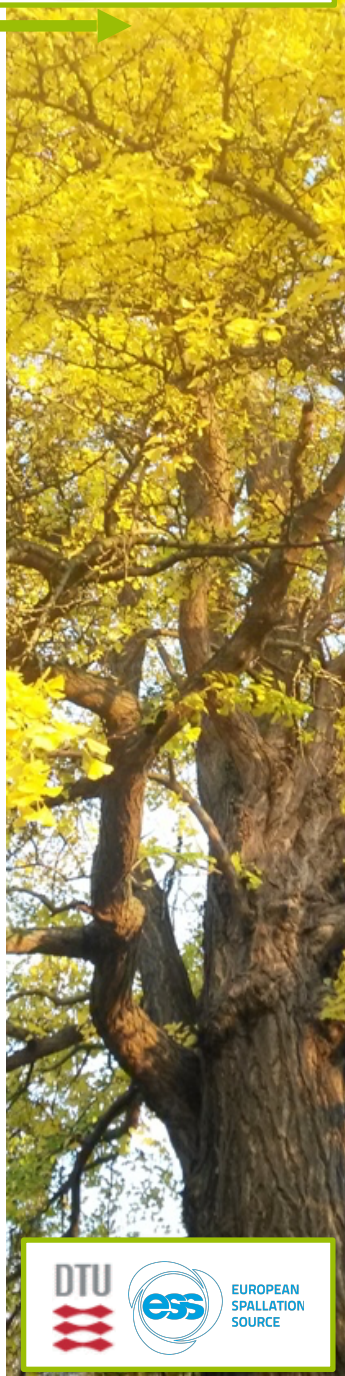
- COMPONENT COPY(H25_1) = COPY(H25_1)
- AT (0,0,L_H25_1+gGap) RELATIVE PREVIOUS
- ROTATED (0,Rh_H25_1,0) RELATIVE PREVIOUS

- 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

Other advanced topics

- Tricks, macros and functions for your components

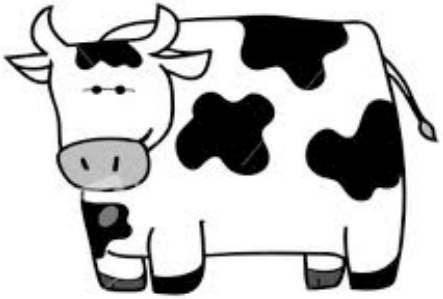




COPY In components:

+

+



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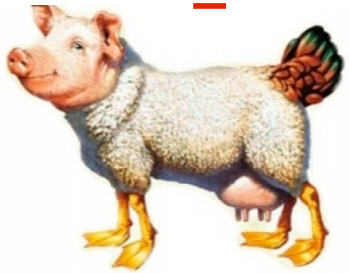


There is a heritage mechanism to create childs of existing components. These are exact duplicates of the parent component, but one may override/extend original definitions of any section.

The syntax for a full component child is

```
DEFINE COMPONENT child_name COPY parent_name
```

This single line will copy all parts of the *parent* into the *child*, except for the documentation header.

As for normal component definitions, you may add other parameters, DECLARE, TRACE, ... sections. Each of them will replace or extend (be catenated to, with the COPY/EXTEND words, see example below) the corresponding *parent* definition. In practice, you could y a component and only rewrite some of it, as in the following example:

```
DEFINE COMPONENT child_name COPY parent_name


SETTING PARAMETERS (newpar1, newpar2)
INITIALIZE COPY parent_name EXTEND
%{
        ...C code to be catenated to the parent_name INITIALIZE ...
%}
SAVE
%{
        ...C code to replace the parent_name SAVE ...
%}
```

Simulation statistics

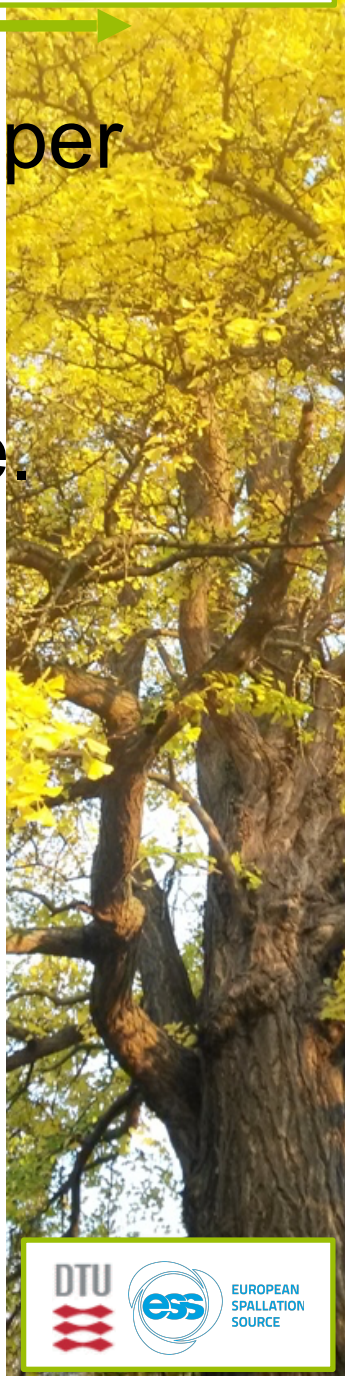
- Neutron weights (intensities) in McStas are "per unit time"
- At a detector bin, N rays with weight p_i arrive. We record:

$$I = \sum_{i=1}^{N} p_i$$

- Intensity

$$E = \sqrt{\frac{N}{N-1}|\sum {p_i}^2 - (\frac{1}{N}\sum p_i)^2|}$$

- Statistical error, root mean square

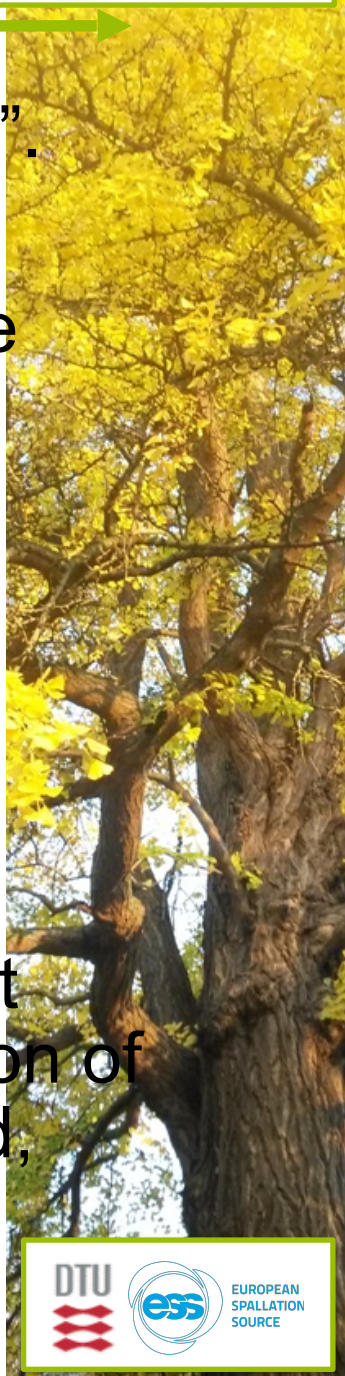


Scaling a simulation to achieve counts

- As noted before, McStas intensities are “per second”.
- A maximal “measurement” or integration time can be defined such that

$$I_m = \alpha_{max} I$$
$$E_m = \sqrt{I_m} \geq \alpha_{max} E$$

- Or in other words, the poisson-law based squareroot error may not become smaller than the scaled version of the statistical error. When a binned monitor is scaled, the minimal E_m for the detector bank to be used.



The end